Varian, Inc.
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# Varian MS Workstation
## Version 6

# Dioxin Reports

QUALITY SYSTEM ISO 9001 CERTIFIED


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# *Quality Systems At Varian, Inc.*

The ISO 9000 series standards were created in Geneva in 1987 to cut through a morass of conflicting quality definitions. These standards define a model for quality assurance systems in product design, development, manufacturing, installation, service, and customer support. They are now the worldwide quality assurance benchmark used to gauge the strength of a company's commitment to quality, and the value of its quality systems.

Various organizations around the world, such as the British Standards Institution (BSI), provide certified, objective auditors to scrutinize quality procedures, product development, manufacturing processes, and customer satisfaction programs. No company can claim ISO 9000 series registration unless it receives a stamp of approval from the demanding quality assessors of BSI or similar accredited examining body. ISO 9000 series registration constitutes an objective third-party report to determine the level of a supplier's commitment to quality.

In 1992, Varian, Inc., Analytical Instruments became registered to the most comprehensive of the ISO 9000 series standards — ISO 9001. ISO 9001 registration means that every stage of our quality system, including product development, manufacturing, final test, shipping, and parts and supplies has been rigorously examined against the most exacting set of internationally recognized standards. It means we live up to a standard of quality that you can count on today, and into the future. Our Quality System has received ISO 9001 certification number FM21797.

The quality systems that earned us ISO 9001 registration have direct benefits for our customers:

- We can speed instruments to you faster than ever before. Emergency orders can be processed even faster.
- We fill your orders promptly and completely.
- We have implemented a system of continuous feedback from our customers — we are aware of your needs today and tomorrow.
- We have improved your productivity by cutting systems failure rates in half and speeding service response time.
- We have embedded continuous improvement into the fabric of our organization so that we can achieve even higher levels of quality in the future.
- We are embedding GLP requirements into our products and services to help you meet your regulatory compliance requirements.

ISO 9001 registration is not enough. For us, quality is defined by our customers. We are not satisfied unless you are satisfied. We are striving to understand customer needs, using independent surveys, user groups, customer advisory boards, and our “Hallmark of Quality” response program, in addition to individual face-to-face customer contact. Our products and our processes are configured to meet those needs.

We know that you are seeking more than the most advanced processes and top-notch applications expertise. You want to join forces with a partner committed to delivering world-class quality, reliability, and value — on time, every time.

QUALITY SYSTEM ISO 9001 CERTIFIED

Our overriding aim is to be that partner.

VARIAN

# *Qualitätssysteme bei Varian, Inc.*

Die Standards der ISO 9000 Serien wurden 1987 in Genf mit dem Ziel geschaffen, das Durcheinander gegensätzlicher Qualitätsbestimmungen zu entwirren. Diese Standards legen ein Modell für Qualitätssicherungssysteme hinsichtlich Produktdesign, Entwicklung, Herstellung, Installation, Service und Kundenbetreuung fest. Sie sind nun die weltweiten Maßstäbe der Qualitätssicherung, die die Anstrengungen eines Unternehmens bezüglich der Qualität und der Bedeutung seiner Qualitätssysteme messen.

Verschiedene Organisationen in der ganzen Welt, wie die British Standards Institution (BSI), stellen ausgebildete, objektive Prüfer zur Begutachtung von Qualitätsmaßnahmen, Produktentwicklung, Herstellungsprozessen und von Programmen zur Erforschung der Kundenzufriedenheit zur Verfügung. Kein Unternehmen kann die ISO 9000 Registrierung beantragen, ohne die Genehmigung von den beauftragten Qualitätsgutachtern der BSI oder einer ähnlichen akkreditierten Stelle erhalten zu haben. Die ISO 9000 Registrierung bildet einen objektiven Bericht von dritter Seite, um den Grad der Qualitätsanstrengung eines Lieferanten zu bestimmen.

1992 wurden die Varian, Inc., Analytical Instruments nach den umfassendsten Standards der ISO 9000 Serie registriert — ISO 9001. Die ISO 9001 Registrierung bedeutet, daß jedes Stadium unseres Qualitätssystems, einschließlich Produktentwicklung, Herstellung, Endkontrolle, Versand, sowie Teile und Zubehör rigoros gegen die anspruchsvollste Serie international anerkannter Standards geprüft worden ist. Das bedeutet, daß wir einen Qualitätsstandard bieten, auf den Sie heute und in Zukunft rechnen können. Unser Qualitätssystem hat die ISO 9001 Zertifikatnummer FM21797 erhalten.

Die Qualitätssysteme der ISO 9001 Registrierung haben für unsere Kunden direkte Vorteile:

- Wir können Instrumente schneller denn je zu Ihnen schicken. Eilbestellungen werden noch schneller durchgeführt.
- Wir erfüllen Ihre Bestellungen pünktlich und vollständig.
- Wir haben ein System kontinuierlichen Informationsrückflusses von unseren Kunden aufgebaut—wir kennen Ihre Anforderungen von heute und von morgen.
- Wir haben Ihre Produktivität durch Halbierung der Systemfehlerraten und durch Verkürzung unserer Reaktionszeit im Service verbessert.
- Wir haben kontinuierliche Verbesserungen in unserer Organisationsstruktur verankert, so daß wir künftig eine noch höhere Qualität erreichen können.
- Wir haben die GLP Anforderungen in unsere Produkte und Dienstleistungen eingeführt, um Ihnen bei der Erfüllung Ihres behördlichen Abnahmeprotokolls zu helfen.

Die ISO 9001 Registrierung ist nicht genug. Für uns wird Qualität durch unsere Kunden definiert. Wir sind nicht zufrieden, wenn Sie es nicht auch sind. Wir bemühen uns, die Anforderungen unserer Kunden durch unabhängige Untersuchungen, Anwendergruppen, Kundenberatungsgremien und unser Antwortprogramm “Gütesiegel der Qualität” zu verstehen, zusätzlich zu persönlichen Kundenkontakten. Unsere Produkte und unsere Prozesse sind so gestaltet, daß sie diese Anforderungen erfüllen.

Wir wissen, daß Sie mehr als fortschrittliche Prozesse und ausgezeichnetes Anwendungswissen suchen. Sie suchen einen Partner, der Qualität von Weltklasse, Verläßlichkeit und Nutzen für Sie liefert— pünktlich und jederzeit.

Unser oberstes Ziel ist, für Sie dieser Partner zu sein.

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# *Systèmes de qualité chez Varian, Inc.*

Les normes ISO série 9000 ont été créées à Genève, en 1987, pour remédier à la confusion dans la définition des normes de qualité. Ces normes définissent un modèle de contrôle de qualité dans le domaine de la conception produit, du développement, de la production, des installations, des services et du support client. Elles constituent à présent la référence mondiale en matière de contrôle de qualité utilisée aux fins d'évaluation du niveau d'engagement d'une entreprise dans ce domaine et la valeur de ses systèmes de qualité.

Plusieurs organisations de par le monde, telle la British Standards Institution (BSI) offrent les services d'auditeurs qualifiés et objectifs, chargés d'examiner les procédures de qualité, le développement de produit, les procédés de fabrication et les programmes de satisfaction du client.

Aucune société ne peut se prévaloir de l'homologation ISO 9000, sans avoir reçu l'approbation des évaluateurs rigoureux de la BSI ou  d'un organisme accréditif similaire. L'homologation ISO 9000 constitue une évaluation objective d'un tiers afin de déterminer le niveau d'engagement d'un fournisseur dans le domaine de la qualité.

En 1992, Varian, Analytical Instruments a reçu l'homologation ISO 9001, normes des plus complètes de la série IS0 9000. En d'autres termes, chaque étape du processus de qualité, notamment le développement produit, la fabrication, le test final, l'expédition et les fournitures de pièces a étés oumis à un contrôle rigoureux par rapport à des normes extrêmement strictes, reconnues au niveau international. Nous sommes donc à même de vous garantir et de maintenir un niveau de qualité. Lesdites procédures ont reçu l'homologation ISO 9001 numéro FM21797.

Les systèmes de qualité qui ont reçu l'homologation ISO 9001 présentent des avantages directs pour nos clients :

- Nous sommes en mesure de vous livrer les instruments et de traiter les commandes en urgence dans des délais record.
- Nous répondons pleinement et de manière rapide à vos commandes.
- Nous avons mis en place un système de feedback continu de la part de nos clients et sommes conscients de vos attentes présentes et futures.
- Nous avons amélioré votre productivité en réduisant de moitié les Temps de panne et en accélérant les temps de réponse.
- Nous avons apporté des améliorations constantes au sein de notre structure, afin d'atteindre des niveaux de qualité optima, à l'avenir.
- Nos produits et services reflètent les exigences BPL pour vous permettre de répondre aux impératifs de respect de la règlementation.

Toutefois, nous ne nous contentons pas de l'homologation ISO 9001. Pour nous, la qualité est définie par nos clients. Nous ne sommes satisfaits que lorsque nos clients le sont. Nous nous efforçons de comprendre vos besoins, à l'aide d'évaluations externes, de groupes d'utilisateurs, de comités de conseil clients, et de notre programme “Hallmark of Quality”, outre les contacts directs que nous établissons avec chacun de nos clients. Nos produits et nos procédés sont conçus pour répondre à vos attentes.

Nous n'ignorons pas que vous recherchez plus que des processus évolués et un savoir-faire d'exception dans le domaine des applications. Vous souhaitez conjuguer vos forces avec un partenaire s'étant engagé à offrir une qualité, une fiabilité et une valeur optimales, au moment où il faut et quand il faut.

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Notre principal objectif : devenir votre partenaire !

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# *I sistemi di qualità della Varian, Inc.*

La serie degli standard ISO 9000 è stata presentata nel 1987 a Ginevra con lo scopo di mettere ordine in un groviglio di definizioni contrastanti sulla qualità. Tali standard definiscono un modello che assicura la qualità nella progettazione, nello sviluppo, nella fabbricazione, nell'installazione e nella manutenzione dei prodotti nonché nel servizio assistenza clienti. Oggi come oggi essi costituiscono il punto di riferimento, a livello mondiale, ai fini della valutazione dell'impegno delle diverse aziende sul fronte della qualità e della validità dei sistemi di qualità da esse adottati.

Diverse organizzazioni internazionali, come la British Standard Institution (BSI), dispongono d'ispettori certificati e imparziali per la valutazione delle procedure di qualità, dello sviluppo dei prodotti, dei processi di fabbricazione e dei programmi di soddisfazione del cliente. Nessuna azienda può asserire d'essere in possesso della certificazione ISO 9000 finché non dispone del marchio d'approvazione concesso dai rigorosi ispettori di qualità della BSI o di altri enti di controllo riconosciuti. La certificazione di conformità agli standard ISO 9000 costituisce un'attestazione imparziale di terzi del grado d'impegno di una determinata azienda nei confronti della qualità.

Nel 1992 la Varian, Inc., Analytical Instruments ha ottenuto l'omologazione allo standard più completo della serie ISO 9000, l'ISO 9001. L'omologazione ISO 9001 significa che ogni singola fase del nostro sistema di qualità - compresi lo sviluppo del prodotto, la fabbricazione, le prove finali, la spedizione, i componenti e le forniture - è stata rigorosamente esaminata a fronte della serie più esigente di standard riconosciuti a livello mondiale, il che significa che rispondiamo pienamente ad uno standard qualitativo sul quale il cliente può contare oggi come nel futuro. Il nostro Sistema di Qualità ha ottenuto la certificazione ISO 9001 col numero FM21797.

I sistemi di qualità per i quali abbiamo ottenuto l'omologazione ISO 9001 comportano dei vantaggi diretti per i nostri clienti, ovvero:

- Siamo in grado di consegnare gli strumenti più rapidamente rispetto al passato, con la possibilità di evadere le richieste d'emergenza con una rapidità ancora maggiore.
- Gli ordini vengono evasi tempestivamente ed in modo completo.
- Abbiamo messo a punto un sistema di riscontro costante con la clientela, in modo da poter essere sempre perfettamente informati sulle esigenze attuali e future del cliente.
- Abbiamo migliorato la produttività del cliente riducendo della metà il tasso di guasti dei sistemi e velocizzando i tempi d'intervento della manutenzione.
- Abbiamo introdotto un costante miglioramento nella nostra struttura organizzativa in modo da poter conseguire in futuro livelli qualitativi ancor più elevati.
- Stiamo adeguando i nostri prodotti e servizi agli standard GLP per poter aiutare i clienti a soddisfare i requisiti di conformità posti loro dagli enti normativi.

Ma l'omologazione ISO 9001 non è tutto. Per quanto ci riguarda, la qualità viene definita dai nostri clienti: noi siamo soddisfatti solo se lo è il cliente. Ci adoperiamo al massimo per comprendere le esigenze del cliente, ricorrendo ad indagini di società private, gruppi di utenti, associazioni di consumatori e con il nostro programma di risposta Hallmark of Quality - il marchio di garanzia di qualità - oltre che col contatto diretto coi singoli clienti. I nostri prodotti ed i nostri processi sono configurati per rispondere a tali esigenze.

Sappiamo che a Voi i processi più avanzati e l'esperienza delle applicazioni di prim'ordine non bastano. Sappiamo che intendete unire le vostre forze con quelle d'un partner impegnato a fornire livelli qualitativi internazionali, affidabilità e valore, in modo tempestivo e costante.

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Quel partner vogliamo essere noi.

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# *Sistemas de calidad en Varian, Inc.*

Las normas ISO 9000 fueron creadas en Ginebra en 1987 para acabar con una multitud de definiciones de calidad contradictorias. Estas normas constituyen un modelo de sistemas de garantía de calidad en el diseño, desarrollo, fabricación, instalación, mantenimiento y asistencia técnica de productos. Se han convertido en el banco de pruebas de garantía de calidad a nivel mundial y miden el grado de compromiso de una empresa con la calidad, así como el alcance de sus sistemas de calidad.

Diversas organizaciones mundiales, como la British Standards Institution (BSI), proporcionan expertos titulados de probada objetividad para investigar procedimientos de calidad, desarrollo de productos, procesos de fabricación y programas de servicio al cliente.

Varian, Inc., Analytical Instruments fue registrada en 1992 con la norma más exhaustiva de la serie ISO 9000: la ISO 9001. La certificación por la norma ISO 9001 significa que todas las etapas de nuestro sistema de calidad, como el desarrollo del producto, la fabricación, las pruebas finales, la expedición, así como los suministros y recambios, han sido examinados rigurosamente respecto a las normas más exigentes reconocidas internacionalmente. Significa que nos comprometemos a mantener un nivel de calidad con el que podrá siempre contar, hoy y en el futuro. Il nostro Sistema di Qualità ha ottenuto la certificazione ISO 9001 col numero FM21797.

Los sistemas de calidad que nos valieron la certificación ISO 9001 representan beneficios directos para nuestros clientes:

- haremos llegar nuestros aparatos más rápidamente que nunca. Podemos cumplir con pedidos urgentes aún más deprisa.
- Atenderemos sus pedidos de forma rápida y completa.
- Aplicamos un sistema de retorno de información permanente con nuestros clientes: siempre somos conscientes de sus necesidades, actuales o futuras.
- Hemos mejorado la productividad de nuestros clientes, disminuyendo el índice de defectos a la mitad y acortando el tiempo de respuesta del servicio de mantenimiento.
- Hemos integrado sistemas de mejora continuada en nuestra organización, de forma que podremos obtener niveles de calidad aún superiores en un futuro.
- Estamos integrando los requerimientos GLP en nuestros productos y servicios para ayudarle a cumplir con requerimientos de conformidad obligatorios.

La conformidad con ISO 9001 no nos basta. Para nosotros, los criterios de calidad los definen nuestros clientes. No estaremos satisfechos hasta que usted lo esté. Intentamos comprender las necesidades de nuestros clientes, a través de entidades independientes, grupos de usuarios, oficinas de asesoramiento a usuarios y nuestro programa de respuesta “Hallmark of Quality”, además de los contactos directos con nuestros clientes. Nuestros productos y procedimientos están diseñados para poder corresponder a sus necesidades.

Sabemos que nuestros clientes buscan más que experiencia en procesos avanzados y aplicaciones punteras. Se trata de unir fuerzas con un socio que se compromete a entregar calidad reconocida a nivel mundial, fiabilidad y valor, a tiempo, siempre.

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Nuestra meta principal es ser ese socio.

# Contents

# Overview

Dioxin Reports is a flexible reporting software package implemented in Microsoft Access 2000. It allows the generation of numerous graphical and text report formats for the analysis of environmental samples for polychlorinated dibenzo-p-dioxins and dibenzofurans by a tandem mass spectrometry (GC/MS/MS) approach.

Dioxin Reports uses data from files processed in MS Workstation Version 6.2 or later. Reports are generated based upon internal standard calculations.

In addition to quantitative reports on Analysis samples, Quality Control and Summary reports can be generated with the software.

There are several different options of numerical and graphical reports for the target compounds and for calculation of the TEQ (toxicity equivalent to 2,3,7,8-Tetrachlorodibenzo-p-dioxin).

The reports can be previewed, printed and or saved as ASCII text files for later retrieval.

The software allows report generation immediately after a sample analysis is completed. Alternatively, reports for a sample or sample list can be easily generated as a post-run operation.

The report templates can be "cloned" to generate a separate template for each type of reporting requirement.

Several Dioxin Reports include fields based on statistical calculations. The calculation of such quantities as average, Relative Standard Deviation (RSD), control limits, and Method Detection Limit (MDL) are based on full-precision values read from MS Workstation data files. The values used in the statistical calculations are reported to less than full precision on reports. An independent recalculation of these statistical quantities based on the lower precision printed values of MS Workstation data files will result in statistical results that differ slightly from Dioxin Reports results that are based on full-precision numbers.

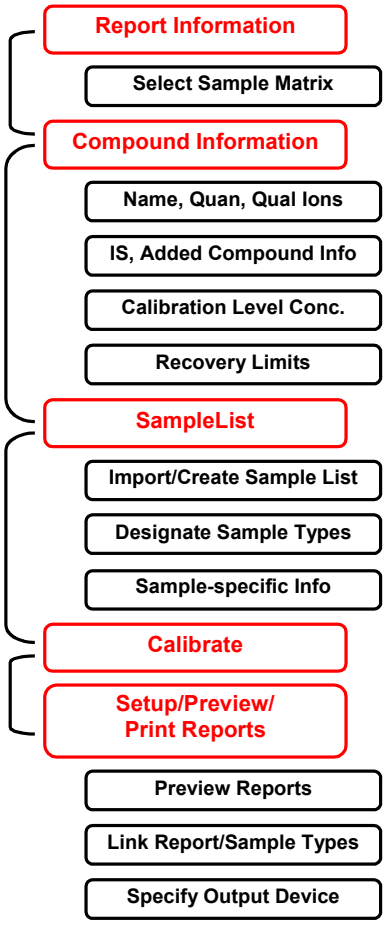
## Help

Immediate context-sensitive help is available throughout in the software. To see help on a specific field in a Dioxin Reports form, position the mouse cursor over the item of interest and click the right mouse button and select the "What's This?" item from the floating menu which then appears.

# Dioxin Reports Components

Dioxin Reports software has five major components, as listed below. These sections interact with each other. Therefore the method should be configured in the order shown below.

1. Report Information
2. Compound Information
3. Sample List
4. Calibrate
5. Setup/Preview/Print Reports




*Overview of Dioxin Reports Software Components*

## Report Information

Pertinent information about the laboratory is entered here. Either a Contract Laboratory Program (CLP) type of output or a two-line title may be chosen as a header for the reports. This is also where the type of sample matrix (Water, Soil, or Tissue) is chosen and this choice will affect the choices in the Sample List form and the reports themselves.

## Compound Information

The Compound Information form contains criteria used in reporting specific target compounds. By default, criteria for the set of C13-labeled and native compounds in EPA Method 1613 have been entered.

On successive lines in the Compound Information form, criteria are set for:

- Compound Name, Compound Class, Quantitation Ion(s), and Qualifier Ions
- The internal standard and its concentration, High/Low Limits for Qualifier Ion Ratios and Relative Retention Times (RRT). Also included here are the Toxicity Equivalency Factor (TEF) and Limit of Detection (LOD) for native compounds.
- Concentrations of this compound in Calibration Levels 1-5
- High/Low Recovery Limits for Initial and Ongoing Precision and Recovery (IPR and OPR), calibration Verification (VER), and Labeled Compound Report (LCR)

## Sample List

The data files to be reported and their attributes are identified in this section.

### *Selection of Files*

Files may be added to this list by any of the following methods:

- Import all existing files from a selected directory
- Import a set of existing files based on a Recalculation List
- Select a single existing data file
- Create a Sample List, entering Sample Ids and Sample Types for files to be acquired later (see automation section)

### *Type of Files*

The sample type of each file must be set in the Sample Type field. The default type is “A” (Analysis). The other sample types available are B (Blank), Q (Quality Control), and V (Verification), and 1-5 (Calibration Levels 1-5). The type specifies how the file will be treated in all types of summary reports.

### *Other Attributes*

Other attributes set on this page are dependent on the Sample Matrix set in the Report Information form. These attributes are printed on report headers and may be used in computing the compound amounts.

## Calibrate

The five level calibration set must be acquired and processed in MS Workstation before the Calibrate operation can be performed. The Compound Information form must have been correctly configured Calibration Levels 1-5 entered into the Sample List.

Clicking the Calibrate button initiates a system calibration. During calibration, the sample list is searched for Sample Types 1 through 5. One file of each type is passed through the calibration calculation associated with the corresponding calibration level concentrations. No more than one file of each calibration level type can be processed in a system calibration. Note that the system calibration is altered only when the Calibration button is clicked on the main form. Preparing a Report on a file labeled 1, 2, 3, 4, or 5 will not change the system calibration. Generating an Initial Calibration Report will also not alter the system calibration. When system calibration is complete, the Initial Calibration Report and an error message log are presented for examination and/or printing. Although the Initial Calibration Report can easily be regenerated, the error message log is lost once closed.

### Setup/Preview/Print Reports

This section controls the configuration of the report formats and the selection of reports to be printed for each sample type. It can be used to preview and/or print individual reports for any file in the Sample List or to print all selected reports for all files in the sample list.

## The MS/MS Approach for Dioxin/Furan Determination

### Basics of MS/MS

Full-scan GC/MS in EI mode is not sufficiently selective to perform trace analysis for dioxins and furans. In part this is because interfering species can coelute with the dioxins and furans and some interferents have common ions with the target dioxin/furan compounds. The interferent ions are slightly different in mass from the target compounds, so high resolution mass spectrometry (HRMS) instruments reduce this problem by focusing the masses of choice more accurately.

The objective here is to take a different approach, GC/MS/MS, to eliminate the chemical interferences in dioxin/furan analysis. The ion trap MS is a different alternative to HRMS but it is capable of MS/MS approaches to sample analysis.

