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How can Waddell Software Development (WSD) improve the performance of your high-resolution mass spectrometry processing system?

High-resolution mass spectrometry analysis for dioxins and PCBs has existed for a number of years. Moreover, a number of different international manufacturers supply instruments that can perform the analysis. However, the demand for isomer speciation has been such that only a handful of laboratories have chosen to actually perform these detailed techniques on a commercial basis. Accordingly, the market has not developed a uniform comprehensive system to do the reporting. Each of the labs involved has developed their own software to address the intricate peculiarities of the processing requirements.

Many labs have opted to use spreadsheet analysis with manual data entry of peak information. Other labs choose to use manufacturer-supplied software (such as OpusQuan) to perform quantitation. Other labs have developed techniques to pass peak information to in-house developed software that does the quantitation in an automated fashion. Still other labs have combined vendor software with post processing to more fully exploit software automation.

In most of these situations, there remain manual processes that can be automated to both generate a more comprehensive reporting format and eliminate human errors that can be attributed to handling large volumes of data. WSD has helped in each of these situations to improve the productivity of the lab.

Listed below are a number of different techniques that WSD has used to reduce turnaround times and increase consistency and quality control for high-resolution dioxin and PCB reporting.

- **Automated data transfer**. Most labs have overcome the networking challenges to be able to transfer information from the instrument over to other computers to process and report the data. Others, unfortunately, have not been able to make this leap. WSD has been able to help some of those smaller labs who hadn't made this productivity leap, without the need to invest in networking equipment.

- **Peak matching**. Several hi-resolution methods specify criterion for Peak co-maximization. WSD has automated much more extensive Peak matching algorithms to allow the laboratories to get more control over the peak matching function.

- **Ether channel flagging**. When interference exists in the diphenylether channel, the corresponding furan channel must be flagged. Often this inspection is done manually, and the flags attached by hand. WSD has automated the identification of interference in the ether channel, and automated the application of flags.

- **Ether channel valleys**. In some packages, Ether Channel flagging has been partially automated. When peaks exist, a flag is applied. WSD has automated the interference identification for both peaks **and valleys.**

- **Combine/consolidate confirms, full screens, dilutions, etc. into reports.** A common problem relates to the necessity to use only selected results from a particular analysis and combine them with results from another analysis of the same sample. WSD as developed straightforward technique to combine all various runs. A typical example would be running a dilution to bring the octa channel under saturation.

- **Noise calculation**. Several labs have questioned the calculation of the noise level by their instrument software. WSD has implemented auxiliary techniques to calculate noise using "means of the extremes" so that the EPA description of noise calculation is most closely followed. With this technology, WSD can adjust noise level calculations to comply with the environment found on most instruments.

- **Blank flagging.** Several methods require that if a specific isomer is found within the batch's QC blank, and, if that isomer is found in any sample (up to a multiple of the blank), it be flagged with a data qualifier. WSD was provided this automated feature and the method specific multiplier specification.

- **Non-standard spiking amounts.** Each analytical method specifies specific spiking amount for internal and recovery standards. However, most labs experience a persistent number of samples where errors are made in wet lab. In some of those cases (as with air samples), the lab may not be able to re-extract. WSD has developed easy, auditable, ways to change the spike amounts and continue with processing.

- **First and last eluters**. Most dioxin and PCB analyses include first and last eluters within the spike mix for a retention time check. WSD has found several ways to integrate this function into its custom programs.

    a. Print chromatogram with print boundaries based on the first and last eluters. Instead of the whole window, our program can make the retention time limits automatically.
    b. Downstream, it can flag peaks outside the first and last eluters, so the operator can use his/her judgment to determine if the peak should be included. For example, a dirty sample might create peaks that elute late, but they would, under normal conditions, be included in the window.
    c. Some software may adjust for first and last eluters. However, WSD has provided for shifts in the first and last eluters' Retention Times based on the shifts of the internal standards.

- **Totals calculation**. Some labs have had problems dealing with non-specific isomers. In particular, there have been problems in handling the different ways in which out-of-ratio peaks (EMPSs) are calculated. WSD has programmed many of the more common approaches such as ignoring, including, adjusting down to theoretical ratio, and several different flagging alternatives.

- **Totals across function groups.** Some instrument settings result in some channels (such as Penta CDF) spanning function groups. Most manufacturer software is unable to merge the peaks from both function groups. WSD has addressed this issue and has allowed several labs to combine peaks from both function groups into one total amount.

- **J and E flagging for specific isomers and totals.** When a specific peak is flagged as being below or above the Initial Calibration dynamic range, the assignment can be straightforward. However, for non-specific peaks, and for totals, the various methods have different requirements for flagging. WSD has addressed and dealt with these combinations.

- **Reporting.** Several labs have had problems converting from manufacturer reporting systems to other reporting systems (such as Crystal Reports, Excel spreadsheets, etc.). WSD has been able to bridge that gap and allow labs to report in the same environment as their other analytical methods. This allows all reports to look the same coming out of the lab.

- **Archiving.** Even with the constant drop in computer disk storage prices, storage is not infinite. WSD has worked with labs to automate the archive of information after the analysis is complete and the information is in the customer's hand. This has allowed for reduced storage requirements and faster storage times.

- **Archive Retrieval.** Archived data may need to be restored so that questions on a specific sample may be answered. Also, a customer way wish to have information for a specific site analyzed over time. As such, information from a number of samples, such as quarterly monitoring samples, may need to be retrieved. WSD has worked with laboratories to accomplish this task with a minimum of operator interaction.

Any modifications to a laboratory's existing procedures should be rigorously validated prior to implementation. WSD provides a comprehensive QC validation program, which is designed to cover this requirement. This QC program is the property of the client and can be repeatedly used to validate any future modifications to their data retrieval/processing system.

Waddell Software Development can help you in any of these areas. There are, of course, a number of other features and capabilities that we've provided to assist in laboratory automation and productivity enhancement. Hardware and corresponding software varies among laboratories. However, the principles defined by US EPA methods requiring high-resolution mass spectrometry are consistent. Waddell Software Development has decades of experience in integrating laboratory analytical processes to meet those method requirements.

To learn more about Waddell Software Development, visit our web site at:
http://www.waddellsoftware.com