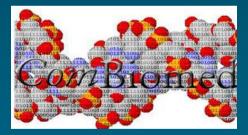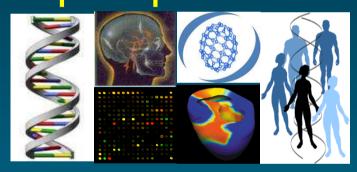Dr. Guillermo López-Campos
Medical NanoBioInformatics Dept.
Institute of Health "Carlos III"
Madrid, SPAIN

Nanoinformatics from the Biomedical Informatics perspective

November 4th, 2010
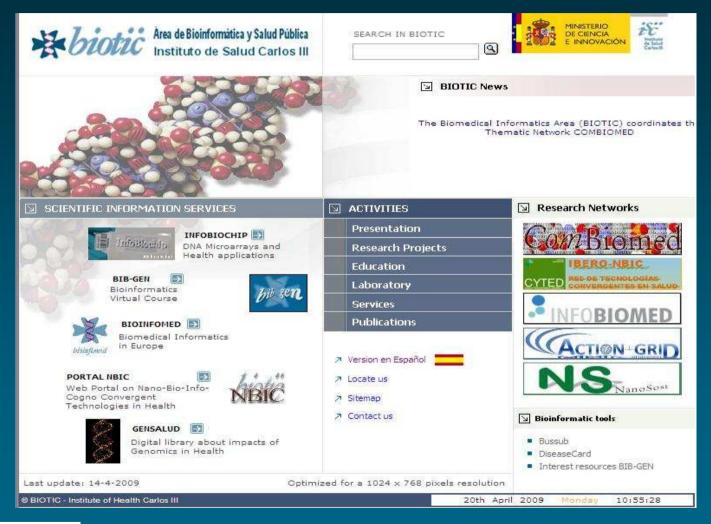Nanoinformatics 2010
Arlington

Outline

- Presentation
- Introduction
- Experiences from Biomedical informatics & reusable tools
- Education
- Ongoing works in Nanoinformatics
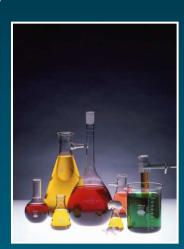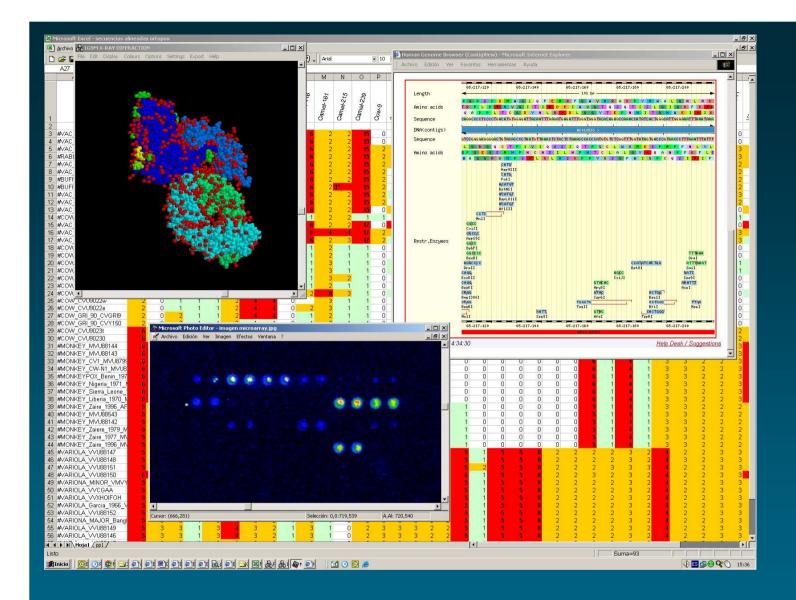- Final remarks

Presentation

http://biotic.isciii.es/

Institute of Health "Carlos III"
Ministry of Science and Innovation

- Public Research Institute
- Scientific and technological support body of the Spanish National Health System
- Competences in:
  - Epidemiology, Public health laboratories
  - Cell therapy and Regenerative Medicine
  - Biomedical research funding and coordination
  - Cooperative research networks
  - National School of Public Health, Health Sciences Library
  - New technologies – Biomedical Informatics and genomics, Nanoinformatics, Telemedicine
  - Pathology oriented research centers (cancer, cardiovascular)
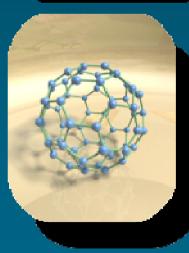
Introduction

New trends towards personalised Medicine

- Genomic (molecular, personalised) medicine

- **Regenerative** medicine/tissue engineering seeks to develop functional cell, tissue, and organ substitutes to repair, replace or enhance biological function that has been lost due to congenital abnormalities, injury, disease, or aging.   NIH Definition, NIBIB, June 2004

- NanoMedicine – Use of nanoscale tools and components for the diagnosis, prevention and treatment of diseases and for understanding their pathophysiology.

    European Science Foundation, Nov. 2005

STEM CELL ANTHOLOGY

Main role of Informatics in Regenerative and Nano Medicine

- **Data on patient**

  - (in ePHR): Data on loss of function, status of immuno-compatibility, tissue characteristics, regeneration by using stem cells or the own tissue, result of application

  - Genomic data for both genotypic classification and phenotypic characterisation.

  - Next generation sequencing - whole human genome. How to access the complete genome sequence so that it can be part of the EMR.