Each point in a GC/MS chromatogram can be reconstructed into a mass spectrum. If, instead of immediately scanning the mass spectrum, all the ions are trapped for a period of time, as they are in ion trap MS, it is possible to apply waveforms to isolate a characteristic ion of a target dioxin or furan species. Interfering ions from coeluting interferents are eliminated by this isolation process, except in the odd event that an interfering species also has a mass spectral ion at the same m/z.

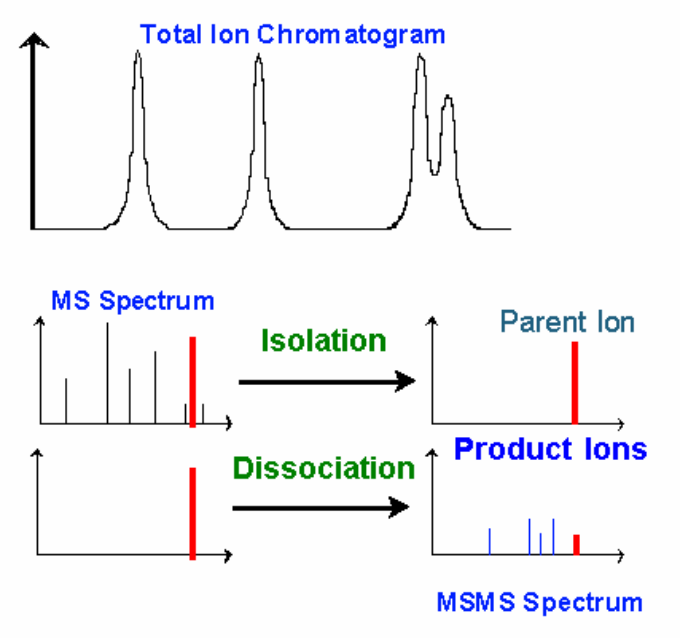
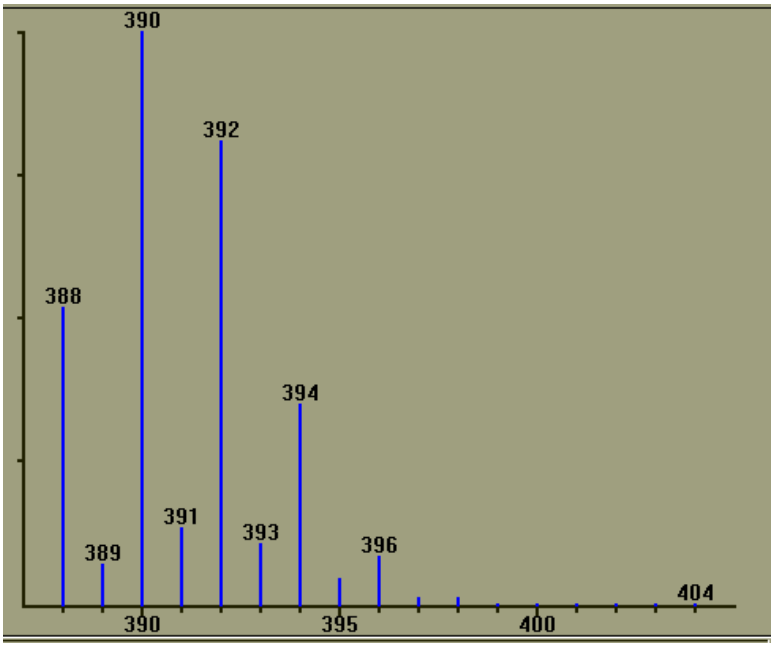



*Illustration of the MS/MS Process*

After the isolation step is completed other waveforms can be applied to dissociate the parent ions by collisions with helium carrier gas from the GC column. This process is called Collision Induced Dissociation (CID) or Collision Assisted Dissociation (CAD). After the CID process, ions are scanned from the ion trap in the normal manner to collect the MS/MS spectrum. The GC/MS/MS method is tailored by Automated Method Development experiments to identify the optimal CID voltage. Even if interference ions comprise a portion of the isolated parent ions they will almost certainly dissociate at different collision energies to product ions of different masses compared to the dioxin or furan parent ions.

## Parent & Product Ions for Dioxins & Furans

As an example of the MS/MS process for dioxins & furans, consider the case of hexachlorodioxins. Using the Isotope Calculator in NIST Library software, one can generate the ion/abundance pattern for the molecular ion cluster. As shown in the accompanying figure, ion abundances are spread over numerous ions in the cluster.

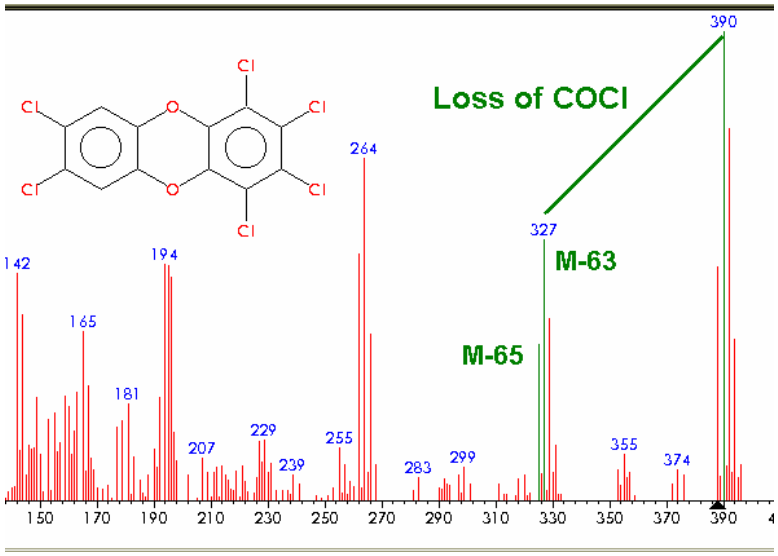



Each of the cluster members is called an isotopomer of the cluster, differing in mass because of differing isotopic content only. The nominal molecular mass (M) is 388, based on the sum of the nominal weights of twelve $^{12}C$ atoms, two $^{16}O$ atoms, two $^{1}H$ atoms, and six $^{35}Cl$ atoms. Note that, mainly because of the negative mass defect of the chlorine atoms, the exact weight of each isotopomer is about 0.2 mass units lower than the nominal mass. The isotopomer at m/z 392 contains a single $^{37}Cl$ atom and is designated the M+2 ion. The ion at 394 is the M+4 ion, and so on.

### *Product Ions for Single Parent Ion Isolation*

What if we chose the isotopomer at the nominal mass m/z 390 as the parent ion for MS/MS? It is always the case that the main CID pathway is the loss of a COCl group. Since the ion at m/z 390 contains one $^{37}Cl$ atom and five $^{35}Cl$ atoms, the chances are 1 in 6 that the COCl loss will be the $CO^{37}Cl$ instead of the $CO^{35}Cl$ fragment. Then the ratio of the Product Ions 325/327 is expected to be 1/5, or 0.2.

When attempting to measure dioxins and furans at very low concentrations it can become difficult to see the two main product ions in the expected ratio, especially if they are expected to differ greatly in abundance.

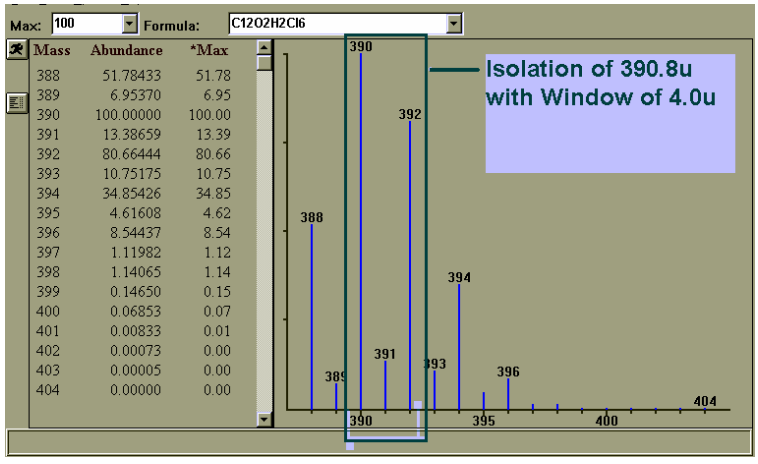



*NIST Mass Spectrum of 1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin*

## *Product Ions for Wider Parent Windows*

To improve the agreement of product ion ratios with expected values and to achieve better Method Detection Limits (MDLs), we have developed the method PCDD_PCDF.mth to allow isolation of a wider parent ion window. The two or three most intense molecular ion isotopomers are isolated and subjected to CID. It is possible to dissociate the entire range of parent ions by applying multiple resonant frequencies to the endcap electrodes. This process is called multifrequency irradiation (MFI).

As shown here, the hexachlorodioxin window has been set up to 4.0 mass units wide, centered about m/z 390.8. That allows efficient isolation of the most intense ions at nominal masses of 390 and 392.




The m/z 390 parent will dissociate to products at (390 - 65 = 325) and (390 - 63 = 327). The parent at 392 will dissociate to product ions at m/z 327 and 329. The relative intensity for each product ion is the sum of contributions from each dissociation channel.

| Parent | Relative Abundance | Loss | Fraction | Product Ion Abundance | Product Ion |
|---|---|---|---|---|---|
| 390 (M+2) | 100.0 | $CO^{37}Cl$ | 1/6 = .167 | 100 * .167 = 16.7 | 325 |
| 390 (M+2) | 100.0 | $CO^{35}Cl$ | 5/6 = .833 | 100 * .833 = 83.3 | 327 |
| 392 (M+4) | 80.66 | $CO^{37}Cl$ | 2/6 = .333 | 80.66 * .333 = 26.9 | 327 |
| 392 (M+4) | 80.66 | $CO^{35}Cl$ | 4/6 = .667 | 80.66 * .667 = 53.8 | 329 |

The most intense product ions will be those at m/z 327 (relative intensity 83.3 + 26.9 = 110.2) and m/z 329 (relative intensity 53.8). The expected product ion ratio is 110.2/53.8 = 2.05.

The PCDD_PCDF_MRM.mth method file has been constructed so that the two or three most intense isotopomers are isolated for each dioxin/furan class.

Qualifier ion ratios have been set in Dioxin Reports to require the ratio of peak areas of the two most intense product ions agree within 25% with the expected isotope ratio.

# Analytical Conditions and Methods

The Dioxin Reports template has been set up by default to process data files collected with the MS Workstation method PCDD_PCDF_MRM that is supplied when the Dioxin Reports option is loaded for the Varian MS Workstation. This section of the manual details the AutoSampler, GC, and MS method sections and provides some suggestions for sample vials, analytical column and other ancillary details.

Using the same column noted here and the same analytical method should provide files that can be processed by Dioxin Reports without significant modification.

## Instrument Configuration

### 8400 AutoSampler [CombiPAL is an alternative]

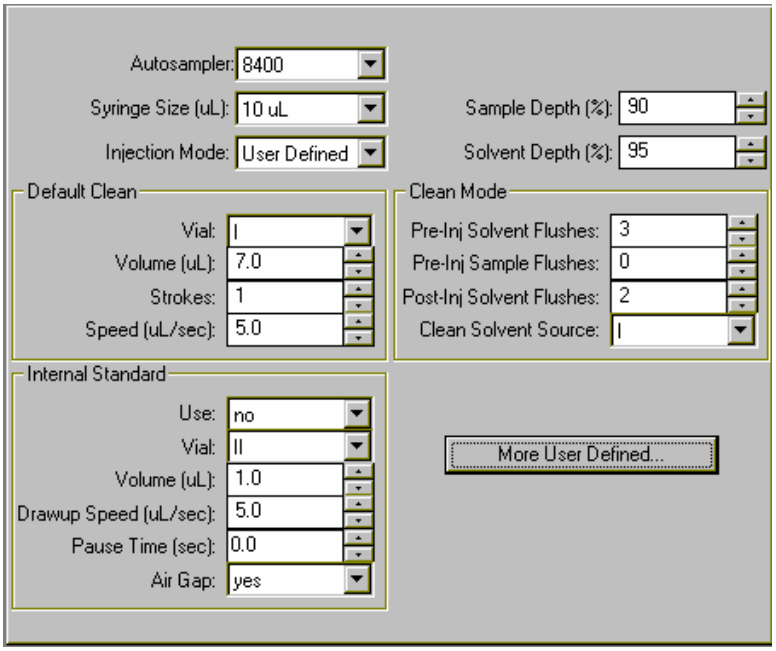
#### *Solvent, Septa, and Sample Vials*

Use ***n-nonane*** as the solvent in both Default Clean and Clean Mode wash vials. Repeated injections from the same calibration standard sample vials can lead to contamination of standards by siloxanes from sample vial or wash vial septa. Some ions in the mass spectra of contaminant peaks are found within the Parent Ion isolation windows for dioxin and furan congeners; artifact peaks from siloxane contaminants can thus appear in the chromatographic results.

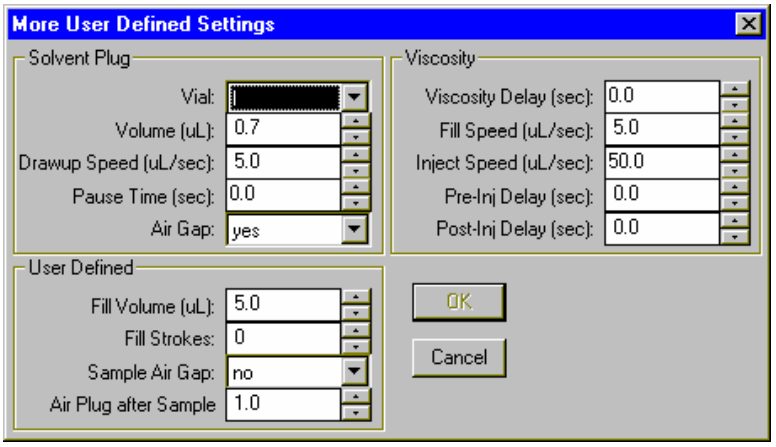
The use of Ultra septa for sample vials will greatly reduce siloxane contamination. The Ultra 9 mm Wide Opening Screw Vial Kit (P/N 392611979) contains 100 vials with these septa already set in the vial cap. Additional Ultra septa can be ordered in packages of 50 (P/N 392611985). For the wash vials of the 8400 AutoSampler, Ultra septa inserted in the 20 mm vial caps may be ordered in packages of 100 (P/N 392611984). The 20 mm Ultra septa alone are also available in packages of 50 (P/N 392611986).

#### *8400AS Software Parameters*

Note that depending on the sample volume, autosampler vial, and insert used you may need to adjust the Sample Depth appropriately.




*8400 AutoSampler Parameters*




*8400 AutoSampler Parameters (More User Defined)*

## 3800/3900 Gas Chromatograph

1177 Injector with Type 1 Electronic Flow Control

Injection Liner: 4-mm Siltek fritted, single gooseneck insert
[Varian PN: RT210462145] (5/pk)
Position insert with the gooseneck down

Injector Septa: Varian 9 mm BTO
[Varian PN: CR298713] (50/pk)

Column: CP-Sil8 Low Bleed MS
50m x 0.25 mm ID x 0.25 μm film thickness
[Varian PN: CP5843]

Septum Purge: 2 mL/min @ 45 psi

## Saturn 2100/2200 Mass Spectrometer

### *Silchrom Electrodes*

| | |
|---|---|
| Trap Temperature: | 220 °C |
| Manifold Temperature | 80 °C |
| Transfer Line Temperature: | 280 °C |

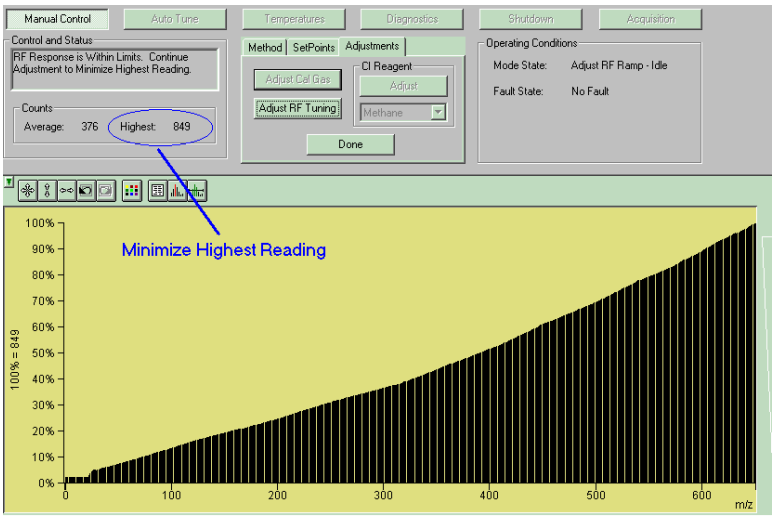
# Tuning the Saturn Mass Spectrometer

## Activate the Standby Method

All AutoTune procedures should be performed while the method PCDD_PCDF_Standby.mth is active. This method is in the Dioxin Data directory of Varian WS. The standby method holds the GC in split mode to keep the injector clean. The column is maintained at 200 °C; this is the optimal temperature for mass calibration and trap function calibration. The helium flow rate is constant at 1.0 mL/min; pressure pulse is (and must be) *OFF* for AutoTune functions.

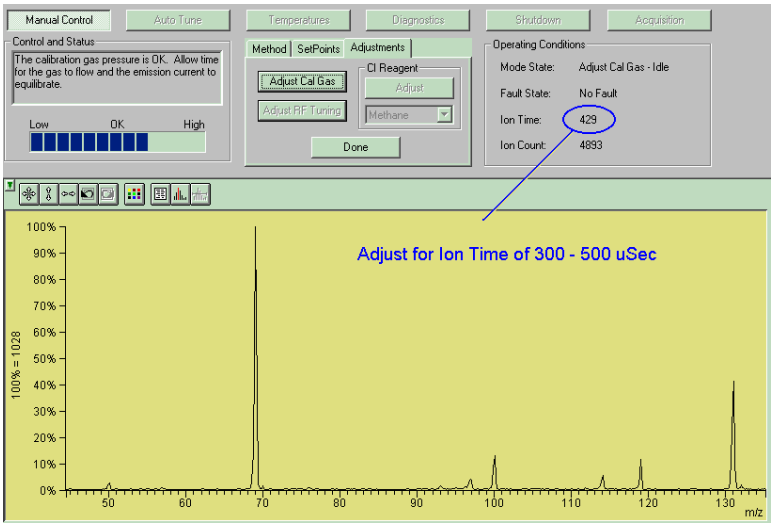
## Adjustments in Manual Control

If RF Adjust has not been run since the last time the ion trap was reassembled, do this adjustment first.




*RF Adjustment in Manual Control*

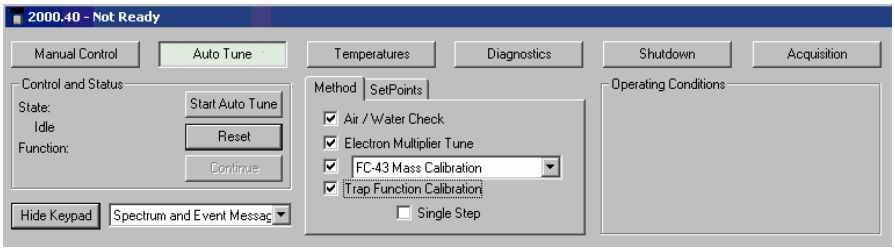
Next, adjust the Calibration Gas. Set the Cal Gas flow so that the Ion Time is between 300 - 500 μsec. This makes the Trap Function Calibration step in AutoTune run smoothly.




*Calibration Gas Adjustment in Manual Control*

## AutoTune

Run all of the tuning routines. Air/Water should be checked every day. Multiplier tune needs to be rerun only if a loss of sensitivity is noted during Dioxin/Furan Verification runs. Trap Function Calibration must be rerun any time Mass Calibration is performed or MS/MS data cannot be collected.




*Auto Tune Dialog*

# The Data Acquisition Method

You will generally need to use several separate data acquisition methods to develop the final dioxin/furan analytical method. The acquisition methods in the Dioxin Data directory of Varian MS have the same gas chromatographic method which has been optimized for the analysis with the CP-Sil8 50m x 0.25 mm ID x 0.25 μm film thickness (Varian P/N CP5843).

## Chemical Standards

Wellington Laboratories has a full line of unlabeled and C13-labeled dioxin and furan standards. The Wellington Catalog and ordering information are both available on-line at:

http://www.well-labs.com

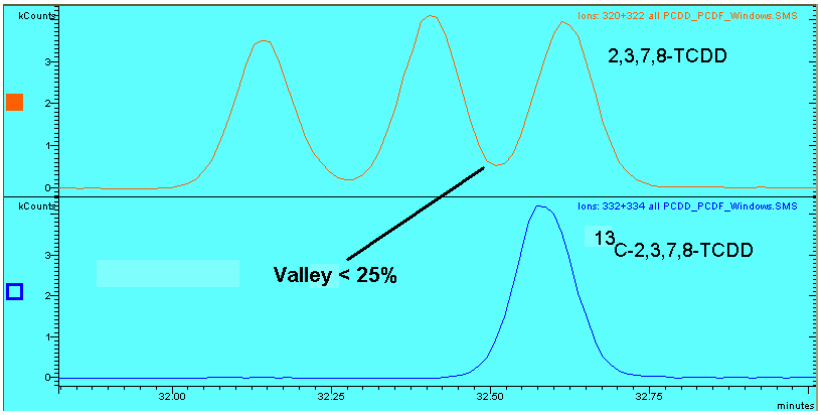
## Full Scan Acquisitions

First you need to run full-scan EI/MS acquisitions for the Windows Defining solution or an Isomer Specificity test mix and for a mid-level (CS3) calibration standard. To acquire full-scan data, activate the method PCDD_PCDF_Windows.mth and place the appropriate sample in the AutoSampler.

Since this is a pressure pulse method, it is necessary to assure that the Septum Purge is calibrated while the pressure pulse is active. This is done from the GC front panel for the 3800 GC; a septum purge flow of 2 mL/min is suggested.

### *Windows or Isomer Specificity Solutions*

Either the Windows Defining solution (Wellington P/N 5CWDS) or the TCDD Isomer Specificity test mix (Wellington P/N 5TCDD) can be used to verify adequate resolution between 2,3,7,8-TCDD and other closely eluting tetra dioxins. The valley between the 2,3,7,8 isomer and any other tetrachlorodioxin must be < 25%. The following figure was taken from a file collected with the PCDD_PCDF_Windows method. Mass chromatograms are displayed for the sums of m/z 320+322 for TCDD and 332+334 for $^{13}$C-TCDD. The 2,3,7,8-TCDD is easily located because the 13C-labeled 2,3,7,8 is included in the solution and coelutes with the unlabeled compound. As you can see, for the chosen chromatographic conditions, the resolution meets the 25% valley requirement.




*Acceptable TCDD Resolution*

### *CS3 Solution*

Collecting a data file of the mid-level CS3 standard with the method PCDD_PCDF_Windows lets you establish the time windows for elution of the 13C-labeled tetrachloro- through octachloro- furans and dioxins. The MS/MS method will be constructed to give the best possible data for the members of each class of target analytes for Dioxin Reports. The time windows for each class are decided based on this data file.

