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Cyber-Enabled Structure Elucidation System

The elucidation of the structure of carbon-based compounds is a ubiquitous component of problem solving in chemical, biological and health-related fields. For example, in the pharmaceutical industry many powerful drugs are derived from limited natural sources incapable of providing required needs. Structure elucidation must precede synthesis and manufacture. The structure of life-threatening toxins must be identified in the search for antidotes. Rapid, reliable and versatile cyber-enabled structure elucidation software can substantially augment productivity in many chemically related projects of research and development.

Researchers at Arizona State University have developed a program called SESAMI (Systematic Elucidation of Structure Applying Machine Intelligence), a comprehensive, computer-based structure elucidation system capable of solving of real-world, complex carbon-based structures rapidly and reliably.

The latest version of SESAMI (2.0), like an experienced chemist, uses the collective spectroscopic properties of a compound of unknown structure as input and directly reducing those data to a very small number of compatible molecular structures, preferably one. The software is built on a platform possessing capabilities in both spectrum interpretation and structure generation. The former produces a set of structural inferences that must be sufficiently rich in information content to dramatically narrow the number of compatible molecular structures, again preferably to one. The structure generator in SESAMI 2.0 is exhaustive and based on an entirely new concept. It is designed to produce all structures compatible with the spectroscopic input, thereby providing the user with the assurance that there is no other molecular structure equally compatible with the input. Thus, SESAMI is not dependent on a data base of structural features. The conversational nature of the program (i.e., efficiency) is enhanced in a number of ways. Structural inferences are used prospectively and very early in the structure generation process, and the program uses redundant, ambiguous and alternative interpretations (i.e., multiple interpretations of the same data) of the spectral data directly without any preprocessing. The structure generator both detects and eliminates highly strained structures prospectively.

This new SESAMI 2.0 system is remarkably efficient and powerful in solving real world, complex structure elucidation problems, overcoming many of the disadvantages observed in other systems. The platform is designed to readily

facilitate expanding SESAMI's versatility and its power.

Potential Applications

- Structure elucidation of complex carbon based compounds
- Drug development
- Research

Benefits and Advantages

- Earlier detection and removal of strained unstable structural features
- Allows for a seamless link between spectral interpretation and structure generation
- Spectrum interpretation is capable of producing a set of substantially rich substructural inferences
- Uses a more efficient structure generator that produces all molecular structures compatible with the input to assure that there are no other structures equally compatible with the input
 - o Extends the applicability of the program and alleviates bottlenecks without the need for additional manpower
- Produces results in a timely manner while avoiding combinatorial explosion
- Operates in either fully automated or interactive mode
- Can elucidate the structures of even complex high molecular weight compounds

For more information about the inventor(s) and their research, please see

[Dr. Munk's Departmental Webpage](#)