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

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ACD/Labs' SMASH Seminar
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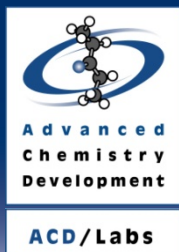
Advanced Chemistry Development, Inc. (ACD/Labs)

Visionary Software

Advancing Research

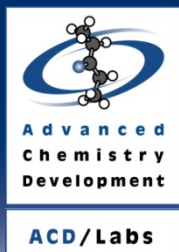
Truth or Myth

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



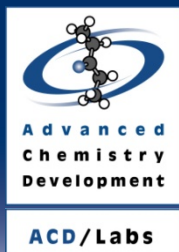
Myth #1

- ❶ Myth – Structure Elucidator is expensive
- ❷ Truth – Structure Elucidator is a component of a suite of tools
 - Processor, database, elucidator, reporter, etc.



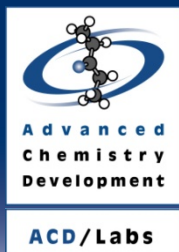
Structure Elucidator Components

- ④ ACD/ChemSketch
- ④ ACD/1D NMR Manager
- ④ ACD/2D NMR Manager
- ④ ACD/MS Manager
- ④ ACD/UV-IR Manager
- ④ ACD/CNMR Predictor
- ④ ACD/HNMR Predictor
- ④ ACD/2D NMR Predictor
- ④ 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

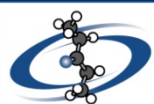
- ❶ Myth - Structure Elucidator will not always reach the correct answer when given all the correct data
- ❷ Truth – Elucidator takes a brute force approach and generates every possibility
 - ❸ Filtering criteria may cause problems but..
 - ❹ In the history of the Elucidator challenge, this has never 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



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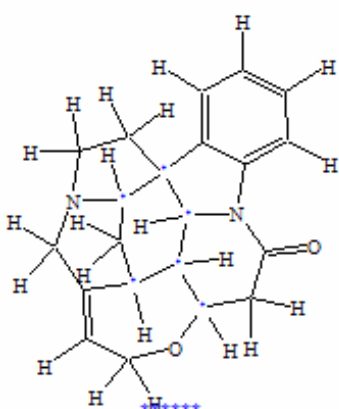
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Stereochemistry

Find Best Stereoisomer

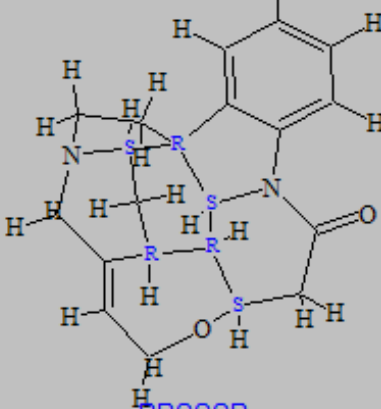
Original Structure

The Best Structure



Created Stereoisomers (Selected/Total) - (0/64) Include Current

E: 83.3863



RRSSSR

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

#	ID	N	N	Volume	Kind	Energy	Dist.
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1 from 64

Optimize All Sort by Energy Select All

Optimize All with NOE Sort by NOE Energy Unselect All

3D Optimization Options... OK Cancel Help

Myth #6

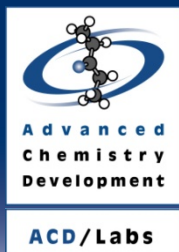
- ❶ Myth – Structure Elucidator is hard to use
- ❷ Truth - It is not EASY to use, but there are plenty of successful users
 - ❸ See any of our past guest speaker's presentations on the subject
 - Scott Smith, Steve Coombes, Gary Martin, Shaun Tennant (2DNMR.com)

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

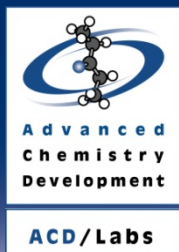
Myth #8

- ❌ 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



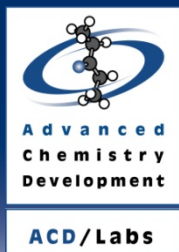
Elucidator Use

- Standard workflow in our software can mean daily use
 - See Steve Coombes' Presentation on our website
 - http://www.acdlabs.com/download/public/2007/ukum2007_nmr_db.zip
- 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