Note that appropriate time segments for each congener class are already set up in the default GC/MS/MS method PCDD_PCDF_MRM if the suggested 50m CPSil 8CB column is used. Note that wherever possible each MS acquisition segment was set up so that data are collected in Multiple Reaction Monitoring (MRM) of only two different Parent Ions. However when the time widows for different classes overlap it is necessary to collect more than two ions in a given segment. For example a single segment is used to collect data for the four unlabeled and C13-labeled hexachloro- dioxins and furans.

## MS/MS Automated Method Development

Although the default MS/MS method supplied (PCDD_PCDF_MRM) has been prepared with suggested Collision Induced Dissociation voltages for each MS/MS segment, the methods PCDD_AMD and PCDF_AMD are provided in case the voltages need to be adjusted. The hexa, hepta, and octa segments for the two methods are set up specifically for dioxin and furan AMD in the two respective methods. Both dioxin and furan segments are available in both methods for tetra and penta classes. These methods are set up to test a range of CID voltages for each target dioxin or furan class.

## Multiple Reaction Monitoring of Dioxins and Furans

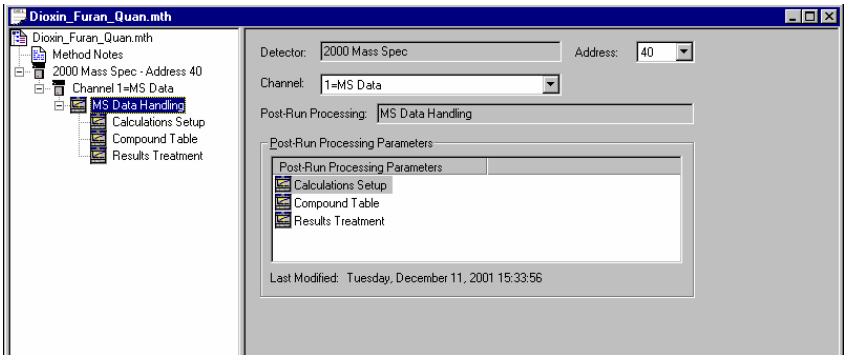
The method PCDD_PCDF_MRM is installed in the Dioxin Data subdirectory in Varian WS. The AutoSampler and GC parameters are identical to the full scan method PCDD_PCDF_Windows. Use this method to acquire all Calibration, Verification, and Analysis files. At least one calibration run must be processed within the MS Workstation as a calibration data point so that the MS Workstation Data Handling method can process files for later use in Dioxin Reports template.

# The Data Handling Method

Dioxin Reports uses the results of data files processed in MS Workstation, Version 6.2. (Data generated with prior versions of the software also can be processed, but first must be converted to the format of Version 6.2.)

Dioxin Reports uses retention times and peak areas from the processed results already stored in the MS workstation data files but does its own calculations for quantitative results and reporting limit tests.

Before using Dioxin Reports, a MS Workstation method (.mth) must be built and used to process Calibration Levels 1-5. The rest of this chapter discusses the use of the MS Workstation Method Builder to build methods for use with Dioxin Reports.




*Sections of the MS Data Handling Method*

The data handling section of the method must be built with great care to deliver the best results.

The Calculation Setup section of the Data Handling method must be properly configured to allow proper identification of all members of each dioxin/furan Class.

In the Compound Table section of the method, the compound identification, integration, calculation and quantitation parameters must be optimized to deliver the best results. Review the compound table integration and identification parameters (peak width, slope sensitivity, tangent %, peak window width, etc.) before the calibration is carried out. It is not necessary to adjust the curve fitting options (including the handling of the origin and the regression weighting parameters) because quantitation is based upon average RRF calculations in Dioxin Reports software.

# Calculations Setup in the MS Workstation (.mth) Method

Use the following settings:

General:

| | |
|---|---|
| Measurement Type: | Area |
| Calibration Type: | External Standard |
| Report Missing Peaks: | Yes (checked) |
| Report Unknown Peaks: | Yes (checked) |
| Normalize Results: | No (not checked) |
| Ignore Calibration Data: | No (not checked) |
| Scale Air Flow Samples: | No (not checked) |

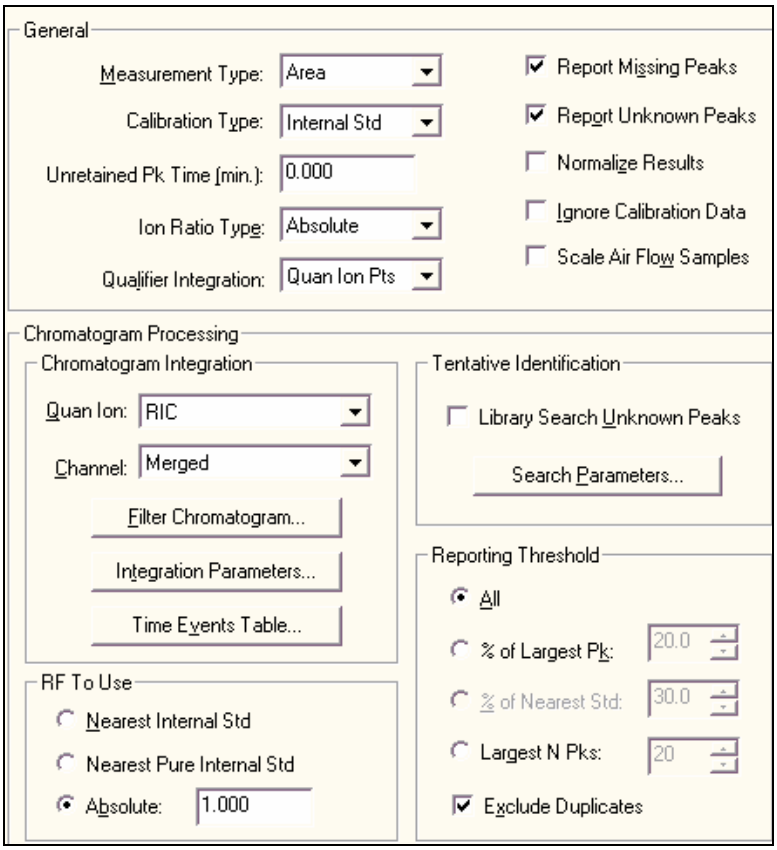
## Chromatogram Processing

Tentative Identification

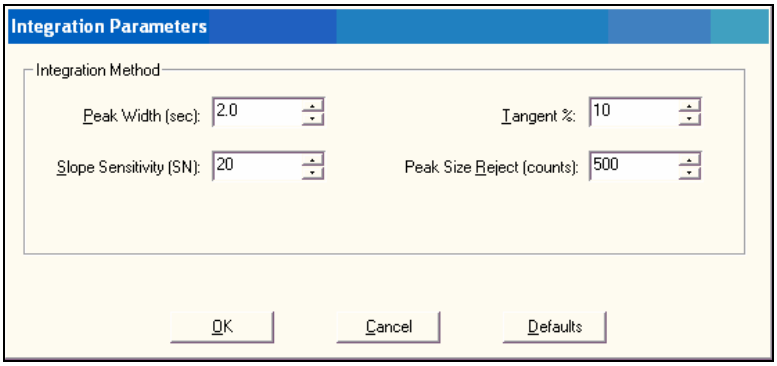
Library Search Unknown peaks: No (Not Checked)

Reporting Threshold

Exclude Duplicates: Yes (Checked)




*Configuration of Calculations Setup dialog in the Method Builder*




*Integration Parameters for Chromatogram Processing*

# Compound Table Setup in the MS Workstation (.mth) Method

The MS/MS method for dioxin analysis is set up to perform EI/MS/MS on each of the following dioxin and furan classes.

| Dioxin Class | Identity | Furan Class | Identity |
|---|---|---|---|
| TCDD | Tetrachlorodioxins | TCDF | Tetrachlorofurans |
| 13C-TCDD | $^{13}$C-labeled-TCDD | 13C-TCDF | $^{13}$C-labeled-TCDF |
| 37C-TCDD | $^{37}$Cl-labeled-TCDD | | |
| PCDD | Pentachlorodioxins | PCDF | Pentachlorofurans |
| 13C-PCDD | $^{13}$C-labeled-PCDD | 13C-PCDF | $^{13}$C-labeled-PCDF |
| HxCDD | Hexachlorodioxins | HxCDF | Hexachlorofurans |
| 13C-HxCDD | $^{13}$C-labeled-HxCDD | 13C-HxCDF | $^{13}$C-labeled-HxCDF |
| HpCDD | Heptachlorodioxins | HpCDF | Heptachlorofurans |
| 13C-HpCDD | $^{13}$C-labeled-HpCDF | 13C-HpCDF | $^{13}$C-labeled-HpCDF |
| OCDD | Octachlorodioxin | OCDF | Octachlorofuran |
| 13C-OCDD | $^{13}$C-labeled-OCDD | | |

Depending upon the retention times observed for each class, between two to four classes may be determined by Multiple Reaction Monitoring in a given time segment of the chromatogram. The Compound Table is set up with three entries for each analyte. In the first entry, the area of the sum of two product ions for each analyte is measured. Then in the successive entries the area of each individual product ion is measured. This allows Dioxin Reports template to evaluate the Qualifier Ion ratios. Although the ultimate processing of the data in Dioxin Reports is via Internal Standard quantitation, all entries in the Compound Table are treated as target compounds.

Reporting of target analytes in Dioxin Reports will be strongly dependent on the parameters set in the Compound Table dialog. Target compounds excluded by these threshold parameters will be excluded from Dioxin Reports. The important considerations in optimizing the data handling method are discussed below for each tab dialog in the data handling method from Compound Attributes to Identification.

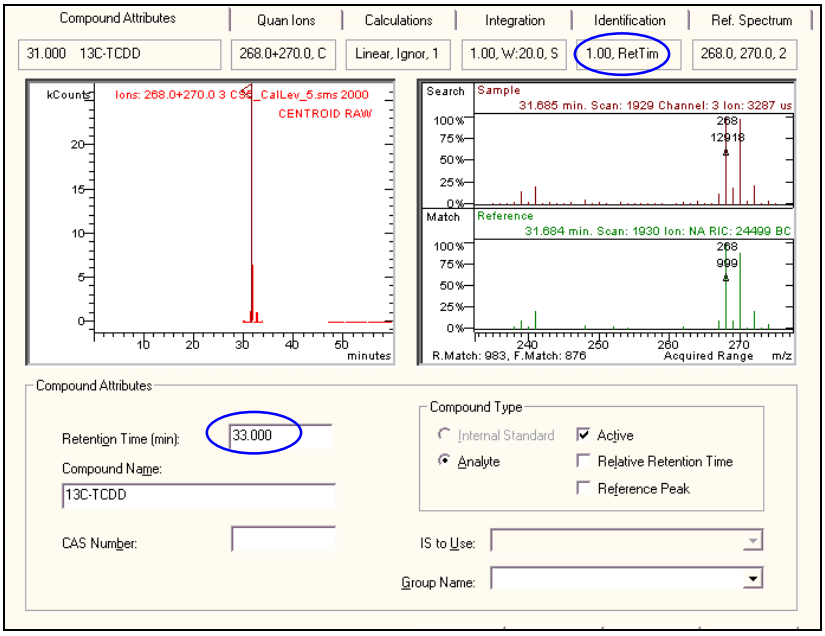
## Compound Attributes Dialog

Several items are worth noting in this dialog. All compounds are treated as analytes. The retention time is the center of the time window for the acquisition segment of the method. The width of the window is set in the Identification tab dialog so that it covers the entire acquisition segment. For example, for TCDF species in Segment 2 of the method, the acquisition segment is from 30 to 32 minutes:

| | Segment Description | Start (min.) | End (min.) | Low Mass (m/z) | High Mass (m/z) | Ionization Mode | Ion Preparation |
|---|---|---|---|---|---|---|---|
| 1 | Fil/Mult Delay | 0.00 | 30.00 | 50 | 650 | None | None |
| 2 | TCDF | 30.00 | 32.00 | 235 | 275 | EI Auto | MRM |
| 3 | TCDD | 32.00 | 34.00 | 250 | 295 | EI Auto | MRM |
| 4 | PCDF | 34.00 | 43.70 | 270 | 295 | EI Auto | MRM |
| 5 | PCDD | 43.70 | 47.00 | 285 | 310 | EI Auto | MRM |

*Acquisition Method Segment for Tetrachlorodioxins*

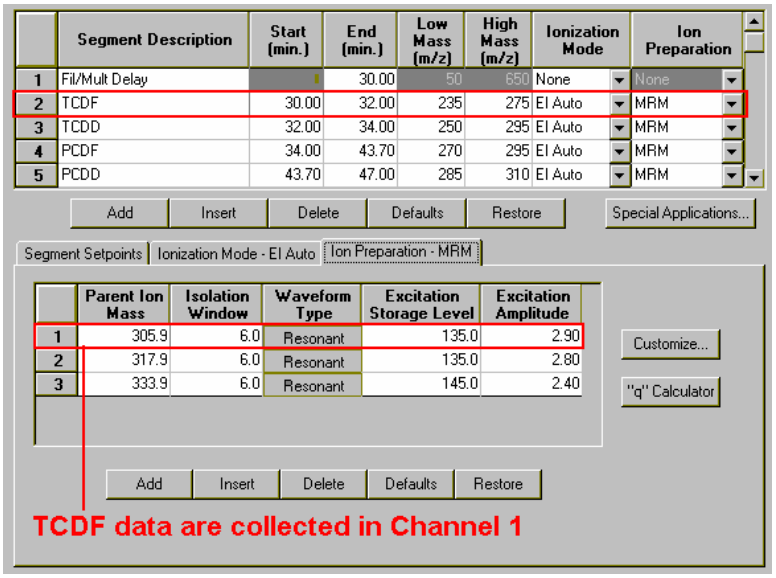
Therefore in the Compound Attributes dialog the retention time is set to the middle of this window. And in the Identification dialog the time window is set to ± 1.00 minute.




*Setting Time Windows Per Acquisition Segment Parameters*

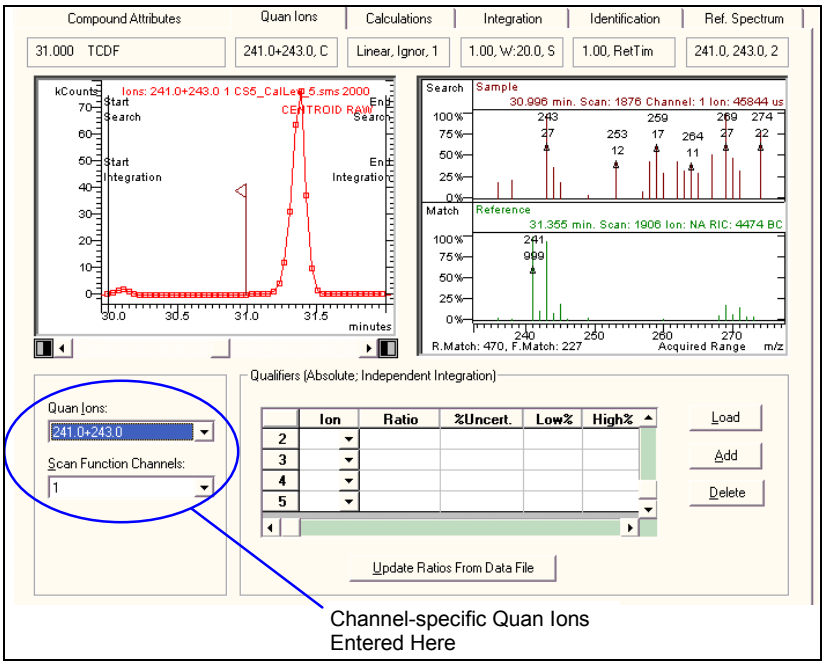
## Quantitation Ions Dialog

The acquisition method designates the MRM Channel in which data for a given compound are collected. For example, here is the acquisition method information for the TCDF segment. The native (non-13C-labeled) TCDF data are collected in Channel 1. The parent ion cluster around m/z 305.9 is dissociated to product ions at m/z 241 and 243.




*MRM Parameters for the Tetrachlorofuran Segment (includes one 13C-TCDD component also)*

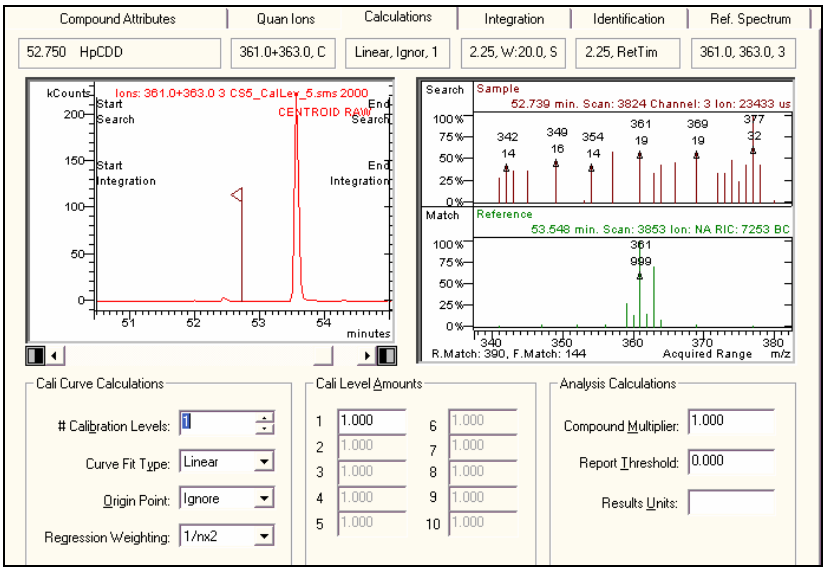
In the Data Handling method, the first entry for TCDF is for the sum of the quantitation ions 241+243. Note that Channel 1 is entered as the Scan Function Channel. The subsequent two entries will be those for 241 and 243 ions alone. Note that no Qualifier Ions are entered in the Data Handling method. All qualifier ion calculations are performed in the Dioxin Reports template.




*Use the appropriate Channel for Data Handling relative to the MRM dialog in the MS acquisition method*

## Calculations Dialog

The Calculations Dialog is set up for a single calibration level. The Data Handling method must be used to process just one of the calibration data files in calibration. The Dioxin Reports template will do the complete calibration outside the Data Handling method. The important thing about data handling is to integrate all the peaks for each data file with consistent integration parameters. Note that the Report Threshold may be entered manually based upon the MDL values from Dioxin Reports calculations.



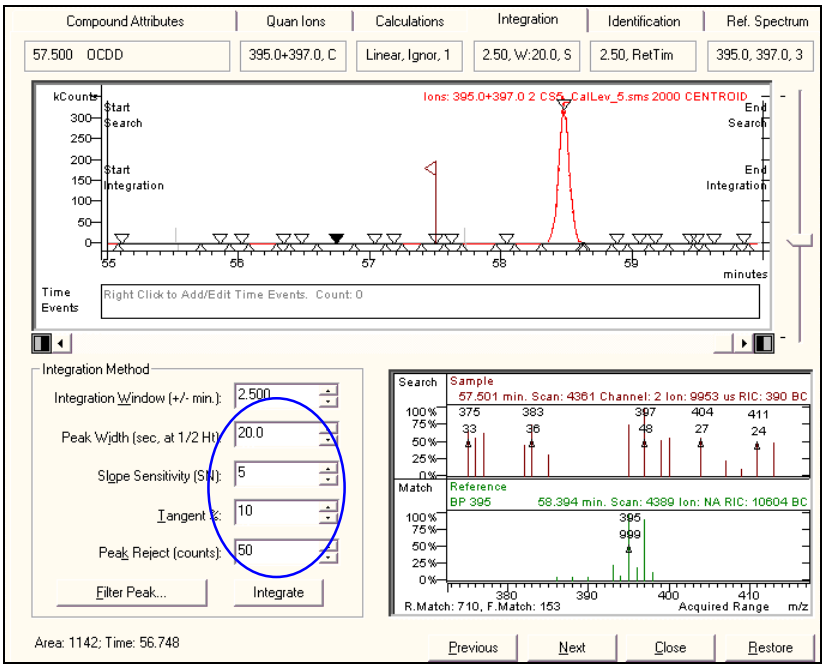

*Only One Calibration Data File Needs to be Processed*

## Integration Dialog

*Please Note: Peak Detection parameters, especially the Peak Width and Slope Sensitivity, must be **IDENTICAL** for all Q1+Q2, Q1, and Q2 compound entries for both the native and $^{13}$C-labeled species of each class.*

Otherwise, there may be failures to identify a peak because one of the entries does not meet retention time agreement requirements in the Dioxin Reports template.

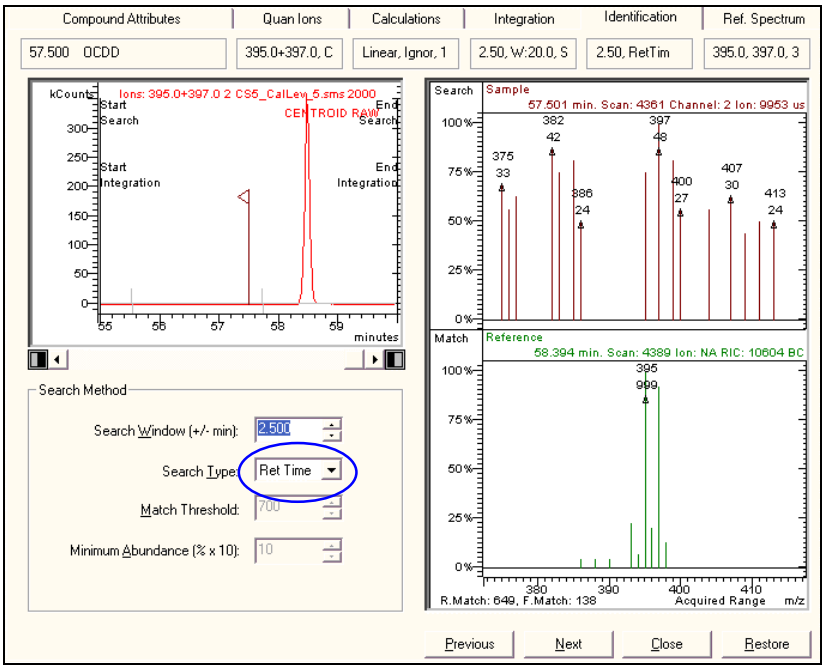
The Peak Area Reject threshold is always set for 50 area counts.




*Integration parameters must match for all native, labeled class members and for both Quantitation and Qualifier Ion entries in the Compound Table*

## Identification Dialog

Identification for all entries is based upon finding peaks within the retention time window for each chromatographic segment. The Expected Retention Time is set to be at the middle of each method segment and the peak window is set up so that the Expected Retention Time ± the Peak Window covers the entire method segment time window. For OCDD, the Expected RT is 57.5 and the Peak Window is 2.5 minutes. The time range for the OCDD segment in the acquisition method is from 55.00 to 60.00 minutes.




