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Collaborative Computational Technologies for Biomedical Research

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Collaborative Computational Technologies For Biomedical Research

Lee Harland, Mark Forster



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Collaborative Computational Technologies for Biomedical Research Sean Ekins, Maggie A. Z. Hupcey, Antony J. Williams, 2011-08-04 Methods Processes and Tools for Collaboration The time has come to fundamentally rethink how we handle the building of knowledge in biomedical sciences today This book describes how the computational sciences have transformed into being a key knowledge broker able to integrate and operate across divergent data types Bryn Williams Jones Associate Research Fellow Pfizer The pharmaceutical industry utilizes an extended network of partner organizations in order to discover and develop new drugs however there is currently little guidance for managing information and resources across collaborations Featuring contributions from the leading experts in a range of industries Collaborative Computational Technologies for Biomedical Research provides information that will help organizations make critical decisions about managing partnerships including Serving as a user manual for collaborations Tackling real problems from both human collaborative and data and informatics perspectives Providing case histories of biomedical collaborations and technology specific chapters that balance technological depth with accessibility for the non specialist reader A must read for anyone working in the pharmaceuticals industry or academia this book marks a major step towards widespread collaboration facilitated by computational technologies

Computational Toxicology Sean Ekins, 2018-02-13 Dieses Buch ist ein wichtiges Referenzwerk für Toxikologen in vielen Bereichen und bietet eine umfassende Analyse molekularer Modellansätze und Strategien der Risikobewertung von pharmazeutischen und Umweltchemikalien Zeigt was mit rechnergestützter Toxikologie aktuell erreicht werden kann und wirft einen Blick auf zukünftige Entwicklungen Gibt Antworten zu Themen wie Datenquellen Datenpflege Behandlung Modellierung und Interpretation kritischer Endpunkte im Hinblick auf Gefahrenbewertungen im 21. Jahrhundert Bündelt herausragende Konzepte und das Wissen führender Autoren in einem einzigartigen Referenzwerk Untersucht detailliert QSAR Modelle Eigenschaften physiochemischer Arzneistoffe strukturbasiertes Drug Targeting die Bewertung chemischer Mischungen und Umweltmodelle Behandelt zusätzlich die Sicherheitsbewertung von Verbraucherprodukten und den Bereich chemische Abwehr und bietet Kapitel zu Open Source Toxikologie und Big Data

Recording Science in the Digital Era Cerys Willoughby, 2019-07-15 For most of the history of scientific endeavour science has been recorded on paper In this digital era however there is increasing pressure to abandon paper in favour of digital tools Despite the benefits there are barriers to the adoption of such tools not least their usability As the relentless development of technology changes the way we work we need to ensure that the design of technology not only overcomes these barriers but facilitates us as scientists and supports better practice within science This book examines the importance of record keeping in science current record keeping practices and the role of technology for enabling the effective capture reuse sharing and preservation of scientific data Covering the essential areas of electronic laboratory notebooks ELNs and digital tools for recording scientific data including an overview of the current data

management technology available and the benefits and pitfalls of using these technologies this book is a useful tool for those interested in implementing digital data solutions within their research groups or departments This book also provides insight into important factors to consider in the design of digital tools such as ELNs for those interested in producing their own tools Finally it looks at the role of current technology and then considers how that technology might develop in the future to better support scientists in their work and in capturing and sharing the scientific record

In vivo Models for Drug Discovery

José Miguel Vela,Rafael Maldonado,Michel Hamon,2014-07-31 This one stop reference is the first to present the complete picture covering all relevant organisms from single cells to mammals as well as all major disease areas including neurological disorders cancer and infectious diseases Addressing the needs of the pharmaceutical industry this unique handbook adopts a broad perspective on the use of animals in the early part of the drug development process including regulatory rules and limitations as well as numerous examples from real life drug development projects After a general introduction to the topic the expert contributors from research driven pharmaceutical companies discuss the basic considerations of using animal models including ethical issues The main part of the book systematically surveys the most important disease areas for current drug development from cardiovascular to endocrine disorders and from infectious to neurological diseases For each area the availability of animal models for target validation hit finding and lead profiling is reviewed backed by numerous examples of both successes and failures among the use of animal models The whole is rounded off with a discussion of perspectives and challenges Key knowledge for drug researchers in industry as well as academia

Managing Scientific Information and Research Data Svetla Baykoucheva,2015-07-14 Innovative technologies are changing the way research is performed preserved and communicated Managing Scientific Information and Research Data explores how these technologies are used and provides detailed analysis of the approaches and tools developed to manage scientific information and data Following an introduction the book is then divided into 15 chapters discussing the changes in scientific communication new models of publishing and peer review ethics in scientific communication preservation of data discovery tools discipline specific practices of researchers for gathering and using scientific information academic social networks bibliographic management tools information literacy and the information needs of students and researchers the involvement of academic libraries in eScience and the new opportunities it presents to librarians and interviews with experts in scientific information and publishing Promotes innovative technologies for creating sharing and managing scientific content Presents new models of scientific publishing peer review and dissemination of information Serves as a practical guide for researchers students and librarians on how to discover filter and manage scientific information Advocates for the adoption of unique author identifiers such as ORCID and ResearcherID Looks into new tools that make scientific information easy to discover and manage Shows what eScience is and why it is becoming a priority for academic libraries Demonstrates how Electronic Laboratory Notebooks can be used to record store share and manage research data Shows how social media and the new

