Uncovering the Truths and Dispelling the Myths Behind ACD/Structure Elucidator

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Advanced Chemistry Development, Inc. (ACD/Labs)
Truth or Myth

- ACD/Structure Elucidator
  - Can solve any structure?
  - Costs a fortune?
  - Will put me out of a job?
- Truth or myth?

Let’s find out...
Myth #1

Myth – Structure Elucidator is expensive

Truth – Structure Elucidator is a component of a suite of tools

Processor, database, elucidator, reporter, etc.
Structure Elucidator Components

- ACD/ChemSketch
- ACD/1D NMR Manager
- ACD/2D NMR Manager
- ACD/MS Manager
- ACD/UV-IR Manager
- ACD/CNMR Predictor
- ACD/HNMR Predictor
- ACD/2D NMR Predictor
- And the Structure Elucidator component
Myth #2

Myth - Elucidations can be performed faster by hand

Truth – In some cases yes. In others no.
The ‘Sweet’ Spot

Very simple compounds are fast manually

Very complex compounds are slow, but may be more successful with Elucidator

If large fragments are known, manual may be faster
Myth #3

Myth - Structure Elucidator will not always reach the correct answer when given all the correct data

Truth – Elucidator takes a brute force approach and generates every possibility

Filtering criteria may cause problems but..

In the history of the Elucidator challenge, this has never happened...
Myth #4

Myth – Structure Elucidator can only solve perfectly prepared data sets

Truth - A ‘Fuzzy Generator’ algorithm is available that allows errors in the peak lists of the HMBC or COSY.

The HSQC and formula need to be correct though.
Myth #5

Myth – Structure Elucidator cannot handle Stereochemistry

Truth – It CAN handle Stereochemistry

After generation, all stereoisomers can be optimized in 3D
Stereochemistry

The Best Structure

C21H22N2O2 C(5),CH(10),CH2(6)

E: 83.3863

RRSSSR
Myth #6

Myth – Structure Elucidator is hard to use

Truth - It is not EASY to use, but there are plenty of successful users

See any of our past guest speaker’s presentations on the subject

Scott Smith, Steve Coombes, Gary Martin, Shaun Tennant (2DNMR.com)
Myth #7

Myth – Structure Elucidator will allow my secretary to solve structures while I am on holiday

Truth – Not really... 😊

- The user needs to be able to solve structures by hand
- The same chemistry rules apply
Myth #8

Myth - If I buy it, I will only use it a couple of times a year

Truth – Users that purchase this product use it all the time!

The components are used independently or with the Elucidator piece
Elucidator Use

Standard workflow in our software can mean daily use

See Steve Coombes’ Presentation on our website


Using our software for processing, databasing and reporting means it will be used daily...
Myth #9

Myth – Structure Elucidator is a black box that solves structures

Truth - This is a collaborative structure solving tool
Elucidation Workflows

Users solve structures in different ways with the software
- Verification (proposed structure)
- Manual Elucidation (processing only)
- Dereplication
- Full Elucidation
The Structure Elucidation Workflow

- All Formats
  - NMR
  - MS
  - UV-IR
  - Chrom

Data Import
The Structure Elucidation Workflow

Manual or Automated

Data Processing
The Structure Elucidation Workflow

- Identify and Assign Known Fragments
  - Database Search
- Work on the Fly
  - Structure Exchange Tool

Interpret Data
The Structure Elucidation Workflow

NMR Predictions

Propose Possible Structures
The Structure Elucidation Workflow

- Confirm Structure
- Fully assign all spectra
The Structure Elucidation Workflow

- Report Template
  - Spectra
  - Tables
  - MCD

Create Report
The Structure Elucidation Workflow

- All-in-One
- Fully Assigned
- Searchable

Build Database
The Structure Elucidation Workflow

- Prediction Training
- Knowledge Management
Hit a Roadblock? Use SE

ACD/Labs Structure Elucidation Engine

Generate Structures  Choose Best Structure

Import  Process  Propose  Report  Database

Propose

ACD/Labs Structure Elucidation Engine
ACD/Structure Elucidator is a suite of software tools

More than the sum of the parts

Manage your knowledge

Partial assignment retention changes everything
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