

International Conference

DATA MANAGEMENT & KNOWLEDGE DISCOVERY

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Intelligent integration of electronic lab data & successful return
on investment for the pharmaceutical and chemical industry

INTERACTIVE WORKSHOPS: 20th April 2009
TWO DAY CONFERENCE: 21th – 22nd April 2009

relexa hotel, Frankfurt am Main, Germany

■ ■ ■ Hear **19** case studies from
leading international companies
and organisations:

- **Bayer HealthCare AG**, Germany
- **Aeterna Zentaris GmbH**, Germany
- **Ariana Pharmaceuticals**, France
- **Intervet GmbH**, Germany
- **eOrganizedWorld LLC**, USA
- **University for Applied Sciences Heilbronn**, Germany
- **Proskauer Rose LLP**, USA
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- **Bodhtree Consulting Limited**, India

Don't miss first to be heard case studies from leading companies on the way from data to knowledge:

- **Intelligent combination of ELN & knowledge management:** Learn how to **reduce time-to-market** by accessing and exchanging **global knowledge**, experiences and data in real-time
- Compare competing **off the shelf** and **in-house solutions** for e-lab data management to **speed up discovery** time for new drugs
- Implement a **global knowledge management scheme** to accelerate your **drug discovery**
- Learn from **real business cases** about efficient **document management systems in R&D** to provide your research department with an **advanced data warehouse**
- Improve the **forecasting of your research** by identifying the latest methods on creating metadata for a **systematic data mining**



Conference-Chairman

Alfred Stefan, Head of Research IT Department,
Abbott GmbH & Co. KG

Highlights

Daniel Caparrós, Head of Information Technology, **Aeterna Zentaris GmbH**

Dr. Daniel Meibom, Medicinal Chemist, Project Manager Pharmacophore Informatics Platform, **Bayer HealthCare AG**

Roman Koetitz, PhD, Senior Research Scientist, Team Leader Data Management **Rhodia "Laboratory of the Future"**

Interactive Workshops

- A: Rollout of a global R&D knowledge management program
- C: Future potentials of ELN and LIMS for R&D processes

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DATA MANAGEMENT & KNOWLEDGE DISCOVERY

Intelligent integration of electronic lab data & successful return on investment for the pharmaceutical and chemical industry

Dear Colleague,

after having completed five successful conferences on the topic **ELN**, we received feedback that the industry is shifting from ELN to **more sophisticated systems**. These include **intelligent data management** with **global knowledge management** and virtual cooperation throughout the **whole discovery process**.

Data management and knowledge discovery have become the **core practices** of every **R&D department** to aid achievement of ambitious goals regarding drug development. After having implemented **LIMS** and **ELN** as necessary databases, pharmaceutical companies are looking **now for potential solutions** regarding knowledge discovery.

For this reason the next step is already determined: Bringing up-to-the-minute knowledge to reality by integrating intelligent **search and analyzing tools** with the latest findings and experiences in the lab. **Text-mining** and **data-mining** not only help to unearth information, but also enable prognoses of new drug discovery. Pooling this worldwide knowledge allows specialists all around the globe to get in touch and share their experiences.

That is why you can't afford to miss IQPC's international conference:

DATA MANAGEMENT & KNOWLEDGE DISCOVERY

Intelligent integration of electronic lab data & successful return on investment for the pharmaceutical and chemical industry

20th – 22nd April 2009, relexa hotel, Frankfurt am Main, Germany

High-level speakers from companies such as **Bayer HealthCare**, **Ariana Pharmaceuticals**, **Allergan**, **Aeterna Zentaris**, **Rhodia Group**, **Abbott** and many more will report about first-hand experiences and latest developments.

Save your place and book now! We are looking forward to meeting you in Frankfurt!

Kind regards

Your
InformationstechnologieIQ Team

Who will you meet?

Representatives from international pharmaceutical and chemical companies as well as clinical research organizations:

- Drug Discovery
- Global Chemistry Leadership Team
- Research IT / R&D IT
- Chemical Research
- Information Discovery
- R&D Computing
- (Medicinal) Chemistry
- Bioinformatics
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SCREENING - Trends in Drug Discovery focuses new trends and developments in drug discovery. It covers all aspects of research as well as strategies of pharmaceutical companies and start-ups. www.gitverlag.com



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Workshop A

10:00 - 13:00

**Rollout of a global R&D knowledge management program**

There is an **accelerating increase** in the quantity of **computer generated information** in R&D. LIMS, ELNs, specialized software, Intranets, Document Management and Records Management products that are replacing traditional paper based programs. The problem is how to **interconnect all of these diverse products** so that information can be abstracted and integrated from all repositories. There are **technical, cultural and performance issues** to be considered.

- What are the conceptual architecture choices?
- Challenges in constructing global systems to share knowledge
- How can you import/export and search across information repositories?
- Considerations in software selections
- How do you measure ROI?