  - Data about the family history of the donor for stem cell therapies

- **Data on biomaterials**:

  - Tissue, material or nano-particle, results, relevant references about the topic

  - It might be chemical information such as molecules, or physical information such as electromagnetic waves, optical information, electrical signal, acoustic waves, mechanical information (mass, speed, acceleration…).
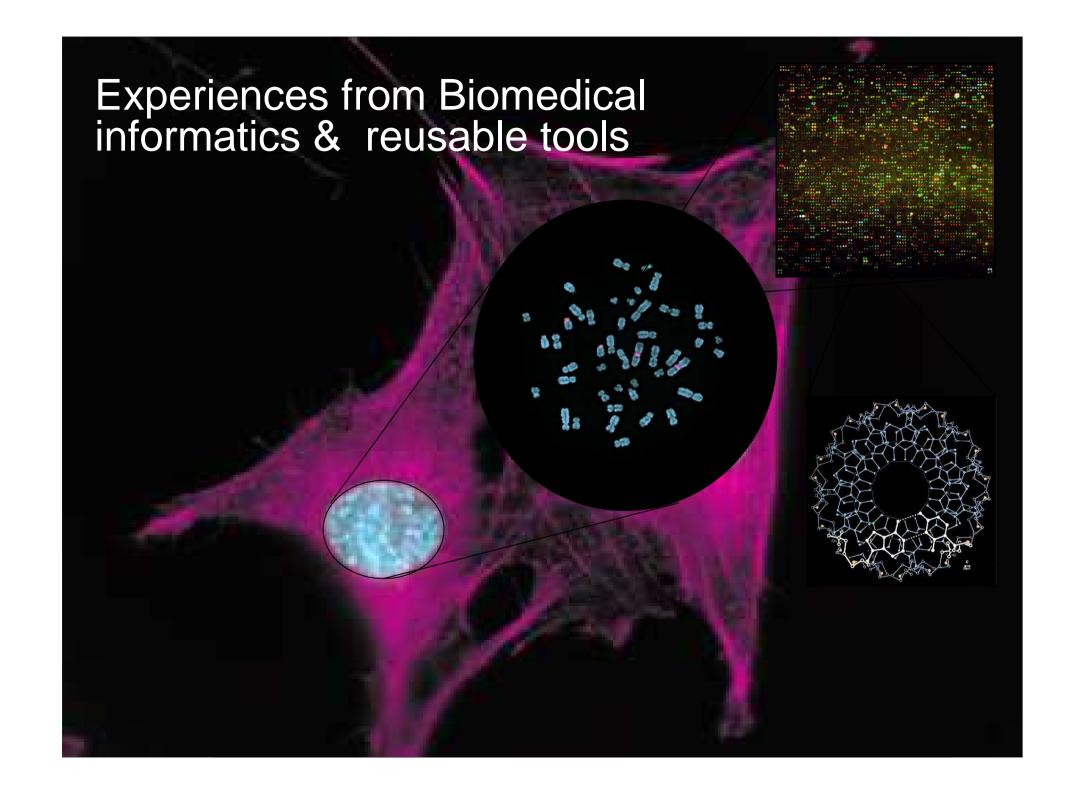
- **Data on biological processes**

  - Metabolic pathways, genes, gene expression, protein structure and post-translational changes.

  - Genes, hormone and growth factors involved in disease and in regenerative process.

  - Optimization of appropriate vectors for specific cell types, including stem and progenitor cells and their use in bioengineered scaffolds and implants;
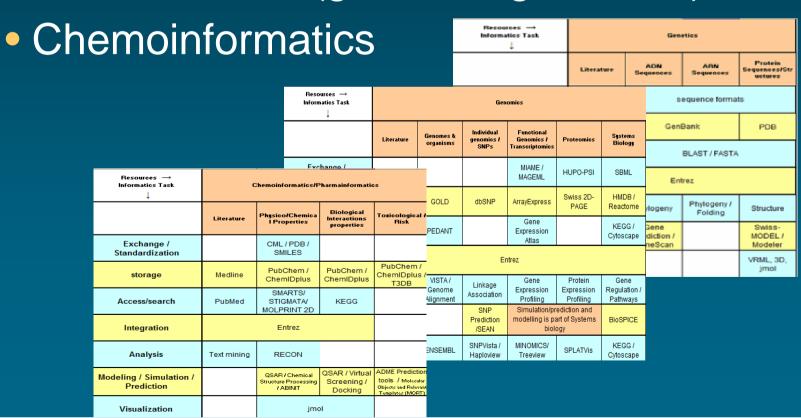
Biomedical Informatics

- Informatics is the science of information

- Information is data plus meaning

- Biomedical informatics is the science of information in the context of biomedicine.

- Informaticians study information (data + meaning).

- Thus, BMI practitioners must understand the context or domain (biomedicine).

- BMI is different¡¡ - The semantic gap between data and meaning is larger than in other fields because biomedicine deals with systems (human beings) which are imperfect, due to evolution and do not respond to an "a priori" design, so many times it is not possible to isolate its component parts and functions.

- Bernstam EV, Smith JW, Johnson TE. (2010) "What is Biomedical Informatics". Journal of Biomedical Informatics; 43 104-110.

- Hersh W. (2009). "A Stimulus to define Informatics and Health Information Technology". BMC Medical Informatics and Decision Making. 9:24.