*Only RT Searching for all entries; Peak Window is half the width of the relevant acquisition segment*

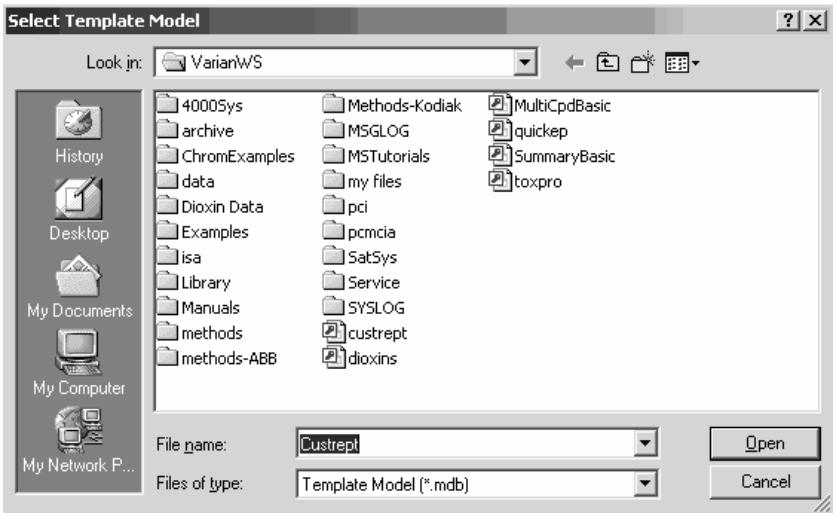
# Start: Main Page

## Launching Dioxin Reports

A MS Workstation method must to be completed and data files must be acquired and processed in MS Workstation before reporting can take place. Please review the sections Analytical Conditions and Methods to configure the data handling section properly.

Dioxin Reports software is launched from the Star Toolbar by pressing the "MS CUSTOM" icon. It also can be started via the Start/Programs/MS Workstation/Custom MS reports path.


**Custom Reports Icon on the Star Toolbar**

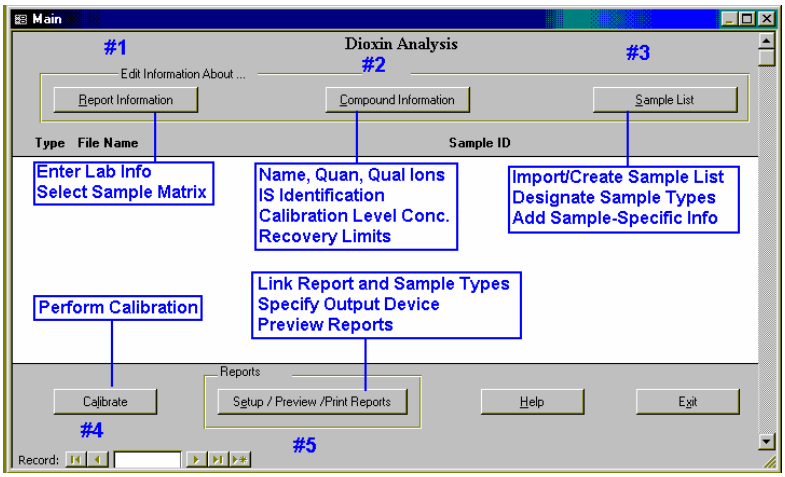



*Selecting the Dioxin Model Template*

When a new report template is being created, select the Dioxins.mdb model template to start a new reporting format. Save the template under a desired name. The template file will have .swt extension.

# Main Page

As discussed in the Overview section, a certain order should be followed when creating a *new Dioxin Reports template*.

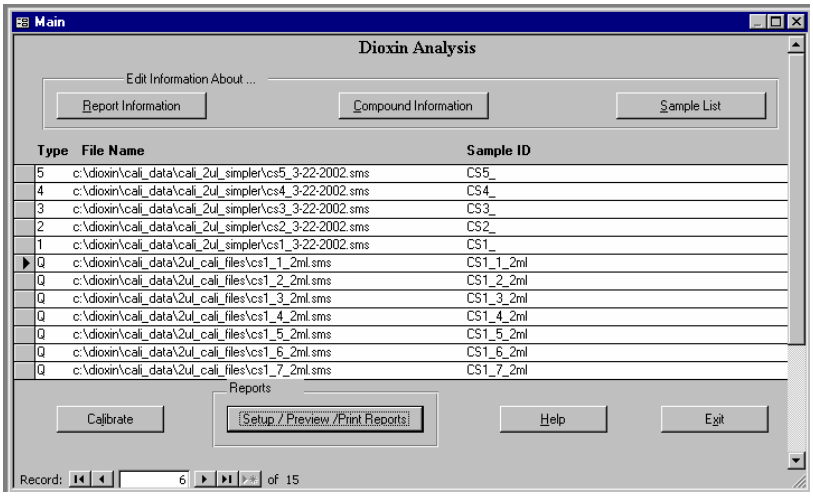



*Main Page of Dioxin Reports*

The first step is usually the configuration of the **Report Information** section.

The **Compound Information** section should be completed in the next step. All compound-specific criteria including QA/QC criteria are specified here for the target analytes and internal standards.

When the *Dioxin Reports* template is entered after the template has been set up, or after completing the actions outlined above, click the **Sample List** button to configure the list of files used to generate the desired reports. The original sample list must include data files for calibration levels 1 through 5. After a Sample List has been created and the Sample List Dialog is closed, the new sample list will be displayed on the Main Page.




*Main Page of Dioxin Reports after Sample List Created*

Click the **Calibrate** button next so that calibration can be performed on the five levels of calibration data files. After Calibration has been performed successfully, you may in the future just choose a desired file to report in the Sample List

Then choose an initial file to be processed by using the mouse to position the black selection triangle in the displayed Sample List. Now click the **Setup/Print/Preview Reports** button to configure report options, preview and print individual reports, or configure and generate report sets to be exported to ASCII files or printed.

# Buttons: Main

## Help

This is the Main Page of the Dioxin Reports template. For Help here or elsewhere in the software, position the mouse cursor over the item of interest and click the right mouse button. Select the "What's This?" item from the floating menu that appears and click on the item you wish to understand.

## Report Information

The **Report Information** dialog is used to select the Sample Matrix and configure report headers. The Sample Matrix setting determines the units to be used in reporting concentrations on the Analysis and TEQ Reports. It also affects the sample list format.

## Compound Information

When clicked the **Compound Information** button opens the Compound form to edit compound-specific information controlling report content.

## Sample List

When clicked the **Sample List** button opens the Sample List form, enabling creation of sample lists and selection a sample file types.

## Calibrate

Clicking the **Calibrate** button initiates calibration of the five calibration levels identified in the Sample List. This operation must be performed before any reports can be prepared. During calibration, the sample list is searched for sample types 1 through 5. One file of each type is passed through the calibration calculation associated with the corresponding calibration level concentrations. No more than one file of each calibration level type can be processed in a system calibration. Note that the system calibration is altered only when the Calibration button is clicked on the main form. Preparing a Report on a file labeled 1, 2, 3, 4, or 5 will not change the system calibration. Generating an Initial Calibration Report will also not alter the system calibration. When system calibration is complete, the Initial Calibration Report and an error message log are presented for examination and/or printing. Although the Initial Calibration Report can easily be regenerated, the error message log is lost once closed.

## Setup/Preview/Print Reports

Clicking the **Setup/Preview/Print Reports** button processes the currently selected file in the sample list displayed on the Main form and then opens the Setup/Preview/Print Reports form. Before clicking on this button, set up the sample list, compound table, and report header, and ensure that the data file on which to report is selected with the black triangle on record selector.

The Setup/Print/Preview Reports form allows report configuration, selection of reporting options, and preview and printing of individual reports. Sets of reports to be prepared for an entire sample list may be configured and report sets generated for printing or export to ASCII files.

Opening this form is the gateway to configuring and printing reports in response to an AutoLink invocation from System Control or printing reports in response to a Star Toolbar print file command.

## Exit

Clicking the **Exit** button causes the Dioxin Reports application to close.

# Fields: Main

The fields shown in this page can not be edited here; they are entered/edited in the Sample List page.

## Sample ID

The **Sample ID** field shows the content of the Sample ID field as set on the Sample List form. See help for the Sample ID field on the Sample List form for additional information. Sample ID is normally the sample name used to acquire the data file. It may be overridden and set to any text string by typing the desired name in the Sample ID field in the Sample List form.

## File Name

The **file name** field contains the full path name of a MS Workstation data file. This field is set on the Sample List form.

## Type

The sample type selects a report profile set for the current sample. Sample Types 1, 2, 3, 4, and 5 specify the corresponding calibration level.

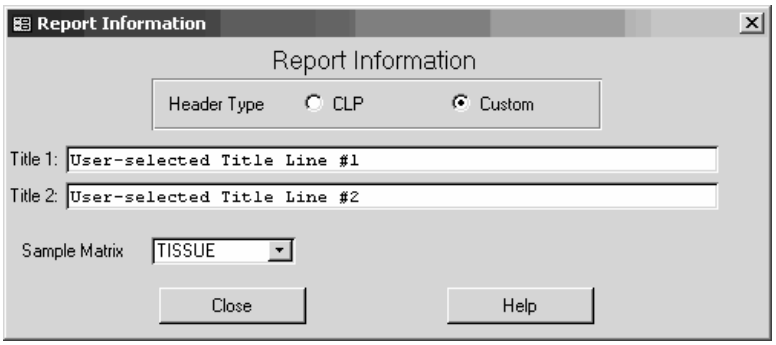
Other sample types are A (Analysis), B (Blank), C (Calibration Verification), and Q (Quality Control).

This field is set in the Sample List form.

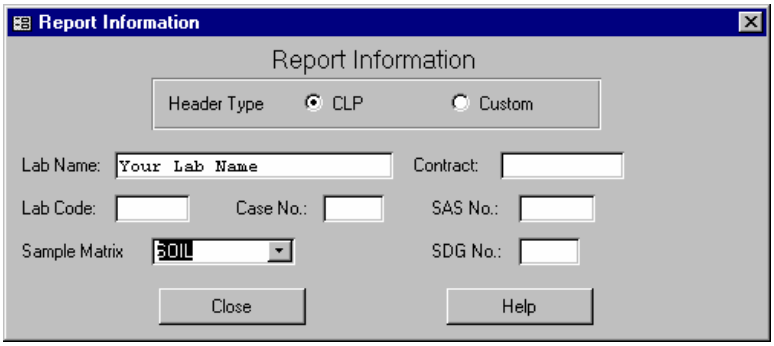
# Report Information

The Report Information settings determine the format and content of report headings. The Sample Matrix setting determines reporting units on the Analysis and TEQ reports, and the parameters shown on the Sample List form. Select the Header Type first, as it controls the information displayed. Right-click the mouse on any field for context-sensitive help.

The two header options are CLP or Custom. In the CLP option the header information content is based on the CLP reporting format. In the custom report, the user has two 60 character title lines which can be filled out as desired. The font size and style are preset. Titles are center aligned with the main report title.




*Custom Report Information Form*




*CLP Report Information form*

# Buttons: Report Information

## Header Type: CLP or Custom

The Header Type radio button group selects between Contract Laboratory Program (CLP) and Custom report headers. The CLP header shows Laboratory Name, Contract, Lab Code, Case No, SAS No, and SDG No. Custom headers offer two centered title lines. The configuration of the Report Information form changes to display the configurable fields for the Header Type selected.

## Help

The Report Information settings determine the format and content of report headings. The Sample Matrix setting determines reporting units on the Analysis and TEQ reports, and the parameters shown on the Sample List form. Select the Header Type first, as it controls the information displayed. Right-click the mouse on any field for context-sensitive help.

## Close

The **Report Information** form is closed when the Close button is clicked and focus is returned to the Main *Dioxin Reports* form.

# Text Boxes: CLP Type Header

## Lab Name

**Lab Name** is a text field of up to 25 characters.

## Contract

**Contract** is a text field of up to 11 characters

## Lab Code

**Lab Code** is a text field of up to 6 characters

## Case No.

**Case Number** is a text field of up to 5 characters

## SAS No.

**SAS Number** (Special Analytical Services Number) is a text field of up to 6 characters.

## SDG No.

**SDG No.** (Sample Delivery Group Number) is a text field of up to 5 characters

### Sample Matrix

The Sample Matrix choices are WATER, SOIL, or TISSUE. The same setting is used for all samples reported. This choice controls the format of the sample list form, the format of the sample header line, and the concentration units shown on the TEQ and Analysis reports.

## Text Boxes: Custom Type Header

### Title 1 text box

The Title 1 field contains the text to be displayed in the top subtitle of the Custom header. The Custom Title 1 field contains a maximum of 60 characters (upper or lower case). The font size and style are preset. Titles are center aligned with the main report title.

### Title 2 text box

The Title 2 field contains the text to be displayed in the bottom subtitle of the Custom header. The Custom Title 2 field contains a maximum of 60 characters (upper or lower case). The font size and style are preset. Titles are center aligned with the main report title.

### Sample Matrix

The Sample Matrix choices are Soil, Water, or Tissue. The choice will affect the format of reports prepared in Dioxin Reports.

# Compound Information

The Compound Table contains all target compound-specific information used for reporting dioxin results. Compound information is presented in several views. The Compound form is organized to display all information about one compound on one form. Selected information for all peaks in the compound table is presented in the **Integration**, **Identification**, **Calibration**, and **Recovery Limits** forms.

Generally it should not be necessary to edit Compound table information on these forms unless target compounds must be added or subtracted from the reporting list. Parameters specific to porting to a new instrument or column are all primarily controlled by the MS Workstation method PCDD_PCDF_MRM.mth and should be configured there first.

The MS Workstation method and the Compound Table in Dioxin Reports must conform to each other, and this table must be internally consistent as follows:

For each class entered in the Compound table, the MS Workstation method must have a corresponding data acquisition channel and segment with an ion preparation method designed to prepare the MS/MS target ions specified for the class. The MS Workstation Data Handling method must be configured to contain three target compound classes for each Dioxin class, one each for Quantitation Ion specification of M1+M2, M1, and M2. The data acquisition segment must span the elution time range for all compounds in the class, regardless of whether the compound is listed as a specific target compound in the Dioxin method. The corresponding data handling target compound should have its retention time set to the midpoint of the data acquisition segment, and the Identification Peak Window should be set to one half the data acquisition segment width. The purpose of this is to acquire and integrate all peaks in the class within the span of this target compound window. Only peaks with areas that exceed the Data Handling Integration Peak Area Reject value will be reported in Dioxin reports.

---

**IMPORTANT:** There must be no more than one MS Workstation method component for each mass specification (M1+M2), M1 and M2 for each data acquisition segment and channel. It is very important that the same peak (same mass spectrum, data handling Channel, and retention time) not be reported more than once in a file.

**IMPORTANT:** The ordering of masses in a mass specification is significant and must be identical in Dioxin compound table and the MS Workstation data handling method Quantitation Ion entry. "264+266" is not the same as "266+264".

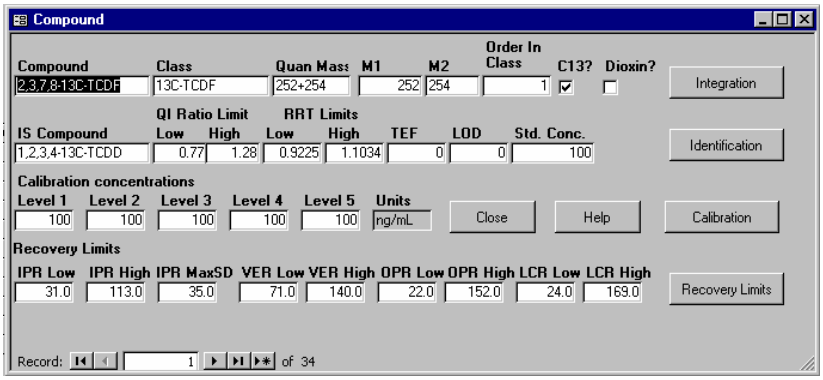
---

The Dioxin compound table must be self-consistent in the following ways.

1. All compounds in the same class must have the same Quantitation Ions, M1 and M2.
2. If C13? is checked, then the Order In Class field must specify the retention time ordering of the target compounds within the class. Taken as a group, these class members must be the largest peaks in the analysis sample class window, and all peak members of the class must be found in each sample.
3. Exact data entry of names and numbers is critical. Text matches are done between Compound and IS Compound, between the class fields of different compounds, and between the Quantitation Ion, M1, and M2 fields and the Quantitation Ion specification in the MS Workstation results.

For information on specific Compound form entry fields, right click the mouse over the field of interest to get context-sensitive help.

If it is required to edit the information for the entire Compound list, it is easiest to click the button for the relevant summary information to perform changes. For example to enter the LOD (Limit of Detection) values, click the **Identification** button to allow access to this field for all compounds.

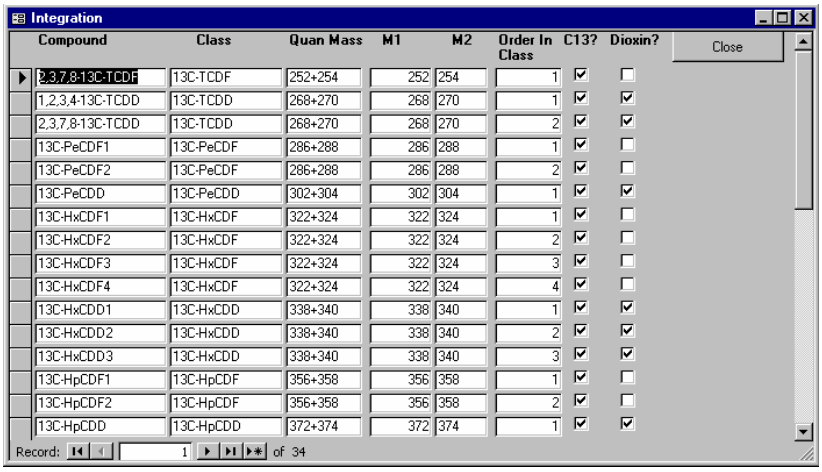



*The Compound Form*

# Buttons: Compound

## Integration

Clicking the Integration button displays the fields on the first line of the compound form for all compounds in the table, in tabular form. This specifically includes the fields Compound, Class, Quantitation Mass, M1, M2, Order in Class, C13?, and Dioxin? In the standard template, the Quantitation Mass is always the sum of the Qualifier Ions, M1 and M2. Order in Class is important when there is more than one 13C-labeled compound in a given class. This specification allows the template to correctly identify each congener. C13? Is checked for all 13C-labeled compounds. Dioxin? Similarly, the Dioxin? Field is only checked if the compound is a dioxin.



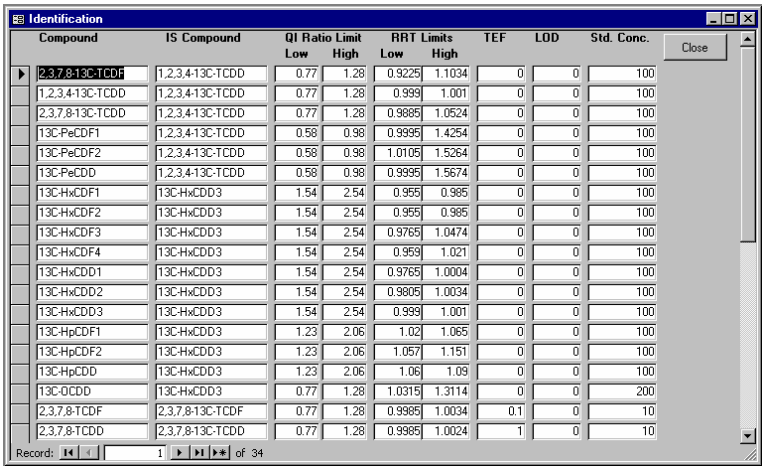

| Compound | Class | Quan Mass | M1 | M2 | Order In Class | C13? | Dioxin? |
|---|---|---|---|---|---|---|---|
| 2,3,7,8-13C-TCDF | 13C-TCDF | 252+254 | 252 | 254 | 1 | ☑ | ☐ |
| 1,2,3,4-13C-TCDD | 13C-TCDD | 268+270 | 268 | 270 | 1 | ☑ | ☑ |
| 2,3,7,8-13C-TCDD | 13C-TCDD | 268+270 | 268 | 270 | 2 | ☑ | ☑ |
| 13C-PeCDF1 | 13C-PeCDF | 286+288 | 286 | 288 | 1 | ☑ | ☐ |
| 13C-PeCDF2 | 13C-PeCDF | 286+288 | 286 | 288 | 2 | ☑ | ☐ |
| 13C-PeCDD | 13C-PeCDD | 302+304 | 302 | 304 | 1 | ☑ | ☑ |
| 13C-HxCDF1 | 13C-HxCDF | 322+324 | 322 | 324 | 1 | ☑ | ☐ |
| 13C-HxCDF2 | 13C-HxCDF | 322+324 | 322 | 324 | 2 | ☑ | ☐ |
| 13C-HxCDF3 | 13C-HxCDF | 322+324 | 322 | 324 | 3 | ☑ | ☐ |
| 13C-HxCDF4 | 13C-HxCDF | 322+324 | 322 | 324 | 4 | ☑ | ☐ |
| 13C-HxCDD1 | 13C-HxCDD | 338+340 | 338 | 340 | 1 | ☑ | ☑ |
| 13C-HxCDD2 | 13C-HxCDD | 338+340 | 338 | 340 | 2 | ☑ | ☑ |
| 13C-HxCDD3 | 13C-HxCDD | 338+340 | 338 | 340 | 3 | ☑ | ☑ |
| 13C-HpCDF1 | 13C-HpCDF | 356+358 | 356 | 358 | 1 | ☑ | ☐ |
| 13C-HpCDF2 | 13C-HpCDF | 356+358 | 356 | 358 | 2 | ☑ | ☐ |
| 13C-HpCDD | 13C-HpCDD | 372+374 | 372 | 374 | 1 | ☑ | ☑ |

*The Integration Form*

## Identification

Clicking the **Identification** button displays the compound name plus all fields on the second line of the compound form for all compounds in the table, in tabular form.

The following fields are displayed for review/editing: Compound, IS Compound, Qualifier Ion (QI) Ratio Low/High Limits, Relative Retention (RRT) Time Low/High Limits, Toxicity Equivalency Factor (TEF). Limit of Detection (LOD), and Standard Concentration. Note that standard concentrations will depend on the type of date file that is currently active. The Qualifier Ion ratios are set to be the expected value ± 25% absolute.



