Cheminformatics Role in Pharmaceutical Industry

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Aug. 23, 2004
ACS
Agenda

- The big picture for pharmaceutical industry
- Current technological/scientific issues
- Types of projects are being tackled today
- Skilled personnel that are needed
Cost of “Finding the Cure”

- **Discovery**
  - Cost to discover one Drug Candidate … $70M
  - Number of successful candidates that go into Development … 1 in 10
  - Duration … 3-5 years

- **Development**
  - Cost to develop and launch a new drug … $800M
  - Duration … 6-12 years

- **Total cost for the latest therapeutic agent …**
... not Priceless

- ... $1.5B for each new drug
- Only 1 in 3 will recoup the R&D investment

The pharmaceutical industry is committed to finding new drugs faster and cheaper
The information pipeline

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DISCOVERY INFORMATICS PLATFORM

Drug Candidate (Knowledge)
What chemical information do pharma scientists need

- What compounds should I make and test
- How do make this compound
- Are there more compounds like this
- Where can I order the reagents
- What is known about this molecule – properties, patents, etc
- What can I predict about this compound
- Is the test library a diverse set of compounds
- What molecules to purchases for the library
- Can this series be synthesized by massive parallel synthesis
- What is the SAR telling me

And I need it all, right now, at my finger tips
Current Issues Cheminformatics

- What is a small molecule
- What is an adequate representation of a sample
- Properties calculations vs measurement
- Scoring functions for “drug-like” molecules
- Docking for ligand binding prediction
- Calculating diversity and similarity
- Where do cheminfo and bioinfo merge
- Tox, ADME and other pieces of the puzzle
- Depiction of structure and visualization of data
- Electronic lab notebooks … still …
Organizational models affect the approach

Where does informatics fit in the organization?

- Is it IT or science
- Is the driver process or invention
- Project versus integrated support
- Big company, small company
Valued skill sets

- Chemistry and computer science a must
  - Conversant in either environment
- Biology, engineering, statistics are a plus
  - Ability to draw upon advances in other areas
- Facilitation & interpersonal skills
  - Share knowledge, not just code; integrate science and IT
- Organizational skills & team orientation
  - Industrialization of the process
Opportunities across the industry

- **Software Vendors** – Develop the tools that used for information management and scientific investigation
- **Data Suppliers** – Provide information and content, as well as tools to manage the data
- **Suppliers** – Vendors of reagents, laboratory supplies and scientific equipment
- **Consultants** – Engagements range from technical developer support, to analyst for strategic informatics decisions
“A” List Resume has...

- Industrial internship or work experience
- Extensive scientific laboratory training
- Examples of algorithm development and application coding achievements
- Examples of process improvements, innovation or scientific accomplishments
- Recommendations on character, initiative and why this person is valuable to the org
Pharma Role of Cheminformatics

- Facilitate process
- Manage the domain knowledge
- Support the integration architecture
- Provide opportunities for innovation
- Contribute to cost reductions