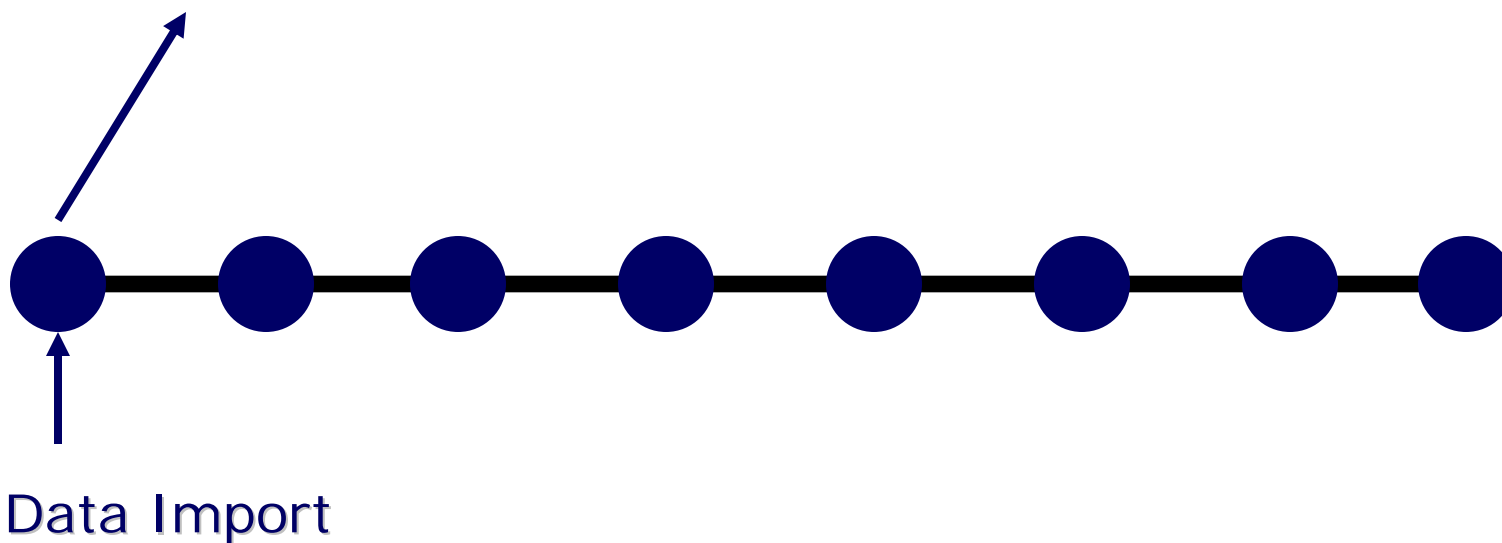
Elucidation Workflows

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