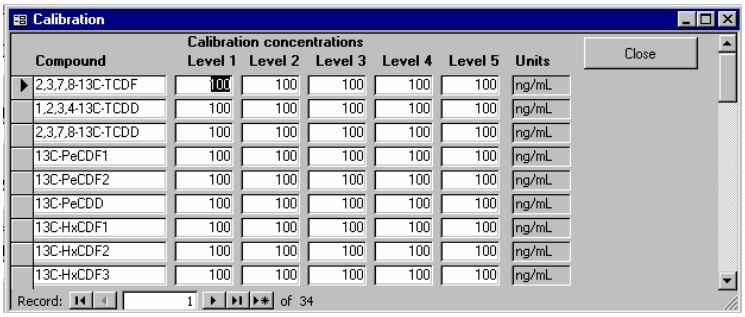

| Compound | IS Compound | QI Ratio Limit Low | QI Ratio Limit High | RRT Limits Low | RRT Limits High | TEF | LOD | Std. Conc. |
|---|---|---|---|---|---|---|---|---|
| 2,3,7,8-13C-TCDF | 1,2,3,4-13C-TCDD | 0.77 | 1.28 | 0.9225 | 1.1034 | 0 | 0 | 100 |
| 1,2,3,4-13C-TCDD | 1,2,3,4-13C-TCDD | 0.77 | 1.28 | 0.999 | 1.001 | 0 | 0 | 100 |
| 2,3,7,8-13C-TCDD | 1,2,3,4-13C-TCDD | 0.77 | 1.28 | 0.9885 | 1.0524 | 0 | 0 | 100 |
| 13C-PeCDF1 | 1,2,3,4-13C-TCDD | 0.58 | 0.98 | 0.9995 | 1.4254 | 0 | 0 | 100 |
| 13C-PeCDF2 | 1,2,3,4-13C-TCDD | 0.58 | 0.98 | 1.0105 | 1.5264 | 0 | 0 | 100 |
| 13C-PeCDD | 1,2,3,4-13C-TCDD | 0.58 | 0.98 | 0.9995 | 1.5674 | 0 | 0 | 100 |
| 13C-HxCDF1 | 13C-HxCDD3 | 1.54 | 2.54 | 0.955 | 0.985 | 0 | 0 | 100 |
| 13C-HxCDF2 | 13C-HxCDD3 | 1.54 | 2.54 | 0.955 | 0.985 | 0 | 0 | 100 |
| 13C-HxCDF3 | 13C-HxCDD3 | 1.54 | 2.54 | 0.9765 | 1.0474 | 0 | 0 | 100 |
| 13C-HxCDF4 | 13C-HxCDD3 | 1.54 | 2.54 | 0.959 | 1.021 | 0 | 0 | 100 |
| 13C-HxCDD1 | 13C-HxCDD3 | 1.54 | 2.54 | 0.9765 | 1.0004 | 0 | 0 | 100 |
| 13C-HxCDD2 | 13C-HxCDD3 | 1.54 | 2.54 | 0.9805 | 1.0034 | 0 | 0 | 100 |
| 13C-HxCDD3 | 13C-HxCDD3 | 1.54 | 2.54 | 0.999 | 1.001 | 0 | 0 | 100 |
| 13C-HpCDF1 | 13C-HxCDD3 | 1.23 | 2.06 | 1.02 | 1.065 | 0 | 0 | 100 |
| 13C-HpCDF2 | 13C-HxCDD3 | 1.23 | 2.06 | 1.057 | 1.151 | 0 | 0 | 100 |
| 13C-HpCDD | 13C-HxCDD3 | 1.23 | 2.06 | 1.06 | 1.09 | 0 | 0 | 100 |
| 13C-OCDD | 13C-HxCDD3 | 0.77 | 1.28 | 1.0315 | 1.3114 | 0 | 0 | 200 |
| 2,3,7,8-TCDF | 2,3,7,8-13C-TCDF | 0.77 | 1.28 | 0.9985 | 1.0034 | 0.1 | 0 | 10 |
| 2,3,7,8-TCDD | 2,3,7,8-13C-TCDD | 0.77 | 1.28 | 0.9985 | 1.0024 | 1 | 0 | 10 |

*The Integration Form*

## Calibration

Clicking the Calibration button displays the compound name plus all fields on the calibration line of the compound form for all compounds in the table, in tabular form.

This allows review/editing of the following fields: Compound, Level 1, Level 2, Level 3, Level 4, and Level 5. Data are already entered in the standard template for the concentrations of all compounds as normally supplied by vendors. The Units field is preset depending upon the choice of Sample Matrix in the Report Information form.

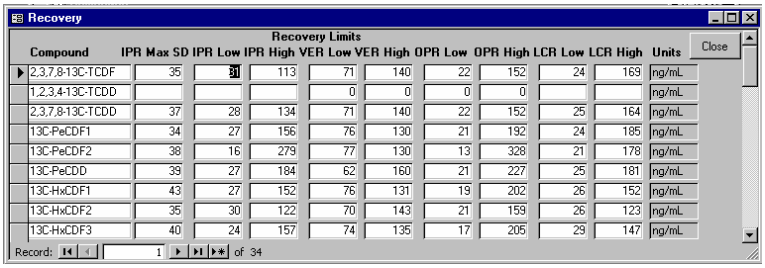



*The Calibration Form*

## Recovery Limits

Clicking the Recovery Limits button displays the Compound Name plus all fields shown on the Recovery Limits line for all compounds in the table, in tabular form.

This allows review/editing of the following fields: Initial Precision and Recovery (IPR), Verification (VER), Ongoing Precision and Recovery (OPR), and Labeled Compound Report (LCR) quality control limits. The values in the standard Dioxin Reports template are consistent with those in the US EPA Method 1613.




*The Recovery Limits Form*

## Close

When the **Close** button is clicked, the Compound form is closed, returning focus to the Main form.

## Help

The Compound Table contains all target compound-specific information used for reporting dioxin results. Compound information is presented in several views. The Compound form is organized to display all information about one compound on one form. Selected information for all peaks in the compound table is

presented in the Integration, Identification, Calibration, and Recovery Limits forms.

For information on specific Compound form entry fields, right click the mouse over the field of interest to get context-sensitive help.

# Fields: Compound

## Compound

The name entered in the Compound field is reported as the compound name in all reports. If this compound is used as an internal standard or as a retention time standard by any other compound in the table, the text in the IS Compound field for that compound must match this Compound text exactly. Note - there is no relationship between the name used for a compound on this form and the name used in a MS Workstation data handling method.

## Class

Class specifies a group of peaks that all share the same Quantitation Mass, M1, and M2 specifications. It applies to all peaks with these same characteristics, whether or not they are listed as specific compounds in this table. If C13? is checked (True), the compounds in the class are in retention time order as specified by the Order in Class field.

## Quan Mass

Quan Mass is the set of quantitation ions for the compound. The peak at the right RT in the mass chromatogram will be integrated and the peak area will be used to compute concentration values in dioxin reports. The Quan Mass can be a single mass or a sum of two masses. Use no spaces in the specification. Use only characters in the set {0123456789+}. The order is important: "123+456" is not the same as "456+123". The mass specification must exactly match the mass specification of the corresponding target compound Quan Ion specification in the MS Workstation data handling section.

## M1

M1 specifies the Qualifier Ion whose intensity is used as the numerator in the Qualifier Ion Ratio. It must match the Quan Ion specified for the corresponding target compound in the MS Workstation data handling method.

## M2

M2 specifies the Qualifier Ion whose intensity is used as the denominator in the Qualifier Ion Ratio. It must match the Quan Ion specified for the corresponding target compound in the MS Workstation data handling method.

## Order in Class

Order in Class specifies the retention time order of this compound relative to other compounds in this class. This feature is only used for C13-labeled compounds.

## C13?

This box must be checked for C13-labeled compounds. Compounds that are checked must be present in every sample, and the set of compounds specified as C13-labeled must have the largest peak areas in the class retention time window.

## Dioxin?

This box must be checked if the compound is a dioxin. This choice will separate dioxins from furans for reporting purposes.

## IS Compound

Enter the name of the internal standard for this compound here.

## QI Ratio Limit Low

QI Ratio Limit Low is the lowest allowed value of the M1/M2 ratio. If the value is lower, peak identification will not be confirmed.

## QI Ratio Limit High

QI Ratio Limit High is the highest allowed value of the M1/M2 ratio. If the value is higher, peak identification will not be confirmed.

## RRT Limit Low

RRT Limit Low is the lowest allowed value for Relative Retention Time compared to that of the IS Compound. If the RRT is lower, the peak will not be identified.

## RRT Limit High

RRT Limit High is the highest allowed value for Relative Retention Time compared to that of the IS Compound. If the RRT is Higher, the peak will not be identified.

## TEF

TEF is the Toxic Equivalency Factor. This is the toxicity of the compound relative to 2,3,7,8-Tetrachlorodibenzo-p-dioxin, which has a TEF of 1.

## LOD

LOD is the Limit of Detection

## Std. Conc.

This is the Standard Concentration in the final extract. For C13-labeled Standard compounds this is the known concentration spiked into each sample. For Native compounds, it is the concentration in the final extract for standard samples (VER, OPR). Typically this is the concentration used in Calibration Level 3.

## Calibration Concentration Level 1

This is the expected concentration of the compound present in Calibration Level 1, expressed as concentration in the final extract.

## Calibration Concentration Level 2

This is the expected concentration of the compound present in Calibration Level 2, expressed as concentration in the final extract.

## Calibration Concentration Level 3

This is the expected concentration of the compound present in Calibration Level 3, expressed as concentration in the final extract.

## Calibration Concentration Level 4

This is the expected concentration of the compound present in Calibration Level 4, expressed as concentration in the final extract.

## Calibration Concentration Level 5

This is the expected concentration of the compound present in Calibration Level 5, expressed as concentration in the final extract.

## Units

This field contains the concentration units for the final extract.

## IPR Low Recovery Limit

This is the lowest acceptable value for Initial Precision and Recovery, expressed as concentration in final extract.

## IPR High Recovery Limit

This is the highest acceptable value for Initial Precision and Recovery, expressed as concentration in final extract.

## IPR Max SD

IPR Max SD is the maximum acceptable value for Standard Deviation of the Initial Precision and Recovery concentration in the final extract.

## VER Low Recovery Limit

VER Low Recovery Limit is the lowest acceptable recovery in a Verification sample, expressed as a concentration in the final extract.

## VER High Recovery Limit

VER High Recovery Limit is the highest acceptable recovery in a Verification sample, expressed as a concentration in the final extract.

## OPR Low Recovery Limit

The OPR Low Recovery Limit is the lowest acceptable recovery in an Ongoing Precision and Recovery sample, expressed as concentration in the final extract.

## OPR High Recovery Limit

The OPR High Recovery Limit is the highest acceptable recovery in an Ongoing Precision and Recovery sample, expressed as concentration in the final extract.

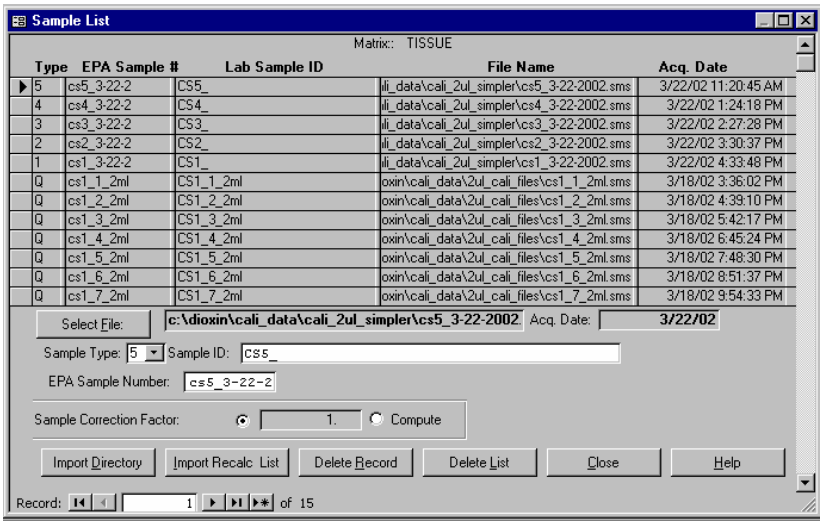
## LCR Low Recovery Limit

The LCR Low Recovery Limit is the lowest acceptable recovery in the Labeled Compound Report, expressed as concentration in the final extract.

## LCR High Recovery Limit

The LCR High Recovery Limit is the highest acceptable recovery in the Labeled Compound Report, expressed as concentration in the final extract.

# Sample List




*The Sample List Form*

The sample list contains sample-specific information that augments the sample information contained in the MS Workstation Sample List or Recalculation List file.

The Sample Type field is used to designate file types for each entry in the Sample List. The choices are Calibration #x (x = 1 to 5), Analysis, Verification, Blank, or Quality Control. It is also possible in this area of the form to label files with a user-selected Sample ID or EPA Sample #. Once Sample List files are labeled appropriately, it is possible to designate the desired reports to be created for each type of file in the Sample List. Also it is possible to select only files of certain types for Summary Reports. See the Report Options section for more details.

The Sample Correction Factor field is used to convert final extract concentration to sample concentration. The factor is defined as [Final extract volume/(sample weight or volume)]. This factor can be configured for calculation in one of two ways. The first, or automatic, option is to use the MS Workstation Sample or Recalculation List multiplier to divisor ratio as the factor. The second option is to manually enter the Sample Wt/Vol and Extract Vol on the Dioxin Sample List form. The currently active multiplier/divisor ratio is shown in the grayed text box in the Sample Correction selection area. To manually enter sample weight or volume and extract volume, select the "Compute" option by clicking on the right radio button and enter the value in the field on the right.

The data files to be reported and their attributes are identified in this section.

# Buttons: Sample List

## Select File

Click the **Select File button** to open the Select File dialog. Use this dialog to select a data file for this entry in the Sample List. The file selected should already have been processed using the same Method used to process the file listed as the Initial Calibration file.

Note: Make sure that the arrow at the left of the sample list table is at an empty line when selecting a new file, otherwise the existing sample entry will be overwritten by the newly selected file.

## Import Directory

Clicking the Import Directory button imports all the MS Workstation data files from the selected directory into the sample list. Values for Sample Correction Factor, Extract Volume, Sample Weight/Volume, % Solids, and % Lipids, as appropriate, are propagated from the first line of the Sample List into each added record as it is imported.

## Import Recalc List

Clicking the Import Recalc List button imports all the MS Workstation data files in the Recalculation list selected by the user into the sample list. The values for Sample Correction Factor, Extract Volume, Sample Weight/Volume, %Solids, and % Lipids, as appropriate, are propagated from the first line of the sample list into each added record as it is imported.

## Delete Record

Clicking the **Delete Record** button will delete (or clear) the currently selected record in the Sample List.

## Delete List

Clicking the **Delete List** button will delete all files in the Sample List.

## Close

Clicking the **Close** button will close the form.

## Help

The sample list contains sample-specific information that augments the sample information contained in the MS Workstation Sample List file. To view context-sensitive help in any part of this form, right-click the mouse and then click the “What’s This” icon on the desired item.

# Fields: Sample List

## Type

The sample type for each data file in the Sample List is selected in this area. The sample type designation will affect the report profile set for each sample. Sample Types 1, 2, 3, 4, and 5 specify the corresponding calibration level. Other sample types are A (Analysis), B (Blank), C (Calibration Verification), and Q (Quality Control).

## EPA Sample Number

The EPA Sample Number is an arbitrary sample identifier. If the field is blank when a file is imported, the EPA Sample Number field will be filled with text derived from the filename. If the field contains text, it will not be overwritten.

## Lab Sample ID

If the Sample ID field is blank when the record is created or set to show a selected file, the Sample ID field is read from the sample data file. If the field is not blank, it is not overwritten. If the objective is to set up a sample list before the data files are created, sample list entries can be created without file entries. In this case enter the Sample ID that will be associated with the soon to be created data file. When the Dioxin Reports application is called through the AutoLink field of MS Workstation System Control Sample or Recalc List, the data file will be automatically linked to the correct sample entry by locating its matching Sample ID entry.

## File Name

The **File Name** field shows the full path name of the data file. This file name is not directly editable, automatically read from the selected file. Click the Select File button to the left of this text box to change this field (by selecting a new file).

## Acq. Date

**Acq. Date** is date of the data file acquisition, as read from the data file. It is not editable.

## Sample Correction Factor

The Sample Correction Factor selects whether the conversion factor from final extract concentration to sample concentration is taken from the MS Workstation Sample List ratio of multiplier to divisor, or is computed from the values for Sample Wt/Vol and Extract Vol entered on this form. This factor affects concentrations shown on the Analysis and TEQ reports. The current sample multiplier to divisor ratio is shown in the grayed text box.

## Sample wt/vol

The sample wt/vol is the sample amount expressed as a weight in kilograms (kg) for SOIL or TISSUE matrices, or a volume in liters (l) for WATER matrices. This field is shown and used only if the Sample Correction Factor is set to "Compute". This field is used as the denominator of the conversion factor from final extract concentration to sample concentration.

## Extract Vol

Extract Vol. is the volume of final extract in milliliters (ml). This field is used as the numerator in the conversion factor from final extract concentration to sample concentration. It is shown and used only if the Sample Correction Factor is set to "Compute".

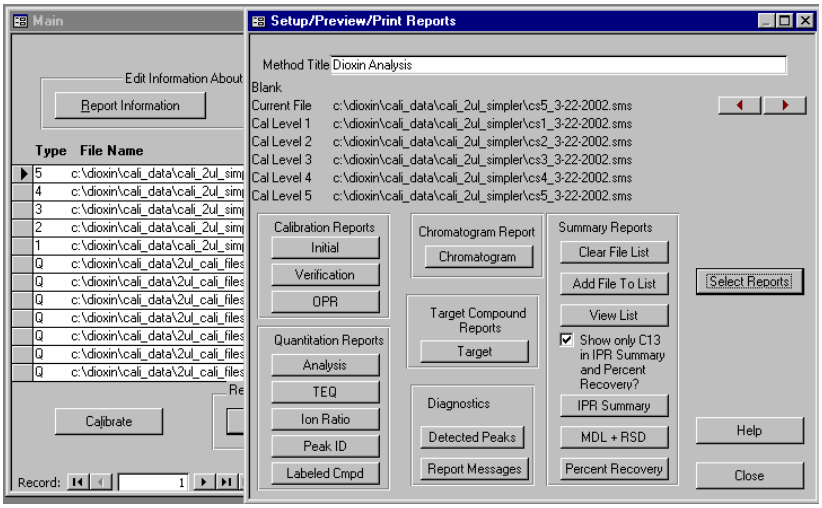
## % Solids

The % Solids is a text field provided to report % Dry Weight when the Matrix Type is SOIL and the Sample Correction Factor is set to "Compute". It is shown on the header of the Analysis and TEQ reports when the Matrix is SOIL, and the Sample Correction Factor is "Compute".

## % Lipids

The % Lipids field is a text field provided to report %Lipids when the Matrix Type is TISSUE and the Sample Correction Factor is set to "Compute". It is shown on the header of the Analysis and TEQ reports when the Matrix Type is TISSUE, and the Sample Correction Factor is "Compute".

# Setup/Preview/Print Reports




*The Setup/Preview/Print Report page. (The sample list page is in the background)*

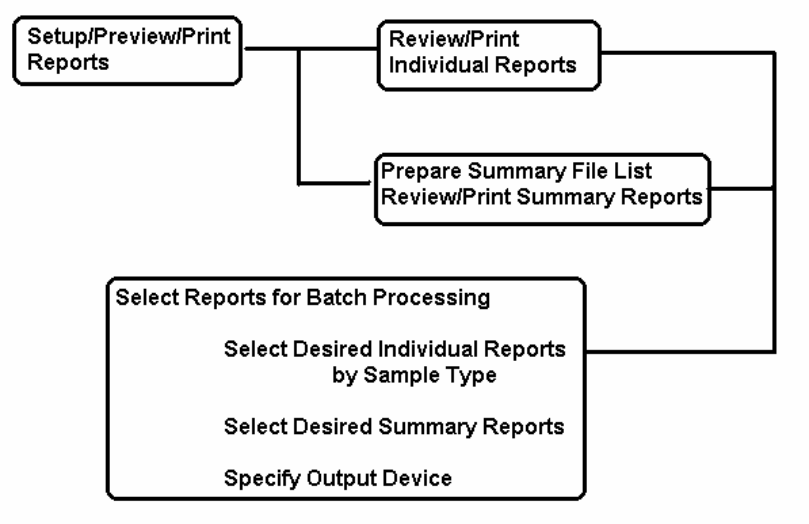
To review this form, the other sections of the template, including the Report Information, Compound Information, Sample List, and Calibrate must have to be completed. This form is used to preview reports based on the current sample. To preview a report, click the report button of interest. For information about a report, click the right mouse button with the cursor on the report button of interest. To print a report that is currently being shown, click the printer icon on the menu bar. To generate text file reports, select a report output profile, or process a sequence of reports based on the sample list, click the Select Reports button.

Summary reports are based on data abstracted from several files. To clear stored summary data, click the Clear File List button. To add the current file data to the summary data, click the Add File to List button. To see the file list of currently stored summary data, click the View List button. To see a summary report based on the currently stored data, click its button. The Initial Calibration Report is based on data generated during calibration processing. Calibration processing is accessed from the main form.

The files shown at the top of this page were selected by creating a sample list and specifying the appropriate sample type in the Sample List form. To see the source file, sample types, and report options controlling specific reports, refer to help for the specific report button described in this section.

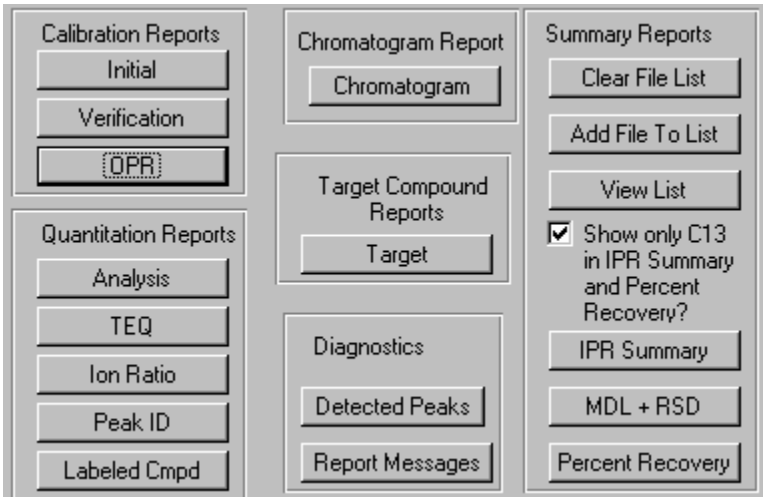
While previewing the individual reports, the current file (displayed in the top part of the page) is the base for the reports. To switch to a different file within the sample list, use the red arrows (upper right corner) to select the next or previous file for review.

To obtain the right report in the right format, follow the actions outlined in the figure below.



