# Computer Elucidation of ICP-MS Spectral Data for the Presence, Identification and Software Correction of Interferences for Qualitative and Quantitative Analysis

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## Overview

➢A new deconvulotion method based on mass spectral peak shape calibration was developed for mixture analysis of overlapped ICP-MS data

➢On a unit mass resolution quadrupole ICP-MS instrument, As at the presence of interference including ArCl , AsH, and Ar2 have been accurately quantified through the spectral accuracy calculation by MassWorks.

## Introduction

Much of ICP-MS development in the last twenty years has centered around collision cells for the physical removal of interferences through reaction chemistry. While quite useful and effective in real world applications, the use of collision cells and the associated chemistry does compromise the analytical sensitivity. In addition, there are interferences that are difficult to remove through chemical reactions even after extensive method development. In this paper, we report a new approach to quantify analyte of interest at presence of interference. Based on peak shape calibration technology, this approach has proved to be very effective to deconvolute overlapped ion signals such as the mixtures of 14C/12C in drug metabolism studies, molecular ions and their fragments (M-H) in EI GC/MS, the parent ions and their oxidized products. Since most of the interference occurred in ICP-MS is known and can be expressed by a chemical formula, the deconvolution can be readily implemented through the mixture search by MassWorks. We will demonstrate the deconvolution of the mixtures of As and the interferences ArCl, AsH, and Ar₂ successfully resulted in accurate identification and quantification of the components in the mixture.

## Methods

➢**Data Acquisition:** All data were acquired in survey mode with a mass range from 0 to 260. The experiments were designed to focus on the studies of As and its isobaric interference ArCl. The raw data of ICP-MS were exported into text data format for MassWorks to process.

➢**MassWorks processing:** All the data were calibrated through a new mass spectral calibration that not only calibrates the m/z axis but, more importantly, calibrates the mass spectral peak shape. With the theoretical mass spectral responses for the ion of interest and possible interference ions known exactly, a multiple linear regression can be applied to any measured mass spectral response after the above calibration to arrive at the relative concentrations of these ions including both the unknown and the interference.

➢**Quantitation of As was performed through calculation of spectral accuracy to obtain its relative concentration at presence of a various of interference.**

## Results and Discussion

**Fig 1. Generation of Calibration with As Standard**



Raw MS
Calibrated MS

| Net Formula | Mono Mass | Closest Centroid | ΔM(mDa) | ΔM(ppm) | Spectral Accuracy |
|---|---|---|---|---|---|
| As | 74.9216 | 74.9211 | -0.5469 | -7.3 | 98.9 |
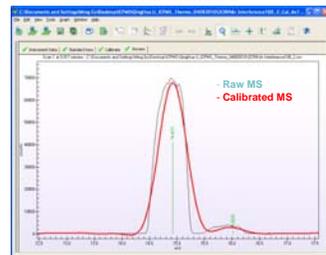
**Fig 2. Application of the Calibration to Composed Spectra**



74.2
Raw Spectrum
Calibrated Spectrum
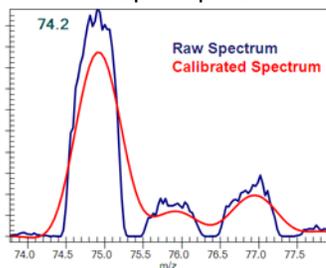
For this application, element As as a standard was used for both mass and peak shape calibration to enable highly accurate isotope pattern matching for mixture analysis. This calibration is then applied to the ICP-MS data files to perform spectral deconvolution to obtain quantitative information of As at the presence of ArCl and other interferences by CLIPS search.

The first analysis was to quantify the As considering the interference of ArCl only since the ArCl was purposed introduced by experiment design. However, the spectral accuracy calculation for such a mixture resulted in poor spectral accuracy at 87.3%. This result indicated other possible interference existed in the mixture which is consistent with the observation of marked peak at m/z 76.

**Fig 3. Spectral Accuracy for As with ArCl as only possible interference**



Calibrated
Fitted w/As & ArCl
Spectral Accuracy=87.2%
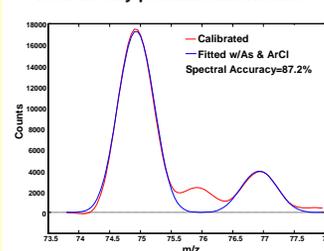
**Fig 4. Spectral Accuracy Calculation Parameters**
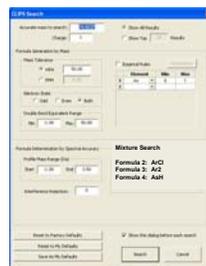


**Fig 5. Spectral Accuracy for As with ArCl, AsH, and Ar₂ as possible interferences**



Calibrated
Fitted w/As, ArCl, AsH & Ar2
Spectral Accuracy=96.4%
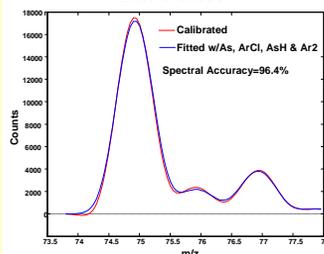
**Fig 6. Theoretical Isotope Distribution of Ar₂**



$^{40}Ar^{40}Ar$ 79.92
x10
$^{36}Ar^{40}Ar$
75.93
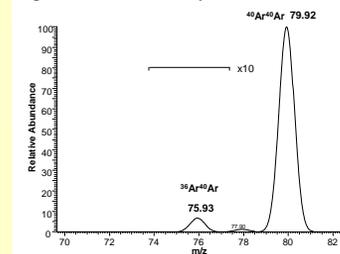
**Fig.7 ID and Quantitation of 4 Components Mixture Spectra**
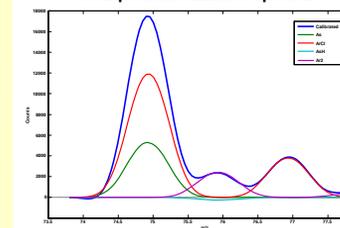


In this well controlled experiment, possible interferences at m/z 76 are likely to be AsH and an isotopic component of $^{36}AR^{40}Ar$ from Ar₂. Although relative intensities of $^{36}Ar^{40}Ar$ are very small compared with those of $^{40}Ar^{40}Ar$ as shown in Fig. 6, their absolute intensities could be significant due to overwhelming intensities of Ar₂. In the second analysi, four comsponents including analyte As and interference of ArCl, ASH, and Ar2 were used for spectral accuracy calculation to determine relative concentration of each of individual component. We obtained high spectral accuracy of 96.3% indicating real decent matching between calibrated and theoretical calculated spectra as shown in Fig. 5. This result shows that ArCl is dominant component with relative concentration about 95%, while As and Ar2 accounts for about 3.5% and 1.5% respectively.

## Conclusions

➢With peak shape calibration generated with As standard, symmetrical and mathematical well defined peak shape can be obtained for all ICP-MS spectra. This allows accurate spectral deconvolution and quantitation of the mixtures containing As, spiked with [ Cl⁻ ], AsH, and $^{36}AR^{40}Ar$.

➢Quantitative analysis of mixture through spectral accuracy calculation employed profile data has advantages over the calculation using centroid data or isotope ratios, which has more degrees of freedom to allow spectral deconvolution of multiple components.

➢Current version of MassWorks can perform three components mixture analysis. In a future release, multiple components, virtually unlimited components can be performed with the spectral deconvolution.

## References

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