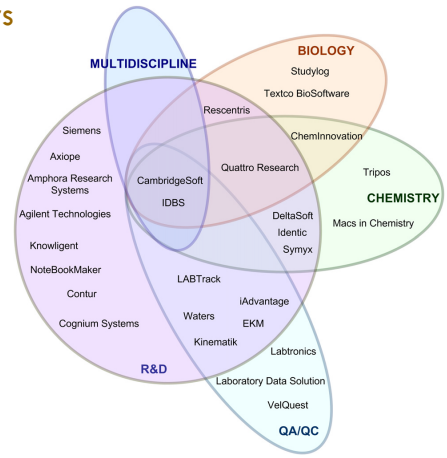
Electronic Notebooks - Why

- Advantages
  - Store all data in an electronic and searchable format
  - Particularly useful for students with poor penmanship
  - Also includes Inventory, Assays, and Biological Data
  - Can access almost anywhere in the world
  - PIs can easily look at all experimental data
  - Can share data between labs easily
  - Teach students/postdocs contemporary methods of record-keeping
  - Some E-notebooks formats can be customized for each lab
  - New E-notebooks are browser based (no software installation)
- Disadvantages
  - Cost ($150-$250/per student each year)
  - Data loss or theft (anything in electronic format is more vulnerable)
  - Requirement for laptop computer & good internet connection
  - Archiving all raw data can be cumbersome (i.e. NMR, TLCs, etc…)

Electronic Notebooks

- 34 vendors



- ChemInnovation Software, Inc. (CBIS)
- Cambridge Soft (Elements)

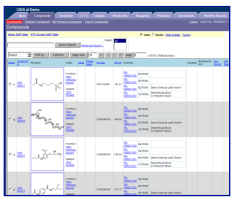
Rubacha, M. et al. *Journal of the Association for Laboratory Automation* **2011**, 90-98.

ChemInnovation Software, Inc

- Company
  - Incorporated in 1996, San Diego, California
  - Missions: Provide Web-based applications for drug R&D
    - Increase productivity
    - Promote data sharing
- Products
  - CBIS
  - Chem4D
- Customers
  - US: J&J, Pfizer, Allergan, Aragon, Celgene , etc
  - Japan: Chugai, Astellas, Taiho, Ryoka, Mitsubishi, Canon, etc
  - China: Sundia, CrownBio , etc
  - Academic: UC (10 campuses), U-Pitt, UND, USC, Sanford-Burnham, City of Hope, etc

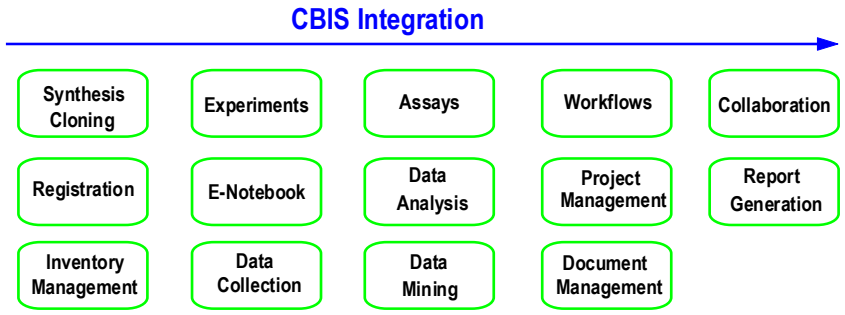
CBIS

- Chemical and Biological Information System (CBIS)
  - Compounds
  - Bio-materials
  - Inventory
  - Assays
  - E-Notebook/Documents



CBIS

Manage and cross-link all types of data



CBIS E-Notebook

- Electronic Records
  - Designs
  - Procedures
  - Results
  - All data files
- Knowledge Database
  - Search text and data
  - Search file content
  - Search structures and sequences
  - Use notebook page as new experiment template

