

LEARNING A NEW LANGUAGE: HOW TO AUTOMATE PROCESSING OF LC-MS DEREPLICATION DATA WITH VISUAL BASIC.

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Automation of repetitive tasks in the processing of natural product extracts results in significant improvements in sample throughput. Fraction collectors and modern HPLC technology greatly reduce the need to separate components by column chromatography employing manual and semi-automatic fraction collection. Liquid handlers can also do much of the post fractionation sample work-up and assay well plate preparation. An area of potential automation often overlooked is the handling of large chromatographic data sets (DAD, MSD) generated by such tasks as sample dereplication. While modern software packages can be used (and are indeed necessary) to process this data they still require user interaction to process one chromatographic data set at a time. The Win32 Application Programming Interface allows for automation of those software packages exposing properties, methods, and events in accordance with the COM+ specification. Here a method for automatically processing spectrometric and spectroscopic dereplication data from multiple marine natural product extracts and automatically querying result sets against the MarinLit database is described. A Win32 programming language is used along with the Bruker Data Analysis and Advanced Chemistry Development SpecManager object libraries to process chromatographic and spectroscopic data, respectively. Using this approach a report is generated using the Cambridgesoft Chemdraw ActiveX control in conjunction with the Microsoft Word object library. This method was successfully applied to a small number of marine sponge extracts known to have a high redundancy of previously identified compounds. It is expected that as the number of samples processed grows beyond more than a handful, significant time savings will be observed with sample dereplication, and potentially a more complete reporting of known compounds.