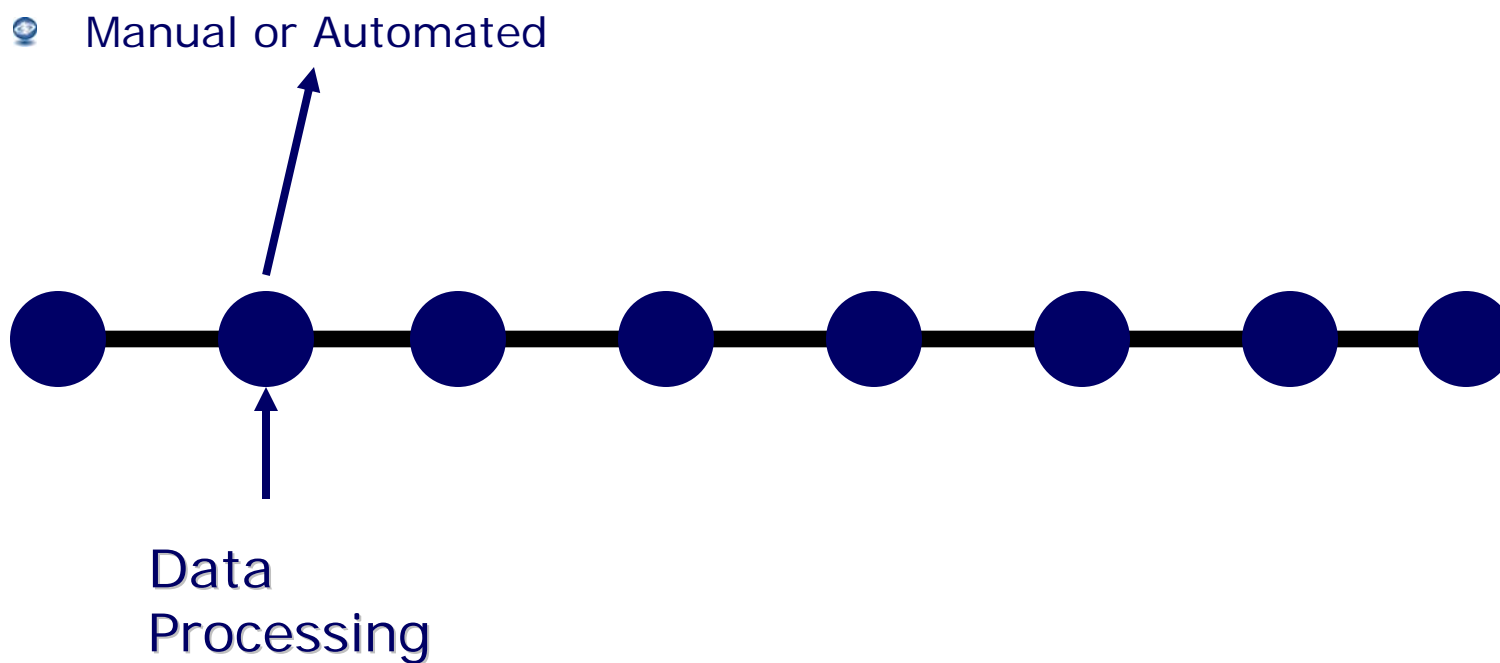
The Structure Elucidation Workflow

☉ All Formats

- ☉ NMR
- ☉ MS
- ☉ UV-IR
- ☉ Chrom

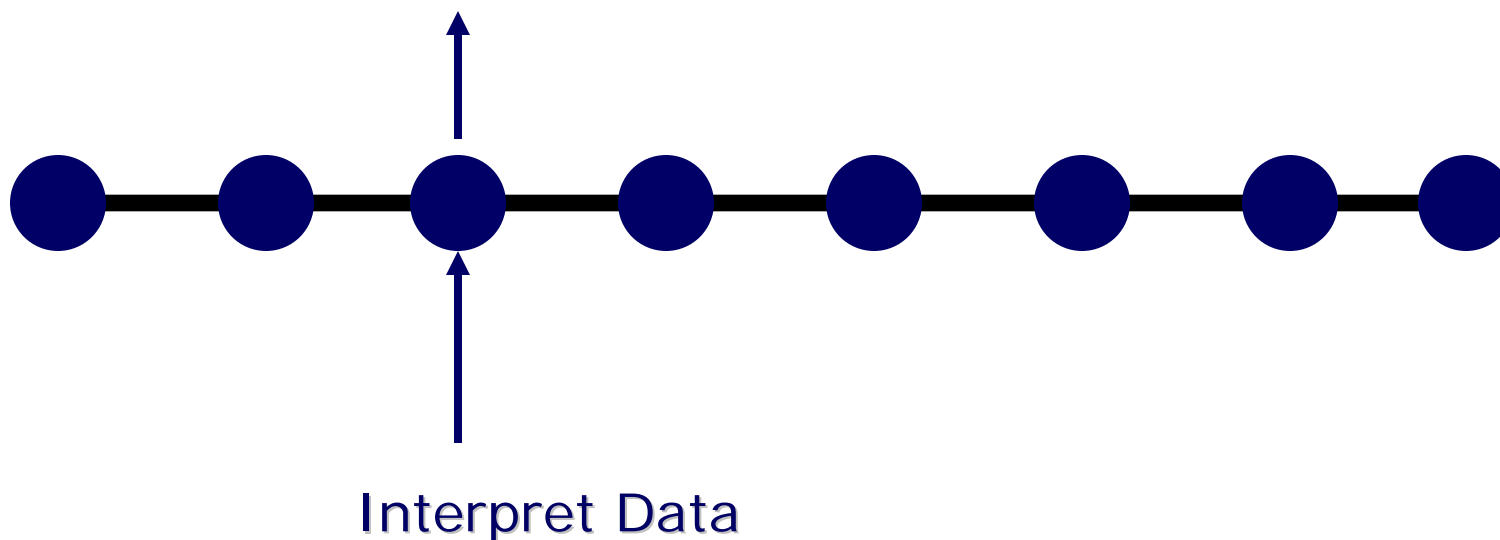


