Departamento Inteligencia Artificial

Nanoinformatics: research and education

Víctor Maojo

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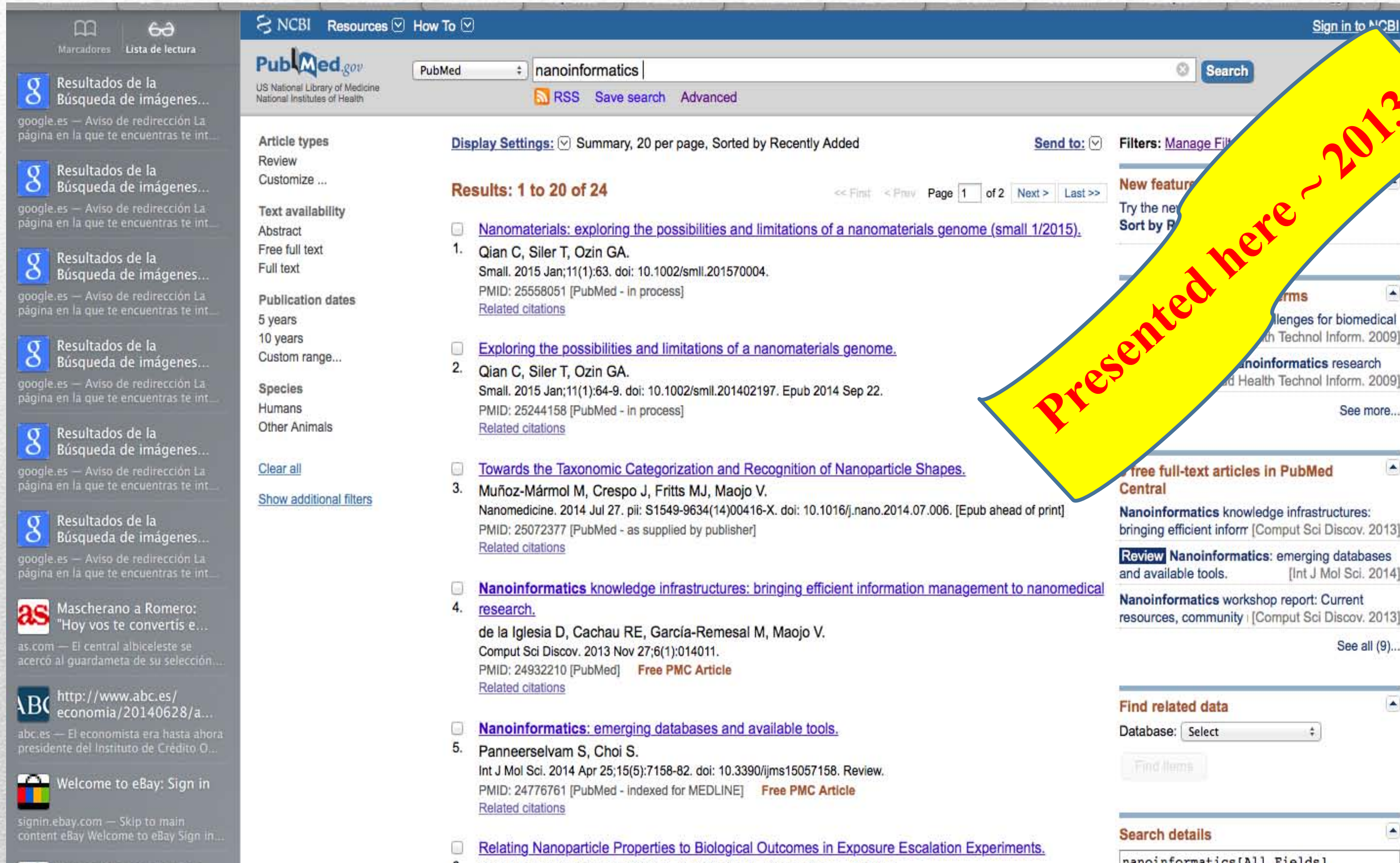
Two parts

- Our own examples of research
- What is Nanoinformatics, with implications for research and education

