

Improved performance of elemental composition determination through true internal calibration on a compact MS system

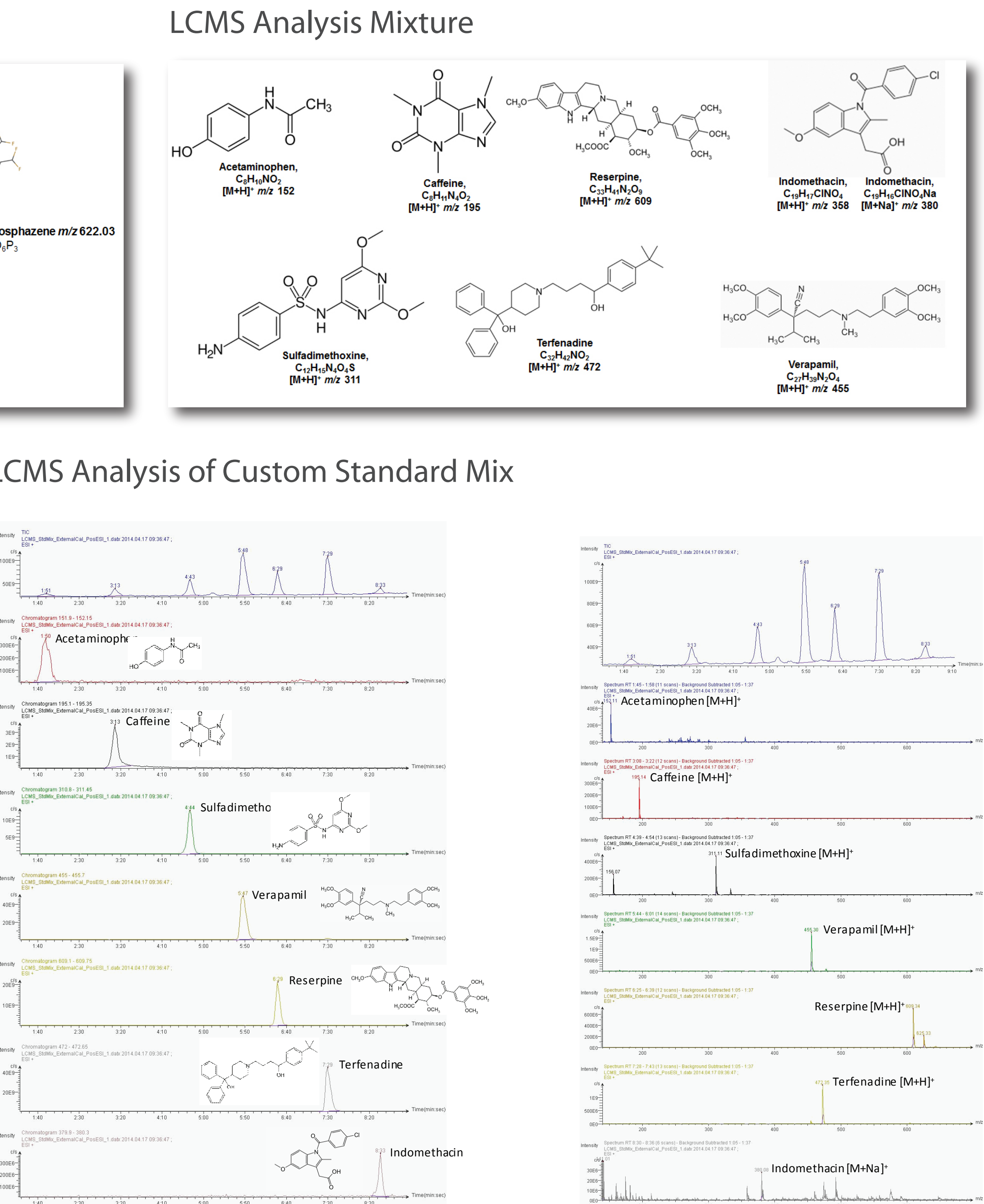
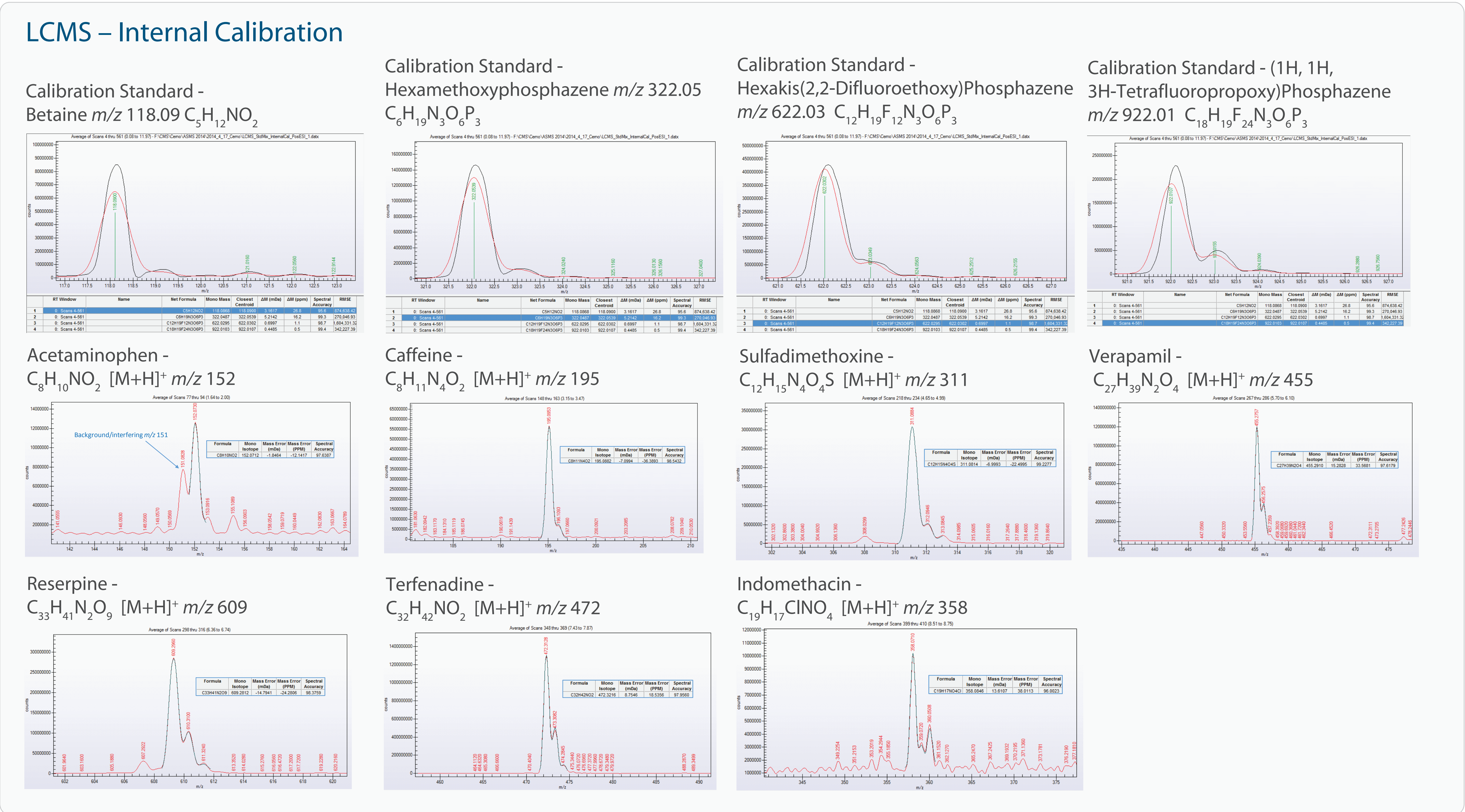
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Introduction

