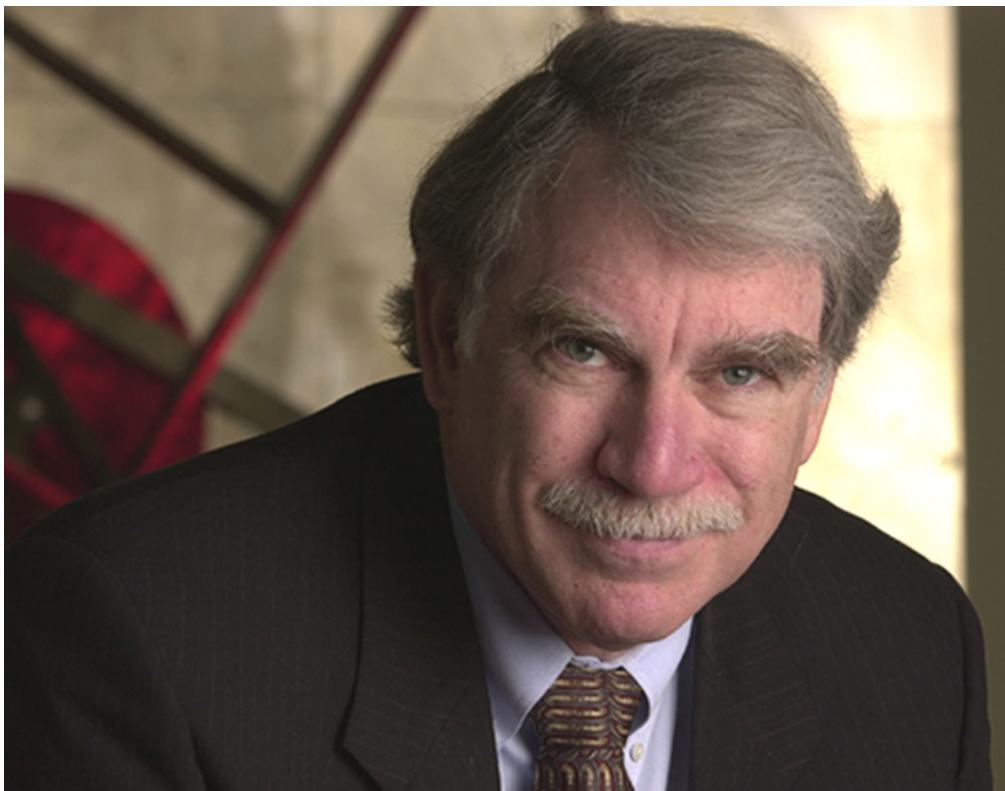


**The Chicago Mass Spectrometry Discussion Group (CMSDG)  
Presents:**

**Dr. Alan Marshall, Director, Ion Cyclotron Resonance  
Program of the National High Magnetic Field Laboratory**



**Accurate Mass Measurement:  
Taking Full Analytical Advantage of Nature's  
Isotopic Complexity**

**Date:** Friday May 6<sup>th</sup>, 2005

**Location:** University of Chicago, Kent Hall 107. Talk to begin at 6:00 pm, refreshments and food at 5:30 pm.

**For directions go to:** <http://maps.uchicago.edu/mainquad/kentlab.html>

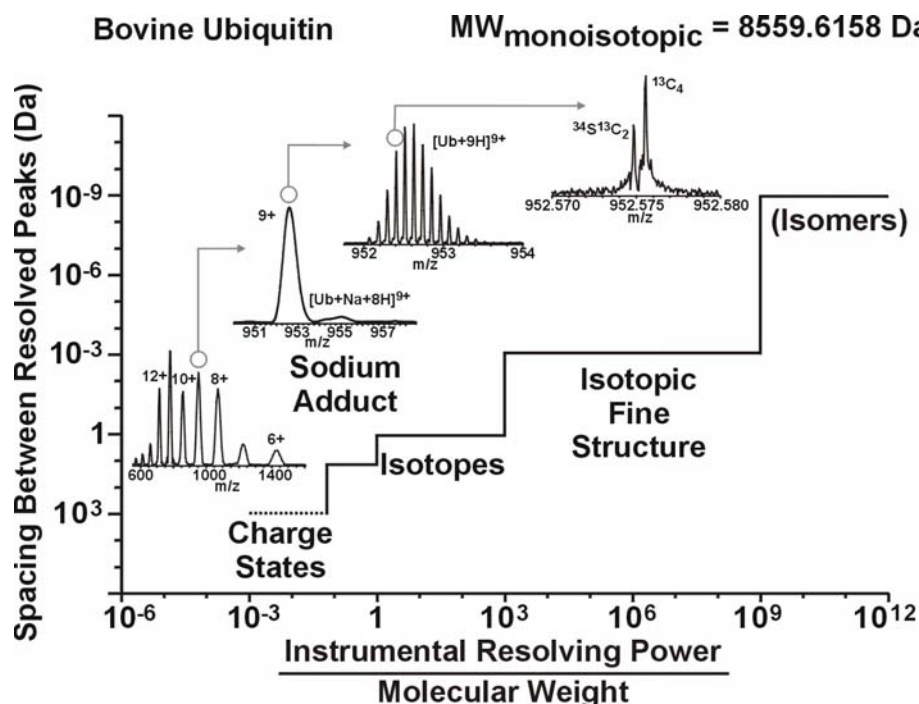
# Accurate Mass Measurement: Taking Full Analytical Advantage of Nature's Isotopic Complexity

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Most mass analysis relies on "nominal" mass accuracy (i.e., to within 1 Da). However, an increasing number of applications are based on much more accurate mass measurement. The Figure shows that mass spectrometric resolution (defined here as the spacing between resolved peaks) does not increase monotonically with increasing spectrometer resolving power for electrosprayed biomolecules. Rather, resolution improves by a series of steps. First, one must resolve different charge states. No additional peaks appear until adducts are resolved, then not again until isotopic peaks are resolved (unit mass resolution), and finally when isotopic "fine structure" (i.e., different elemental compositions of same nominal mass) is resolved. The easiest way to apprehend the advantages of Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is that it effectively extends the onset of each "plateau" in Figure 1 to ~100 times higher mass than with any other mass analyzer.



**Mixtures and Elemental Compositions.** High mass resolving power ( $m/\Delta m_{50\%} > 300,000$  over a wide mass range) offers two major advantages. First, it becomes possible to separate complex mixtures without prior chromatographic or gel separation. Second, elemental composition may be determined from accurate (to ~1 ppm) mass measurement alone for unknown molecules up to ~1,000 Da. Examples from environmental, petrochemical, analytical, and biological problems will be presented, including world records for mass resolution.

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