

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 related 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 (e.g. drug purity), the system for computer-assisted elucidation is structured as:

CASE Methodology

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

1. Obtain experimental data to extract knowledge
 - Molecular Formula
 - Masses
 - Chemical name
 - Substructure
 - Spectroscopy
 - Green Synthesis
 - Special synthesis
2. Search structure space to derive all possible structures
3. Ranklist based on all criteria
 - Molecular formula

Case Illustrations



Figure 2: An ACD/LABS CASE software panel displaying the identification procedure in use of related data associated with ACD/LABS. During elucidation, the software displays information for assigned spectra and structure, highlighting those which are likely to be accurate.

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Database Generation



Figure 3: A Molecular Connectivity Database (MCD) is created automatically during data interpretation. This can be used both for de novo elucidation, or to perform an elucidation based on proposed structure.

Ranking the Best Candidates

Using the selected properties of a substance Molecular Weight, the entropy of the structure space can be gained for possible structures which agree with the experimental data. The software automatically evaluates all structural possibilities, and then ranks the best candidates by giving based on the difference between the experimental and proposed structure data.



Figure 4: A list of possible structures, ranked by their calculated chemical data. Structures highlighted are highlighted based on their agreement with the experimental data.

Report Generation and Statistics

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

1. Structures and Weight list
 - 200,000 assigned chemical structures
2. Molecular Weight list
 - 200,000 structures
 - 4,400,000 structural fragments
3. Chemicals list
 - 20,000,000 structural compounds with Mol. Wt. 10-100, 100-200, 200-300
4. Chemistry of Natural Products
 - 200,000,000 compounds
5. Masses
 - 2,000,000 compounds having masses
6. Formulae
 - 2,000,000 compounds having masses and higher

The Structure Elucidation Challenge

Between 2000 and 2011, 112 different samples were submitted from various industries as challenges to the ACD/LABS Structure Elucidation system (1). The structures determined ranged from 100 to 1000 g/mol, with the largest of all the samples that contained complex structures determining the correct structure (Figure 5).



Figure 5: The number of samples weight or molecular challenge submitted to ACD/LABS.



Figure 6: The number of structural possibilities generated by ACD/LABS Structure Elucidation from data (100-1000 g/mol).

In one recent example, Molecular Weightable Data was able to determine the structure of a large, symmetrical drug isolate by ACD/LABS (2) generating 99 structural isomers with the presence of a substance (Figure 7).



Figure 7: The successful structure of substance 2.

Case Systems

Modern CASE systems such as ACD/LABS Structure Elucidation provide the necessary capability necessary to create chemical structures for complex molecules based on readily available data such as mass, first atomic composition, and elemental analysis. These systems, and their associated systems, offer the most use of 2,000,000,000 data which also contain the information of many structural isomers with the structure, to our structural systems.



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Computer Assisted Structure Elucidation

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Computer Assisted Structure Elucidation:

Contemporary Computer-Assisted Approaches to Molecular Structure Elucidation Mikhail E Elyashberg, Antony Williams, Kirill Blinov, 2015-11-09 Computer Assisted Structure Elucidation CASE systems are a combination of software algorithms and tools to support and enable chemists and spectroscopists engaged in the process of molecular structure elucidation via the analysis of spectroscopic data These expert systems dramatically reduce the time associated with structure elucidation and improve the reliability of the results Contemporary Computer Assisted Approaches to Molecular Structure Elucidation describes the principles on which these expert systems for spectroscopic structure elucidation are based and concisely explains the algorithmic concepts behind the programs The authors use their own personal experiences in the development of the Structure Elucidator StrucEluc CASE software system to discuss the present state of the art in computer assisted structure elucidation Scientists that are presently using CASE systems will be interested in the algorithms and modern approaches and for organizations that are currently using the StrucEluc platform the book is designed to help researchers understand the strategies behind CASE as well as details regarding the StrucEluc platform For scientists that have never used CASE systems they will now have access to all necessary information to understand CASE systems for mastering this new and very effective approach to structure elucidation The authors overall goal in writing this book is to produce the must read definitive text that will represent the results of decades of work to develop computer assisted structure elucidation software systems CASE systems are now powerful software tools commonly outperforming and correcting human interpretations of data This book will also provide an historical perspective of the work of the founding fathers of the technique and identify the challenges that have been overcome to produce modern CASE systems