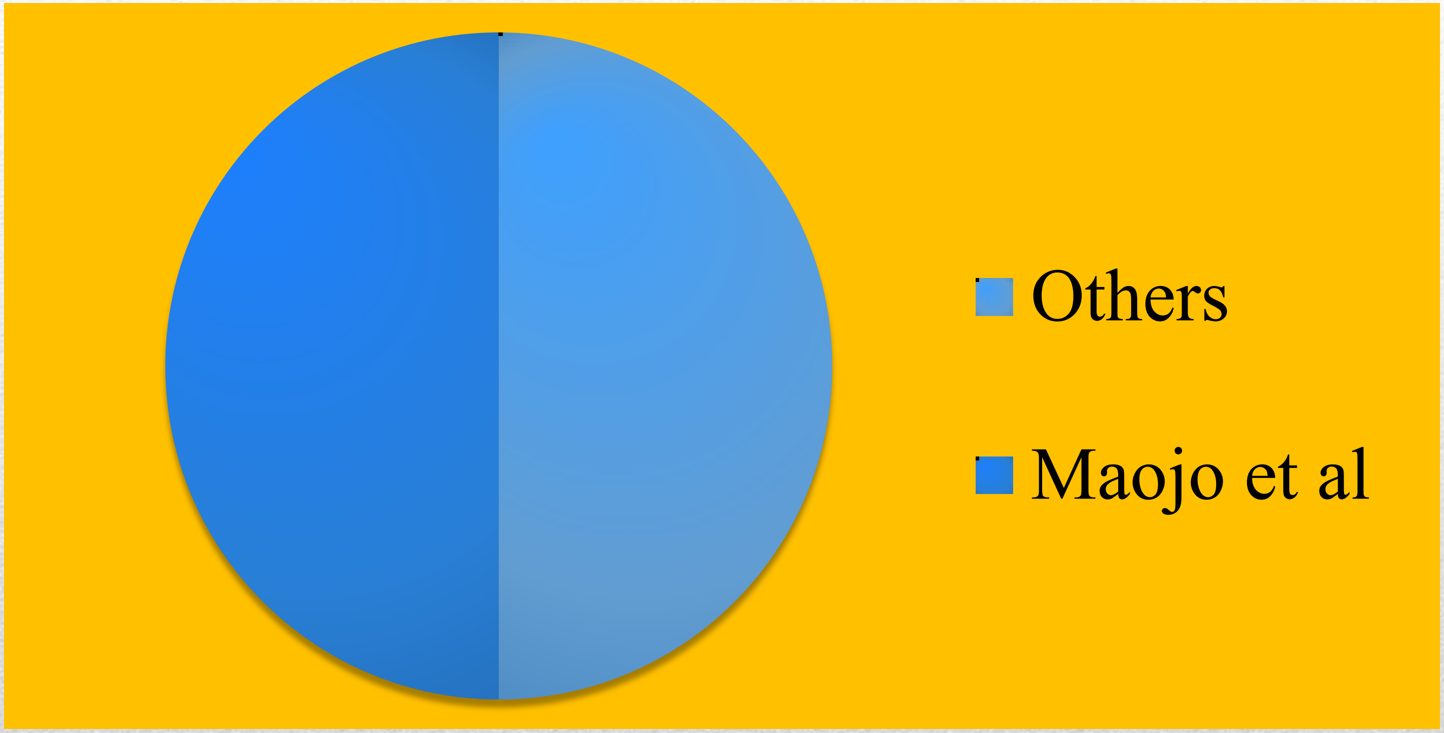
Thousands of citations in nano, but…

what about "Nanoinformatics", by searching Pubmed and the ISI Web of Science?

"Nanoinformatics" in Pubmed: just 24 hits after 7+ years…



Victor Maojo, UPM, June 2, 2016



Some of my informatics colleagues think that nanoinformatics is my weird creation!!