The Structure Elucidation Workflow

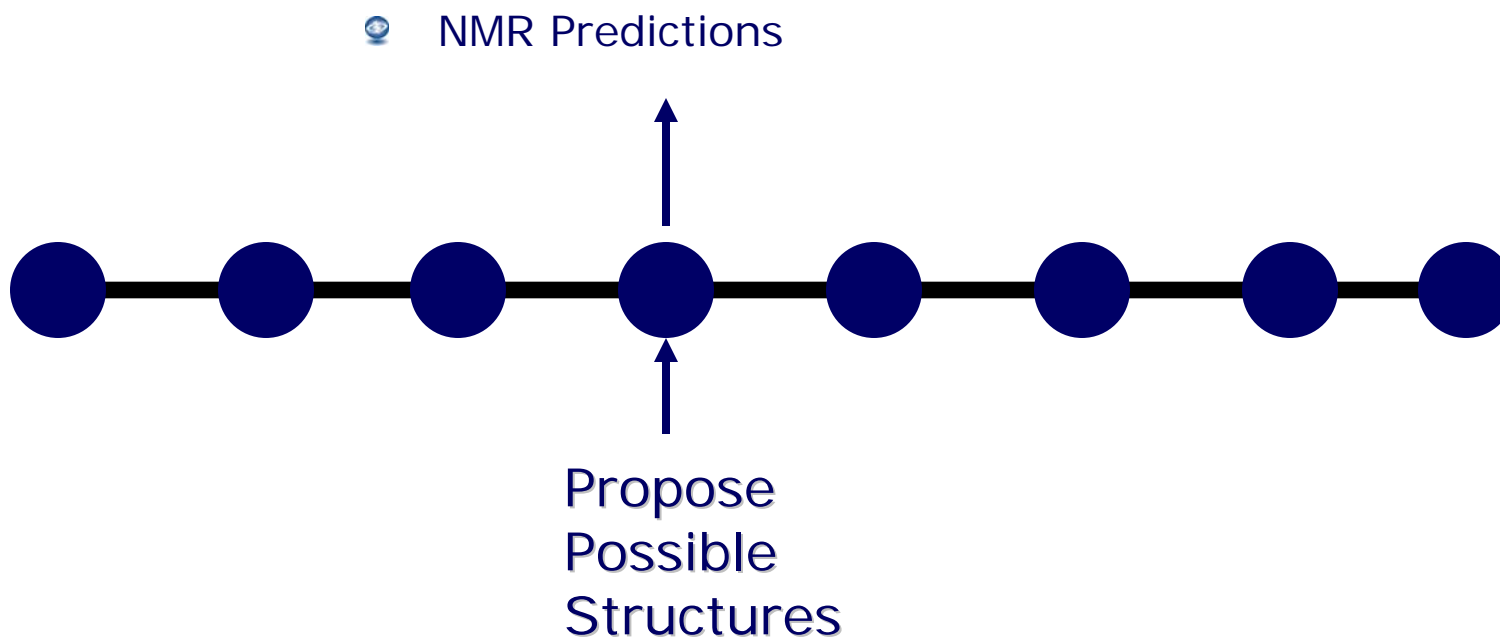


The Structure Elucidation Workflow