- Groth DP and MacKie-Mason JK. (2010) "Why an Informatics degree?" Communications of the ACM. 53 (2) 26-28

Experiences from Biomedical informatics & reusable tools

Framework for Nanoinformatics

Identify tools and applications in different fields covered by Biomedical informatics
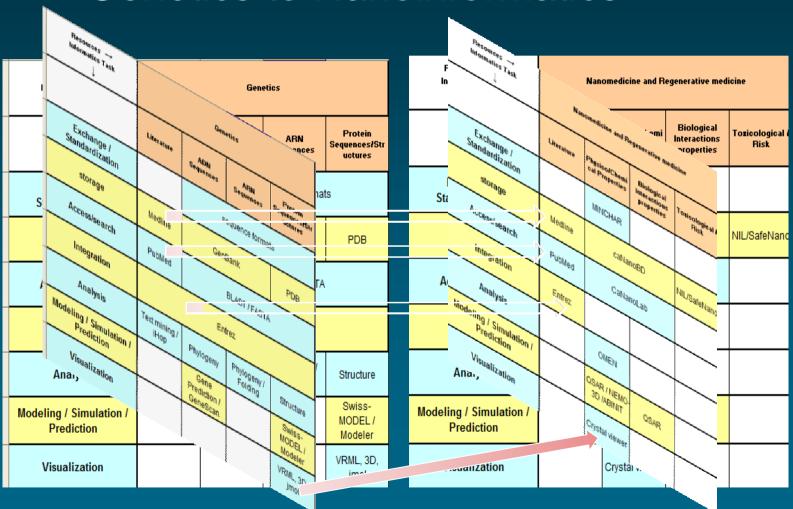
- Bioinformatics (genetics, genomics)
- Chemoinformatics

Resources → Informatics Task ↓		Genetics			
		Literature	ADN Sequences	ARN Sequences	Protein Sequences/Structures
					sequence formats
				GenBank	PDB
				BLAST / FASTA	
				Entrez	
				Phylogeny / Folding	Structure
				Gene Prediction / GeneScan	Swiss-MODEL / Modeler
					VRML, 3D, jmol

Resources → Informatics Task ↓		Genomics					
		Literature	Genomes & organisms	Individual genomics / SNPs	Functional Genomics / Transcriptomics	Proteomics	Systems Biology
Exchange /					MIAME / MAGEML	HUPO-PSI	SBML
	GOLD	dbSNP	ArrayExpress	Swiss 2D-PAGE	HMDB / Reactome
PEDANT			Gene Expression Atlas		KEGG / Cytoscape
		Entrez				
VISTA / Genome Alignment	Linkage Association	Gene Expression Profiling	Protein Expression Profiling	Gene Regulation / Pathways
SNP Prediction /SEAN	Simulation/prediction and modelling is part of Systems biology		BioSPICE
ENSEMBL	SNPVista / Haploview	MINOMICS/ Treeview	SPLATVis	KEGG / Cytoscape

Resources → Informatics Task ↓	Chemoinformatics/Pharmainformatics			
	Literature	Physico/Chemical Properties	Biological Interactions properties	Toxicological & Risk
Exchange / Standardization		CML / PDB / SMILES		
storage	Medline	PubChem / ChemIDplus	PubChem / ChemIDplus	PubChem / ChemIDplus / T3DB
Access/search	PubMed	SMARTS/ STIGMATA/ MOLPRINT 2D	KEGG	
Integration	Entrez			
Analysis	Text mining	RECON		
Modeling / Simulation / Prediction		QSAR / Chemical Structure Processing / ABINIT	QSAR / Virtual Screening / Docking	ADME Prediction tools / Molecular Objects and Relevant Templates (MORT)
Visualization		jmol		

Resources → Informatics Task ↓	Literature	Physico/Chemical Properties	Biological Interactions properties	Toxicological / Risk	Clinical effects
Data Generation – NM Synthesis					
Validation - Characterization					
Exchange/Standardization	1. NanoCollaboratory 2. ANSI NSP(American National Standards Institute's Nanotechnolovy Standards Panel) 3. ISO TC 229				
Storage	1. NBI Nanomaterial-biological interactions Knowledgebase 2. CaNanoBD			1. TOXNET	
Storage	1. TOXNET 2. MEDLINE 3. NTIS (National Technical Information Service) 4. NIOSH: CDC-Centers for Disease Control and Prevention 5. ICON EHS Database				
Portals	1. NanoForum 2. NanoHub				
Portals	1. SNN Safer Nanomaterials and Nanomanufacturing Initiative 2. National Institute for Occupational Safety and Health (NIOSH). 3. InterNano		1. SNN Safer Nanomaterials and Nanomanufacturing Initiative 2. NBI Nanomaterial-biological interactions	1. National Institute for Occupational Safety and Health (NIOSH).	
Collaboration	1. ICON International Council on Nanotechnology 2. NanoHub				
Collaboration	1. INTERNANO (National Nanomanufacturing Network(NNN)) 2. NanoMedNet 3. International nanotechology and society network 4. NBI Nanomaterial-biological interactions			1.SAFENANO: Ilustration Acknowledgement 2. NanoMedNet	
Access/Search	1. CaNanoLab				
Access/Search	1.PUBMED 2.TOXLINE 3. University of Albertas Libraries 4. NIOSH NIL: Nanoparticle Information Library			1. SAFENANO: Publication database search	
				1.TOXLINE	
Integration					
Analysis		1. Quantum Dot Lab 2. NEMO 3-D			
Modeling/Simulation		1. Hyperchem 2. Quantitative structure-activity relationship modeling (QSAR) 3. CananoBD 4. BioSensorLab 5. Quantum Dot Lab 6. HidrophobicityLab			
Prediction					
Visualization					

