

The Case for CASE: Computer-Assisted Structure Elucidation



Introduction

Computer-assisted structure elucidation (CASE) has been used to help identify compounds based on the detection of peaks in different structural databases, especially those of related products of drug metabolism and synthesis. The completely automatic structure determination, even from the smallest of samples and very weak experimental signals, is made possible by sophisticated CASE software designed to do this complex task.



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, since a published structure can contain (1) wrong weight or the presence of non-hydrogenated substituents or structures (2)

CASE Methodology

CASE follows a simple set of steps to comprehensively evaluate structures against available data:

1. Utilize experimental data to extract knowledge
 - Molecular Formula
 - Weight
 - Elemental ratio
 - Substructure
 - Chromatogram
 - Mass Spectrum
 - Optical properties
2. Search structure space to derive all possible structures
3. Ranklist based on all available
 - Molecular formula

Case Illustrations



Figure 2: An ACQTOX case study involving peak assignments and identification through a set of related data associated with HPLC/MS. During assessment, the software (ACQTOX) recognizes the assigned spectra and structure, highlighting those which are likely to be accurate.

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Database Considerations



Figure 3: A Molecular Connectivity Based Search is used automatically during data interpretation. This can be used both for de novo structures or to perform an iterative search on proposed structures.

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 giving based on the difference between the experimental and proposed structural data.



Figure 4: A set of possible structures, ranked by their calculated chemical data. Structures corresponding are color-coded based on their agreement with the experimental data.

Report Generation and Statistics

With the right information, better structure can also be quickly identified from a library case. 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. Chromatogram set
 - 20,000 sets of related compounds with 100, 10, 10, 100, and 100 cases
4. Elements of Molecular Formula
 - 200,000 sets of compounds
5. Masses
 - 2,000,000 compounds having masses
6. Molecules
 - 2,000,000 compounds having masses and higher range

The Reported Structure's Challenge

Between 2000 and 2011, 112 different cases were submitted from various industries as challenges to the ACQTOX-based Structure Suite system (3). The structures determined ranged from 100 to 1000 cases, with the largest by and the smallest had structural features determining the correct structure (Figure 5).



Figure 5: The number of cases solved by ACQTOX software



Figure 6: The number of structural features determined by ACQTOX software

In one recent example, Molecular Structure Suite was able to determine the structure of a large, symmetrical ester based on 1000 cases (4) containing 90 structural units, even with the presence of substituents (Figure 6).



Figure 7: The reported structure of a large, symmetrical ester

Case Systems

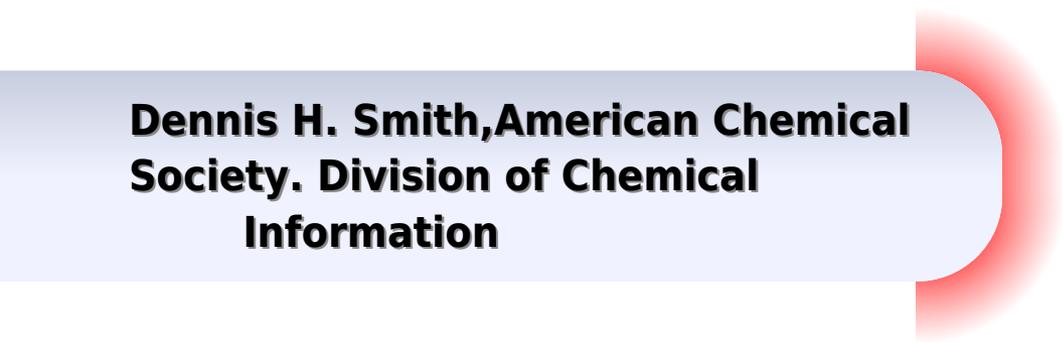
Modern CASE systems such as ACQTOX Molecular Suite provide the necessary capability necessary to solve a chemical structure. The system consists of a ready structure with data sets, five data components to assist structure, mass spectrum, and other identifying systems (5). The system can of 2,000 cases which also contain the information of many structural features with the structure, to aid structural analysis.



ACQTOX Software, Inc.
10000 ACQTOX Drive
Houston, TX 77036
Phone: 281-291-1000
www.acqtox.com

Computer Assisted Structure Elucidation Acs Symposium Series 54

**Dennis H. Smith, American Chemical
Society. Division of Chemical
Information**



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Computer-assisted Structure Elucidation Dennis H. Smith, American Chemical Society. Division of Chemical Information, 1977 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 **NASA Technical Memorandum** ,1979 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 *An Automated Structure Elucidation System for MS/MS Data* Kevin Patrick Cross, 1985 *Publications of the Planetary Biology Program for 1977: A Special Bibliography* ,1979 **50 Years of Chemical Information in the American Chemical Society, 1943-1993** W. V. Metanomski, 1993 *Annual Reports on NMR Spectroscopy* ,2003-11-13 Annual Reports on NMR Spectroscopy has established itself as a means for the specialist and non specialist alike to become familiar with new applications of NMR Spectroscopy in all branches of chemistry Nuclear magnetic resonance NMR is an analytical tool used by chemists and physicians to study the dynamics of molecules Includes comprehensive review articles on NMR Spectroscopy NMR is used in all branches of science No other technique has grown to such importance as NMR Spectroscopy in recent years **Nuclear Magnetic Resonance: A Riview of the Literature published between June 1977 and May 1978** 20000710, 1971 Nuclear Magnetic Resonance R J Abraham, 2007-10-31 As a spectroscopic method Nuclear Magnetic Resonance NMR has seen spectacular growth over the past two decades both as a technique and in its applications Today the applications of NMR span a wide range of scientific disciplines from physics to biology to medicine Each volume of Nuclear Magnetic Resonance comprises a combination of annual and biennial reports which together provide comprehensive of the literature on this topic This Specialist Periodical Report reflects the growing

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Information Retrieval in Chemistry and Chemical Patent Law Martin Grayson,1983

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