CBIS E-Notebook Formats

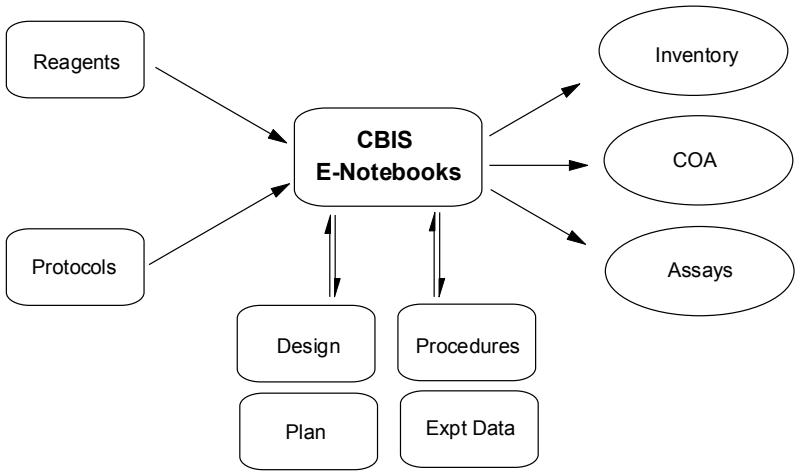
- Generic Experiments
  - Section, paragraph
  - Text
  - Image
  - Table (load Excel file)
  - Attachments
- Pre-defined Template
  - Chemical reactions
    one-step, multi-steps, parallel reactions
  - Plasmid cloning

Chemical Reaction E-Notebooks

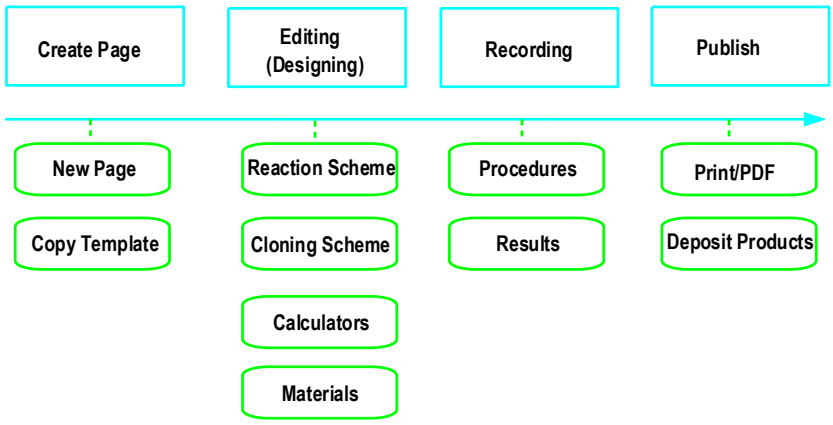
- Define Reaction
  - Draw reaction scheme with Chem4D
  - Or specify reactants and products separately using Java Script tool or any drawing program
  - Add reactants/solvents from CBIS Reagents module
- Design Experiment
  - Specify limiting reagent
  - Auto-calculate millimols, amounts, volumes
- Procedures and results
  - Upload analytical data files
  - Deposit products to CBIS Inventory module
  - Sign/approve pages and save as locked PDF files

CBIS E-Notebooks

Fully integrated with other CBIS Applications

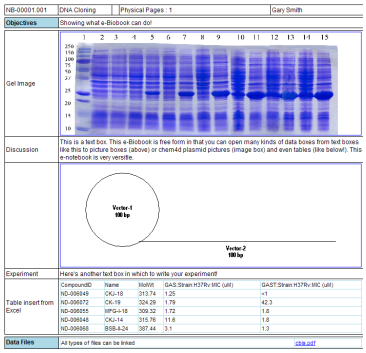


CBIS E-Notebook Workflow



CBIS E-Notebook Advantages

- Fully Customizable
- Link to raw materials (other modules)
  - Bio-reagents
  - Clones/Proteins
- Direct deposit to inventory modules
  - Batch ID
- COA Generation
- Search all fields
  - Properties
  - Structures or sequences
  - File Contents
- Access Control



CBIS E-Notebook Advantages

- Rich features and user-friendly
- Web UI supports all browsers and most mobile devices
- Hosted at ChemInnovation site or run on campus server
- Competitive cost

Other Popular CBIS Modules Deployed at Universities

- Chemical Inventory Management and Safety Report
- Chemical Stock Room Management
  - Ordering and receiving
  - Purchasing by PI or grad students