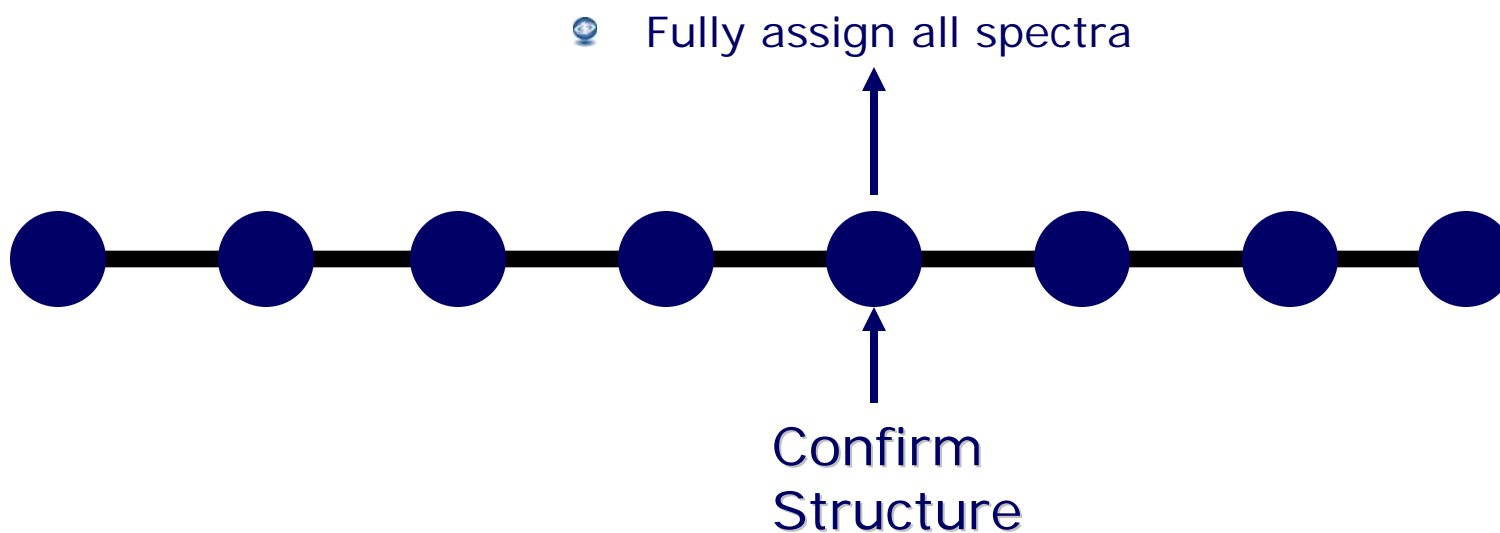
- Identify and Assign Known Fragments
 - Database Search
- Work on the Fly
 - Structure Exchange Tool