area of Altmetrics increase researchers visibility and measure attention to their research Directs to sources for datasets Provides directions on choosing and using bibliographic management tools Critically examines the metrics used to evaluate research impact Aids strategic thinking and informs decision making *Grid and Cloud Computing: Concepts and Practical Applications* F. Carminati, L. Betev, A. Grigoras, 2016-05-31 The distributed computing infrastructure known as the Grid has undoubtedly been one of the most successful science oriented large scale IT projects of the past 20 years It is now a fully operational international entity encompassing several hundred computing sites on all continents and giving access to hundreds of thousands of CPU central processing unit cores and hundreds of petabytes of storage all connected by robust national and international scientific networks It has evolved to become the main computational platform many scientific communities This book presents lectures from the Enrico Fermi International School of Physics summer school Grid and Cloud computing Concepts and Practical Applications held in Varenna Italy in July 2014 The school aimed to cover the conceptual and practical aspects of both the Grid and Cloud computing The proceedings included here are divided into eight chapters with chapters 1 2 3 and 8 covering general applications of Grid and Cloud computing in various scientific fields while chapters 4 5 6 and 7 discuss specific technical areas of Grid and Cloud structures The book will be of interest to all those whose work involves the use of the Grid or Cloud computing **Handbook of Human Computation** Pietro Michelucci, 2013-12-04 This volume addresses the emerging area of human computation The chapters written by leading international researchers explore existing and future opportunities to combine the respective strengths of both humans and machines in order to create powerful problem solving capabilities The book bridges scientific communities capturing and integrating the unique perspective and achievements of each It coalesces contributions from industry and across related disciplines in order to motivate define and anticipate the future of this exciting new frontier in science and cultural evolution Readers can expect to find valuable contributions covering Foundations Application Domains Techniques and Modalities Infrastructure and Architecture Algorithms Participation Analysis Policy and Security and the Impact of Human Computation Researchers and professionals will find the Handbook of Human Computation a valuable reference tool The breadth of content also provides a thorough foundation for students of the field The Semantic Web - ISWC 2013 Harith Alani, Lalana Kagal, Achille Fokoue, Paul Groth, Chris Biemann, Josiane Xavier Parreira, Lora Aroyo, Natasha Noy, Chris Welty, Krzysztof Janowicz, 2013-10-16 The two volume set LNCS 8218 and 8219 constitutes the refereed proceedings of the 12th International Semantic Web Conference ISWC 2013 held in Sydney Australia in October 2013 The International Semantic Web Conference is the premier forum for Semantic Web research where cutting edge scientific results and technological innovations are presented where problems and solutions are discussed and where the future of this vision is being developed It brings together specialists in fields such as artificial intelligence databases social networks distributed computing Web engineering information systems human computer interaction natural language processing and the social sciences Part 1 LNCS 8218

contains a total of 45 papers which were presented in the research track They were carefully reviewed and selected from 210 submissions Part 2 LNCS 8219 contains 16 papers from the in use track which were accepted from 90 submissions In addition it presents 10 contributions to the evaluations and experiments track and 5 papers of the doctoral consortium

Collaborative Innovation in Drug Discovery Rathnam Chaguturu, 2014-03-28 Can academia save the pharmaceutical industry The pharmaceutical industry is at a crossroads The urgent need for novel therapies cannot stem the skyrocketing costs and plummeting productivity plaguing R D and many key products are facing patent expiration Dr Rathnam Chaguturu presents a case for collaboration between the pharmaceutical industry and academia that could reverse the industry's decline Collaborative Innovation in Drug Discovery Strategies for Public and Private Partnerships provides insight into the potential synergy of basing R D in academia while leaving drug companies to turn hits into marketable products As Founder and CEO of iDDPartners focused on pharmaceutical innovation Founding president of the International Chemical Biology Society and Senior Director Discovery Sciences SRI International Dr Chaguturu has assembled a panel of experts from around the world to weigh in on issues that affect the two driving forces in medical advancement Gain global perspectives on the benefits and potential issues surrounding collaborative innovation Discover how industries can come together to prevent another Pharma Cliff Learn how nonprofits are becoming the driving force behind innovation Read case studies of specific academia pharma partnerships for real life examples of successful collaboration Explore government initiatives that help foster cooperation between industry and academia Dr Chaguturu's thirty five years of experience in academia and industry managing new lead discovery projects and forging collaborative partnerships with academia disease foundations nonprofits and government agencies lend him an informative perspective into the issues facing pharmaceutical progress In Collaborative Innovation in Drug Discovery Strategies for Public and Private Partnerships he and his expert team provide insight into the various nuances of the debate

Open Source Software in Life Science Research Lee Harland, Mark Forster, 2012-10-31 The free open source approach has grown from a minor activity to become a significant producer of robust task orientated software for a wide variety of situations and applications To life science informatics groups these systems present an appealing proposition high quality software at a very attractive price Open source software in life science research considers how industry and applied research groups have embraced these resources discussing practical implementations that address real world business problems The book is divided into four parts Part one looks at laboratory data management and chemical informatics covering software such as Bioclipse OpenTox ImageJ and KNIME In part two the focus turns to genomics and bioinformatics tools with chapters examining GenomicsTools and EBI Atlas software as well as the practicalities of setting up an omics platform and managing large volumes of data Chapters in part three examine information and knowledge management covering a range of topics including software for web based collaboration open source search and visualisation technologies for scientific business applications and specific software such as DesignTracker

and Utopia Documents Part four looks at semantic technologies such as Semantic MediaWiki TripleMap and Chem2Bio2RDF before part five examines clinical analytics and validation and regulatory compliance of free open source software Finally the book concludes by looking at future perspectives and the economics and free open source software in industry Discusses a broad range of applications from a variety of sectors Provides a unique perspective on work normally performed behind closed doors Highlights the criteria used to compare and assess different approaches to solving problems

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