Making the Jump: Moving from Research into Chemical informatics

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Where is the knowledge?
  - Lost in the information

Where is the information?
  - Lost in the data

Where is the data?
  - Lost in the database!!
So why is cheminformatics important?

- Google web search – UMIST – M.Sc in Cheminformatics
- The storage, manipulation, presentation and application of chemical and biochemical information lie at the heart of contemporary scientific research. All chemical, fine chemical, biochemical, agrochemical, and pharmaceutical industry is increasingly reliant upon electronic data management and application both 'in house' and for interfacing with external information sources.
So what is it?

- Software tools
- Basic molecular modeling
- Laboratory information management systems (LIMS)
- Database management tools
- Chemical database systems (including spectral and reaction systems)
- Statistics and chemometrics
- Laboratory automation and instrument interfacing
- Automated synthesis
- High throughput screening
- High-performance computing tools and their role in chemical research
- Structure coding systems (including nomenclature)
- Electronic chemical publishing systems
- Chemical patent information sources.
So who can be involved?

- Well, it depends on what you want to do
- Chemists, biologists, scientists, software engineers, computer programmers
- BS, MS, Ph.D.
- The list is almost endless
Careers out there?

- Chemical companies
- Publishing
- Software
Chemical Industry

- Chemical information services
  - Corp. dbs, inventory systems, experimental handling, LIMS

- Applications
  - Searching dbs, designing, running & managing experiments, analyzing results, mining data

- Libraries
  - Patents
  - Journals
  - Reference works, books
Publishing

- Journals
- Patents
- Reference works, books
- Writers
- Editors
So what about me?

- I am not *that* David A. Evans
  - Nor *that* David A. Evans
  - But I am this David A. Evans

- University of Bath (UK) – B.Sc. Chemistry
- University of Bath (UK) – Ph.D. – Computational Chemistry – modeling multi-component lipid bilayers
- NYU – Post-doc – computational studies on self-assembling systems
- Oxford Molecular Group – Collaborative Discovery Group, contract research for drug discovery
- MDL Information Systems, Inc. – Product Marketing
I like chemistry
But ....
  * I don’t like nasty cancerous dangerous chemicals
  * They are
    • Nasty
    • Cancerous
    • Dangerous
Computers are not
Greg was right

- Networking is fantastic
- Everywhere I’ve been so far:
  - I found out about my Post-doc from a friend who had been my undergraduate demonstrator
  - I found out about my first job from a friend at my first internship job
  - I found out about this job from a friend I’d done my Ph.D with
So what do I do now?

- I work for MDL Information Systems
- MDL is the leading supplier of discovery informatics solutions to the life sciences and chemical industries and academia
- I am a Product Manager
- I have a Ph.D. in Chemistry and I do marketing!!
- Other plus points
- I am British but ….
But Seriously ..... 

- Back to software and making it
- I am a Product Manager
Software Houses

- Engineers
- Testers
- Technical communicators
- Support people
- Product Management & Marketing
- Sales and sales support
And finally ....
I have to plug my own company ..... ;-) 

- So, check us out
- Or ....
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- Or ....
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