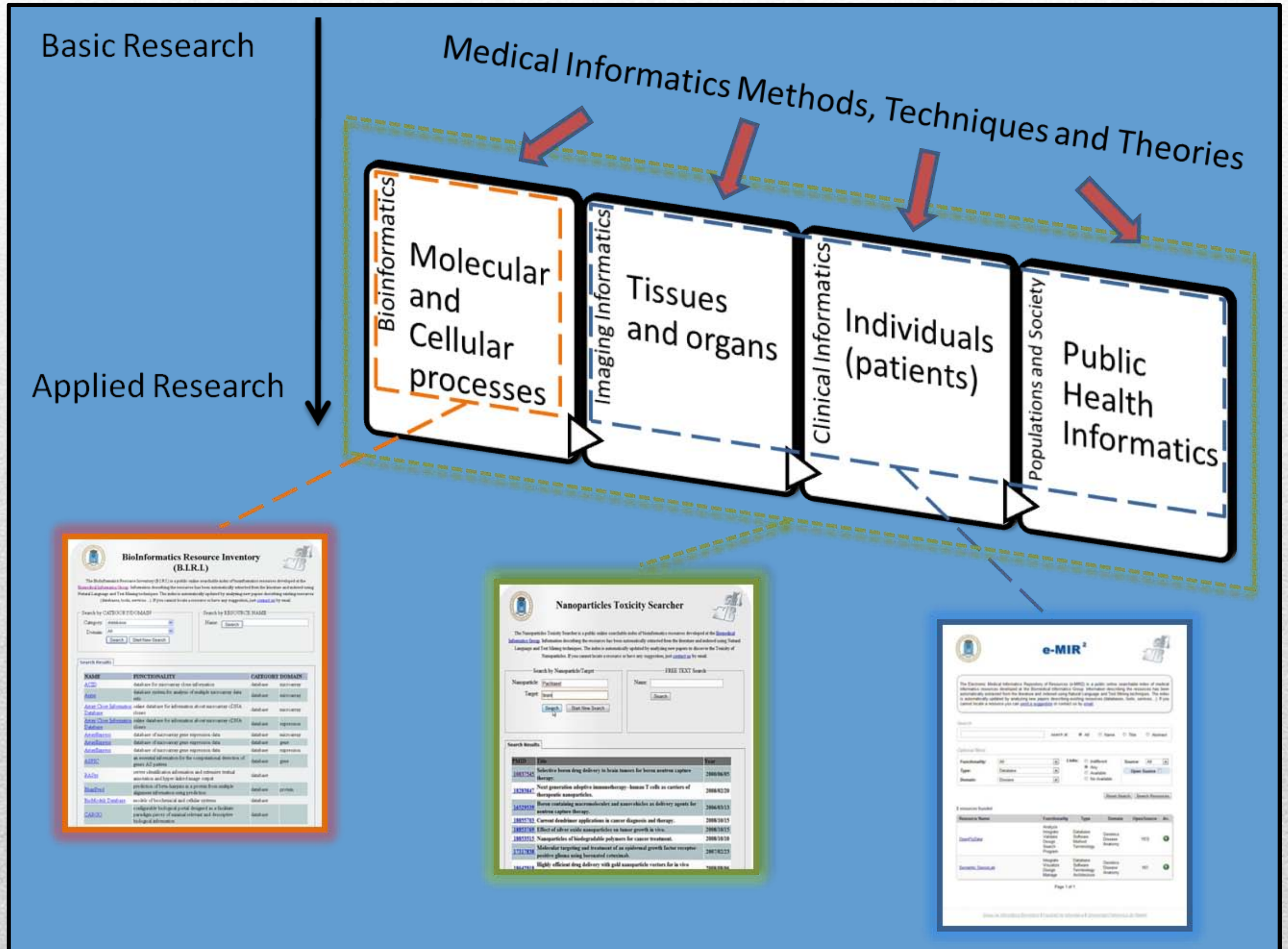
Recent publications on nanoinformatics

- Muñoz-Mármol M, Crespo J, Fritts MJ, Maojo V. Towards the Taxonomic Categorization and Recognition of Nanoparticle Shapes. Nanomedicine. 2015

- de la Iglesia D, García-Remesal M, Anguita A, Muñoz-Mármol M, Kulikowski C, Maojo V. A machine learning approach to identify clinical trials involving nanodrugs and nanodevices from ClinicalTrials.gov. PLoS One. 2014 Oct 27;9(10):e110331

- García-Remesal M, García-Ruiz A, Pérez-Rey D, de la Iglesia D, Maojo V. Using nanoinformatics methods for automatically identifying relevant nanotoxicology entities from the literature. Biomed Res Int. 2013;2013:410294.