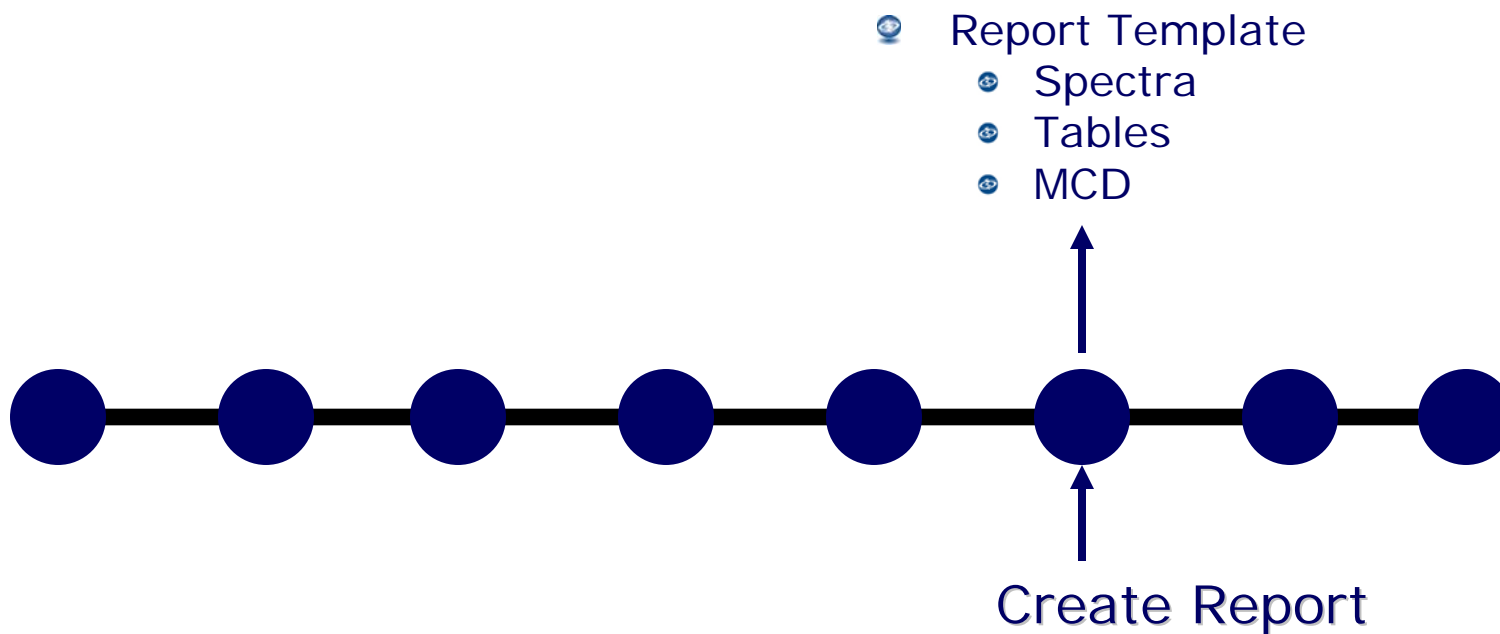
The Structure Elucidation Workflow

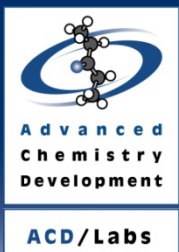


The Structure Elucidation Workflow

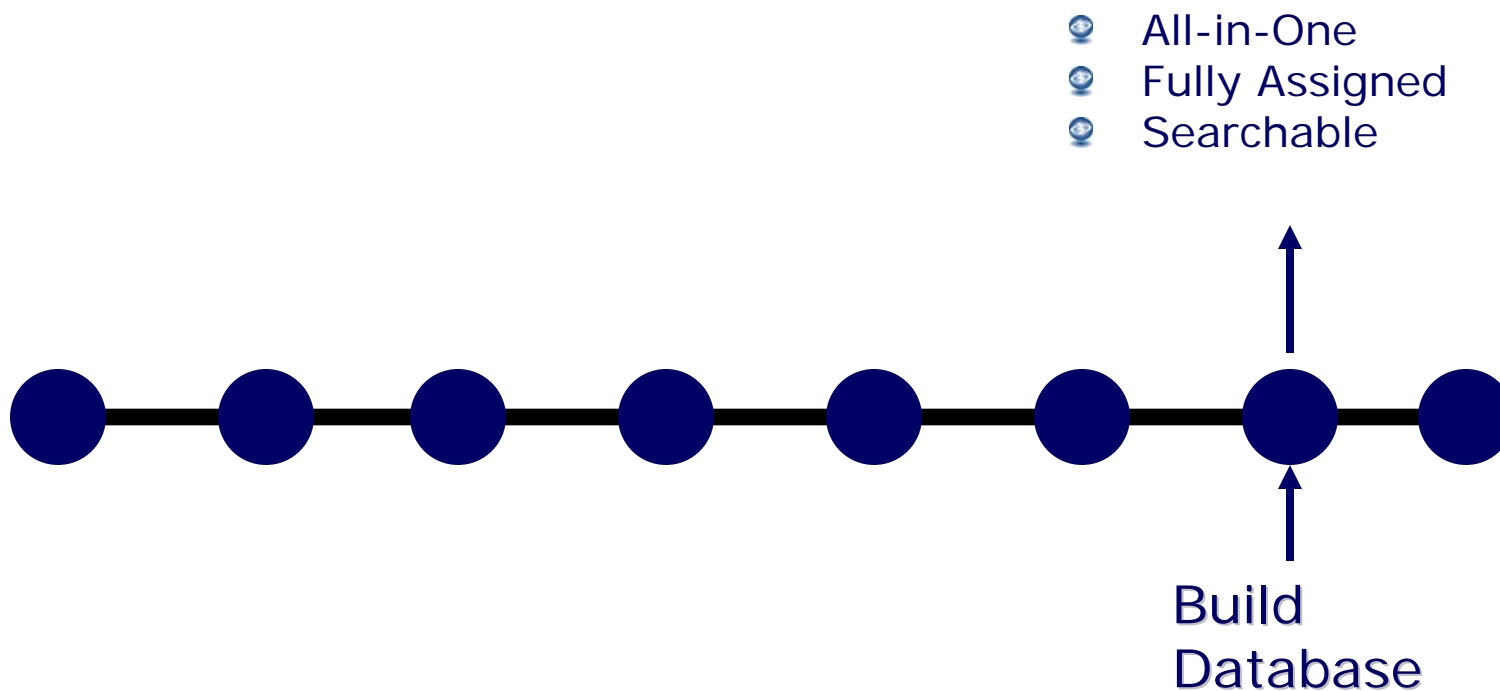


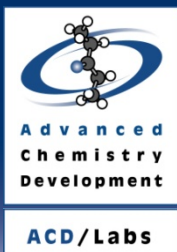
