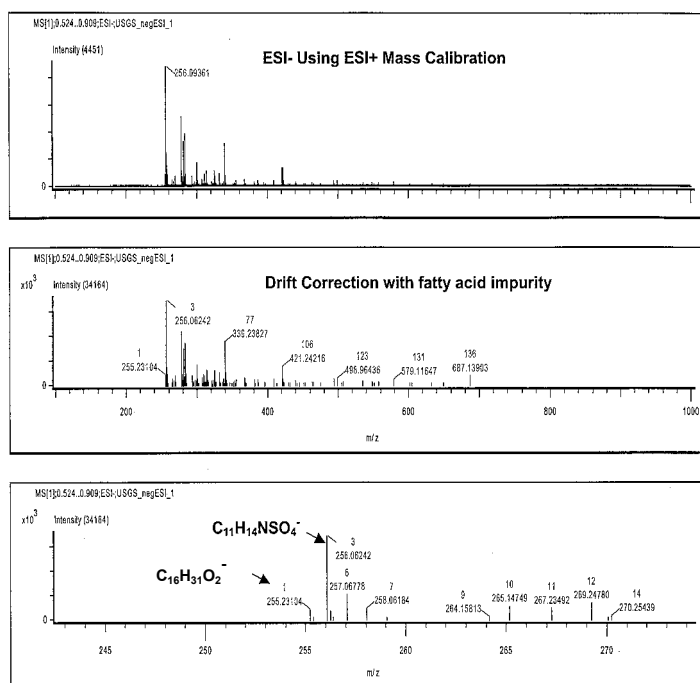


# AccuTOF™

## Using a Positive-Ion Calibration for an Exact Mass Measurement in Negative-Ion Mode

The *AccuTOF* makes it very easy to obtain exact mass measurements and determine elemental compositions. The mass spectra shown below were acquired with the electrospray ion source operated in negative-ion mode. The mass calibration was acquired the previous day in positive-ion mode. After changing the mass spectrometer polarity and retuning, a stearic acid impurity (present in the methanol) was used as a single-point drift correction “lock mass” to determine the elemental composition of the analyte peak at  $m/z$  256.06242 and the palmitic acid impurity at  $m/z$  256.23104. The error was less than 0.002 u.



Sample  
courtesy of  
Mike  
Thurman and  
Imma Ferrer  
-- USGS

Measured (u)	Theoretical (u)	Composition	Difference (mmu)
256.06242	256.06435	$C_{11}H_{14}NSO_4^-$	-1.93
255.23104	255.23240	$C_{16}H_{31}O_2^-$	-1.36