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Computer-Based Structure Elucidation from Spectral Data Mikhail E. Elyashberg, Antony J. Williams, 2015-02-27 Here the authors introduce readers to solving molecular structure elucidation problems using the expert system ACD Structure Elucidator They explain in detail the concepts of the Computer Assisted Structure Elucidation CASE approach and point out the crucial role of understanding the axiomatic nature of the data used to deduce the structure Aspects covered include the main blocks of the expert system and essential features of the mathematical algorithms used Graduate and PhD students as well as practicing chemists are provided with a detailed explanation of the various practical approaches depending on available spectral data peculiarities and the complexity of the unknown structure This is supported by a large number of real world completed examples most of which are related to the structure elucidation of natural product molecules containing unusual skeletons Dedicated software and further supplementary material are available at www.acdlabs.com TeachingSE

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important new algorithms for solving problems in structural chemistry It is a review of problems related to the representation and manipulation of chemical data illustrated with various approaches to their solutions

Computer-assisted Structure Elucidation Using Automatically Acquired [¹³C NMR Rules Stanford University. Computer Science Dept. Heuristic Programming Project, G. M. Schwenzer, T. M. Mitchell, 1977

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Applied Chemoinformatics Thomas Engel, Johann Gasteiger, 2018-06-05 Edited by world famous pioneers in chemoinformatics this is a clearly structured and applications oriented approach to the topic providing up to date and focused information on the wide range of applications in this exciting field The authors explain methods and software tools such that the reader will not only learn the basics but also how to use the different software packages available Experts describe applications in such different fields as structure spectra correlations virtual screening prediction of active sites library design the prediction of the properties of chemicals the development of new cosmetics products quality control in food the design of new materials with improved properties toxicity modeling assessment of the risk of chemicals and the control of chemical processes The book is aimed at advanced students as well as lectures but also at scientists that want to learn how chemoinformatics could assist them in solving their daily scientific tasks Together with the corresponding textbook

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Progress in the Chemistry of Organic Natural Products 116 A. Douglas Kinghorn, Heinz Falk, Simon Gibbons, Yoshinori Asakawa, Ji-Kai Liu, Verena M. Dirsch, 2021-10-26 This volume describes several highly diverse subjects Chapter 1 explores marine biodiscovery of the North eastern Atlantic off the coast of Ireland as a model for best practice in research The second chapter investigates Brazilian Chemical Ecology and examples of insect plant communication studies that are mediated by natural products demonstrate the beautiful interconnectedness of species in a biome Our third chapter comprises the advances in the science of the sesquiterpene quinone perezone which in 1852 was the first natural product isolated in crystalline form in the New World The last two chapters are from a Vietnamese group and the first of these follows the phytochemistry pharmacology and ethnomedical uses of the genus Xanthium which produces interesting sulfur and nitrogen containing natural products Finally the genus Desmos is discussed where an overview of its constituent natural products and their in vitro pharmacological potential is described

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Development of a System for Computer-assisted Structure Elucidation of Small Organic Compounds Michael Wenk, 2023*

Anthropic Awareness Csaba Szantay Jr., 2015-06-25 Anthropic Awareness The Human Aspects of Scientific Thinking in NMR Spectroscopy and

Mass Spectrometry blends psychology philosophy physics mathematics and chemistry describing a human centered philosophy of the essence of scientific thinking in the natural sciences and in everyday life It addresses the reasons why we are prone to make errors in our conclusions and how to avoid such mistakes also exploring a number of the mental traps that can lead to both individual mistakes and mass misconceptions The book advocates that by understanding the nature of these mental traps we can adopt tactics to safely evade them It includes Illustrative examples of common scientific misunderstandings and mental traps in both the theory and real life application of NMR spectroscopy and mass spectrometry Provides strategies on how to deal with molecular challenges and instrument limitations Presents multiple applications of small molecule structure elucidation using NMR MS IR and UV Explores critical topics including anthropic awareness AA NMR Spectroscopy mass spectrometry scientific thinking and more Includes tactics on how to Improve quality control and data interpretation skills while minimizing data analysis time and increasing confidence in results Presents coverage on tactics to optimize experimental NMR parameters and enhance NMR vocabulary *Pharmaceutical Analysis* David C Lee, Michael L. Webb, 2009-02-12 The use of analytical sciences in the discovery development and manufacture of pharmaceuticals is wide ranging From the analysis of minute amounts of complex biological materials to the quality control of the final dosage form the use of analytical technology covers an immense range of techniques and disciplines This book concentrates on the analytical aspects of drug development and manufacture focusing on the analysis of the active ingredient or drug substance It provides those joining the industry or other areas of pharmaceutical research with a source of reference to a broad range of techniques and their applications allowing them to choose the most appropriate analytical technique for a particular purpose The volume is directed at analytical chemists industrial pharmacists organic chemists pharmaceutical chemists and biochemists

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