Charlie Sodano, PhD, Founder, **eOrganizedWorld, USA**

Workshop C

14:00 - 17:00

**Future potentials of ELN and LIMS for R&D processes**

There is a **growing need** for increased **automation in the R&D process**. **Data management** has become an essential component of R&D. The last few years has seen increased adoption of ELN and LIMS solutions by R&D centres across the world. It is essential to understand the **potentials of ELN and LIMS** in the R&D process and their role in increasing **efficiency and reducing the costs of R&D** processes.

- Translation of ELN and LIMS capabilities in the broader perspective
- Identifying new avenues of application
- Would interconnectivity help in maximizing potential?
- Is there a need of integrating ELN and LIMS with the business process?
- What are the trends in the need for customized solutions?

Eramangalath Sujith, Team Lead and Senior Analyst, **Frost & Sullivan, UK**

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Symyx Technologies
415 Oakmead Parkway,
94085 Sunnyvale, CA, USA
Phone: 1-408-764-2000
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Amphora Research Systems Ltd.
PO Box 3940 Bracknell,
Berkshire, RG42 2XN, UK
Phone: +44 (0)845 2300160
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STARLIMS Europe
Endeavour House, 98 Waters Meeting Road
Bolton, Lancs, BL1 8SW, UK
Phone: +44 (0) 1204 546 700
Fax: +44 (0) 1204 546 701
Email: joe.peden@starlims.com
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Bodhtree Consulting Limited
8-2-351/N/1, Road No: 2,
500034 Banjara Hills, Hyderabad 34 AP, India
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DATA MANAGEMENT & KNOWLEDGE DISCOVERY

Intelligent integration of electronic lab data & successful return on investment for the pharmaceutical and chemical industry

CONFERENCE DAY ONE | Tuesday, 21st April 2009

8:30 Registration & coffee

9:00 Chairman's welcome & opening address

Alfred Stefan,

Head of Research IT Department,

Abbott GmbH & Co. KG, Germany

From knowledge discovery to business development: Latest developments and future trends for accelerated drug discovery9:10 **Strategic market overview of LIMS-ELN in drug discovery**

- Applications of ELN-LIMS in drug discovery
- Market trends in ELN-LIMS
- Forecasts for the European market
- Vendor landscape – What is offered? Who is offering?

Eramangalath Sujith,

Team Lead and Senior Analyst,

Frost & Sullivan, UK

9:55 **Legal implications of knowledge discovery – How to file patents safely?**

- The potential effects of global knowledge sharing in your company on patent validity
- The importance of ELN records as legal documents
- Using ELN records to obtain and support patents
- Giving up your ELN records in US litigation

Colin Sandercock, Partner,

Proskauer Rose LLP, USA

10:40 Refreshment break & networking

11:10 **Lessons from the edge: Think now or pay later**

- Common misunderstandings between record managers and scientists
- Practical steps for your organisation to reduce costs and risks in record creation
- Experiences from implementations
- Comparing different industries and countries
- Happiness & harmony throughout

Simon Coles, Chief Technical Officer,

Amphora Research Systems, UK

Knowledge discovery systems: On the way to the perfect e-lab data management11:55 **An integrated approach to informatics – Bayer HealthCare Pharmacophore Informatics Platform**

- Data integration & retrieval
- Conversion of data into information & knowledge
- Data sharing
- Project management support

Dr. Daniel Meibom,

Medicinal Chemist, Project Manager Pharmacophore Informatics Platform,

Bayer HealthCare AG, Germany

12:40 Networking lunch

14:10 **Decision support: From data to knowledge**

- Definition of scientific objectives and observations
- Data generation and plausibility analysis
- Data analysis and decision support
- Putting the scientific user in the center
- Use case: From scientific objective to a scientific decision

Brunhilde Markus, Analyst & Software Developer,

Intervet GmbH, Germany

14:55 **Where do ELN and LIMS fit in the infrastructure?**

- What is and ELN - R&D, QC, MES, LES, EN?
- Do EN and LIMS not compete?
- Do companies need both?
- Envisaged solution

Joe Peden, General Manager for Europe,

STARLIMS Europe Ltd., UK

15:40 Refreshment break & networking

Enhanced data warehousing in drug discovery and substance development16:10 **Scientific data management life cycle**

- Software updates & new releases
- Problems of software customizations
- Data integration in heterogeneous environments
- ETL and data warehouse

Daniel Caparrós, Head of Information Technology,
Aeterna Zentaris GmbH, Germany**HIGHLIGHT**16:55 **Information architecture for integrated e-laboratory**

- Application standardization
- Processes harmonization
- System integration
- Customer satisfaction for increasing productivity and compliance
- Informatics investments

Joseph Kofman, PhD, Director,
R&D Information Services,
Allergan Inc, USA17:40 **R&D worldwide – Making knowledge management work throughout the whole discovery team**

- Corporate knowledge management as a global challenge
- Stakeholder of a globally unified informatics architecture
- Required support from the management board
- Managing the communication: How to make different departments cooperate?
- Standardising formats, user rights during the harmonisation of a global roll out

Chairman:

Alfred Stefan, Head of Research IT Department,
Abbott GmbH & Co. KG, Germany

Panelists:

