

Some Reflections on the Past and Future

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Overview

- Personal technology milestones
- What's happening to the publishing industry?
- What's happening to the pharma industry?
- Why prediction of the future is dangerous...
- ...some predictions nevertheless

Personal technology milestones

- 1964 – Birmingham University acquired its first mainframe computer
- 1965 – I learnt to program in Fortran II
- 1967 – I learnt to program in Assembler
- 1970 – first computer typeset publication
- 1972 – my first VAX mail message
- 1979 – my first email id (on CAS mail)

Personal technology milestones

- 1980 – experienced my first conference call
- 1981 – acquired my first fax machine
- 1982 – gave my first online demonstration
- 1983 – acquired my first microcomputer
- 1986 – development of STN Express
- 1989 – first aware of the internet

Personal technology milestones

- 1993 – first web browser launched
- 1996 – acquired my first mobile phone
- 1997 – launched ChemWeb.com
- 1998 – organised first virtual conference
- 2001 – acquired my first digital camera
- 2002 – first private email address
- 2004 – KC company website launched

Technology as an enabler

- Review of my technology milestones shows how much has changed in 50 years
- When I was at school, I had to walk 100m to a red phone box to call my girlfriend
- Now, I run a business from my home, hold video conferences, remain in constant contact with world and chemical news, etc.
- My social life has become a hybrid of contacts between real and virtual friends

Technology as an enabler

- Scientific publishing is now predominantly an online business
- Telecommunications enable global companies and their operations
- Spare capacity in networks reduces costs, enables outsourcing, and leads to completely new business models – the world is flat – companies can become virtual companies

What is happening to the publishing industry?

- Continued growth in numbers of journals and articles published is fuelled by the 'publish or die' syndrome and the growth of science in China, India, etc.
- Technology has enabled a shift from print to predominantly electronic publishing in the last 15 years
- Electronic paper still predominates but semantic markup is making an impact

What is happening to the publishing industry?

- Library funding crisis has led to a demand for new business models
- Open access publishing (gold and green) continues to advance but, in chemistry, it is still far from making a major impact (ACS)
- Outsourcing to the Phillipines and India is reducing the production costs for typesetting and indexing

What is happening to the pharmaceutical industry?

- Increased regulation has raised the cost of bringing a new drug to market
- Patent system protects drugs but the effective life times of patents are too short so the pharma industry seeks to stretch artificially the life of a patent
- Resurgence of the generic drugs industry is caused by the desire of governments to reduce the costs of the health service.

What is happening to the pharmaceutical industry?

- Production of drugs has already largely been outsourced to India
- Pharma companies are increasingly outsourcing their research to China and India and closing or reducing research centres in the UK
- Mergers and acquisitions – 48 members of PhRMA in 1988 was reduced to 11 by 2011

CAOCI – a case study

- CAOCI – the Commercially Available Organic Chemicals Index began life as a collaborative project proposed in 1972/73 by some members of CNA(UK)
- ICI Plant Protection Division created a prototype and six companies agreed to collaborate and project started in 1974
- Original members were Pfizer, Glaxo (incl. Allen & Hanbury's), Boots, ICI, Beecham and Wellcome

CAOCI – a case study

- The project ran for 5 years and in 1979 the CAOCI file was handed to Fraser Williams
- The file contained 120,000 records, representing 42,000 different chemicals from 48 supplier catalogues
- Chemical structures were coded in WLNs and was searchable within ICI using CROSSBOW
- In mid 1980s, the file was acquired by MDL and became ACD

CAOCI – a case study

It is instructive to look at the fate of some of the original participants:

- In 1993, ICI demerged its pharma and agrochemicals divisions to form Zeneca
- In 1995, Glaxo acquired Wellcome and BASF acquired Boots
- In 1999, Astra and Zeneca merged
- In 2000, GlaxoWellcome and SmithKline Beecham merged

CAOCI – a case study

...and Pfizer now comprises the following companies

- Warner Lambert (Agouron, Farmitalia, Jouvénal, Parke-Davis)
- Pharmacia (Monsanto, Searle, Sugén, Upjohn)
- Wyeth (American Cyanamid, American Home Products, A.H.Robins, Genetic Institute)

CAOCI – a case study

The chemical/cheminformatics software industry has also seen a few mergers:

Acclerys now comprises the following former companies: MSI (Biodesign, Cambridge Molecular Design, Polygen, Biosym, Biocad), Synopsys, Oxford Molecular (Biostructure, CAChe, Chemical Design, HDI, PSI (Fein Marquart), GCG, Intelligenetics, Cambridge Combinatorial), Synomics, SciTegic, Symyx (MDL (ORAC, OHS)), Contur Software AB

Why prediction of the future is dangerous...

