

Inchl at Wiley

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View expressed herein are my own and are not necessarily those of my employer.



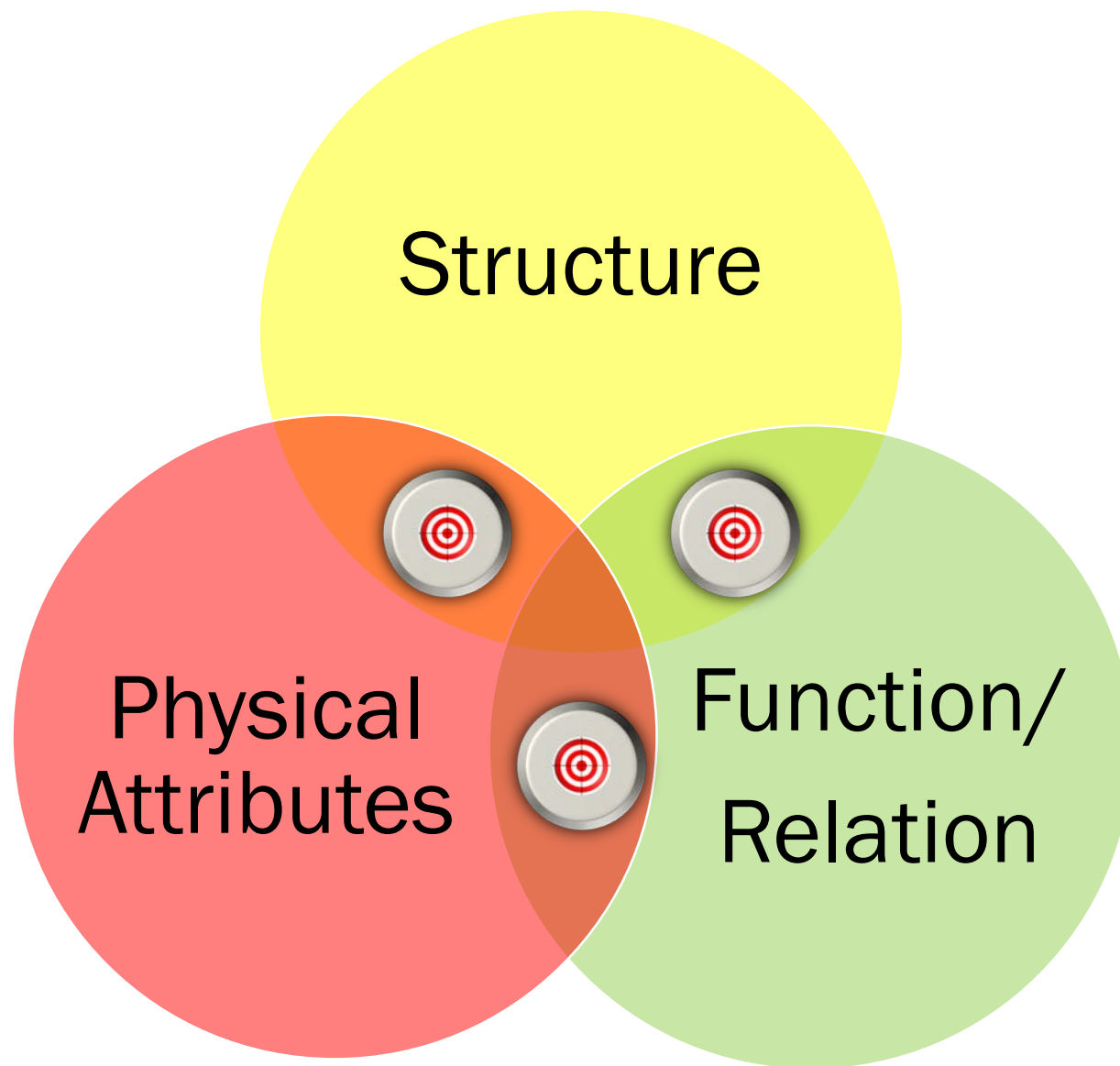
Wiley Science Solutions

Improve Human Health and Welfare

We do this chiefly through spectroscopic data collections

Dealing With Unknowns

- Measurable attributes
- Function or relation
- Structure
- Life Sciences/Clinical
- Molecular Medicine





Most Identifiers Have Gaps

Mol files can't handle
certain molecule types

InChI – organometallics,
stereochemistry

Isotopic handling (chiefly
software)

Mixtures

Actively Used Identifiers

Generic Public Identifiers

- PubChem CID
- InChI
- Mol V-3000
- J-CAMP DX
- IUPAC systematic name

Internal Identifiers

- Wiley Spectrum ID
- Wiley JCAMP-CS (can handle many more attributes than Mol V-3000)
- Wiley JCAMP-DX (JCAMP-DX on steroids)

Identifiers We Don't Actively Discard

Proprietary Identifiers

- KEGG
- CAS RN
- CAS Systematic Name
- etc.

What's Missing from InChI

What InChI Should Do

- ~~Polymers~~
- Organometallics
- Inorganics
- Mixtures
- Tautomers
- Isotopes

Done Elsewhere

- Large Molecules (HELM)
- Anything beyond 2-D

Compound Search

Simple and Fast

- >3m compounds
- Structure, synonyms
- Response in milliseconds

Links out

- Wiley Online Library
- PubChem, PubMed
- NCBI Cross Database
- Others (Google, Bing)

Coming Soon

- Links to Spectra/Search
- Polymers and Large Molecules
- Metabolism/large molecules

Thank you for your time

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