LC/MS Application in the Drug Discovery

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Liquid chromatography (LC) combined with mass spectrometry (MS) creates an ideal analytical tool for the laboratory. The high-performance liquid chromatography (HPLC) has been the laboratory tool of choice for separating, analyzing, and purifying mixtures of organic compounds since the 1970s. An HPLC column can separate almost any mixture that can be dissolved. A mass spectrometer can ionize the separated peak solution and provide a molecular weight for each peak component. An LC/MS/MS system can fragment the parent ion into a distinctive fragmentation pattern and can separate the daughter ions for identification and quantitation. The characteristic fragmentation pattern from each parent ion can be identified by comparison to fragmentation patterns produced by standard computerized databases. There are currently three principal application areas in LC/MS, but the technique has much wider potential application and is in fact already being applied to a variety of fields. The first main area is compound discovery and identity confirmation in pharmaceutical manufacturing or drug discovery. The second application area, called *proteomics,* is protein structure determination by LC/MS. A growing subset of these studies is in the field of DNA/RNA structure studies; although the name is not in common use currently, an appropriate term would be *nucleomics*. The third area of application is in metabolite and trace contaminates studies. Our main interest here is the compound discovery; anyone doing organic synthesis or isolating compounds from biological sources has an interest, first, in establishing the activity of the compound, then its molecular weight, and finally, the compound's definitive structure. In this study we will focus step by step on the identification and characterization of new drugs from the medicinal plant *Solandra grandiflora* using LC/MS.