Mapping and identifying reusable tools in Nanoinformatics
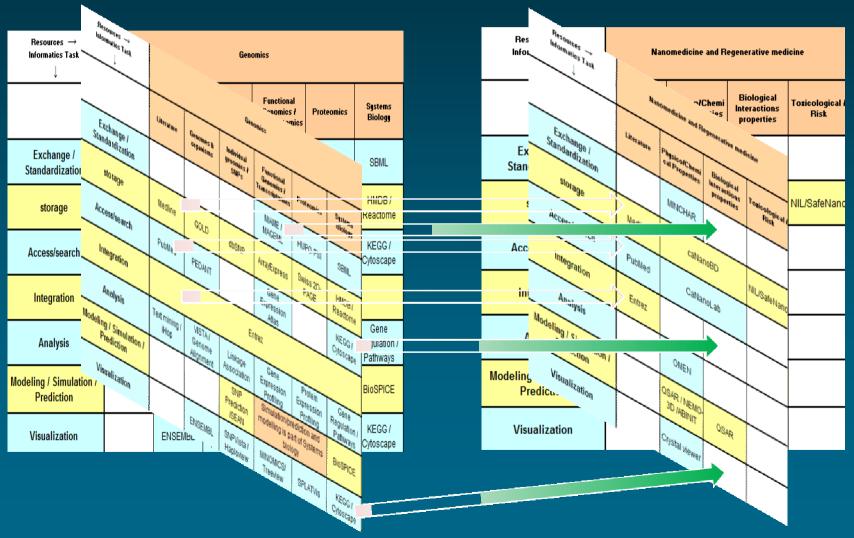
- Genetics to Nanoinformatics

Mapping and identifying reusable tools in Nanoinformatics
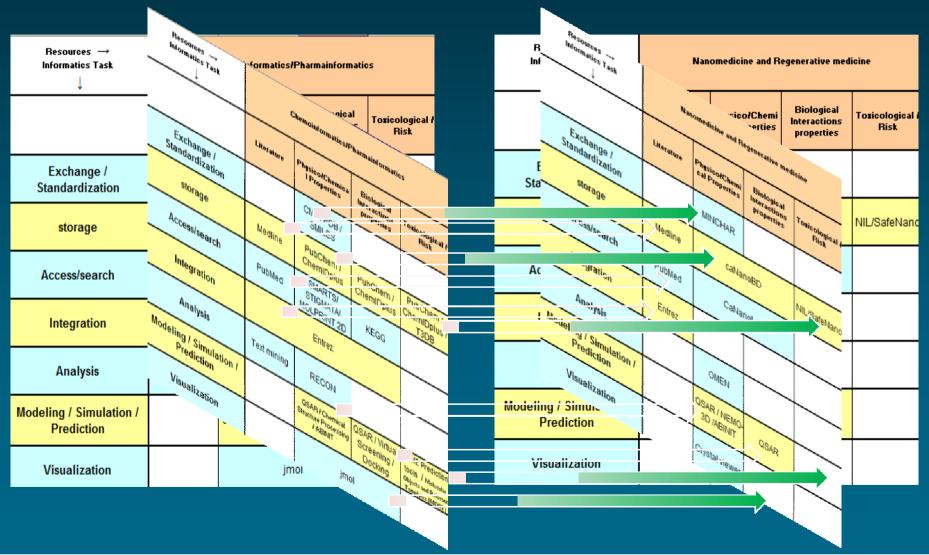
Genomics to Nanoinformatics

Mapping and identifying reusable tools in Nanoinformatics
Chemoinformatics to Nanoinformatics

Experiences from BMI

Development of Standards

- PDB (Protein Data Bank) and PDB format

- MIAME/MAGEML experience

  – Development of a set of standards for data storage, data exchange, ontologies…

  – MIAME (Minimal Information About a Microarray Experiment) describes the whole process of conducting microarray experiments

Experiences from BMI

Development of standards

- MIAME/MAGEML experience
  - Focused in 6 main areas
    - Raw data from microarray experiment
    - Final processed data for the set of reactions done in the whole experiment
    - Essential sample annotation
    - Experimental design including sample data relationships
    - Sufficient Information describing the array
    - Essential laboratory and data processing

Experiences from BMI

Development of Standards

- MIAME/MAGEML experience
  - Required by publishers as a condition to publish microarray experiments

A non-exhaustive list of journals requiring MIAME compliant data as a condition for publishing microarray based papers
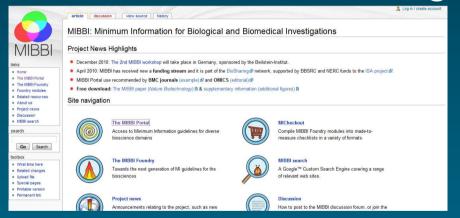
If you know of any other journals or wish to amend the below list, please email us.

