

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 formulas, especially those of unusual products of drug metabolism and reactions. The completely automatic structure determination, even from the smallest of samples and very faint experimental spectra, is made possible by sophisticated CASE software designed to do the necessary calculations.



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 structural complexity, including bond types, functional groups, and other information on connectivity. However, even in published structures the number of atoms might be too small for computer-assisted elucidation to structure it.

CASE Methodology

CASE follows a simple set of steps to computer-assisted structure elucidation: generate possible structures.

1. Generate experimental data to extract knowledge
 - Molecular Formula
 - Masses
 - Chemical shifts
 - Subgroups
 - Connections
 - Green Regions
 - Special features
2. Search structure space to derive all possible structures
3. Ranklist based on best fit
 - Ranked structural data

Case Illustrations



Figure 2. An ACQTOX case study involves peak assignments and fragmentation through a set of related table structures with MS/MS data. During assignment, the software displays visualizations for assigned spectra and structure, highlighting those which are likely to be accurate.

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Automated Generation



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 iteration about the proposed structure.

Ranking the Best Candidates

Using the selected properties of a substance's Molecular Formula, 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 using based on the difference between the experimental and proposed structural data.



Figure 4. A set of possible structures, ranked by their calculated chemical shift features. Structure assignments are color-coded based on their agreement with the experimental data.

Report Generation and Statistics

With the right information, better structure lists can be quickly identified from thousands more. The following table shows the statistics using ACQTOX software:

1. ACQTOX case study set
 - 200,000 assigned chemical structures
2. Molecular Formula set
 - 200,000 structures
 - 4,400,000 structural fragments
3. Chemical shift
 - 20,000,000 structural connections with ^{13}C , ^{15}N , ^{17}O , and ^{31}P NMR
4. Entropy of Molecular Formula
 - About 200,000 compounds
5. Masses
 - 21,000 compounds having masses
6. Results
 - 2,000,000 experimental assignments and higher range

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The Reported Elucidation Challenge

Between 2000 and 2011, 112 different cases were submitted from various industries as challenges to the ACQTOX-based Structure Suite system. (2) The structures determined ranged from 100 to 1000 atoms, with the largest of all the submitted test cases being determined by the correct structure (Figure 5).



Figure 5. The number of molecules sought in elucidation challenges submitted to ACQTOX.



Figure 6. The number of structural possibilities generated by ACQTOX-based Structure Suite from 2000-2011.

In one recent example, Molecular Formula Suite was able to determine the structure of a large, symmetrical dendrimer by Structure A (3) generating 99 structural units even with the presence of unknowns (Figure 7).



Figure 7. The successful structure of dendrimer A.

Case Systems

Modern CASE systems such as ACQTOX Molecular Suite provide the necessary capability necessary to create chemical structures the complex molecules found in reality. Structure Suite can also, find other compounds in great numbers, even thousands, and then calculating systems effects. The system can of 2,000,000 cases which also contain the combination of many structural formulas into the structure, to get structural results.



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Computer Assisted Structure Elucidation

Bonnie Lynn Webber, Nils J. Nilsson



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 is 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

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 **Computer-assisted Structure Elucidation** Dennis H. Smith, American Chemical Society, Division of Chemical Information, 1977 **Computer-assisted Structure Elucidation** Craig Alan Shelly, 1978 [Computer-assisted Structure Elucidation](#) Neil A. B. Gray, 1986 Drawing on a wide range of recent research this book introduces the most

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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Elyashberg, Antony J. Williams, 2015 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 **Computer-assisted Structure Elucidation** Dennis H. Smith, 1977

Computer Chemistry Mario Marsili, 2017-07-28 Computer Chemistry illustrates the methods and philosophies of how a computer can be instructed to understand chemical facts formulas and rules It focuses on discussions of all of the major sections in both theoretical framework and practical application through examples It includes the Synthesis Design Systems for the simulation of chemical reactions the Structure Elucidation Systems for the interpretation of spectral data the Molecular Modelling Systems for the visualization of chemical structures and the calculation of physico chemical parameters

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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Readings in Artificial Intelligence Bonnie Lynn Webber, Nils J. Nilsson, 2014-05-12 *Readings in Artificial Intelligence* focuses on the principles methodologies advancements and approaches involved in artificial intelligence The selection first elaborates on representations of problems of reasoning about actions a problem similarity approach to devising heuristics and optimal search strategies for speech understanding control Discussions focus on comparison with existing speech understanding systems empirical comparisons of the different strategies analysis of distance function approximation problem similarity problems of reasoning about action search for solution in the reduction system and relationship between the initial search space and the higher level search space The book then examines consistency in networks of relations non resolution theorem proving using rewriting rules for connection graphs to prove theorems and closed world data bases The manuscript tackles a truth maintenance system elements of a plan based theory of speech acts and reasoning about knowledge and action Topics include problems in reasoning about knowledge integration knowledge and action models of plans compositional adequacy truth maintenance mechanisms dialectical arguments and assumptions and the problem of control The selection is a valuable reference for researchers wanting to explore the field of artificial intelligence

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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

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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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Fundamental Concepts Fidele Ntie-Kang, 2020-02-24 Vol 1 of Chemoinformatics of Natural Products presents an overview of natural products chemistry discussing the chemical space of naturally occurring compounds followed by an overview of computational methods

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