Mass Spectrometry

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1 INTRODUCTION

> "It is a fundamental tenet of chemistry that the structural formula of any compound contains coded within it all that compound's chemical, physical and biological properties." (Katritzky, Karelson and Lobanov, 1997)

If we accept this statement as philosophical truth, the determination of the structure of organic molecules is of paramount interest. Determining the structure will permit determining all other properties of the molecule. Therefore, methods for determining structure are important. Mass spectrometry has become one of the premier methods for determining organic structure, and is generally the first line of experimentation done (if not the only experimentation necessary) for determining the structure of organic molecules. Mass spectrometry, coupled especially with liquid chromatography (normal or reverse phase), is a foundation experimental technique in any structure elucidation effort, and in drug metabolism in particular. The combination of high-resolution chromatography, for handling complex mixtures, and the structural specificity and sensitivity for detecting low-level components of mass spectrometry—both in low relative abundance in a mixture and low absolute amounts of analyte—is unsurpassable for tackling such problems. Sometimes it is sufficient to solve the problem. Always it is necessary to have done the experiments to provide solid foundation for subsequent required work—by isolation, NMR, synthesis, and so on—to finally arrive at the answer.

> "Why learn anything about spectral interpretation when the computer can do all the work? The answer to this question is simple, as most conscientious users quickly realize. The library search often does not provide a realistic answer or (worse) may provide an answer that looks correct but is not. Even software programs that profess to 'interpret' unknown spectra can only provide probable answers. After that, you are left to your own devices." (Smith, 2004)

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