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- “X-rays will prove to be a hoax.” (Lord Kelvin, 1883)
- “Radio has no future.” (Lord Kelvin, 1897)
- “Fooling around with alternating current is a waste of time. Nobody will use it, ever.” (Thomas Edison , circa 1900)

Why prediction of the future is dangerous...

- “Stocks have reached what looks like a permanently high plateau.” (Prof. Irving Fisher of Yale, on October 17, 1929, just before the stock market crashed)
- “I think there is a world market for maybe five computers.” (Thomas Watson, Chairman of IBM, 1943)
- “We don’t like their sound. Groups of guitars are on their way out.” (Decca Records executive, 1962)

Why prediction of the future is dangerous...

- “I want to assure you that I have never felt better about the prospects for the company.” (Enron CEO Ken Lay, after selling \$160 million of his own company stock, August 14, 2001)
- “Companies come and go. It’s part of the genius of capitalism.” (Paul O’Neill, Treasury secretary, on the collapse of Enron, January 14, 2002)

Why prediction of the future is dangerous...

- “There is no reason for any individual to have a computer in their home.” (Ken Olson, President, Digital Equipment Corporation, 1977)
- “640K ought to be enough for anybody.” (Bill Gates, 1981)
- “Open Access is evil.” (Commercial & Society Publishers, 2005)

...some predictions nevertheless

Publishing industry:

- Open access publishing will become the predominant business model within ten years
- Some abstracting and indexing services will disappear or mutate
- There will be more mergers of publishers
- One or more major publishers will be owned by an Indian company

...some predictions nevertheless

Pharma industry

- The number of new chemical entities approved each year will remain about the same
- The trend to outsource research to India and China will continue
- There will be more mergers
- One or more major pharma companies will be owned by an Indian company

...some predictions nevertheless

Software industry

- HTML5 will be released in the 21st century
- New software paradigms will emerge
- New companies will appear and old companies will merge or die
- BRIC countries (or African countries) will dominate the industry

...some predictions nevertheless

Pre-competitive and open collaborative efforts will thrive and some of the following will succeed:

Data, Models and Software Becoming More Accessible- free, Precompetitive and Open Efforts - Collaboration



Innovative Medicines Initiative



Environment Directorate

Environment Directorate

Chemical Safety

- Agricultural Pesticides and Biocides
- Assessment of Chemicals
- Chemicals Testing - Guidelines
- Good Laboratory Practice
- Risk Management of Installations and Chemicals
- Safety of Manufactured Nanomaterials

Biodiversity, Water and

Home: Assessment of Chemicals

About Publications & Documents

The OECD QSAR Toolbox

What does the Toolbox do?

Download the Toolbox

Guidance Documents and Training Materials

Public Discussion Forum

An Overview of Phase 2 development of the Toolbox

SUMMARY

Drug discovery sources

Expressing integration companies

To address Pharmacology needed to all users



MetaPrint2D-React metabolic product predictor

University of Cambridge > Department of Chemistry > Unilever Centre for Molecular Science Informatics

Query Structure

Enter SMILES string:

Advanced options

Fingerprint matching

Set the similarity strictness of the fingerprint match

- Loose (2, 1.0, 1.0, 1.0, 1.0, 0.75, 0.5, 0.25)
- Default (3, 0.5, 1.0, 1.0, 1.0, 0.75, 0.5, 0.25)
- Strict (4, 0.1, 1.0, 1.0, 1.0, 1.0, 0.5, 0.25)
- Custom (set the values below)

Number of exact levels:

Similarity threshold:

First weight:

Second weight:



ABOUT

WORKING GROUPS

INDUSTRY CHALLENGES

Does every life science company really need its own...
We sure hope not!

See what we're working on.

Industry Challenges

Precompetitive Collaboration

SESL

Seq

Upcoming Events

- 12 September 2011 - Pistoia Alliance Annual General Meeting
- 15-16 September 2011 - 9th Pharmaceutical Conference

Lowering barriers to R&D innovation



The Pistoia Alliance is a not-for-profit, precompetitive science company...

OECD harmonised

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Thank you!

Any questions?