- American Physiological Society journals
- Anaerobe
- Antioxidants & Redox Signaling
- Arteriosclerosis, Thrombosis and Vascular Biology
- Biochemical Journal
- Bioinformatics

  - Extensions were proposed to cover specific aspects
    - MIAME CGH, MIAME ChIP-on-Chip, MIAME Plant, MIAME TOX/Env

Experiences from BMI

Development of Standards

- MIBBI – Minimum Information for Biological and Biomedical investigations

- ISA (Investigation/Study/Assay)

Experiences from BMI

Annotation

- DAS/ENSEMBL experience
  - DAS (Distributed Annotation System). Method to integrate and visualize disparate data sources (DAS servers) in a DAS client.
  - Consists in a data exchange specification, Interaction data servers and visualization clients
  - DAS registry ensures the interoperability among DAS servers and clients around the world

Experiences from BMI

Annotation

- DAS/ENSEMBL experience
  - Originally designed for sequence annotation (ENSEMBL), different extensions are designed for other data types
  - DAS1.6E Proteins - STRUCTURES, alignments, INTERACTIONS
    - SPICE is an application for projecting protein annotations onto 3D structures (http://www.efamily.org.uk/software/dasclients/spice/)
    - DASMI is an integration portal for protein interaction data. (http://www.dasmi.de/)

Experiences from BMI
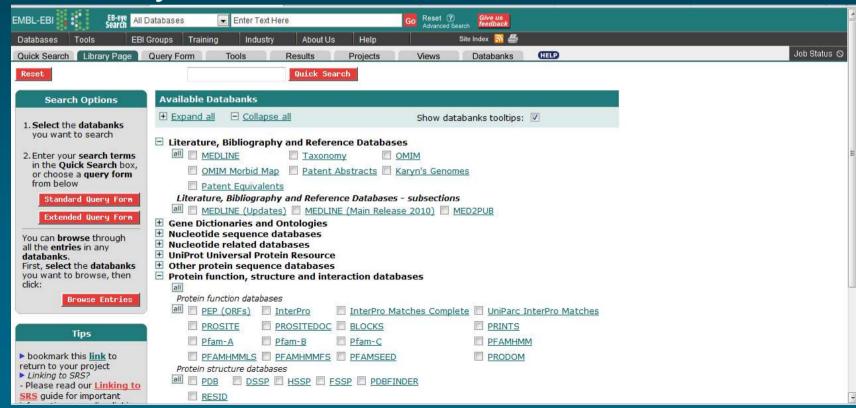
Data Integration

- SRS system
  - Integrates different databases and tools
  - Uses a single interface
  - It is possible to query simultaneously all the integrated databases
  - It's possible to integrate proprietary data with publicly available data

Experiences from BMI

Data Integration

- SRS system

Experiences from BMI
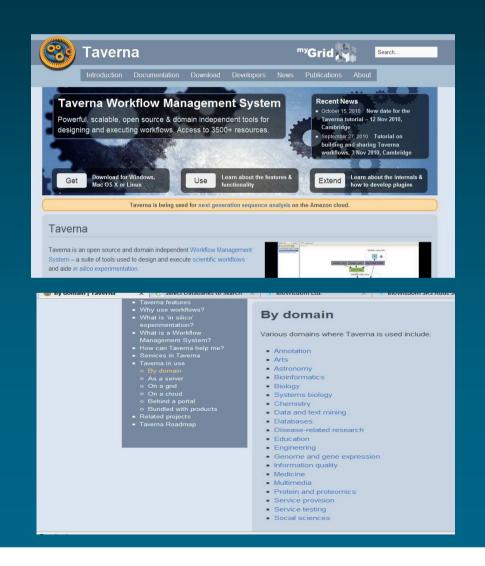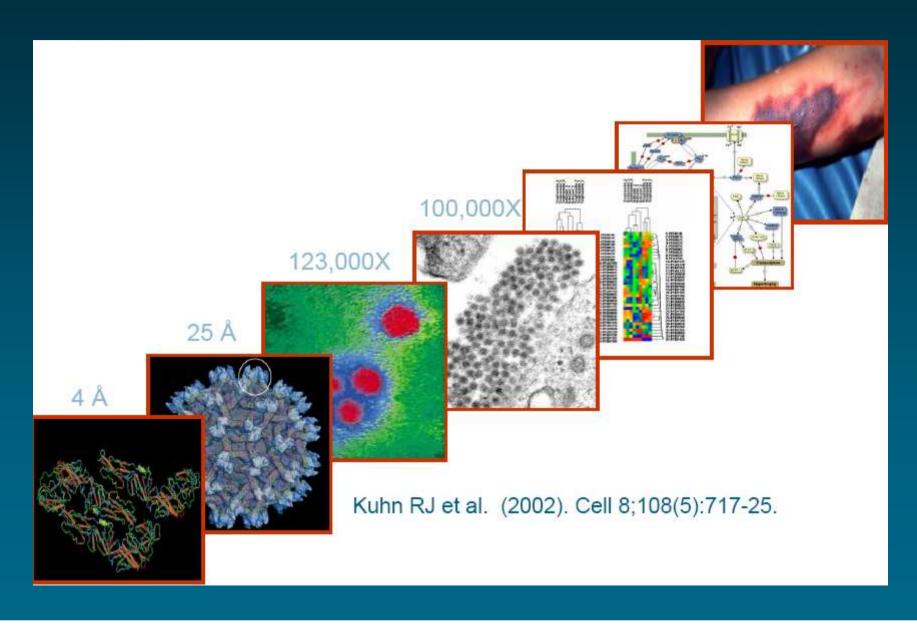
Workflows

- Taverna
  - Workflow management system
  - Extensively used in Biomedical Informatics

Experiences from BMI

Kuhn RJ et al. (2002). Cell 8;108(5):717-25.

Education

Horizontal activities
Education

Mantas J, Ammenwerth E, Demiris G, Hasman A, Haux R, Hersh W, Hovenga E, Lun KC, Marin H, Martin-Sanchez F, Wright G; IMIA Recommendations of the International Medical Informatics Association (IMIA) on Education in Biomedical and Health Informatics. First Revision. Methods Inf Med. 2010 Jan 7;49(2):105-120.

