

# Electronic Lab Notebooks & Digital Data Management

ELN User Group  
UCSD

Session sponsored in part by GSA

# Agenda

- Introduction and brief overview of ELN technology
- Icebreaker
- Questions and Answers
- Setting future goals
  
- Setting up a Network

# Our Purpose

- To help students and researchers adopt and use ELN technology
- To improve awareness of ELN's and to show that there is a growing demand
- To facilitate acceptance of ELN's and to help set standards and guidelines for ELN implementation

# A common grad student experience:

The professor walks in, wakes you up and asks for a gel you ran last year. It happens to everyone— which would you prefer?



OR

Welcome Demo!

 [Advanced Search](#)

# Who Needs an ELN

- Students
- Researchers
- Anyone who needs traceable records
- Anyone regularly producing numbers or who keeps regular notes
- Most everyone

# Advantages of ELN's

- Faster to type for most
- Clarity and legibility
- Easy to store electronic data (images, spreadsheets etc.)
- Searchability
- Organization
- Access (network or web)
- Collaboration and data sharing
- Security
- Third party verification for IP
- Portfolio/Request-For-Proposal Documents

# Barriers to ELN's

- Paper is Status Quo
- Legal questions
- Momentum (early adoption is hard)
- Still few options
- Lack of awareness
- Lack of standards and guidelines
- In Academia, Need vocal supporters

# 5 Major Types of ELN's

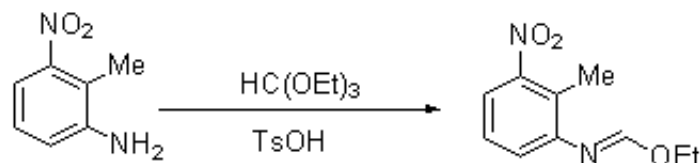
- Packages
  - Software based
  - Web based
- Custom
  - In House
  - Outsourced
- Process or Pipeline Based

# Software ELN's

- Bought as a package and installed on individual computers
- Pros: Several choices, specific applications, control over data, witnessing can be automated
- Cons: Often discipline-specific, expensive, update costs, software specific, extra effort to network or make external backups
- Examples: Labtrack, Infotrieve, Cambridgesoft's E-Notebook, others
- Other: HTML notebooks



## Reaction



## Reactants &amp; Products

	Name	MF	Limit?	MW	Equivalents	Moles	Sample Mass	% Wt
1	2-methyl-3-nitroaniline	C7H8N2O2	Yes	152.151	1	1000 mmol	152 g	100.0
2	triethyl orthoformate	C7H16O3	No	148.200	1	1350 mmol	200 g	100.0
3	p-toluenesulfonic acid	C7H8O3S	No	172.202	0.006	6 mmol	1 g	100.0

	Name	MF	Actual Mass	Actual Mol	Yield	Purity	MW
1	(E)-ethyl N-(2-methyl-3-nitrophenyl)formimidate	C10H12N2O	184 g	778 mmol	78%	88%	208.214

## Solvents

	Name	Solvent Ratio	Volume
1	p-toluenesulfonic acid	1	1000 ml

## Reaction Conditions

Reaction Molarity	1 mol/l
Pressure	100 atm
Temperature	120 °C

## Preparation

## AutoText

- Standard
- ... Addition Funnel
- ... Addition Syringe
- ... Distillation
- ... Heat Solvent
- ... Wash