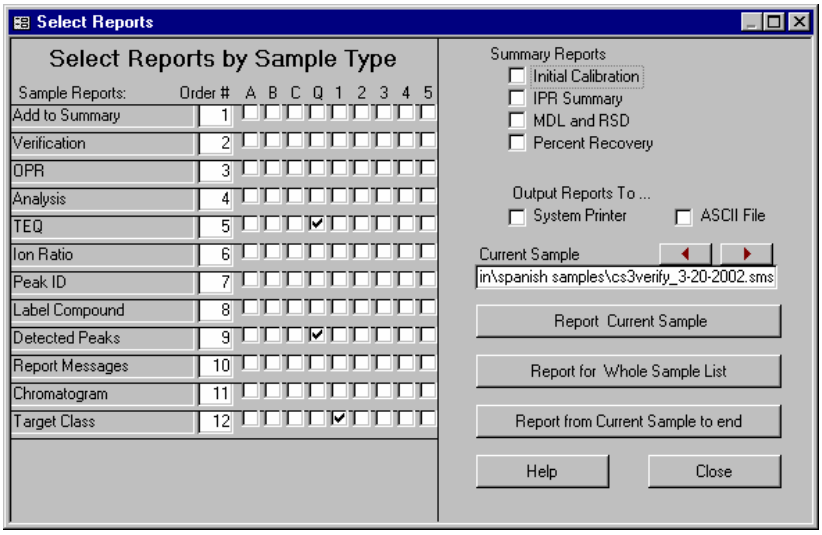

*Order of Operations in the Setup/Preview/Print page*

After specifying the reporting options the individual and summary reports maybe reviewed.




*Individual Report Review* *Summary Report Review*

The report generated by clicking on these buttons is shown in a later part of this section, where these reports are discussed in more detail.




*Select Reports for Batch Processing*

## Calibration Reports

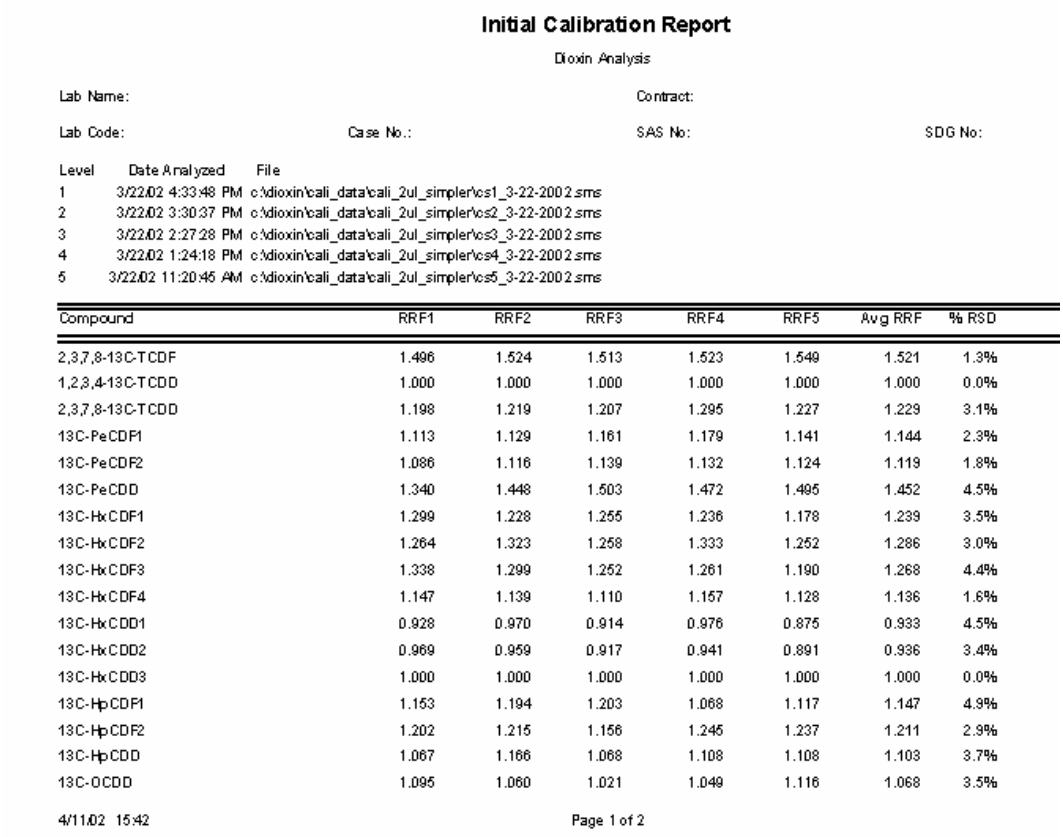
Three different reports may be selected for calibration:

1. Initial
2. Verification
3. Ongoing Precision and Recovery (OPR)

### *Initial Calibration Report*

**Purpose:** Shows Compound Name, Relative Response Factor, average RRF, and percent relative standard deviation (%RSD) for all compounds.

**Settings:** Compound Name, Calibration Levels, IS Compounds, C13?, Sample Table sample type 1-5



**Initial Calibration Report**

Dioxin Analysis

Lab Name: Contract:

Lab Code: Case No.: SAS No: SDG No:

| Level | Date Analyzed | File |
|---|---|---|
| 1 | 3/22/02 4:33:48 PM | c:\dioxin\cali_data\cali_2ul_simpler\cs1_3-22-2002.sms |
| 2 | 3/22/02 3:30:37 PM | c:\dioxin\cali_data\cali_2ul_simpler\cs2_3-22-2002.sms |
| 3 | 3/22/02 2:27:28 PM | c:\dioxin\cali_data\cali_2ul_simpler\cs3_3-22-2002.sms |
| 4 | 3/22/02 1:24:18 PM | c:\dioxin\cali_data\cali_2ul_simpler\cs4_3-22-2002.sms |
| 5 | 3/22/02 11:20:45 AM | c:\dioxin\cali_data\cali_2ul_simpler\cs5_3-22-2002.sms |

| Compound | RRF1 | RRF2 | RRF3 | RRF4 | RRF5 | Avg RRF | % RSD |
|---|---|---|---|---|---|---|---|
| 2,3,7,8-13C-TCDF | 1.496 | 1.524 | 1.513 | 1.523 | 1.549 | 1.521 | 1.3% |
| 1,2,3,4-13C-TCDD | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.0% |
| 2,3,7,8-13C-TCDD | 1.198 | 1.219 | 1.207 | 1.295 | 1.227 | 1.229 | 3.1% |
| 13C-PeCDF1 | 1.113 | 1.129 | 1.161 | 1.179 | 1.141 | 1.144 | 2.3% |
| 13C-PeCDF2 | 1.086 | 1.116 | 1.139 | 1.132 | 1.124 | 1.119 | 1.8% |
| 13C-PeCDD | 1.340 | 1.448 | 1.503 | 1.472 | 1.495 | 1.452 | 4.5% |
| 13C-HxCDF1 | 1.299 | 1.228 | 1.255 | 1.236 | 1.178 | 1.239 | 3.5% |
| 13C-HxCDF2 | 1.264 | 1.323 | 1.258 | 1.333 | 1.252 | 1.286 | 3.0% |
| 13C-HxCDF3 | 1.338 | 1.299 | 1.252 | 1.261 | 1.190 | 1.268 | 4.4% |
| 13C-HxCDF4 | 1.147 | 1.139 | 1.110 | 1.157 | 1.128 | 1.136 | 1.6% |
| 13C-HxCDD1 | 0.928 | 0.970 | 0.914 | 0.976 | 0.875 | 0.933 | 4.5% |
| 13C-HxCDD2 | 0.969 | 0.959 | 0.917 | 0.941 | 0.891 | 0.936 | 3.4% |
| 13C-HxCDD3 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.0% |
| 13C-HpCDF1 | 1.153 | 1.194 | 1.203 | 1.068 | 1.117 | 1.147 | 4.9% |
| 13C-HpCDF2 | 1.202 | 1.215 | 1.156 | 1.245 | 1.237 | 1.211 | 2.9% |
| 13C-HpCDD | 1.067 | 1.166 | 1.068 | 1.108 | 1.108 | 1.103 | 3.7% |
| 13C-OCDD | 1.095 | 1.060 | 1.021 | 1.049 | 1.116 | 1.068 | 3.5% |

4/11/02 15:42 Page 1 of 2

## *Calibration Verification Report*

**Purpose:** Compares calculated concentrations in Verification samples to Recovery Limits and gives Pass/Fail result. Use Sample Table sample type C for this report.

**Settings:** Compound Name, Standard Conc., IS Compounds, C13?, Recovery Limits VER Low and High

**Calibration Verification Report**

Lab Name: Contract:

Lab Code: Case No: SAS No: SDG No:

File: c:\dioxin\spanish samples\cs3verify_3-20-2002.sms Date Acquired: 3/20/02 9:31:19 PM

| Compound | Low Limit | Concentration | High Limit | Units | P/F |
|---|---|---|---|---|---|
| 2,3,7,8-TCDF | 8.4 | 9.0 | 12.0 | ng/mL | Pass |
| 2,3,7,8-TCDD | 7.8 | 9.4 | 12.9 | ng/mL | Pass |
| 1,2,3,7,8-PeCDF1 | 41.0 | 51.2 | 60.0 | ng/mL | Pass |
| 2,3,4,7,8-PeCDF2 | 41.0 | 47.1 | 60.0 | ng/mL | Pass |
| 1,2,3,7,8-PeCDD | 39.0 | 46.2 | 65.0 | ng/mL | Pass |
| 1,2,3,4,7,8-HxCDF1 | 45.0 | 51.4 | 56.0 | ng/mL | Pass |
| 1,2,3,6,7,8-HxCDF2 | 44.0 | 46.2 | 57.0 | ng/mL | Pass |
| 1,2,3,7,8,9-HxCDF3 | 45.0 | 50.1 | 56.0 | ng/mL | Pass |
| 2,3,4,6,7,8-HxCDF4 | 44.0 | 47.6 | 57.0 | ng/mL | Pass |
| 1,2,3,4,7,8-HxCDD1 | 39.0 | 49.3 | 64.0 | ng/mL | Pass |
| 1,2,3,6,7,8-HxCDD2 | 39.0 | 54.5 | 64.0 | ng/mL | Pass |
| 1,2,3,7,8,9-HxCDD3 | 41.0 | 65.2 | 61.0 | ng/mL | Fail |
| 1,2,3,4,6,7,8-HpCDF | 45.0 | 45.1 | 55.0 | ng/mL | Pass |
| 1,2,3,4,7,8,9-HpCDF | 43.0 | 43.2 | 58.0 | ng/mL | Pass |
| 1,2,3,4,6,7,8-HpCDD | 43.0 | 49.6 | 58.0 | ng/mL | Pass |
| OCDF | 63.0 | 113.5 | 159.0 | ng/mL | Pass |
| OCDD | 79.0 | 107.6 | 126.0 | ng/mL | Pass |
| 2,3,7,8-13C-TCDF | 71.0 | 101.7 | 140.0 | ng/mL | Pass |
| 2,3,7,8-13C-TCDD | 71.0 | 99.4 | 140.0 | ng/mL | Pass |
| 13C-PeCDF1 | 76.0 | 99.5 | 130.0 | ng/mL | Pass |

## *Ongoing Precision and Recovery Report*

**Purpose:** Shows Compound Name, concentrations and recovery limits for OPR samples. Use Sample Table sample type Q for this report.

**Settings:** Compound Name, Standard Conc., IS Compounds, C13?, OPR Low and High

**Ongoing Precision And Recovery Report**

Lab Name: Contract:

Lab Code: Case No: SAS No: SDG No:

File: c:\dioxin\spanish samples\cs3verify_3-20-2002.sms Date Acquired: 3/20/02 9:31:19 PM

| Compound | Low Limit | Concentration | High Limit | Units | P/F |
|---|---|---|---|---|---|
| 2,3,7,8-TCDF | 7.5 | 9.0 | 16.0 | ng/mL | Pass |
| 2,3,7,8-TCDD | 6.7 | 9.4 | 16.0 | ng/mL | Pass |
| 1,2,3,7,8-PeCDF1 | 40.0 | 51.2 | 67.0 | ng/mL | Pass |
| 2,3,4,7,8-PeCDF2 | 34.0 | 47.1 | 80.0 | ng/mL | Pass |
| 1,2,3,7,8-PeCDD | 35.0 | 46.2 | 71.0 | ng/mL | Pass |
| 1,2,3,4,7,8-HxCDF1 | 36.0 | 51.4 | 67.0 | ng/mL | Pass |
| 1,2,3,6,7,8-HxCDF2 | 42.0 | 46.2 | 65.0 | ng/mL | Pass |
| 1,2,3,7,8,9-HxCDF3 | 39.0 | 50.1 | 65.0 | ng/mL | Pass |
| 2,3,4,6,7,8-HxCDF4 | 35.0 | 47.6 | 78.0 | ng/mL | Pass |
| 1,2,3,4,7,8-HxCDD1 | 35.0 | 49.3 | 82.0 | ng/mL | Pass |
| 1,2,3,6,7,8-HxCDD2 | 38.0 | 54.5 | 67.0 | ng/mL | Pass |
| 1,2,3,7,8,9-HxCDD3 | 32.0 | 65.2 | 81.0 | ng/mL | Pass |
| 1,2,3,4,6,7,8-HpCDF | 41.0 | 45.1 | 61.0 | ng/mL | Pass |
| 1,2,3,4,7,8,9-HpCDF | 39.0 | 43.2 | 69.0 | ng/mL | Pass |
| 1,2,3,4,6,7,8-HpCDD | 35.0 | 49.6 | 70.0 | ng/mL | Pass |
| OCDF | 63.0 | 113.5 | 170.0 | ng/mL | Pass |
| OCDD | 78.0 | 107.6 | 144.0 | ng/mL | Pass |
| 2,3,7,8-13C-TCDF | 22.0 | 101.7 | 152.0 | ng/mL | Pass |
| 2,3,7,8-13C-TCDD | 22.0 | 99.4 | 152.0 | ng/mL | Pass |
| 13C-PeCDF1 | 21.0 | 99.5 | 192.0 | ng/mL | Pass |
| 13C-PeCDF2 | 13.0 | 104.4 | 328.0 | ng/mL | Pass |

# Quantitation Reports

Five different quantitation reports can be selected:

1. Analysis
2. TEQ
3. Ion Ratio
4. Peak ID
5. Labeled Compound

## *Analysis Report*

**Purpose:** Shows Compound Name, Area, Concentration or Recovery, TEQ, and Ion Ratio for Total Class, Native, and Labeled Compounds.

**Settings:** Compound Name, Standard Conc., Ion Ratio Low & High Limit, Sample Matrix, IS Compound, C13?, Sample Wt/Vol, Extract Vol, Multiplier/Divisor, %Lipids, %Solids, Sample Correction Factor, TEF

**Dioxin Analysis Report**

Lab Name: Contract:

Lab Code: Case No: SAS No: SDG No:

File: c:\dioxin\spanish samples\r_47_01.sms Date Acquired: 3/15/02 9:44:42 AM

Matrix: WATER Dilution Factor: 1.000 Units: pg/L

| Compound | R.T. | Area | Recovery | Concentration | TEQ | Ion Ratio | P/F |
|---|---|---|---|---|---|---|---|
| 1,2,3,4-13C-TCDD | 31.664 | 31086 | 100.0% | | | 1.020 | Pass |
| 2,3,7,8-13C-TCDD | 32.628 | 12436 | 32.5% | | | 1.026 | Pass |
| 13C-PeCDD | 44.073 | 17001 | 37.7% | | | 0.778 | Pass |
| 13C-HxCDD1 | 49.386 | 4089 | 27.8% | | | 0.632 | Fail |
| 13C-HxCDD2 | 49.501 | 5053 | 34.3% | | | 0.000 | Fail |
| 13C-HxCDD3 | 49.783 | 15744 | 100.0% | | | 0.000 | Fail |
| 13C-HpCDD | 53.548 | 4543 | 26.1% | | | 0.000 | Fail |
| 13C-OCDD | 58.420 | 9927 | 29.5% | | | 1.092 | Pass |
| 2,3,7,8-13C-TCDF | 31.315 | 16417 | 34.7% | | | 1.018 | Pass |
| 13C-PeCDF1 | 40.150 | 11607 | 32.6% | | | 0.840 | Pass |
| 13C-PeCDF2 | 43.193 | 5947 | 17.1% | | | 0.937 | Pass |
| 13C-HxCDF1 | 48.352 | 13882 | 71.2% | | | 1.933 | Pass |
| 13C-HxCDF2 | 48.503 | 13403 | 66.2% | | | 2.081 | Pass |
| 13C-HxCDF3 | 49.195 | 6097 | 30.5% | | | 0.000 | Fail |
| 13C-HxCDF4 | 50.132 | 5859 | 32.8% | | | 0.000 | Fail |
| 13C-HpCDF1 | 52.008 | 5156 | 28.6% | | | 1.406 | Pass |
| 13C-HpCDF2 | 54.298 | 6002 | 31.5% | | | 1.515 | Pass |
| 2,3,7,8-TCDD | 32.632 | 291 | | 1.742 | 1.742 | 1.646 | Fail |
| 1,2,3,7,8-PeCDD | 44.100 | 154 | | 0.959 | 0.480 | 0.000 | Fail |
| 1,2,3,4,7,8-HxCDD1 | 49.382 | 165 | | 2.940 | 0.294 | 0.000 | Fail |
| 1,2,3,6,7,8-HxCDD2 | 49.512 | 607 | | 8.823 | 0.882 | 1.737 | Pass |
| 1,2,3,7,8,9-HxCDD3 | 49.789 | 435 | | 6.505 | 0.650 | 1.154 | Fail |
| 1,2,3,4,6,7,8-HpCDD | 53.562 | 9320 | | 207.460 | 2.075 | 1.777 | Pass |
| OCDD | 58.436 | 86278 | | 1653.427 | 1.653 | 1.085 | Pass |
| 2,3,7,8-TCDF | 31.340 | 826 | | 4.873 | 0.487 | 1.006 | Pass |
| 1,2,3,7,8-PeCDF1 | 40.163 | 273 | | 2.554 | 0.128 | 0.750 | Pass |

## *TEQ Report*

**Purpose:** Shows Compound Name, Concentration, and TEQ for Native and Total Class.

**Settings:** Compound Name, Standard Conc., IS Compound, C13?, Sample Matrix, Sample Wt/Vol, Extract Vol., Sample Correction Factor, Multiplier/Divisor, %Solids, %Lipids, TEF

**Toxic Equivalent Summary Report**

Lab Name: Contract:

Lab Code: Case No: SAS No: SDG No:

File: c:\dioxin\spanish samples\r_47_01.sms Date Acquired: 3/15/02 9:44:42 AM

Matrix: WATER Dilution Factor: 1.000 Units: pg/L

| Compound | Concentration | TEQ |
|---|---|---|
| 2,3,7,8-TCDD | 1.742 | 1.742 |
| 1,2,3,7,8-PeCDD | 0.959 | 0.480 |
| 1,2,3,4,7,8-HxCDD1 | 2.940 | 0.294 |
| 1,2,3,6,7,8-HxCDD2 | 8.823 | 0.882 |
| 1,2,3,7,8,9-HxCDD3 | 6.505 | 0.650 |
| 1,2,3,4,6,7,8-HpCDD | 207.460 | 2.075 |
| OCDD | 1653.427 | 1.653 |
| 2,3,7,8-TCDF | 4.873 | 0.487 |
| 1,2,3,7,8-PeCDF1 | 2.554 | 0.128 |
| 2,3,4,7,8-PeCDF2 | 3.494 | 1.747 |
| 1,2,3,4,7,8-HxCDF1 | 3.498 | 0.350 |
| 1,2,3,6,7,8-HxCDF2 | 3.020 | 0.302 |
| 1,2,3,7,8,9-HxCDF3 | 10.567 | 1.057 |
| 2,3,4,6,7,8-HxCDF4 | 1.293 | 0.129 |
| 1,2,3,4,6,7,8-HpCDF | 20.090 | 0.201 |
| 1,2,3,4,7,8,9-HpCDF | 3.932 | 0.039 |
| OCDF | 44.786 | 0.045 |
| Total TCDF | 14.323 | |
| Total TCDD | 9.959 | |
| Total PeCDF | 53.493 | |
| Total PeCDD | 7.781 | |
| Total HxCDF | 48.518 | |
| Total HxCDD | 57.337 | |
| Total HpCDF | 76.681 | |
| Total HpCDD | 409.232 | |
| Total OCDF | 71.233 | |
| Total OCDD | 1694.864 | |
| | Total TEQ | 12.261 |

## *Ion Ratio Report*

**Purpose:** Shows Compound Name, M1, M2, M1+M2, Ion Ratio for all compounds. Shows Pass/Fail for ion ratio requirements.

**Settings:** Compound Name, M1, M2, Quan Mass, IS Compounds, Standard Conc., C13?, Ion Ratio Limit Low & High

**Ion Ratio Report**

Lab Name: Contract:

Lab Code: Case No: SAS No: SDG No:

File: c:\dioxin\spanish samples\r_47_01.sms Date Acquired: 3/15/02 9:44:42 AM

| Compound | RT | M1 | M2 | Low Limit | Ion Ratio | High Limit | P/F |
|---|---|---|---|---|---|---|---|
| 2,3,7,8-13C-TCDF | 31.315 | 252 | 254 | 0.770 | 1.018 | 1.280 | Pass |
| 1,2,3,4-13C-TCDD | 31.664 | 268 | 270 | 0.770 | 1.020 | 1.280 | Pass |
| 2,3,7,8-13C-TCDD | 32.628 | 268 | 270 | 0.770 | 1.026 | 1.280 | Pass |
| 13C-PeCDF1 | 40.150 | 286 | 288 | 0.580 | 0.840 | 0.980 | Pass |
| 13C-PeCDF2 | 43.193 | 286 | 288 | 0.580 | 0.937 | 0.980 | Pass |
| 13C-PeCDD | 44.073 | 302 | 304 | 0.580 | 0.778 | 0.980 | Pass |
| 13C-HxCDF1 | 48.352 | 322 | 324 | 1.540 | 1.933 | 2.540 | Pass |
| 13C-HxCDF2 | 48.503 | 322 | 324 | 1.540 | 2.081 | 2.540 | Pass |

## *Peak ID Report*

**Purpose:** Shows Compound Name, Retention Time and Relative Retention time for M1, M2, M1+M2, along with RRT Limits Low and High. Shows Pass/Fail relative to RRT requirements.