Lopez-Campos G, Lopez-Alonso V, Martin-Sanchez F. (2010) Training Health Professionals in Bioinformatics. Experiences and Lessons Learned. Methods Inf Med. 49:(3):299-30

Fernando Martin-Sanchez, 07

Ongoing work on NI

NanoSpain
Red Española de Nanotecnología

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NanoSpain: Members

Update

Nanotechnology Activities Survey in Spain

Name of the Laboratory	nBIOTIC
Department	Área de Investigación en Bioinformática Médica y Tecnologías Convergentes
Institution	Instituto de Salud Carlos III
Institution (Acronym)	ISCIII
Contact Person (e-mail)	MARTIN SANCHEZ, Fernando
Address	Ctra. Majadahonda a Pozuelo, Km. 2
Country	Spain
Phone	+34918223219
Fax	+34918223259
Website	http://biotic.isciii.es
Main Research Areas	* Nanoinformatics * Nanosafety * Nanoparticles * Nanomedicine

Participating Projects
* Action-Grid - Roadmap - Nanoinformatics - http://www.action-grid.eu/
Coordinator: Fernando Martin-Sanchez: Comisión Europea (**200.000 €**)

* NanoSost - Hacia una nanotecnologia segura, responsable y sostenible
Coordinator: Fernando Martin-Sanchez: MICINN (**80.000 €**)

* Ibero-NBIC - Red Iberoamericana de Tecnologóías Convergentes (NBIC) en Salud
Coordinator: Fernando Martin-Sanchez: CYTED (**80.000 €**)

Three more relevant publications within 20...
* López-Alonso Victoria; Hermosilla-Gimeno Isab...
GRID: assessing the impact o - Annual Symposiu...

* 3. Fernando Martín-Sanchez, Victoria López-A...
Knowledge Management for Nanoinfor - "Knowled...
Jain (Eds). KES 2008 LNAI Volume 5178/2008 Se...

* 2. Altman RB, Balling R, Brinkley JF, Coiera E...
Martin-Sanchez F, Mihalas GI, - Methods Inf Med...

Instruments and equipment available
* Robot Spotter para fabricación de microarrays
* Escaner 2 laser para revelado de microarrays
* Escaner 4 laser para revelado de microarrays

funding 2006-2009 (In thousand Euro)

	MEC/MITYC	CC.AA...			
2006	0	0			
2007	0	0			
2008	28000	0	100000	0	120000
2009	56000	0	100000	20000	176000

NANOMED
SPAIN
PLATAFORMA ESPAÑOLA DE NANOMEDICINA

Misión y Objetivos | Organización | Participantes | Documentos | Enlaces | Actualidad

🔍 **Buscador** | buscar... | ok

Instituto de Salud Carlos III

Bioinformatica Médica y Tecn. Convergentes (NBIC)

El Área de Bioinformática Médica y Tecnologías Convergentes se creó en 1998, como respuesta a la creciente necesidad del Instituto de Salud Carlos III de formar un equipo que se encargara de investigar y desarrollar los modelos y métodos de información que facilitaran la comprensión y el uso de los nuevos enfoques de la medicina basada en la genómica. Entre sus funciones actuales destaca la de facilitar el conocimiento de las nuevas tecnologías (NBIC, Nano-Bio-Info-Cogno-Tecnologías) y su convergencia para su aplicación en la investigación, práctica clínica y salud pública, desde la perspectiva del tratamiento integrado de la información biomédica.

Las líneas de trabajo actuales de la Unidad que se centran en las Nanotecnologías y Tecnologías Convergentes (NBIC) EN SALUD son:

Proyectos Nacionales
▪ BIOTIC-NBIC: Convergencia de tecnologías bioinformáticas basadas en microarrays y su aplicación en el campo de las enfermedades infecciosas.
▪ PROYECTO ESTRATÉGICO SINGULAR NANOSOST: Hacia una nanotecnología sostenible, responsable y segura. En la que el área de Bioinformática Médica y Tecn. Convergentes (nBIOTIC) tiene como objetivo el desarrollo de una metodología para la elaboración de un sistema de gestión del riesgo frente a nanopartículas, que garantice un nivel permanente de

...Informatics between the European Union,
...er para la Comisión Europea en el que se
...as sinergias con la Informática

...e se incluyen biólogos, farmacéuticos,
...ortante actividad de asesoría técnica y de
...co sobre los siguientes temas:
...CNOLOGÍAS CONVERGENTES (NBIC) EN
...cional de Salud, lleva a cabo los
...lógica y prospectiva, -asesoría
...onsable de la gestión del laboratorio de

http://biotic.isciii.es

IBERO-NBIC
RED DE TECNOLOGÍAS CONVERGENTES EN SALUD
CYTED

Ibero-American network of Converging Technologies NBIC in Health
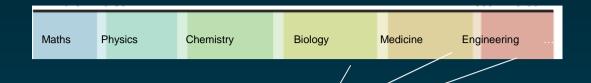
- **Objetive:** The objective is to contribute to the creation of a wide community of scientists and technologists in the Iberoamerican area who know, develop and assess applications of Convergence of NBIC Technologies in health from a multidisciplinary and global integration perspective. The aim is to promote synergies between countries, disciplines and methodologies, paying special attention to the social impact of these new developments.
- **Finantial:** CYTED
- **Duration:** 2009-2012
- **Partners:** 11 reseach groups of 7 diferents countries.

