

# InterAction Meeting 2005, Basel

## November 9, Morning

### Session 1 Life Science Innovation Café - Confidence in Safety

09.30-10.45 Moderated by Victor Newman (KnowledgeWorks) with Saad Shakir (Drug Safety Research Unit, UK), James Averback (Life Science Integration Partners), and Barry Hardy (Douglas Connect)

### Session 2 Protein Folding & Dynamics, chaired by Wilfred van Gunsteren (ETH-Zürich)

08.30 Overviews & Goals, Barry Hardy (Douglas Connect)  
 08.50 Chair's Introductory Remarks, Wilfred van Gunsteren (ETH-Zürich)  
 09.00 Dynamics of Protein Binding, Reaction and Structural Change, Jeremy Smith (University of Heidelberg)  
 09.30 All Atom Protein Folding with Stochastic Optimization Methods, Wolfgang Wenzel (University of Karlsruhe)  
 10.00 Protein Dynamics Measured by Triplet-Triplet Energy Transfer, Thomas Kiefhaber (University of Basel)  
 10.30 Coffee Break  
 11.00 Aspects of beta-Peptide Folding from Molecular Dynamics Simulation, Xavier Daura (University of Barcelona)  
 11.30 Structure Determination of Native and Non-Native Protein Conformations Using NMR-Derived Restraints, Michele Vendruscolo (University of Cambridge)  
 12.00-13.00 Panel Discussion

### Session 3 Knowledge Management in R&D, chaired by Robert Scoffin (CambridgeSoft)

08.40 Overview & Goals, Barry Hardy (Douglas Connect)  
 08.50 Chair's Introductory Remarks, Robert Scoffin (CambridgeSoft)  
 09.00 ABCD and Combinatorial Library Design, Alan Gibbs (Johnson & Johnson Pharmaceutical Research & Development)  
 09.30 Assembly, Distribution, & Retrieval of Biological Information in Drug Discovery, Kim Henrick (Eur. Bioinformatics Inst.)  
 10.00 Pharmaceutical Development and the Use of Electronic Lab Notebooks, Michael Swartz (CambridgeSoft)  
 10.30 Coffee Break  
 11.00 Global Roll-Out of an Electronic Notebook at Schering, Rolf Jautelat (Schering)  
 11.30 Aggregation, Filtering and Alerting of Scientific Information from Multiple Sources, Mark Sharp (Corpora)  
 12.00-13.00 Panel Discussion

## November 9, Afternoon

### Session 4 Knowledge Management in R&D (cont'd)

14.00 Ontologies: Real Applications in Pharma, Steve Gardner (Biowisdom)  
 14.30 Molecular Architecture to Prepare Structures with Desired Properties, Ulrich Jordis (Vienna University of Technology)  
 15.00 Global Information Integration in R&D, Pierre Allemand (Symyx-Intelligence)  
 15.30 Coffee Break  
 16.00 Strategic Knowledge Management in Life Science Research, Victor Newman (KnowledgeWorks)  
 16.30 Knowledge Management Methodologies and Auditing for Electronic Lab Notebook Implementations, Barry Hardy (Douglas Connect) and Jeff Spitzner (Rescentris)  
 17.00-18.00 Panel Discussion

### Session 5 Virtual Screening, Docking & Scoring, chaired by Miklos Vargyas (Chemaxon)

14.00 Chair's Introductory Remarks, Miklos Vargyas  
 14.15 Pattern Recognition and Grid Computing in Discovery, Graham Richards (University of Oxford)  
 14.45 The Issue of Protein Flexibility in Docking-Based Virtual Screening, Xavier Barril (Vernalis)  
 15.15 Coffee Break  
 15.45 Discovery of Cell-Permeable Non-Peptide Inhibitors of beta-Secretase by High Throughput Docking and Continuum Electrostatic Calculations, Amedeo Caffisch (University of Zürich)  
 16.15 Beyond Ligand Flexibility: Improvement & Validation of rDock for Structure-Based Drug Design, David Morley (Enspir Discovery)  
 16.45 Structure-Based Identification of GPCR Ligands by High-Throughput Docking, Didier Rognan (University of Strasbourg)  
 17.15-18.00 Panel Discussion

### Session 6 Confidence in Safety, chaired by Saad Shakir (Drug Safety Research Unit, UK), with Barry Hardy (Douglas Connect), Sidney Kahn (PvRM), A. Leander Fontaine (Pharmaceutics) and Peter Elkin (Mayo Clinic)

14.00-15.30 Roundtable Discussion

### Session 7 Combating Drug Counterfeiting and Trafficking, chaired by Sebastian Bloch & Ulrich Meier (Sun Microsystems) with Hellmuth Broda (Sun Microsystems), Dietrich Heinicke (CADAC) and Jim McKiernan (McKiernan Associates)

16.00-18.00 Panel Presentation & Discussion

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**November 10, Morning**

**Session 8** **Applying Complex Systems & Organisational Development Approaches to Life Science Product Development & Drug Safety Decisions**, chaired by Jim Cook (Volutio) and Barry Hardy (Douglas Connect), with David Snowden (The Cynefin Centre), Adam Filler (Denison Europe) and Thomas Kell (Heidrick & Struggles)

09.00-12.30 Discussion (Coffee Break 10.30 -11.00)