**Settings:** Compound Name, M1. M2, Quan Mass, IS Compounds, C13?, RRT Limits Low & High

**Peak Identification Report**

Lab Name: Contract:

Lab Code: Case No: SAS No: SDG No:

File: c:\dioxin\spanish samples\r_47_01.sms Date Acquired: 3/15/02 9:44:42 AM

| | M/Z | | Retention Time | | | | Relative Retention Time | | | | Limits | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Compound | M1 | M2 | M1+M2 | M1 | M2 | Ref. Peak | Ref RT | M1+M2 | M1 | M2 | Low | High | P/F |
| 2,3,7,8-13C-TCDF | 252 | 254 | 31.315 | 31.313 | 31.317 | 1,2,3,4-13C-TCDD | 31.664 | 0.989 | 0.989 | 0.989 | 0.922 | 1.103 | Pass |
| 1,2,3,4-13C-TCDD | 268 | 270 | 31.664 | 31.661 | 31.669 | 1,2,3,4-13C-TCDD | 31.664 | 1.000 | 1.000 | 1.000 | 0.999 | 1.001 | Pass |
| 2,3,7,8-13C-TCDD | 268 | 270 | 32.628 | 32.629 | 32.627 | 1,2,3,4-13C-TCDD | 31.664 | 1.030 | 1.030 | 1.030 | 0.989 | 1.052 | Pass |
| 13C-PeCDF1 | 286 | 288 | 40.150 | 40.148 | 40.152 | 1,2,3,4-13C-TCDD | 31.664 | 1.268 | 1.268 | 1.268 | 1.000 | 1.425 | Pass |
| 13C-PeCDF2 | 286 | 288 | 43.193 | 43.195 | 43.147 | 1,2,3,4-13C-TCDD | 31.664 | 1.364 | 1.364 | 1.363 | 1.011 | 1.526 | Pass |
| 13C-PeCDD | 302 | 304 | 44.073 | 44.075 | 44.071 | 1,2,3,4-13C-TCDD | 31.664 | 1.392 | 1.392 | 1.392 | 1.000 | 1.567 | Pass |
| 13C-HxCDF1 | 322 | 324 | 48.352 | 48.353 | 48.352 | 13C-HxCDD3 | 49.783 | 0.971 | 0.971 | 0.971 | 0.955 | 0.985 | Pass |
| 13C-HxCDF2 | 322 | 324 | 48.503 | 48.505 | 48.506 | 13C-HxCDD3 | 49.783 | 0.974 | 0.974 | 0.974 | 0.955 | 0.985 | Pass |

## *Labeled Compound*

**Purpose:** Reports recovery of C13 Label compound in analysis samples and Pas/Fail per recovery requirements.

**Settings:** Compound Name, Standard Conc, IS Compounds, C13?, LCR Recovery Limits Low & High

**Labeled Compound Recovery Report**

Lab Name: Contract:

Lab Code: Case No: SAS No: SDG No:

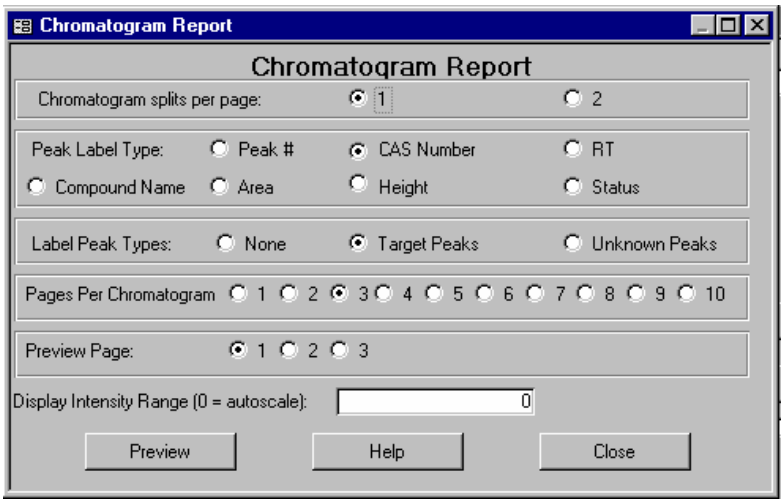
File: c:\dioxin\spanish samples\r_47_01.sms Date Acquired: 3/15/02 9:44:42 AM

| Compound | % Recovery | Concentration | Low Limit | High Limit | Units | P/F |
|---|---|---|---|---|---|---|
| 2,3,7,8-13C-TCDF | 34.7% | 34.7 | 24.0 | 169.0 | ng/mL | Pass |
| 2,3,7,8-13C-TCDD | 32.5% | 32.5 | 25.0 | 164.0 | ng/mL | Pass |
| 13C-PeCDF1 | 32.6% | 32.6 | 24.0 | 185.0 | ng/mL | Pass |
| 13C-PeCDF2 | 17.1% | 17.1 | 21.0 | 178.0 | ng/mL | Fail |
| 13C-PeCDD | 37.7% | 37.7 | 25.0 | 181.0 | ng/mL | Pass |
| 13C-HxCDF1 | 71.2% | 71.2 | 26.0 | 152.0 | ng/mL | Pass |
| 13C-HxCDF2 | 66.2% | 66.2 | 26.0 | 123.0 | ng/mL | Pass |
| 13C-HxCDF3 | 30.5% | 30.5 | 29.0 | 147.0 | ng/mL | Pass |
| 13C-HxCDF4 | 32.8% | 32.8 | 28.0 | 136.0 | ng/mL | Pass |
| 13C-HxCDD1 | 27.8% | 27.8 | 32.0 | 141.0 | ng/mL | Fail |
| 13C-HxCDD2 | 34.3% | 34.3 | 28.0 | 130.0 | ng/mL | Pass |
| 13C-HpCDF1 | 28.6% | 28.6 | 23.0 | 140.0 | ng/mL | Pass |
| 13C-HpCDF2 | 31.5% | 31.5 | 28.0 | 143.0 | ng/mL | Pass |
| 13C-HpCDD | 26.1% | 26.1 | 23.0 | 140.0 | ng/mL | Pass |
| 13C-OCDD | 29.5% | 59.0 | 34.0 | 313.0 | ng/mL | Pass |

# Chromatogram Report

Note: The Chromatogram Report is an artifact of the EnviroPro software reporting package and is not useful for interpreting and reporting Dioxin/Furan data files.

The **Chromatogram Report** form configures parameters used to construct the multi page Chromatogram Report. This report shows a chromatogram trace, whose time axis has been scaled to be between 9 inches and 180 inches in length. When the Chromatogram Report is printed under the control of the "Select Reports" form, through System Control Automation, or from the Star Toolbar Data File Operations-Print MS Report menu, all pages of the multi page report will be generated. Using the Chromatogram Report form individual pages of the report may be shown and printed.




### *Close*

Click the **Close** button to close the Chromatogram Report form.

### *Preview*

Click the **Preview** button to display the page of the multi page Chromatogram Report selected in the "Preview Page" group.

### *Chromatogram Splits Per Page*

The **Chromatogram Splits per Page** group selects either one 5.5" high by 9" wide chromatogram section per page or two 2.75" high by 9" wide chromatogram sections per page. The time range displayed in each section is determined by the formula [length of the data acquired in the file(minutes)]/[[Chromatogram splits per page]*[Pages per Chromatogram]].

### *Peak Label Type*

The **Peak Label Type** group selects the type of text label that is to be shown on peaks in the chromatogram trace.

### *Label Peak Type*

The **Label Peak Type** group selects the type of peaks to label with the information selected in the "Peak Label Type" group. Select "None" to disable peak annotation. Select "Target Peaks" to label peaks defined in the Method Compound Table. Select "Unknown Peaks" to label peaks that are integrated using parameters in the Calculation Setup page of the Method Editor.

### *Pages per Chromatogram*

The **Pages per Chromatogram** group selects the number of pages in the Chromatogram Report. The chromatogram time axis length may be scaled from 9 inches (1 page per chromatogram, 1 Chromatogram split per page) to 180 inches (10 pages per chromatogram, 2 chromatogram splits per page).

### *Preview Page*

The **Preview Page** group selects the page of the multi page Chromatogram Report to display when the Preview button is clicked.

### *Display Intensity Range*

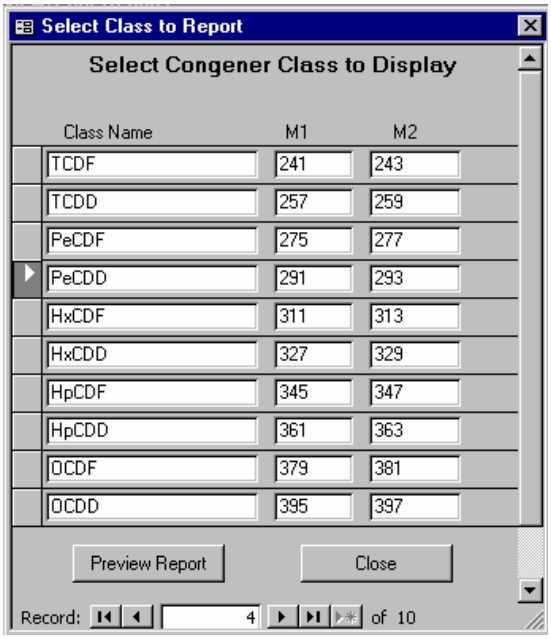
The **Display Intensity Range** text box controls the vertical (amplitude) scale of the Chromatogram Report. If it is set to 0, the scale is automatically set so that the largest peak on any page of the report will be approximately full scale. The scale is fixed to the same value for all pages of the report. If the field is set to a non-zero value, then the range of all pages of the report will be from zero to the value specified. This field is always set in units of counts even though the range of most reports is typically labeled in thousands of counts.

# Target Compound Reports

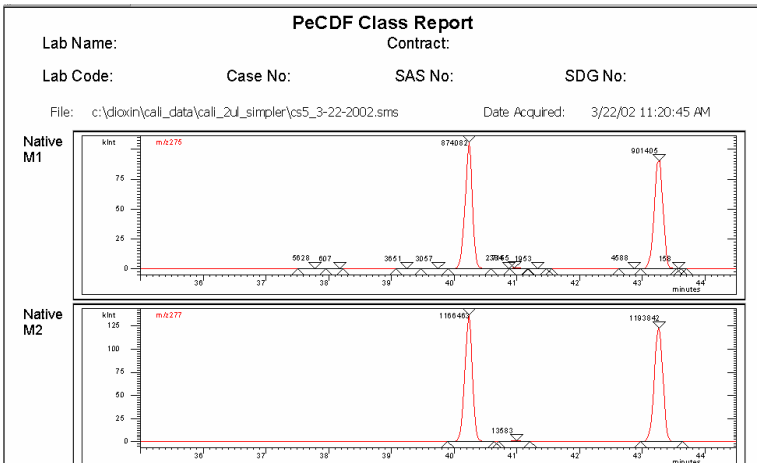
Clicking the Target button opens the Select Class to Report form so that graphical Congener Class reports may be viewed and printed.

## Select Class to Report

To preview a compound class report, click on the record selector button of the compound record and then click Preview Report.



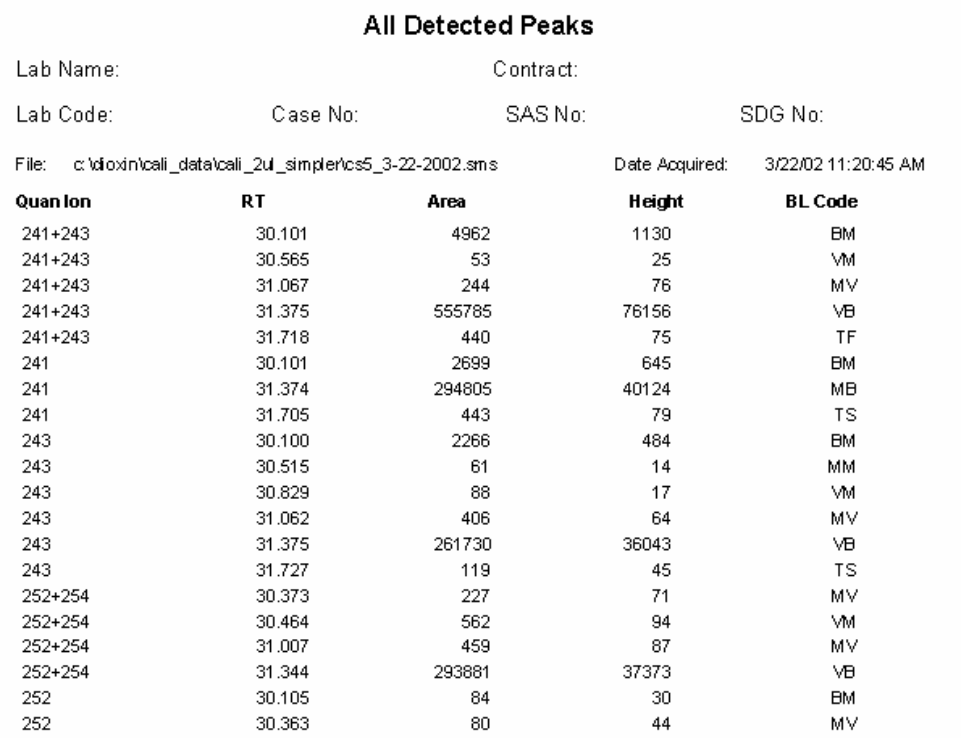

*The Select Class to Report Form*




*Example: Pentachlorofuran Class Report*

# Diagnostics Reports

### *Detected Peaks Report*



**All Detected Peaks**

Lab Name: Contract:

Lab Code: Case No: SAS No: SDG No:

File: c:\dioxin\cali_data\cali_2ul_simple\cs5_3-22-2002.sms Date Acquired: 3/22/02 11:20:45 AM

| Quan Ion | RT | Area | Height | BL Code |
|---|---|---|---|---|
| 241+243 | 30.101 | 4962 | 1130 | BM |
| 241+243 | 30.565 | 53 | 25 | VM |
| 241+243 | 31.067 | 244 | 76 | MV |
| 241+243 | 31.375 | 555785 | 76156 | VB |
| 241+243 | 31.718 | 440 | 75 | TF |
| 241 | 30.101 | 2699 | 645 | BM |
| 241 | 31.374 | 294805 | 40124 | MB |
| 241 | 31.705 | 443 | 79 | TS |
| 243 | 30.100 | 2266 | 484 | BM |
| 243 | 30.515 | 61 | 14 | MM |
| 243 | 30.829 | 88 | 17 | VM |
| 243 | 31.062 | 406 | 64 | MV |
| 243 | 31.375 | 261730 | 36043 | VB |
| 243 | 31.727 | 119 | 45 | TS |
| 252+254 | 30.373 | 227 | 71 | MV |
| 252+254 | 30.464 | 562 | 94 | VM |
| 252+254 | 31.007 | 459 | 87 | MV |
| 252+254 | 31.344 | 293881 | 37373 | VB |
| 252 | 30.105 | 84 | 30 | BM |
| 252 | 30.363 | 80 | 44 | MV |

**Title:** All Detected Peaks

**Purpose:** This report shows all peaks imported into the Dioxin Report application, which includes all integrated peaks that exceed the minimum area specification for their class. All Detected Peaks is primarily a diagnostic report used to identify problems in peak identification. This report helps to discern whether the problem lies within the dioxin application or within MS Workstation Data Handling.

**Settings:** MS Method Data Handling Compound Table settings, particularly RT, Quan Ions, Scan Function Channel, Peak Area Reject, Peak Window, Slope Sensitivity, and Peak Width control peak integration.

## *Report Messages*

**Messages Generated By The Last Report Processed**

| | |
|---|---|
| File Name | c:\dioxin\cali_data\cali_2ul_simple\cs5_3-22-2002.sms |
| Type: | Warning: Multiple Peaks found in M1 + M2 ID Window |
| Detail | 1,2,3,6,7,8-HxCDD2 327+329 RT Window49.389 to 49.731. Peak identified at 49.417 |
| File Name | c:\dioxin\cali_data\cali_2ul_simple\cs5_3-22-2002.sms |
| Type: | Warning: Multiple Peaks found in M1 ID Window |
| Detail | 1,2,3,6,7,8-HxCDD2 327 RT Window49.389 to 49.731. Peak identified at 49.523 |
| File Name | c:\dioxin\cali_data\cali_2ul_simple\cs5_3-22-2002.sms |
| Type: | Warning: Multiple Peaks found in M2 ID Window |
| Detail | 1,2,3,6,7,8-HxCDD2 329 RT Window49.389 to 49.731. Peak identified at 49.414 |
| File Name | c:\dioxin\cali_data\cali_2ul_simple\cs5_3-22-2002.sms |
| Type: | Warning: Multiple Peaks found in M1 + M2 ID Window |
| Detail | 1,2,3,7,8,9-HxCDD3 327+329 RT Window49.612 to 50.473. Peak identified at 49.808 |
| File Name | c:\dioxin\cali_data\cali_2ul_simple\cs5_3-22-2002.sms |
| Type: | Warning: Multiple Peaks found in M1 ID Window |
| Detail | 1,2,3,7,8,9-HxCDD3 327 RT Window49.612 to 50.473. Peak identified at 49.808 |
| File Name | c:\dioxin\cali_data\cali_2ul_simple\cs5_3-22-2002.sms |
| Type: | Warning: Multiple Peaks found in M2 ID Window |
| Detail | 1,2,3,7,8,9-HxCDD3 329 RT Window49.612 to 50.473. Peak identified at 49.808 |

**Title:** Messages Generated by the Last Report Processed

**Purpose:** This report shows errors and warnings generated when the Dioxin Reports software performs the peak identification and concentration calculation process.

**Settings:** Compound Table Calibration Levels, IS Compounds, Sample Table sample type 1-5, and all Integration and Quantitation parameters on the Dioxin Compound Information Form.

# Summary Reports

There are three summary reports available for reporting:

1. IPR Summary
2. MDL&RSD
3. Percent Recovery

Typically the box “Show only C13 in IPR and Percent Recovery?” is checked because the data are relevant only for these compounds.

To prepare summary reports, it is necessary to create a list of files to be used in the reports. There are three buttons to help you create or remove summary report lists:

### *Clear File List*

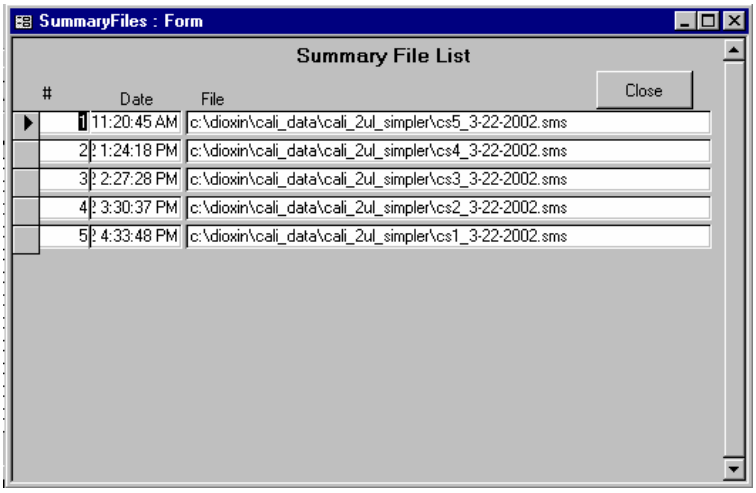
Clicking the **Clear File List** button will erase all stored summary information except that for Initial Calibration.

### *Add File to List*

Clicking the **Add File to List** button adds information from the current file into tables so that the file can be reported on the IPR Summary, MDL & RSD and/or Percent Recovery Summary Reports. Note that to save time the Sample List should be prepared in such a way that the desired files can be added sequentially.

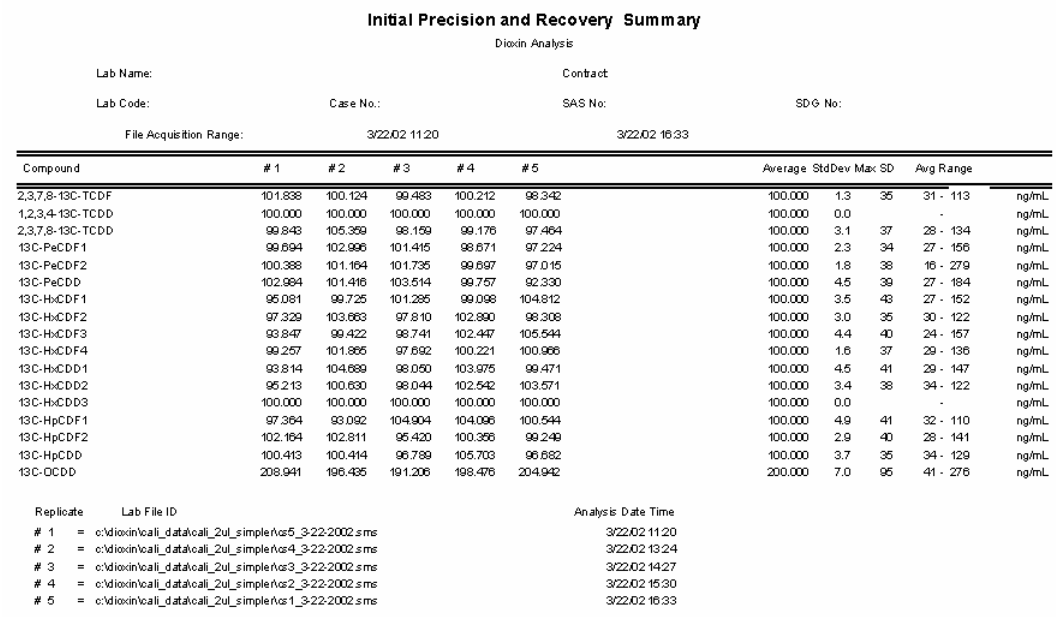
### *View List*

Clicking the View List button displays a list of the files currently available for viewing on the Summary Reports.




