Experiences with Knowledge and Data Sharing at Lhasa Limited

Philip Judson
philip.judson@blubberhouses.net
Introduction

- Sharing knowledge
- Sharing data
- Current situation
LHASA program

- Chemical synthesis planning
- Not cost effective for a single company to expand the knowledge base on its own
- Need to share knowledge about chemistry
Beware of geeks bearing gifts

- Give away secrets to the competition?
- Wreck patenting prospects?
- Be accused of forming an illegal cartel?
- Get ripped off by a software house?
Conditions to be met

- Share only non-sensitive information
- Each donate equally
- Donations become shared property
- Each member has rights for own use
Conditions to be met

- Fair terms for new members
- Fair terms for small organisations
- Fair terms for academics
Lhasa Limited

- Owned by its members and not for profit
- Members control projects
- Full members
  - Contribute knowledge
- Associate members
  - Pay for access
- Academic and non-academic membership
- Fair terms for new members
DEREK

- Share knowledge about toxicity alerts
- Developed internally by Schering Agrochemicals Limited
- Donated to Lhasa Limited and Harvard to be used for knowledge sharing
- Superseded by Derek for Windows
Past practice in toxicology

- In-house or exclusive contract
- Highly confidential
- Release to regulators only to the extent required by law
- No publication
Did the ideas work?

About 20 organisations joined the LHASA chemistry project
  • Full commitment to knowledge sharing

About 130 organisations now use Derek for Windows
  • They fund knowledge development at Lhasa
  • Many of them donate knowledge from their own research
First proposals on sharing data

- Mid 1990s
- Save costs
- Reduce use of animals
  - A goal in itself
  - PR benefits
- Kathy Stitzel, David Tennant and others
Yes, but…

At the start of the LHASA and DEREK projects people doubted that companies would be willing to share knowledge.

In the event they have done so.
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But sharing data is different.
Synthetic chemistry knowledge
Synthetic chemistry data

Chemical reactions and structures are shown with various molecular structures and chemical formulas. The reactions involve specific temperatures and solvents, indicated by 'x °C' and 'Solvent y', respectively. The yield of the reaction is given as 87%.
Toxicology knowledge

Potential skin sensitiser

\[ Y = N, CH \]
\[ R = F, Cl, OMe, CN \]
Potential skin sensitizer

$Y = N, CH$
$R = F, Cl, OMe, CN$

Skin sensitizer -
Data: xxxxxxxxxx

xxxxxxxxxx
xxxxxxxxxx
xxxxxxxxxx
xxxxxxxxxx
ITIC - a pilot project

- International Toxicology Information Centre
- Coordinated by ILSI
- Technical work done by Lhasa
- 3 year project ended in 2004
ITIC - a pilot project

Demonstration database system

Contained published data in a form suitable for (Q)SAR work

Contained a small amount of proprietary data to demonstrate that sharing is possible in principle

Vitic

- Full scale project
- Collect and share published data in a form suitable for (Q)SAR
- Share appropriate proprietary data
Changing regulations

- HPV data publication
- REACH data sharing for registration
- GHS, REACH, US EPA and FDA - increasing use of (Q)SAR

Urgent need for industry to act on its own initiative
What data can be shared?

- Data from old projects
  - May be hard to compile
  - May not be consistent with current standards

- Data on fully patented products
  - Already technically in the public domain but often hard to access

- Production intermediates
- Formulants and excipients
Production intermediates

- Many used by more than one company
- Their use is not secret
- Testing is needed for worker safety and for registration packages if the intermediates are potential contaminants of final products
- These compounds do not have proprietary value for the companies doing the tests - the costs are lost money
Production intermediates project

Joining terms

- Donate Ames test data for 50 compounds

Current ongoing terms

- Donate Ames test data for 20 compounds (or potentially data from other tests)

Flexibility

- Donations can be reduced for small companies
Excipients project

- Pilot project initiated by members of EFPIA (European Federation of Pharmaceutical Industry Associations)
- Ongoing support from EFPIA
- Currently sponsored by eleven organisations
Excipients project

- In-house
- On-line
- “Pay as you go” option planned for small users
- Membership terms open to negotiation
Current knowledge sharing projects

- Derek for Windows
  - Mammalian (mainly) toxicity
- Meteor
  - Mammalian metabolism
- MEPPS
  - Environmental biodegradation
- Chemical Degradation
  - Degradation of pharmaceutical formulations during storage
Current data sharing projects

- Vitic general toxicity data project
- Production intermediates
- Formulants and excipients
Where next

- Expand data sharing for REACH compliance
- Expand use of shared data for (Q)SAR work to support regulatory requirements
- Develop intelligent software to link knowledge and data about toxicity, ecotoxicity, metabolism, and biological and chemical degradation
Conclusion

Knowledge sharing and data sharing are now realities

- Helping to meet scientific ideals
- You have to put effort into negotiations with legal and business departments but if you set up the right collaborative structure you will succeed
- Big cost savings, PR benefits, and competitive advantage to companies who participate