SPECTRUM OF BIOMEDICAL KNOWLEDGE IN INTERNET

Maths | Physics | Chemistry | Biology | Medicine | Engineering | …

RSS feeds

BIKMAS SYSTEM
(Biomedical
Information
Knowledge
Management
Antena
System)

Archive of topics

USES (several formats and applications)

Webs (Combiomed, NanoSost)

Courses (Lain Entralgo, ISCIII)

News (for I+S, Ibero-NBIC)

Scientific Documents (White Paper, artículos)

biotic Àrea de Bioinformàtica y Salud Pública
Instituto de Salud Carlos III

BIKMAS2.0

BioTic

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Archivo Editar Ver Historial Marcadores Herramientas Ayuda

http://10.15.60.216:8080/web/bioinfo/nanomedicina

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Navigation

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- CONVERGENT TECHNOLOGIES
- BIOMEDICAL INFORMATICS
- HORIZONTAL ASPECTS

RSS NANOMEDICINE

NANO letters
6/28/09 11:46 PM
Observation of Optical Spin Symmetry Breaking in Nanoapertures
6/25/09 3:15 PM

Nano Letters, Volume 0, Issue 0, Articles ASAP (As Soon As Publishable).

Propulsion of Gold Nanoparticles with Surface Plasmon Polaritons: Evidence of Enhanced Optical Force from Near-Field Coupling between Gold Particle and Gold Film

ACS Nano
6/28/09 11:48 PM
Spin Gapless Semiconductor–Metal–Half-Metal Properties in Nitrogen-Doped Zigzag Graphene Nanoribbons
6/25/09 3:17 PM

ACS Nano, Volume 0, Issue 0, Articles ASAP (As Soon As Publishable).

Fabrication, Self-Assembly, and Properties of Ultrathin AlN/GaN Porous Crystalline Nanomembranes: Tubes, Spirals, and Curved Sheets

Terminado

News - RSS feeds - any format

Blogs

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diseasecard

Welcome to DiseaseCard Tool

>Search for a disease

| | Submit |

○ by disease name ○ by omim number ○ by gene symbol

>List of available diseases

>DiseaseCard Forum

DiseaseCard is an information retrieval tool for accessing and integrating genetic and medical information for health applications. Resorting to this integrated environment, clinicians are able to access and relate diseases data already available in the Internet, scattered along multiple databases. Diseasecard was developed by University of Aveiro Bioinformatics Group in collaboration with the Institute of Health Carlos III Bio-Computing and Public Health Unit. The use of DiseaseCard is subject to the following disclaimer and warning.

Endorsement:

diseasecard

Disease Forum

Collapse Disease Nodes

Cystic fibrosis
- References
- Pathology
- Drugs
- Clinical Trials
- Genetic Tests and Labs
- Pharmaco. Research
- Disorders and Mutations
- Polymorphism
- Nucleotide Sequence
- Chromosomal Local.
- Gene
- Nomenclature
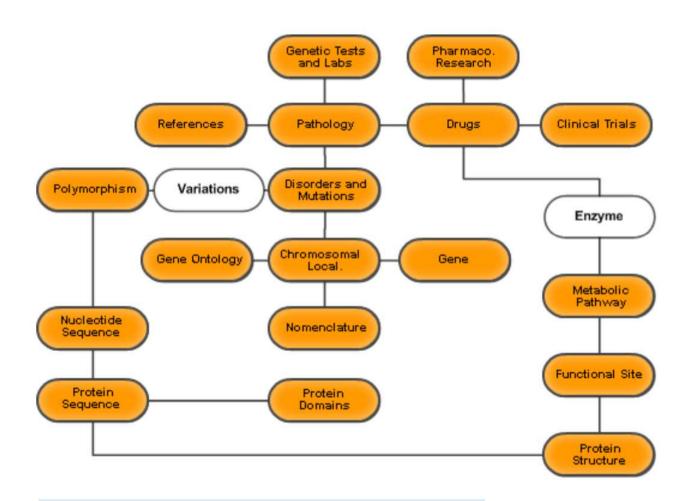- Enzyme
- Metabolic Pathway
- Functional Site
- Protein Structure
- Protein Sequence
- Protein Domains
- Gene Ontology
- Variations