A recently introduced and more economical Quadrupole compact mass spectrometer affording unit mass resolution was used to achieve elemental composition determination of unknown compounds through instrument line shape calibration technology. Briefly, this comprehensive mass spectral technology calibrates not only *m/z* values, but more importantly, the mass spectral peak shape. Consequently, symmetrical and mathematically well-defined mass spectral peak shape is obtained to allow accurate mass measurement on unit resolution mass spectra even when the monoisotopic peak (A) is overlapped with the corresponding A+1 peak. In addition to the high mass accuracy thus achieved, the high spectral accuracy available from a quadrupole system allows for exact isotope modeling to achieve elemental composition determination, much like one would achieve with a high resolution MS system such as TOF or qTOF. In this work, both external and internal calibration standards were investigated with their respective mass accuracy as well as the effectiveness of elemental composition determination.

Results



Summary

Compound	External Calibration (mDa)	Internal Calibration (mDa)
Acetaminophen	-9.35	-1.85
Caffeine	-21.30	-7.10
Sulfadimethoxine	11.20	-7.00
Verapamil	55.28	15.28
Reserpine	26.81	-14.79
Terfenadine	42.05	8.75
Indomethacin*	54.06	13.61

Conclusion

With the novel instrument line shape calibration technology embedded in the MassWorks software, the expression compact mass spectrometer can achieve sufficient high mass and spectral accuracy to enable elemental composition determination of unknown compounds or for compound confirmation. While the utilization of internal calibration requires additional experimental setup, it does provide better mass accuracy to help minimize false positives when compared to external calibrations.