

The Case for CASE: Computer-Assisted Structure Elucidation



Introduction

Computer-assisted structure elucidation (CASE) has been used to help identify compounds isolated by the detection of novel or difficult structural isomers, especially those of unusual products of drug metabolism and synthesis. The completely automatic structure determination, even from the smallest of samples, has now become a reality. Systems like ACD/LABS are designed to do this in a very efficient way.



Figure 1: The large number of possible isomers for some relatively small organic molecules.

Modern CASE algorithms give ever-increasing amounts of information about a substance's structure, such as its molecular weight, formula, and other information on composition. However, when a particular structure has been found (it gives weight to the system for computer-assisted elucidation of structure) it

CASE Methodology

ACD/LABS is simply one of many computer-assisted systems designed to help elucidate structure.

1. Obtain experimental data to extract knowledge
 - Molecular Formula
 - Masses
 - Chemical shifts
 - Substructures
 - Connections
 - Green Synthesis
 - Special features
2. Search structure space to derive all possible structures
3. Ranklist based on all criteria
 - Ranked structural list

Case Illustrations



Figure 2: An ACD/LABS CASE software panel displaying the fragmentation pathway of an oil of essential oils. The molecule was identified using ACD/LABS. During elucidation, the software displayed isomers that fit the experimental data and structure, highlighting those which are likely to be accurate.

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Automated Elucidation



Figure 3: A Molecular Connectivity Matrix (MCM) is created automatically during data interpretation. This can be used both for de novo elucidation, or to perform an elucidation check on proposed structures.

Ranking New Bond Candidates

Using the advanced properties of substructure Molecular Weights, the priority of the structure space can be guided for possible structures which agree with the experimental data. The software automatically evaluates all structural possibilities, and then ranks the bond candidates by giving weight to the difference between the experimental and proposed structural data.



Figure 4: A list of proposed structures, ranked by their calculated Molecular Weight Difference. Structures highlighted are color-coded based on their agreement with the experimental data.

Report Generation and Statistics

With the right information, better decisions can also be quickly identified from structure lists. The following table shows the statistics using ACD/LABS software:

1. Structures and Weight list
 - 200,000 assigned chemical structures
2. Molecular Weights list
 - 200,000 structures
 - 4,400,000 structural fragments
3. Chemicals list
 - 20,000 new structural compounds with Mol. Wt. 100, 150, and 200
4. Summary of Molecular Properties
 - 200,000 new compounds
5. Masses
 - 2,000,000 compounds having masses
6. Formulae
 - 2,000,000 compounds having formulae and higher range

The Reported Elucidation Challenge

Between 2000 and 2011, 112 different samples were submitted from various industries as challenges to the ACD/LABS Structure Elucidation system (10). The structures determined ranged from 100 to 1000 g/mol, with the largest of all and the toughest that contained complex substituents and several stereocenters (Figure 5).



Figure 5: The number of molecules versus molecular weight of samples submitted to ACD/LABS.



Figure 6: The number of structural possibilities generated by ACD/LABS Structure Elucidation from these 112 g/mol (11).

In one recent example, Molecular Weights Software was able to determine the structure of a large, symmetrical ester isolate by ACD/LABS (12) containing 20 structural units even with the presence of stereocenters (Figure 7).



Figure 7: The reported structure of compound 12.

Case Systems

Modern CASE systems such as ACD/LABS Structure Elucidation provide the necessary capability to identify structures in novel chemical libraries. The complete workflow, from the initial structure list to the final structure, is automated. The system can handle up to 2,000,000 compounds and generate the structure of many structural isomers with the structure, to our knowledge, of any compound.



ACD/LABS
 www.acdlabs.com

Computer Assisted Structure Elucidation

Katrin Zwirgmaier



Computer Assisted Structure Elucidation:

Computer Assisted Structure Elucidation Book Review: Unveiling the Magic of Language

In a digital era where connections and knowledge reign supreme, the enchanting power of language has become more apparent than ever. Its ability to stir emotions, provoke thought, and instigate transformation is really remarkable. This extraordinary book, aptly titled "**Computer Assisted Structure Elucidation**," written by a very acclaimed author, immerses readers in a captivating exploration of the significance of language and its profound effect on our existence. Throughout this critique, we will delve to the book is central themes, evaluate its unique writing style, and assess its overall influence on its readership.

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