Times

8

**B***I*

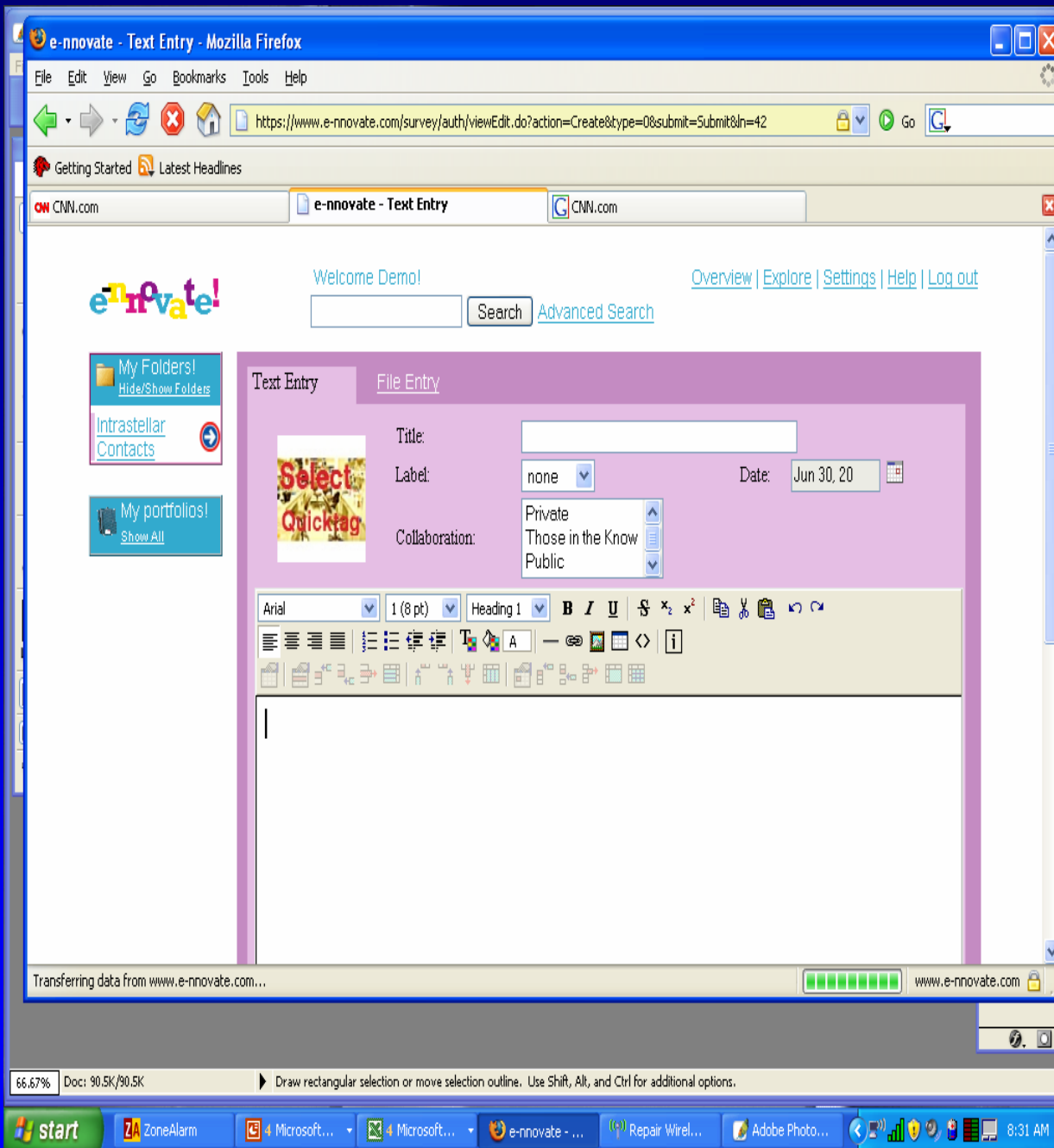
A 1-L, one-necked, round-bottomed flask, fitted with a Claisen condenser protected with freshly distilled triethyl orthoformate (200 g, 1350 mmol), p-toluenesulfonic acid (1 g, 6 mmol), and 2-methyl-3-nitroaniline (152 g, 1000 mmol). The solution is heated to 120°C and all of the ethanol is removed by azeotropic distillation. The residue is purified by fractional vacuum distillation at 156-158°C/6 mm, the product is a solidifying oil, mp 57-58°C.

Modified from *Organic Syntheses*, CV 8, 493

E-notebook

# Web Based ELN's

- Online ELN's
- Pros: Access from anywhere, automatic updates, secure backups, *not restricted by software or platform*, long distance collaborations, less expensive, automatic witnessing
- Cons: Lower storage capability, subscription based (still less expensive)
- Examples: e-nnovate



E-nnovate

# In House

- Do it yourself
- Pros: Very specific/specialized, control over data, cheap
- Cons: Time consuming, errors can show up too late, guidelines for in-house applications are yet unclear, not a good option for non-programmers
- Examples: Your MS-word file, that thing you wrote in C and abandoned, more effective programs your CSE friend wrote

# Outsourced

- Bring someone in to design your application
- Pros: Custom made, usually powerful, saves time and trouble
- Cons: Can be expensive and often contract based, hard to update or make additions, usually not for academics
- Examples: IT firms and consultants, most current ELN providers offer custom designs

# Process or Pipeline

- Intention is to mine for and process data, not just store it, a likely big element of future ELN's
- Pros: Highly visual, built-in data analysis, simplified mining
- Cons: Often lacks simpler functions, more than the average user needs, still in development stages
- Example: The UCSD Supercomputer Project

# Note

- Don't forget that your lab notebooks are only partly for you, they are also for your
  - PI's
  - Colleague's
  - Successors (Overcoming the legacy effect)
  - IP conflicts and applications

# Future Directions

- Hands free note-taking
- Tablet PC's
- Compatibility of ELN's with pocket devices

# Sources for ELN Information

- UCSD Outreach (developing an info base)
- Office of Tech Transfer (guidelines)
- Atrium Research (Offer a not cheap business case, some info for free)
- CENSA for industry info
- Web search (after you type 'failure' into google feeling lucky)

# Club/Networking Possibilities

- Meetings/meals (bimonthly)
- Email list
- Setup a message board
- Private connections



# Storage

- Paper doesn't last forever and is subject to fire/water damage or loss
- Writeable media have a limited lifespan (especially when warm)
- Storage devices become obsolete
- Two solutions
  - Continuous backup (ie managed server)
  - Combination of approaches

If you do need a hard copy



# LIMS and ELNs Defined

- LIMS: Laboratory Information Management Systems
  - Automated tracking of specimens, experiments and data generated from those experiments.
  - The goal is to manage large quantities of similar information
- ELN: Electronic Lab Notebooks
  - Acts as a repository of ideas, experiments, data and discussion
  - More flexible and geared towards intellectual property generation

# Things To Keep In Mind



- How repetitive are your experiments? Do they involve a serial set of similar tests?
- How many people are involved and at what level?
- How much creativity and knowledge generation is involved?
- Level of training and adaptation resistance

# 21 CFR 11

- The acceptance of electronic documents with electronic signatures as valid in regulatory fulfillment
- Very important if work is to be ultimately submitted to organizations such as FDA
- Most ELN have features that make them “more” 21 CFR 11 compliant
- You must evaluate the features and their compliance level in the context of your organizational needs. Seek legal counsel.

# 21 CFR 11 'Some' Features



- Traceable, auditable access logs
- Identity verification using passwords
- Documented electronic signatures (with identity verification)
- Server security features
- See federal agency or rule documents for more specifics