Summary List Viewed by Clicking View List Button

# IPR Summary Report



**Initial Precision and Recovery Summary**

Dioxin Analysis

Lab Name: Contract:

Lab Code: Case No.: SAS No: SDG No:

File Acquisition Range: 3/22/02 11:20 3/22/02 16:33

| Compound | #1 | #2 | #3 | #4 | #5 | Average | StdDev | Max SD | Avg Range | |
|---|---|---|---|---|---|---|---|---|---|---|
| 2,3,7,8-13C-TCDF | 101.838 | 100.124 | 99.483 | 100.212 | 98.342 | 100.000 | 1.3 | 35 | 31 - 113 | ng/mL |
| 1,2,3,4-13C-TCDD | 100.000 | 100.000 | 100.000 | 100.000 | 100.000 | 100.000 | 0.0 | | - | ng/mL |
| 2,3,7,8-13C-TCDD | 99.843 | 105.359 | 98.159 | 99.176 | 97.464 | 100.000 | 3.1 | 37 | 28 - 134 | ng/mL |
| 13C-PeCDF1 | 99.594 | 102.996 | 101.415 | 98.571 | 97.224 | 100.000 | 2.3 | 34 | 27 - 156 | ng/mL |
| 13C-PeCDF2 | 100.388 | 101.164 | 101.735 | 99.697 | 97.015 | 100.000 | 1.8 | 38 | 16 - 279 | ng/mL |
| 13C-PeCDD | 102.984 | 101.416 | 103.514 | 99.757 | 92.330 | 100.000 | 4.5 | 39 | 27 - 184 | ng/mL |
| 13C-HxCDF1 | 95.081 | 99.725 | 101.295 | 99.098 | 104.812 | 100.000 | 3.5 | 43 | 27 - 152 | ng/mL |
| 13C-HxCDF2 | 97.329 | 103.663 | 97.810 | 102.899 | 98.308 | 100.000 | 3.0 | 35 | 30 - 122 | ng/mL |
| 13C-HxCDF3 | 93.847 | 99.422 | 98.741 | 102.447 | 105.544 | 100.000 | 4.4 | 40 | 24 - 157 | ng/mL |
| 13C-HxCDF4 | 99.257 | 101.865 | 97.692 | 100.221 | 100.966 | 100.000 | 1.6 | 37 | 29 - 136 | ng/mL |
| 13C-HxCDD1 | 93.814 | 104.689 | 98.050 | 103.975 | 99.471 | 100.000 | 4.5 | 41 | 29 - 147 | ng/mL |
| 13C-HxCDD2 | 95.213 | 100.630 | 98.044 | 102.542 | 103.571 | 100.000 | 3.4 | 38 | 34 - 122 | ng/mL |
| 13C-HxCDD3 | 100.000 | 100.000 | 100.000 | 100.000 | 100.000 | 100.000 | 0.0 | | - | ng/mL |
| 13C-HpCDF1 | 97.364 | 93.092 | 104.904 | 104.096 | 100.544 | 100.000 | 4.9 | 41 | 32 - 110 | ng/mL |
| 13C-HpCDF2 | 102.164 | 102.811 | 95.420 | 100.356 | 99.249 | 100.000 | 2.9 | 40 | 28 - 141 | ng/mL |
| 13C-HpCDD | 100.413 | 100.414 | 96.789 | 105.703 | 96.682 | 100.000 | 3.7 | 35 | 34 - 129 | ng/mL |
| 13C-OCDD | 208.941 | 196.435 | 191.206 | 198.476 | 204.942 | 200.000 | 7.0 | 95 | 41 - 276 | ng/mL |

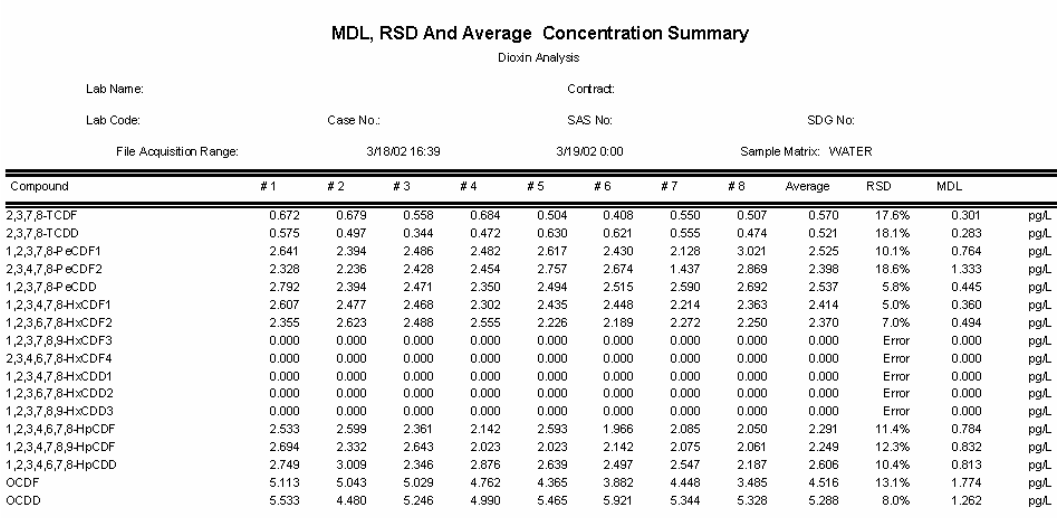
| Replicate | | Lab File ID | Analysis Date Time |
|---|---|---|---|
| # 1 | = | c:\dioxin\cali_data\cali_2ul_simple\cs5_3-22-2002.sms | 3/22/02 11:20 |
| # 2 | = | c:\dioxin\cali_data\cali_2ul_simple\cs4_3-22-2002.sms | 3/22/02 13:24 |
| # 3 | = | c:\dioxin\cali_data\cali_2ul_simple\cs3_3-22-2002.sms | 3/22/02 14:27 |
| # 4 | = | c:\dioxin\cali_data\cali_2ul_simple\cs2_3-22-2002.sms | 3/22/02 15:30 |
| # 5 | = | c:\dioxin\cali_data\cali_2ul_simple\cs1_3-22-2002.sms | 3/22/02 16:33 |

**Title:** Initial Precision and Recovery Summary

**Purpose:** Shows recovery of up to 30 replicates, the average concentration and standard deviation, the allowable standard deviation and range of recovery.

**Settings:** IPR Recovery Limits, MaxSD, High and Low recovery, Show only C13 label peaks on summary reports?, Recovery concentrations are determined by C13?, ISCompound, Standard Conc, and the initial calibration.

# MDL & RSD Report



**MDL, RSD And Average Concentration Summary**

Dioxin Analysis

Lab Name: Contract:

Lab Code: Case No.: SAS No: SDG No:

File Acquisition Range: 3/18/02 16:39 3/19/02 0:00 Sample Matrix: WATER

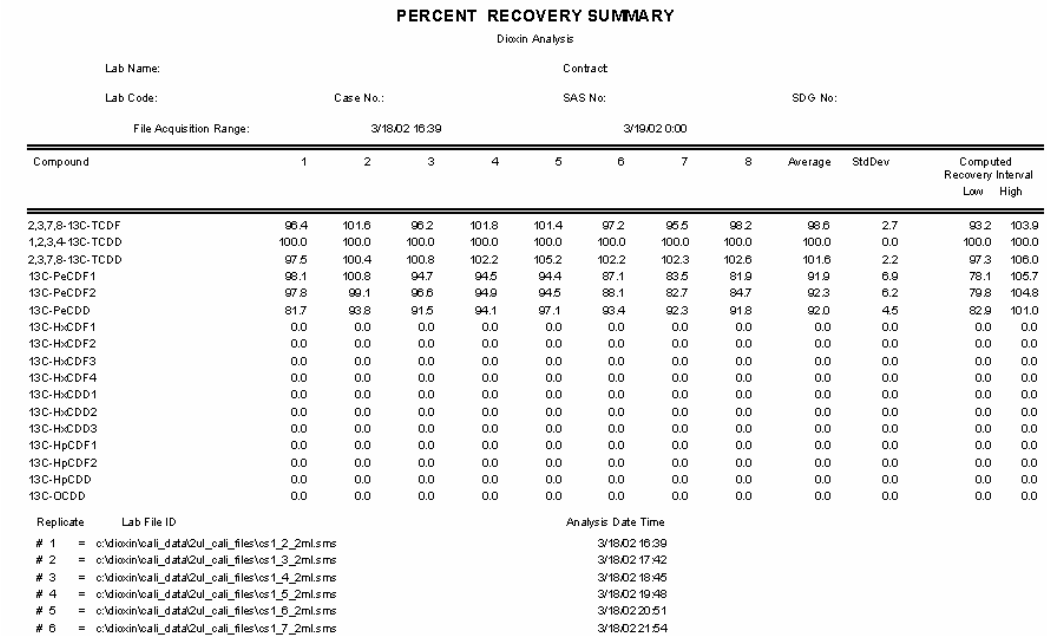
| Compound | #1 | #2 | #3 | #4 | #5 | #6 | #7 | #8 | Average | RSD | MDL | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2,3,7,8-TCDF | 0.672 | 0.679 | 0.558 | 0.684 | 0.504 | 0.408 | 0.550 | 0.507 | 0.570 | 17.6% | 0.301 | pg/L |
| 2,3,7,8-TCDD | 0.575 | 0.497 | 0.344 | 0.472 | 0.630 | 0.621 | 0.555 | 0.474 | 0.521 | 18.1% | 0.283 | pg/L |
| 1,2,3,7,8-PeCDF1 | 2.641 | 2.394 | 2.486 | 2.482 | 2.617 | 2.430 | 2.128 | 3.021 | 2.525 | 10.1% | 0.764 | pg/L |
| 2,3,4,7,8-PeCDF2 | 2.328 | 2.236 | 2.428 | 2.454 | 2.757 | 2.674 | 1.437 | 2.869 | 2.398 | 18.6% | 1.333 | pg/L |
| 1,2,3,7,8-PeCDD | 2.792 | 2.394 | 2.471 | 2.350 | 2.494 | 2.515 | 2.590 | 2.692 | 2.537 | 5.8% | 0.445 | pg/L |
| 1,2,3,4,7,8-HxCDF1 | 2.607 | 2.477 | 2.468 | 2.302 | 2.435 | 2.448 | 2.214 | 2.363 | 2.414 | 5.0% | 0.360 | pg/L |
| 1,2,3,6,7,8-HxCDF2 | 2.355 | 2.623 | 2.488 | 2.555 | 2.226 | 2.189 | 2.272 | 2.250 | 2.370 | 7.0% | 0.494 | pg/L |
| 1,2,3,7,8,9-HxCDF3 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | Error | 0.000 | pg/L |
| 2,3,4,6,7,8-HxCDF4 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | Error | 0.000 | pg/L |
| 1,2,3,4,7,8-HxCDD1 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | Error | 0.000 | pg/L |
| 1,2,3,6,7,8-HxCDD2 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | Error | 0.000 | pg/L |
| 1,2,3,7,8,9-HxCDD3 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | Error | 0.000 | pg/L |
| 1,2,3,4,6,7,8-HpCDF | 2.533 | 2.599 | 2.361 | 2.142 | 2.593 | 1.966 | 2.085 | 2.050 | 2.291 | 11.4% | 0.784 | pg/L |
| 1,2,3,4,7,8,9-HpCDF | 2.694 | 2.332 | 2.643 | 2.023 | 2.023 | 2.142 | 2.075 | 2.061 | 2.249 | 12.3% | 0.832 | pg/L |
| 1,2,3,4,6,7,8-HpCDD | 2.749 | 3.009 | 2.346 | 2.876 | 2.639 | 2.497 | 2.547 | 2.187 | 2.606 | 10.4% | 0.813 | pg/L |
| OCDF | 5.113 | 5.043 | 5.029 | 4.762 | 4.365 | 3.882 | 4.448 | 3.485 | 4.516 | 13.1% | 1.774 | pg/L |
| OCDD | 5.533 | 4.480 | 5.246 | 4.990 | 5.465 | 5.921 | 5.344 | 5.328 | 5.288 | 8.0% | 1.262 | pg/L |

**Title:** MDL, RSD and Average Concentration Summary

**Purpose:** Shows up to 30 replicate concentrations per compound, as stored in the summary table. Also shows the average concentration, Relative Standard Deviation (RSD), and the Method Detection Limit (MDL).

**Settings:** Show only C13 Label peaks on summary reports?, C13?, IS Compound, Standard Conc., and the initial calibration.

## Percent Recovery



PERCENT RECOVERY SUMMARY

Dioxin Analysis

Lab Name: Contract:

Lab Code: Case No.: SAS No: SDG No:

File Acquisition Range: 3/18/02 16:39 3/19/02 0:00

| Compound | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | Average | StdDev | Computed Recovery Interval Low | High |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2,3,7,8-13C-TCDF | 98.4 | 101.6 | 98.2 | 101.8 | 101.4 | 97.2 | 95.5 | 98.2 | 98.6 | 2.7 | 93.2 | 103.9 |
| 1,2,3,4-13C-TCDD | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 0.0 | 100.0 | 100.0 |
| 2,3,7,8-13C-TCDD | 97.5 | 100.4 | 100.8 | 102.2 | 105.2 | 102.2 | 102.3 | 102.6 | 101.6 | 2.2 | 97.3 | 106.0 |
| 13C-PeCDF1 | 98.1 | 100.8 | 94.7 | 94.5 | 94.4 | 87.1 | 83.5 | 81.9 | 91.9 | 6.9 | 78.1 | 105.7 |
| 13C-PeCDF2 | 97.8 | 99.1 | 96.6 | 94.9 | 94.5 | 88.1 | 82.7 | 84.7 | 92.3 | 6.2 | 79.8 | 104.8 |
| 13C-PeCDD | 81.7 | 93.8 | 91.5 | 94.1 | 97.1 | 93.4 | 92.3 | 91.8 | 92.0 | 4.5 | 82.9 | 101.0 |
| 13C-HxCDF1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-HxCDF2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-HxCDF3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-HxCDF4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-HxCDD1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-HxCDD2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-HxCDD3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-HpCDF1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-HpCDF2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-HpCDD | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13C-OCDD | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

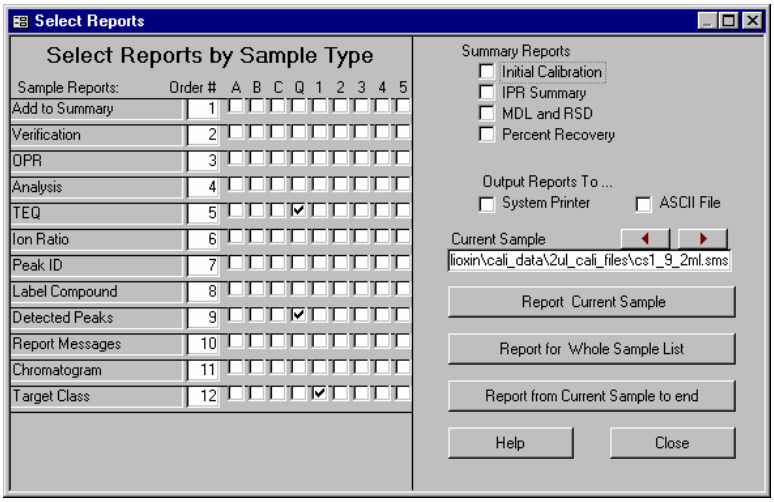
| Replicate | Lab File ID | Analysis Date Time |
|---|---|---|
| # 1 = | c:\dioxin\cali_data\2ul_cali_files\cs1_2_2ml.sms | 3/18/02 16:39 |
| # 2 = | c:\dioxin\cali_data\2ul_cali_files\cs1_3_2ml.sms | 3/18/02 17:42 |
| # 3 = | c:\dioxin\cali_data\2ul_cali_files\cs1_4_2ml.sms | 3/18/02 18:45 |
| # 4 = | c:\dioxin\cali_data\2ul_cali_files\cs1_5_2ml.sms | 3/18/02 19:48 |
| # 5 = | c:\dioxin\cali_data\2ul_cali_files\cs1_6_2ml.sms | 3/18/02 20:51 |
| # 6 = | c:\dioxin\cali_data\2ul_cali_files\cs1_7_2ml.sms | 3/18/02 21:54 |

**Title:** Percent Recovery Summary

**Purpose:** Shows up to 30 replicate percent recoveries, their average, standard deviation, and computed recovery intervals.

**Settings:** Show only C13 Label peaks on summary reports?, C13?, IS Compound, Standard Conc. and the initial calibration.

# Select Reports




The Select Reports form is used to configure profiles of the reports to be printed for each sample type, to select the Summary Reports to be printed after printing a sequence of reports, to select report destinations, and to trigger processing of report sequences.

To configure a report profile, on the left side of the form, check the reports that should be processed for each sample type. A report that has a checkmark will be generated when a data file of the sample type corresponding to the column caption is processed. The "Add to Summary" row does not generate a report. If selected, it adds results from the file being processed to the summary report data.

Reports are sent to the system default printer if the System Printer box is checked. ASCII text files are generated if the ASCII file box is checked.

The path and name of the current sample data file is shown in the Current Sample box.

Clicking Report Current Sample generates report processing selected for the file shown using its sample type. Report for Whole Sample List and Report for Current Sample to End process the indicated files from the sample list and then process the selected summary reports.

For more information right click the mouse with the cursor on the item of interest.

# Output Reports To Check Boxes

## System Printer

If the System Printer box is checked, when reports are output they will be sent to the printer selected as the default printer in Start->Settings->Printers.

## ASCII File

If the ASCII File box is checked, when reports are output they will be stored as files with the same path as the data file. The ASCII report filename will be the data file name plus three additional characters that define the report type. The extension will be ".txt". The three-letter character codes are:

VER Calibration Verification Report

OPR Ongoing Precision and Recovery Report

ANL Dioxin Analysis Report

TEQ Toxic Equivalent Summary Report

INT Ion Ratio Report

PKI Peak Identification Report

LCR Labeled Compound Recovery Report

PKS All Detected Peaks Report

XCP Messages Generated by the last report processed

Summary Reports will have the path of the template that generated them. The ASCII report will have the name of the template plus three added characters to indicate the report type. The file extension is ".txt" The three-letter character codes are:

ICC Initial Calibration

IPR Initial Precision and Recovery

MDL MDL, RSD and Average Concentration Summary

OPR Percent Recovery Report

Example where the template is c:\varianws\Dioxin Data\Dioxins.swt and the MS Workstation data file c:\varianws\Dioxin Data\soil34.sms:

The Dioxin Analysis Report will be:

- C:\varianws\Dioxin Data\soil34ANL.txt

The Initial Calibration Report will be:

- C:\varianws\DioxICC.txt

# Buttons: Select Reports

## Report Current Sample

If the Report Current Sample button is clicked, reports specified for the Sample Type of the currently selected sample file will be generated to the selected output destinations.

## Report for Whole Sample List

If the Report for Whole Sample List button is clicked, the sample list will be traversed. For each sample, the reports selected for the sample type of the sample will be sent to the selected output destinations. After the Sample List has been processed, the selected summary reports will be sent to the selected output destinations.

## Report for Current Sample to End

If the Report for Current Sample to End button is clicked, the sample list is traversed from the current sample to the end. For each sample, the reports selected for the sample type of the sample will be sent to the selected output destinations. After the Sample List has been processed, the selected summary reports will be sent to the selected output destinations.

## Left and Right Arrows

Click the Left Arrow to move the current sample to the prior Sample List position. Click the Right Arrow to move the current sample to the next Sample List position.

## Close

Clicking here will close the Select Reports form.

# Sample Reports Fields

## Current Sample

The Current Sample field displays the path and name of the currently active sample in the Sample List. Use backward and forward arrows to scroll through the files in the Sample List.

## Order #

Order number is the sequential order in which this report will be printed. The order may be edited.

## A

If this box is checked the Sample Report indicated on the left will be generated when files of Sample Type A (Analysis) are processed. "A" is the default sample type.

## B

If this box is checked the Sample Report indicated on the left will be generated when files of Sample Type B (Blank) are processed.

## C

If this box is checked the Sample Report indicated on the left will be generated when files of Sample Type C (Calibration Verification) are processed.

## Q

If this box is checked the Sample Report indicated on the left will be generated when files of Sample Type Q (Quality Control) are processed.

## 1

If this box is checked the Sample Report indicated on the left will be generated when files of Sample Type 1 (Calibration Level 1) are processed.

## 2

If this box is checked the Sample Report indicated on the left will be generated when files of Sample Type 2 (Calibration Level 2) are processed.

## 3

If this box is checked the Sample Report indicated on the left will be generated when files of Sample Type 3 (Calibration Level 3) are processed.

## 4

If this box is checked the Sample Report indicated on the left will be generated when files of Sample Type 4 (Calibration Level 4) are processed.

## 5

If this box is checked the Sample Report indicated on the left will be generated when files of Sample Type 5 (Calibration Level 5) are processed.

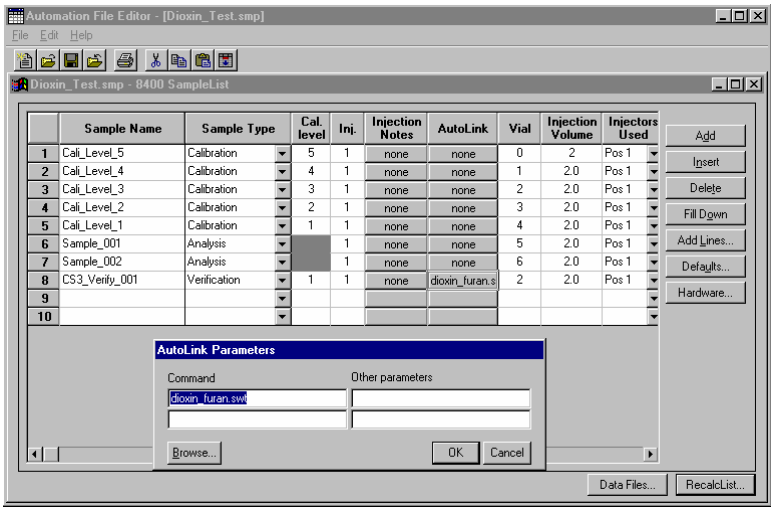
# Automation

Before online reporting can take place, the reporting template (.swt) must be completed. The Laboratory Information, Method setup, Compound Information, Sample List and Reporting specifications must be set up. The name of this completed Dioxin Reports template (.swt) will be used in the Auto Link field of the Sample List of the core MS Workstation software.

Note: So that the Autolink invocation works correctly, it is best not to use spaces in the name of the Dioxin Reports template. Use the underscore (_) sign to separate words in the template name.

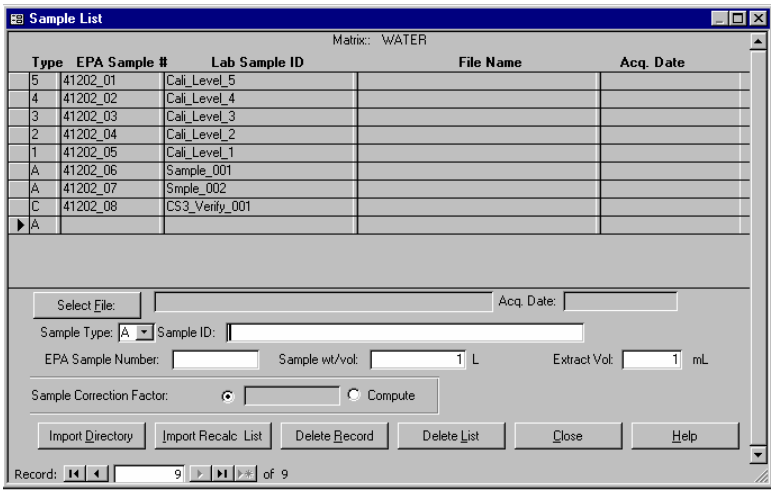
Dioxin Reports output may be generated immediately after the file acquisition is completed. If this is the desired report generation format, the Sample List used in System Control of the MS Workstation to execute data acquisition and the Sample List in Dioxin Reports must be coordinated.

## Sample List in MS Workstation Software




Complete the Sample List for data acquisition, specifying unique sample names. In the Auto Link field enter the name of the Dioxin Reports template to be used for reporting once the acquisition is completed.

## Sample List in Dioxin Reports




The sample list in the Dioxin Reports template (*.swt) used in the Auto Link field must be filled out properly. The "Sample Name" specified in the automation sample list file should be entered into the white "Sample ID" field in the lower part of the Sample List form. This name will then be displayed in the "Lab Sample ID" field in the Dioxin Reports Sample List. The Lab Sample ID will be the link between the data files to be acquired and the reporting specifications for them in Dioxin Reports. The other sample parameters (EPA sample number, date received on the form shown above) also may be entered for each sample when the Dioxin Reports Sample List is created.