The Structure Elucidation Workflow



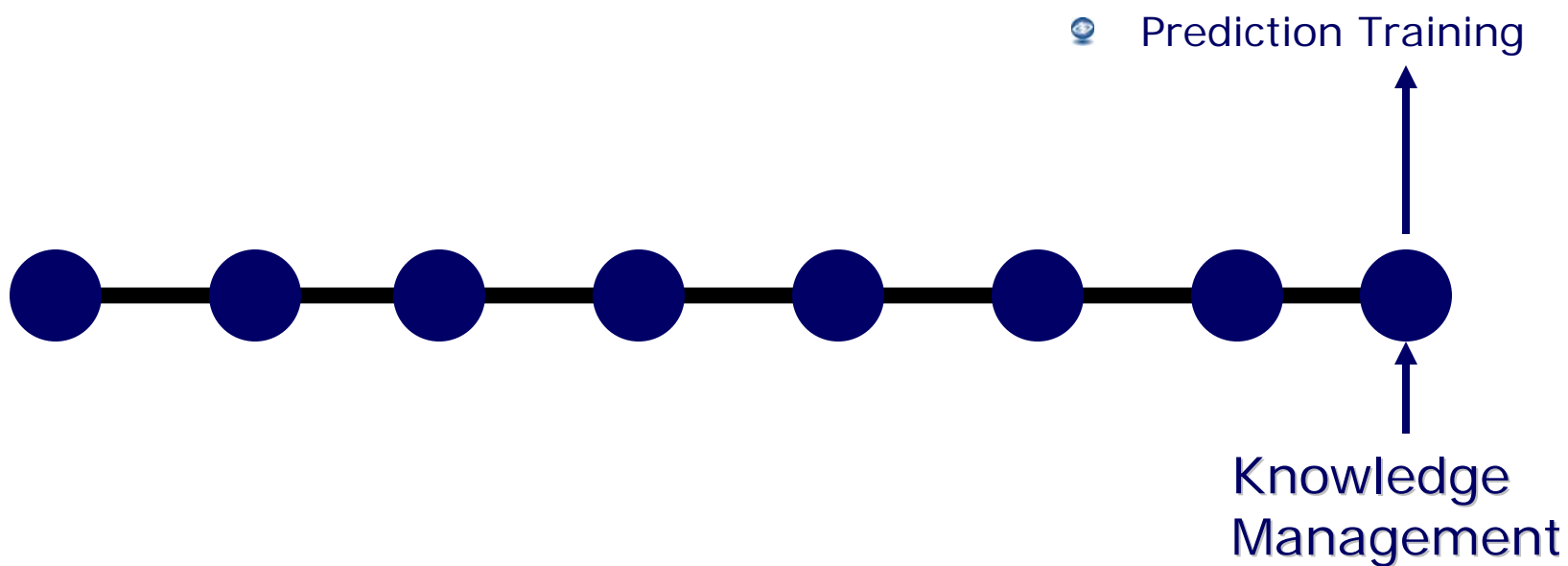


The Structure Elucidation Workflow



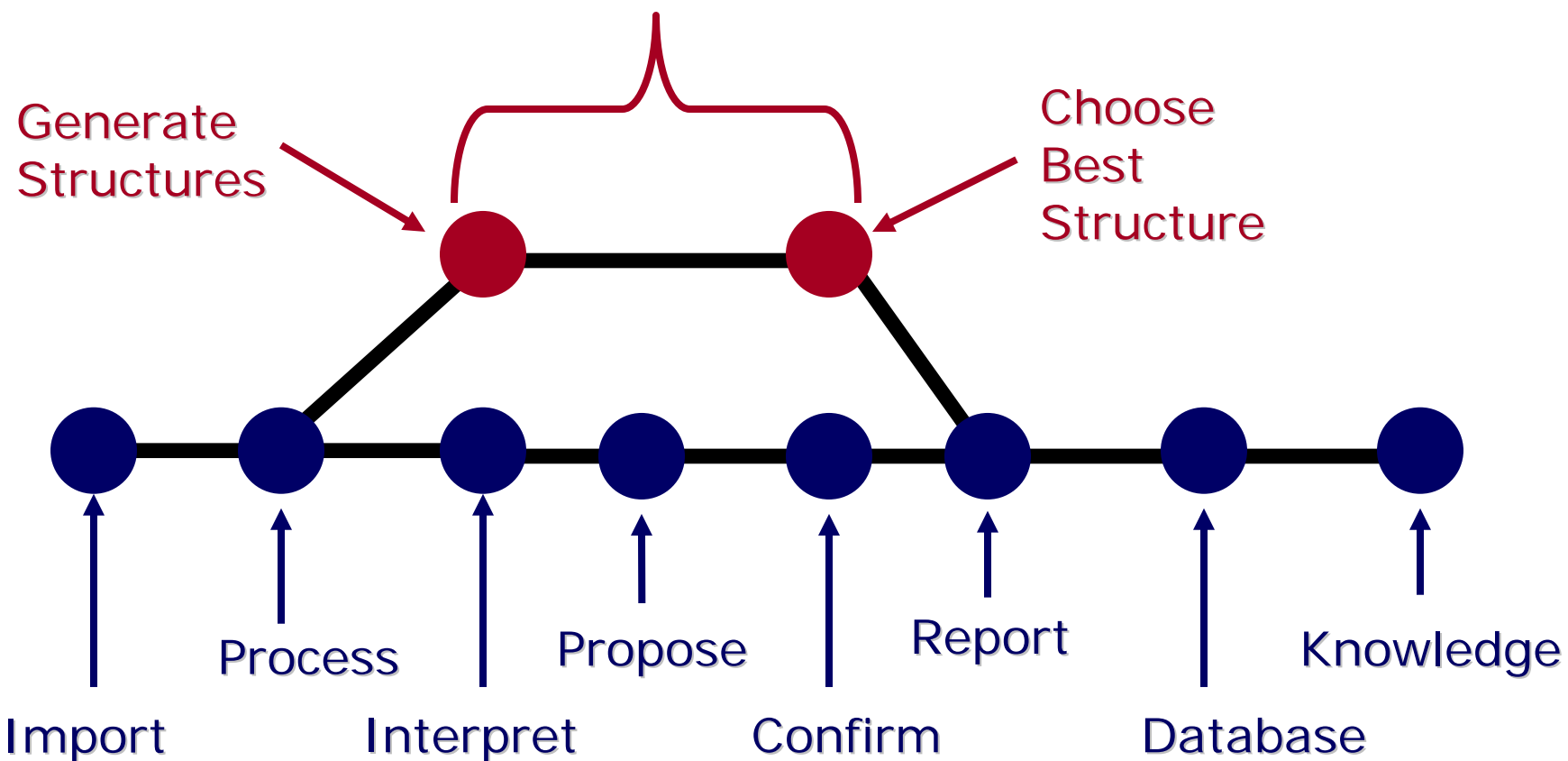


The Structure Elucidation Workflow



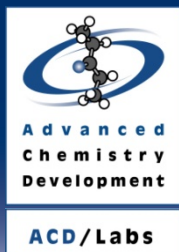
Hit a Roadblock? Use SE

ACD/Labs Structure Elucidation Engine



Summary

- ④ ACD/Structure Elucidator is a suite of software tools
- ④ More than the sum of the parts
 - ④ Manage your knowledge
 - Partial assignment retention changes everything



Acknowledgments

 Kirill Blinov

 Ryan Sasaki