

# 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!!

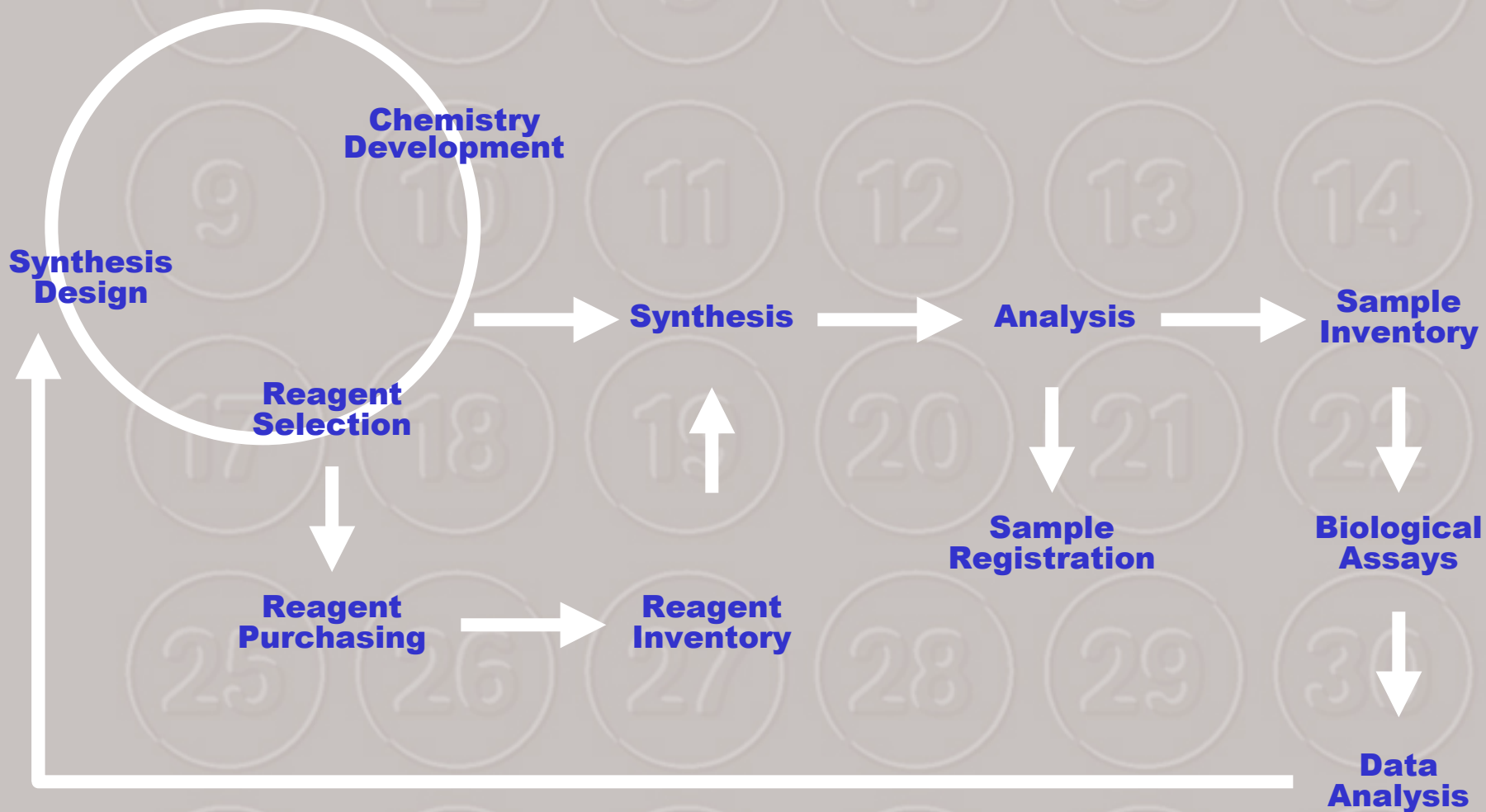
# So why is cheminformatics important?

- ▶ 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.

# Library Planning & Synthesis Workflow



# 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 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



- ▶ 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

# Greg was right

- ▶ 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



# Product Marketing

		Business Case	Product Definition	Advertising		
Distinctive Competence	Sales Analysis	Buy, Build or Partner	Positioning	Press		
Market Research	Trend Analysis	Pricing	Sales Process	Speaking Engagements		
Technology Assessment	Product Profitability	Thought Leaders	Roll-out Process	Lead Generation		
<b>Market Analysis</b>	<b>Quantitative Analysis</b>	<b>Strategic Planning</b>	<b>Product Planning</b>	<b>Promotional Comm.</b>	<b>Internal Comm.</b>	<b>Sales and other support</b>
Prospect Problems	Win/Loss Analysis	Innovation	Product Contract	Presentation	White Papers	"Special" Calls
Competitive Review			External Specification	Demonstration	Cost Justification	Seminars & Tradeshow
			Implementation	Brochures & Fact Sheet	News Flash	Corporate Visit
				Newsletter	Competitive Write-up	Phone Support

Strategic

Tactical

# 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
- ▶ <http://www.mdli.com/>
- ▶ Or ....
- ▶ [Jobs@mdli.com](mailto:Jobs@mdli.com)
- ▶ Or ....
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