

## ACD/Structure Elucidator: A Timeline

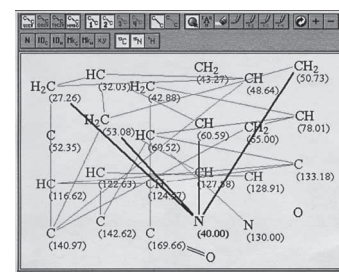
ACD/Labs' mission over the last decade was to take on the daunting challenge of structure elucidation in an unbiased fashion, by leveraging the technological enhancements in computer science as well as the sophisticated algorithms available in ACD/Labs core software offerings to deliver the best CASE system on the market.

With over a decade of product development spanning 10 software versions between 1998–2011 (version 3.5–version 12), Structure Elucidator is the most peer-reviewed system in scientific literature.

This timeline shares our most notable milestones since the initial release of the product in 1998.

First peer-reviewed article describing Structure Elucidator, with the unique ability to build sets of fragments containing no common atoms if structure generation with known methods fails.  
[Elyashberg et al., \*Autom. Inf. Manage.\* 1999, 34, 15-30.](#)

Structure Elucidator development continues with the ability to generate structures from 2D NMR spectra, allowing elucidation of heavier molecules.  
[Bilnov et al., \*Fresenius J. Anal. Chem.\* 2001, 369, 709-714.](#)

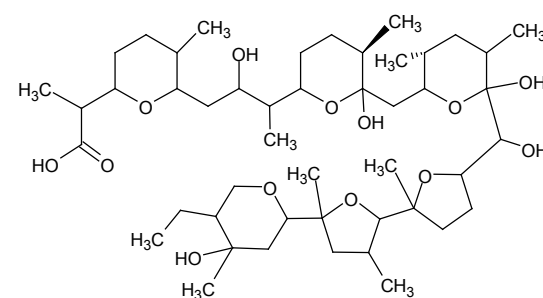


1999

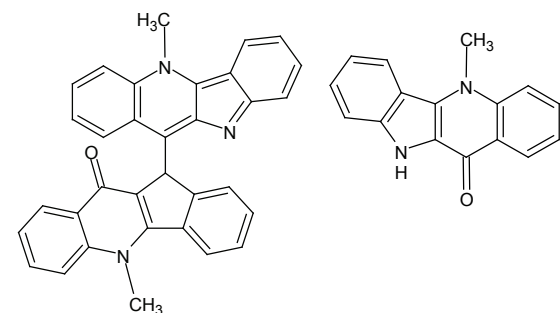
2001

2002

Structures of 60 natural products of up to 65 skeletal atoms are successfully determined by Structure Elucidator.  
[Elyashberg et al., \*J. Nat. Prod.\* 2002, 65, 693-703.](#)



Structure Elucidator is used to determine the structure of degradants of a nonacyclic alkaloid, including an unexpected rearrangement product.  
[Martin et al., \*J. Heterocyclic Chem.\* 2002, 39, 1241-1250.](#)



Real-World Applications

## Identifying Mixture Components at Very Low Concentrations

Anna Codina et al. have reported one of the first examples of computer-assisted structure elucidation of volatile impurities isolated by prep-GC. A combination of the proposed in silico methods and instrumentation were successful even in cases where the total amount of material is of the order of 60 nmol.

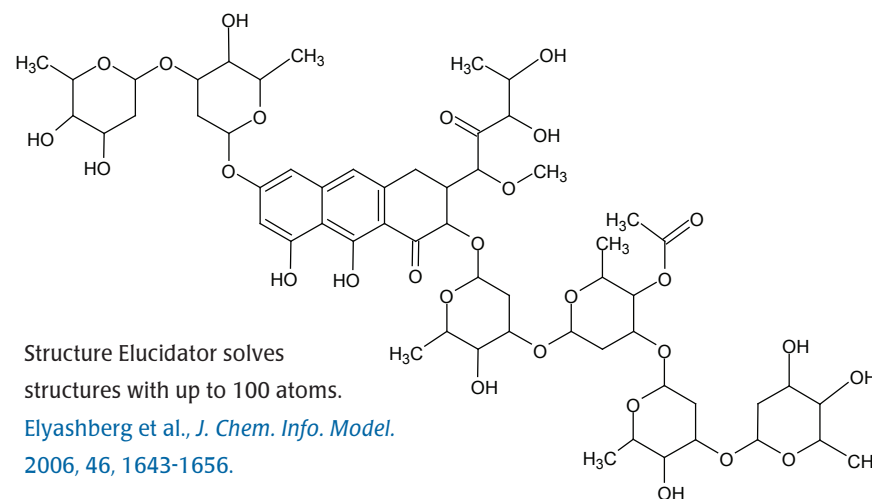
The authors state, "We are of the opinion that for relatively small organic molecules, the combined computational approach can nowadays be faster and more thorough than the expert spectroscopist. Thus, despite there being many instances in the literature describing CASE as an expert system to assist in solving difficult problems, we prefer to use it for the relatively routine investigations so that the expert can focus on complex elucidations involving mixtures, weak data, and/or with several peaks overlapping."

