Resources, Strategies, and Tactics for Identifying Unknowns

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Outline of Presentation

- Key Resources
- Data from the Lab
- Simplified Flowchart
- Types of Searches for Each Resource
- Converting Lab Data to Search Strategies
- Sample Searches
- Help
Key Resources

- Start With These Resources
  - SDBS Integrated Spectral Database for Organic Compounds
  - Properties of Organic Compounds (POC)
  - Sigma-Aldrich Online Catalog or Aldrich Spectral Tables

- If Haven’t Found Unknown, Then Use
  - Dictionary of Organic Compounds (DOC)
  - ACD’s Spectral Prediction Software

- Comprehensive Resources for More Info
  - Beilstein via Reaxys
  - SciFinder on the web
Types of Data from the Lab

- **Data from Lab:**
  - Spectral Data
  - Hetero Atoms
  - Functional Groups or Substructures
  - “Family” for Substance
  - MP/BP Data

- **Search Strategy:**
  - Search spectral peaks as a range of values or draw structure to view predicted spectra
  - Enter presence or range of values in molecular elements or molecular formula field
  - Draw or use shortcuts and templates
  - Tricky to search, instead look at chemical names in search results
  - Search data as range in MP/BP field to allow for error/variation between lab values and sources.