STEM Research Literacy

Are We Adequately Preparing Our STEM Graduates for Positions in Laboratory Research in Academia and Industry?

Graeme Whitley
Agenda

- What Prompted This?
- Wiley Science Solutions
- Wiley Spectra Lab
What Prompted This
Self-Perception Versus Employer Perception

“new graduates are not equipped to function in the work place and are not meeting employers’ expectations”

Inside Higher Education
Where do Life Science graduates end up working?

https://www.census.gov/dataviz/visualizations/stem/stem-html
Why This Matters

Laboratory Workers Have an Outsized Impact

- 70% of clinical diagnoses are the result of a clinical lab test
- Forensic science is a key component of our criminal justice system
- ~70% of R&D is corporate
  - Wiley has plenty examples of corporate teams spending months and years on problems that can be solved in minutes with the right tools.
Working With Data

We Are All Data Scientists

In whatever field a life science student ends up in, in all likelihood, it will involve working with and interpreting data.

• Manipulating data, statistical analyses
• Problem solving – job #1 learning to not reinvent the wheel.
  – Having current and modern resources helps
  – Understanding limitations of “CopyLeft” resources that can’t be used in industry

Wiley Science Solutions

Inspiring Possibilities
Improving Human Health and Welfare

Intelligent Services
Spectroscopy

What is it good for?
- Compound identification
- Targeted and untargeted screening
- Compound quantification
- Typically using isotopic labeling
- Mixture analysis

Where is it used?
- Quality assurance, anti-counterfeiting
- Deformation, mixture analysis
- Clinical lab tests, biomarker development
- Criminalistics, toxicology
- Disaster response
- R&D – anything to do with molecules.
- Metabolomics/lipidomics
Why Spectroscopic Data?

Think of it as a set of sensory organs for Science and Medicine

- Modern instrument systems kick out significant amounts of data
- Traditionally students and researchers spend a lot of time at the bottom of the pyramid
- CDS’s help coalesce information to create knowledge
- Students and researchers spend more time on higher-level interpretation
What Do Academic Libraries Currently Use?

- Paper collections
  - Aldrich, Sadtler, Wiley, others
- Image banks
  - CAS, ChemSpider, PubChem
- Often left up to departments

Problems
- These are 1970s solutions to big-data problems
- This is NOT the way research is expected to be performed
- Lack of exposure to commercial solutions results in unfamiliarity with methods and thinking used in industry and government
Wiley Spectra Lab
The world’s largest spectral database – takes the guesswork out of identifying unknowns

Wiley Spectra Lab is an expert spectral data system that uses empirical spectral data and advanced software to help chemists, toxicologists, and life scientists confidently identify chemical substances.
Wiley Spectra Lab
Flexible Deployment

Cloud
Desktop
Server
Local Instruments
Data Collections

Wiley Publishes and Distributes the Largest Collections of Evaluated Spectra in the World

Mass Spectrometry

• ~2m spectra
• Wiley, METLIN, specialty libraries, Antibase

NMR

• 833,000 spectra
• Multiple atomic centers
• The basis for advanced prediction (Machine learning)

Vibrational Spectroscopies

• 334,000 spectra
• ATR-IR, Raman, UVVIS, FT-IR and Near-IR spectra.
• Aldrich Libraries – coming soon!
Scientific Methods Continue to Evolve

20th Century
1. PCR
2. Manual identification
3. Molecular modeling

21st Century
1. NGS
2. Search Algorithms, machine learning, Black Box AI, White Box AI
3. HTS, rational drug design
Wiley Spectra Lab SaaS

IP authentication

- IP Authentication
- Campus-Wide
- Comprehensive
- 3 Collections
Wiley Spectra Lab Desktop
Powerful, One interface, Research Grade

- Employs powerful algorithms
- "White Box" AI
- analyses and AI decisions are explained
- users can override AI
Spectral Interpretation Has Changed

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<th>Old Method</th>
<th>Current Method</th>
<th>Wiley Spectra Lab</th>
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https://www.wsslabs.com/ssr_login.php

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Other Resources
Agilent, ACD/Labs, Bio-Rad