Overview
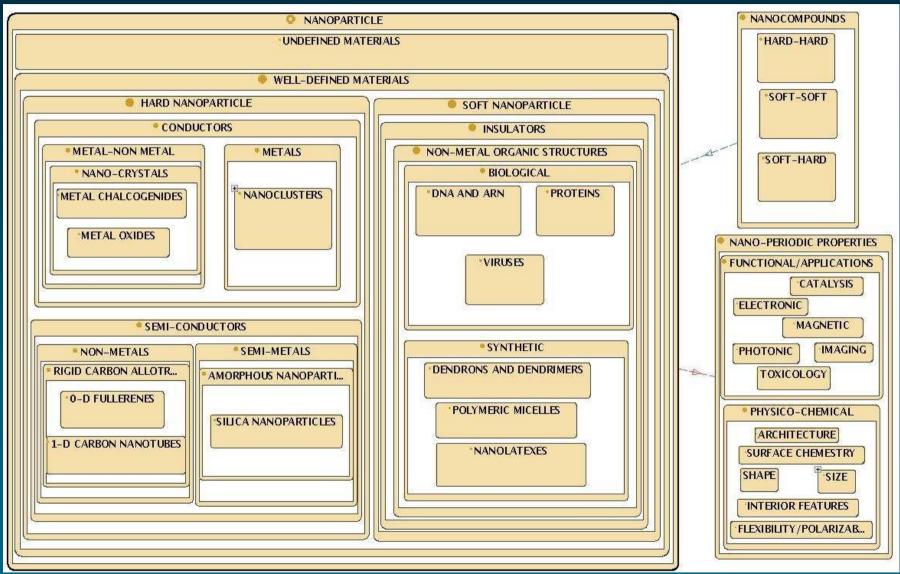
Disease omim code 219700

Other Names	• Cystic fibrosis lung disease, modifier of
	• Cystic fibrosis

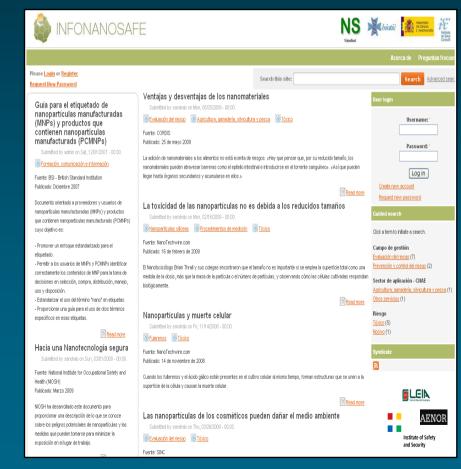# D. TOMALIA'S PERIODIC CLASSIFICATION NANONTOLOGY

D. Tomalia "In quest of a systematic framework for unifying and defining nanoscience". J Nanopart Res (2009) 11:1251–1310

INFONANOSAFE - Communication of the risk in the context of the nanotechnology

Objectives

- To spread news, guides and good practices relative to the safety in the use of the nanotechnology.

- To be the website of reference into Spanish on nanosafety.
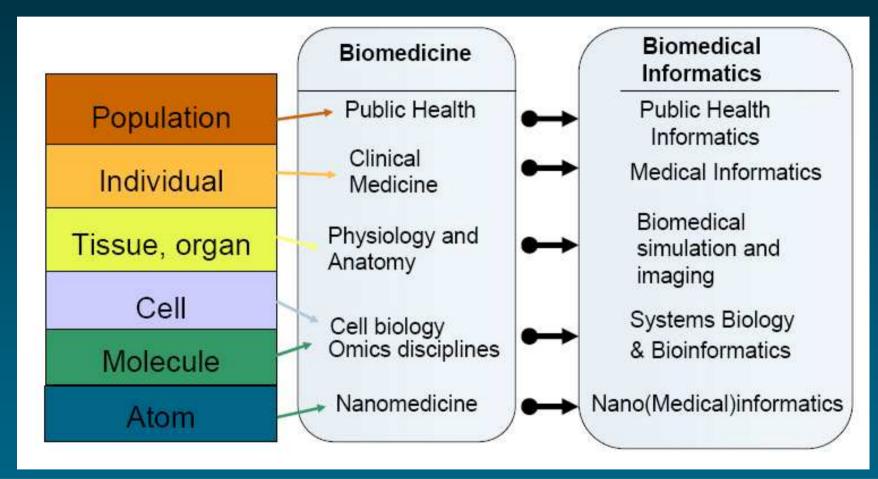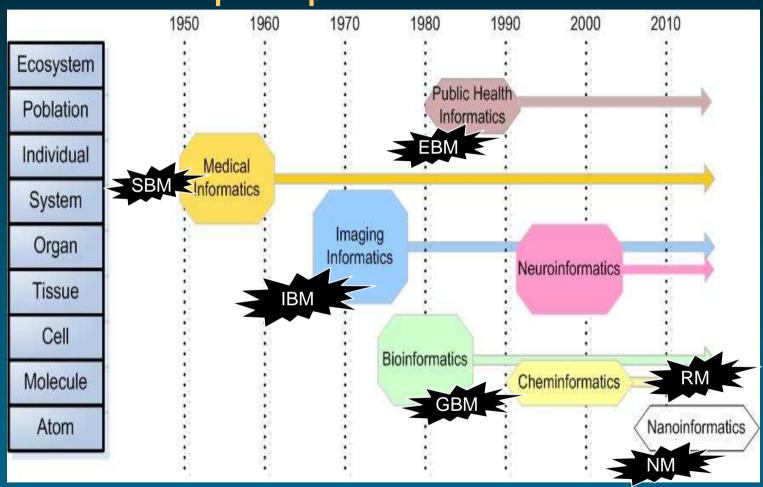
Conclusions

Final remark:
BMI - from particle to population

Altman RB, Balling R, Brinkley JF, Coiera E, Consorti F, Dhansay MA, Geissbuhler A, Hersh W, Kwankam SY, Lorenzi NM, Martin-Sanchez F, Mihalas GI, Shahar Y, Takabayashi K, Wiederhold G. "Commentaries on Informatics and medicine: from molecules to populations". Methods Inf Med. 2008;47(4):296-317. PMID: 18690363

Final remark: a chronological perspective for BMI

López-Alonso Victoria; Hermosilla-Gimeno Isabel; Lopez-Campos Guillermo; Maojo Victor; Martin-Sanchez Fernando J. "Action GRID: assessing the impact of Nanotechnology on Biomedical Informatics". AMIA Annual Symposium Proceedings 2008,

Medical NanoBioinformatics Dept.
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THANK YOU FOR
YOUR ATTENTION !!!