



Integrating Cheminformatics and Spectroscopy to Elucidate the Structures of Natural Products

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This is a talk I gave at the 5th Brazilian Conference on Natural Products as part of my “spare time” activities and to remain engaged with my passion of NMR, structure elucidation and computational spectroscopy applications

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The structure elucidation of natural product structures from analytical data, specifically NMR and MS, remains a major challenge. With an enormous palette of NMR experiments to choose from, and supported by breakthrough technologies in hardware, the generation of high quality data to enable even the most complex of natural product structures to be determined is no longer the major hurdle. The challenge is in the analysis of the data. We are in a new era in terms of approaches to structure elucidation: one where computers, databases, and a synergy between scientists and algorithms can offer an accelerated path forward. Software tools are capable of digesting spectroscopic data to elucidate extremely complex natural products. Scientists can now elucidate chemical structures utilizing multinuclear chemical shift data, correlation data from an array of 2D NMR experiments and utilize existing data sets for the purpose of dereplication and computer-assisted structure elucidation. With the explosion of online data especially, in public databases such as PubChem and ChemSpider, many tens of millions of chemical structures are available to seed fragment databases to include in the elucidation process. This presentation will provide an overview of how cheminformatics and chemical databases have been brought together to assist in the identification of natural products. It will include an examination of the state-of-the-art developments in Computer-Assisted Structure Elucidation.

Cheminformatics and the Structure Elucidation of Natural Products from **US Environmental Protection Agency (EPA)**