Speakers of the day

Panel Discussion

18:20 Closing remarks of the chairman and end of conference day one

8:30 Registration & coffee

9:00 Chairman's welcome
Alfred Stefan, Head of Research IT Department,
Abbott GmbH & Co. KG, Germany**Data mining: On the way to successful knowledge discovery**9:10 **Effective data mining for decision support**

- Knowledge discovery requires systematic hypothesis generation and management
- Systematic identification of rules and associations
- "What if" scenarios
- Linking each rule with the raw data
- Examples from discovery and development

Mohammad Afshar, Chief Executive Officer,
Ariana Pharmaceuticals, France

9:50 **Improving ELN Workflows and Information Capture to Facilitate Information Driven R&D**

- Optimizing workflows around secure IP capture within the laboratory is a primary business goal for ELN investments. Essential in optimizing the IP capture is enabling information to be 'pushed' into the workflow of the scientist and captured in context to the experiment. If information is captured correctly ELNs can provide a far greater return on investment than time savings and workflow optimization.
- Together ELN's and researchers turn data into information and knowledge. Knowledge that can be accessed and shared across the enterprise and re-used to drive innovation, reduce experimental costs and improve experimental results.
- This presentation explores and provides demonstrations for how information from across the enterprise can be rapidly pulled into to a notebook experiment and the information stored in a fully shareable repository that enables scientists to search across unstructured and structured data.

Francis Bennett, Director, Product Marketing,
Symyx Technologies Europa AG, Switzerland

10:30 Refreshment break & networking

11:00 **Data integration – Simplified, with MIDAS**

- Existence of molecule data at different stages
 - Inception
 - Patent analysis
 - Under development
 - Clinical trials
 - File pending approval
 - Sales
 - Integration of molecule data from disparate systems across stages
 - Presenting the "single version of truth" about molecule
- Raghavan VSR Madabhushi, Head - SOA – DW,
Bodhtree Consulting Limited, India

11:40 **Data mining: Limits and opportunities**

- Data mining and the knowledge discovery process
- Typical data mining tasks
- Basic prerequisites: When does data mining work?
- The annoying part: Preparing the data
- The exciting part: Learning from data

Prof. Dr. Carsten Lanquillon, Chair Holder,
Institute for Informatics,
University for Applied Sciences Heilbronn, Germany

12:20 **Data mining in complex data repositories**

- Data mining in distributed environments
- Privacy preservation and data anonymization
- Data mining und object complexity
- Object-, comparison- and pattern-based approaches

- Context specific evaluation

Matthias Schubert, PhD,
Academic Councilor,
Ludwig-Maximilians-University Munich, Germany

13:00 Networking luncheon

14:30 **Data mining with sharepoint und search server**

- Integration of a sharepoint and a search server
- How to increase the acceptance of a sharepoint?
- Searching, finding and assuring the access to various resources
- Particular compliance challenges in the pharmaceutical sector
- Conclusions

Walter Steinsdorfer,
Group Lead IT,
Trion Pharma GmbH, Germany

15:10 **Architectural patterns of the biological data warehouse**

- Computational infrastructure
- Impact of staying current
- Utilizing the "user" resource
- Case study: ObjectLinks – A framework for taming wild mining-tools

Armin Ollig,
Director Information Technologies,
Biofrontera, Germany

15:50 Refreshment break & networking

Visualization techniques for advanced data understanding

16:10

**High throughput chemistry: Data management challenges and solutions**

- Data types and amount generated by HT equipment
- Automated image processing: A powerful tool to extract quantitative data
- How to keep track of raw, processed and meta HT-data
- Perspective: Database of product properties

Roman Koetitz, PhD,
Senior Research Scientist, Team Leader Data Management,
Rhodia "Laboratory of the Future", France

16:50

**A picture is worth more than a thousand words**

- Data visualization tools can reveal unexpected insights and relationships in the analysis from large and complex datasets without requiring complicated mathematical calculations or statistics. Through a more holistic analysis of whole data sets, or filtered data, in context with alternative data sources render possible intuitive informed decision making.
- Examples will be given how the integration of visualization tools into the analysis workflow facilitates multi dimensional assay optimization and positives selection in small molecule screening campaigns.
- Improvements achieved will be highlighted by means of the hit selection, when systematic errors introduced by the applied technologies are evaluated and corrected. These methods are generally applicable and also provide an excellent platform for explaining complex data sets to non expert customers.

Jan Selig, Senior Technical Officer,
Chemical Biology Core Facility,
European Molecular Biology Laboratory (EMBL) Heidelberg AG, Germany

17:30 Closing remarks of the chairman and end of the conference

DATA MANAGEMENT & KNOWLEDGE DISCOVERY

20th – 22nd April 2009 relexa hotel, Frankfurt am Main, Germany

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Please indicate choice of workshop on Monday, 20. April 2009

Workshop A | Workshop C

A: Rollout of a global R&D knowledge management program
C: Future potentials of ELN and LIMS for R&D processes



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- Increase your **productivity in R&D** by understanding the **potentials of ELN and LIMS** and learn how to search across **different information repositories**
- Discover how to guarantee long term data storage safely in a native environment to allow **reliable traceability** and **re-use of data**
- Learn how to solve **compliance & legal issues** to **secure patent protection** and pave the way to market authorisation

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