A "resourceome": Inventories of resources across medical, bio and nanoinformatics



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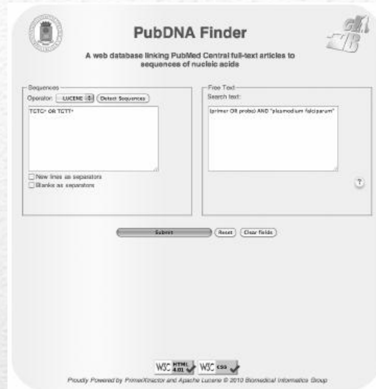
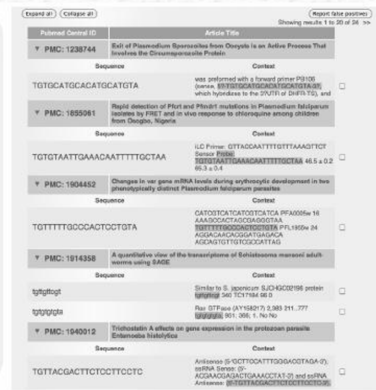
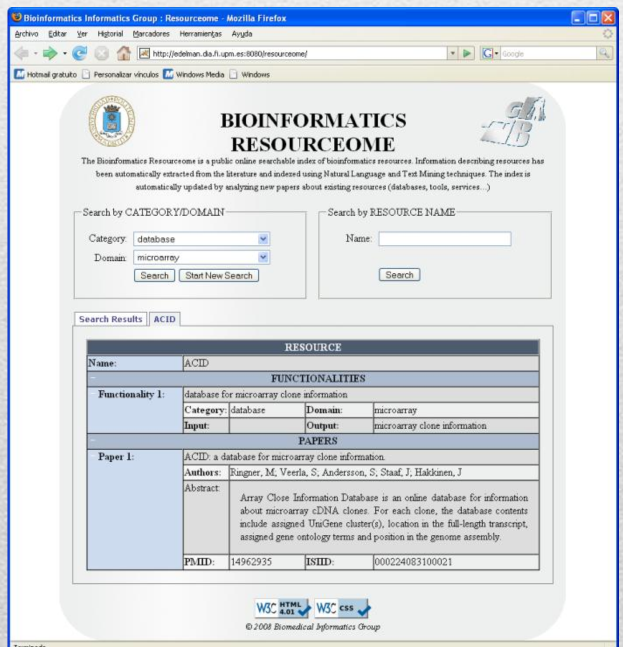
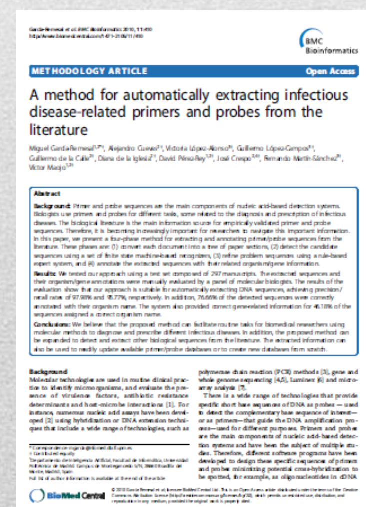
BIRI: text mining for automatically creating inventories of bioinformatics resources