[Anna Codina et al., \*Anal. Chem.\*, 2010, 82, 9127-9133](#)

Structure Elucidator's efficient processing of 2D NMR is found to be necessary to elucidate complex natural compounds, and significantly faster than other systems.  
[Elyashberg et al., \*J. Chem. Inf. Comp. Sci.\* 2004, 44, 771-792.](#)

A CASE review article is published citing ACD/Structure Elucidator as the most promising achievement in terms of practical applicability of all CASE systems available.  
[Steinbeck, \*Nat. Prod. Rep.\* 2004, 21, 512-518.](#)

2004



Structure Elucidator solves structures with up to 100 atoms.  
[Elyashberg et al., \*J. Chem. Info. Model.\* 2006, 46, 1643-1656.](#)

2006

2007

Fuzzy Structure Generation is introduced, capable of delivering a correct solution in the presence of an unknown number of non-standard correlations with unknown lengths in 2D NMR data.  
[Elyashberg et al., \*J. Chem. Info. Model.\* 2007, 47, 1053-1066.](#)

2008

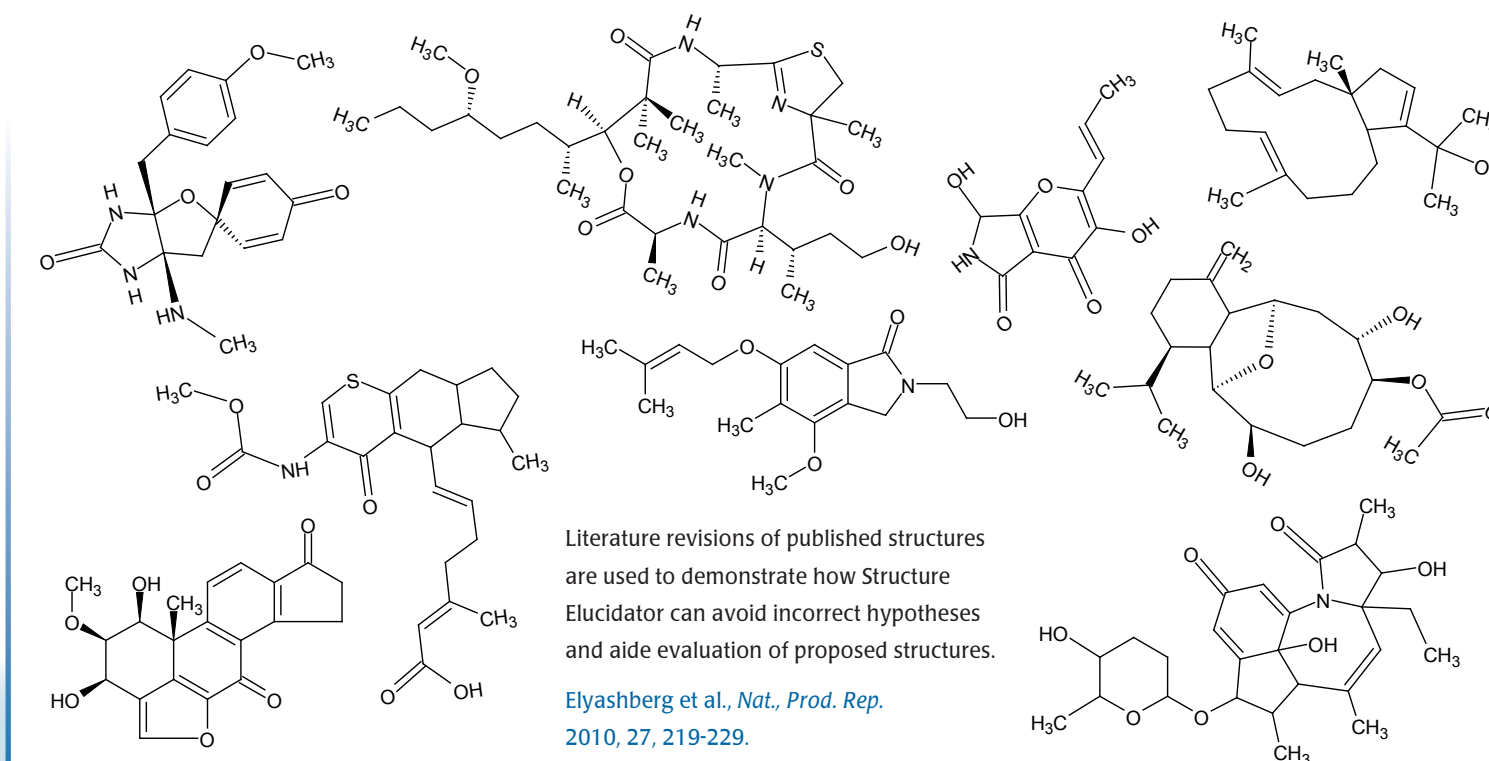
Structure Elucidator found to be the most advanced commercial expert tool, encompassing all features of other products but with even more advanced functionality.  
[Elyashberg et al., \*Prog. Nucl. Magn. Reson. Spectrosc.\* 2008, 53, 1-104](#)

2010

M. Elyashberg's 2009 CASE review paper featuring Structure Elucidator is still the most accessed paper from the Journal of Cheminformatics.  
[Elyashberg et al., \*J. Cheminf.\*, 2009, 1-3.](#)

Contemporary Computer-Assisted Approaches to Molecular Structure Elucidation, a book featuring Structure Elucidator and describing the state-of-the-art in CASE systems is accepted for publication.  
[M. Elyashberg, A. Williams, K. Blinov, \*Royal Soc. Chem.\*](#)

2011



Literature revisions of published structures are used to demonstrate how Structure Elucidator can avoid incorrect hypotheses and aide evaluation of proposed structures.  
[Elyashberg et al., \*Nat., Prod. Rep.\* 2010, 27, 219-229.](#)

Impurity

Coming Soon

The next generation of Structure Elucidator, an integral part of the ACD/Spectrus family of products.