**Session 9** **Drug Discovery Innovation, chaired by Alan Gibbs (Johnson & Johnson)**

08.30 Overview & Goals, Barry Hardy (Douglas Connect)

08.40 Chair's Introductory Remarks, Alan Gibbs

09.00 Metabolomics for White Biotechnology, Lars M.Blank, (University of Dortmund & Institute for Analytical Sciences)

09.30 Analysis Based on Molecular Diversity, Steve Boyer (IBM)

10.00 Analytical Strategies for the Identification of Biomarkers in Biological Fluids Gérard Hopfgartner (University of Geneva)

10.30 Coffee Break

11.00 A New Clustering Algorithm for General Metric Spaces, Alan Gibbs (Johnson & Johnson)

11.30 Biosensor Platform Based on Magnetic Nano-Beads, Jeroen H. Nieuwenhuis (Philips Research)

12.00-13.00 Panel Discussion

**Session 10** **Applications of Machine Learning & Graph Mining in Drug Discovery, chaired by Stefan Kramer (Techn.Univ.München)**

08.40 Chair's Introductory Remarks, Stefan Kramer

09.00 Graph-Theoretic Procedures for Searching Databases of Molecular Structures, Peter Willett (University of Sheffield)

09.30 Lazy-Structure-Activity-Relationships (Lazar) for the in-silico Prediction of Chemical Carcinogenicity, Christoph Helma (University of Freiburg)

10.00 Finding Discriminative Substructures Using Elaborate Chemical Representation, Joost N. Kok (Leiden University)

10.30 Coffee Break

11.00 Alignment-free Potential Pharmacophore - Point Descriptors for "Informed" Similarity Searching, Gisbert Schneider (Johann Wolfgang Goethe-University)

11.30 Mining of Molecular Fragments with Wildcards, Michael Berthold (Univ. Konstanz)

12.00-13.00 Panel Discussion

**Session 11** **Computational Biochemistry, chaired by Alessandro Curioni (IBM Zürich Research Ctr)**

08.40 Overview & Goals, Barry Hardy (Douglas Connect)

08.50 Chair's Introductory Remarks, Alessandro Curioni

09.00 On the Art of Computing the Infra Red Spectra of Molecules in the Condensed Phase, Paul Tavan (University of Munich)

09.30 Application of Hybrid QM/MM Methods to the Simulation of Biological Systems, Ursula Roethlisberger (Swiss Federal Institute of Technology, Lausanne)

10.00 Kinetic Isotope Effects for Enzyme-Catalysed Methyl Transfer, Ian Williams (University of Bath)

10.30 Coffee Break

11.00 Determination of the Catalytic Reaction Pathways in Urate Oxidase Using Quantum Chemistry Tools, Gerald Monard (Université Henri Poincaré. Nancy)

11.30 The Role of Quantum Mechanics in Structure-Based Drug Design, Ken Merz (University of Florida)

12.00-13.00 Panel Discussion

**Abstracts can be seen on <http://innovationwell.net> or <http://echeminfo.com>**

## InterAction Meeting 2005, Basel

**November 10, Afternoon**

**Session 12 Knowledge-based Intellectual Property Management, Auditing and Investment, chaired by Ronald Layden (Venture Valuation), with Rudolf Gygax (Novartis Venture Fund), Gerard Farmer (Alfomec International Regulatory Consultants), Antonino Cattaneo (Lay Line Genomics) and Stefan Odenthal (Arthur D. Little)**

14.00 Chair's Introductory Remarks, Ronald Layden

14.10 Discussion

15.30 Coffee Break

16.00-17.30 Discussion

**Session 13 Web-based Services in Drug Design, chaired by Kim Henrick (European Bioinformatics Institute)**

13.50 Overview & Goals, Barry Hardy (Douglas Connect)

14.00 Chair's Introductory Remarks, Kim Henrick

14.10 The Representation of Chemical Structures and Its Application to Property Prediction, Johann Gasteiger, (Uni. Erlangen-Nürnberg)

14.40 Investigating Chemical Trends in the Context of Ligand-Protein Complexes by Using Online Data Analysis Directly on the Web, Dimitris Dimitropoulos, (European Bioinformatics Institute)

15.10 Open Archives as a Route for the Capture, Dissemination & Access to Chemical Information, Simon Coles (Univ. Southampton)

15.40 Coffee Break

16.10 Identification of Biological Units in Protein Crystals, Eugene Krissinel (European Bioinformatics Institute)

16.40 SWISS-MODEL Server & Repository: Web-based Ressources for Comparative Protein Structure Modeling and their Application in Drug Discovery, Torsten Schwede (University of Basel)

17.10-18.00 Panel Discussion

**Session 14 Biosensors and Nanopores, chaired by Nick Quirke (Imperial College, London)**

14.00 Overview & Goals, Barry Hardy (Douglas Connect)

14.10 Chair's Introductory Remarks, Nick Quirke

14.20 Continuous-Flow Electrophoresis, IEF and ITP on Chip, Joachim Franzke (Inst. for Analytical Sciences Dortmund and Berlin)

14.50 Microfluidic Systems for Controlled Production of Small Molecules & Nanoparticles, Andrew de Mello (Imperial College, London)

15.20 Coffee Break

15.45 Simulating Nanoflows, Nick Quirke (Imperial College, London)

16.15 Thermophoresis Between Solids: A Molecular Dynamics Study of Gold Nanoparticles Confined and Thermally Driven through Carbon Nanotubes, Jens Walther (ETH-Zürich)

16.45-17.30 Panel Discussion

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