PubDNA Finder: searching automatically DNA sequences in the literature

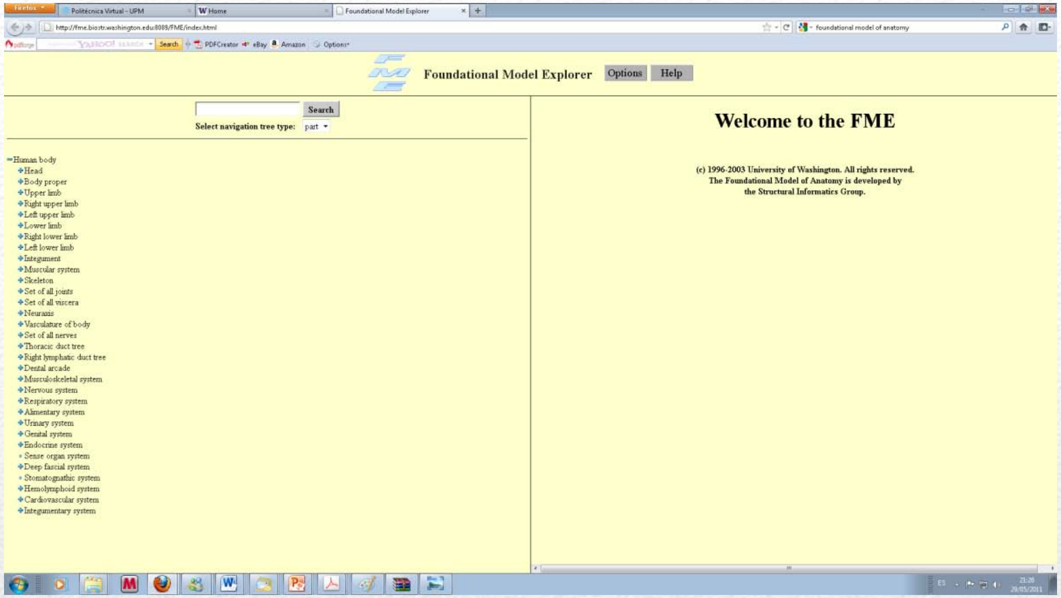




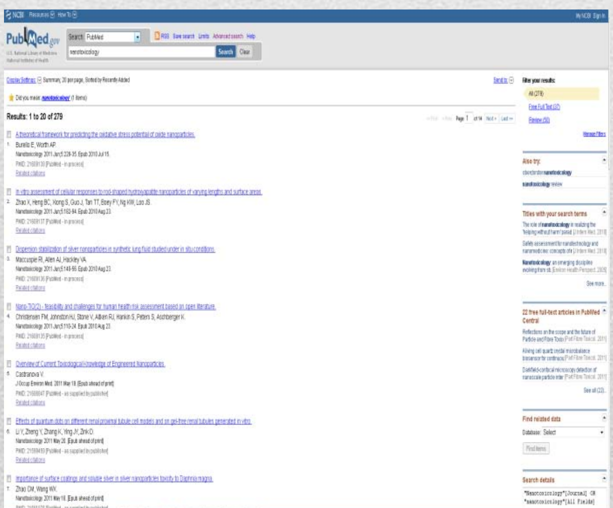




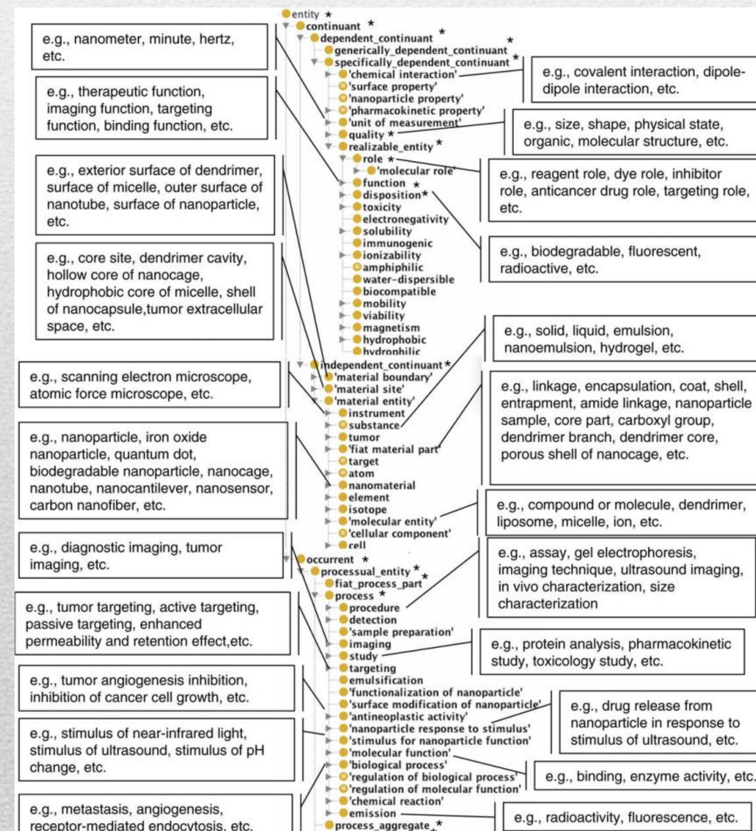
Papers published in BMC Bioinformatics (2) and Bioinformatics (1)



The Foundational Model of Anatomy (FMA)



Establishing links with the literature

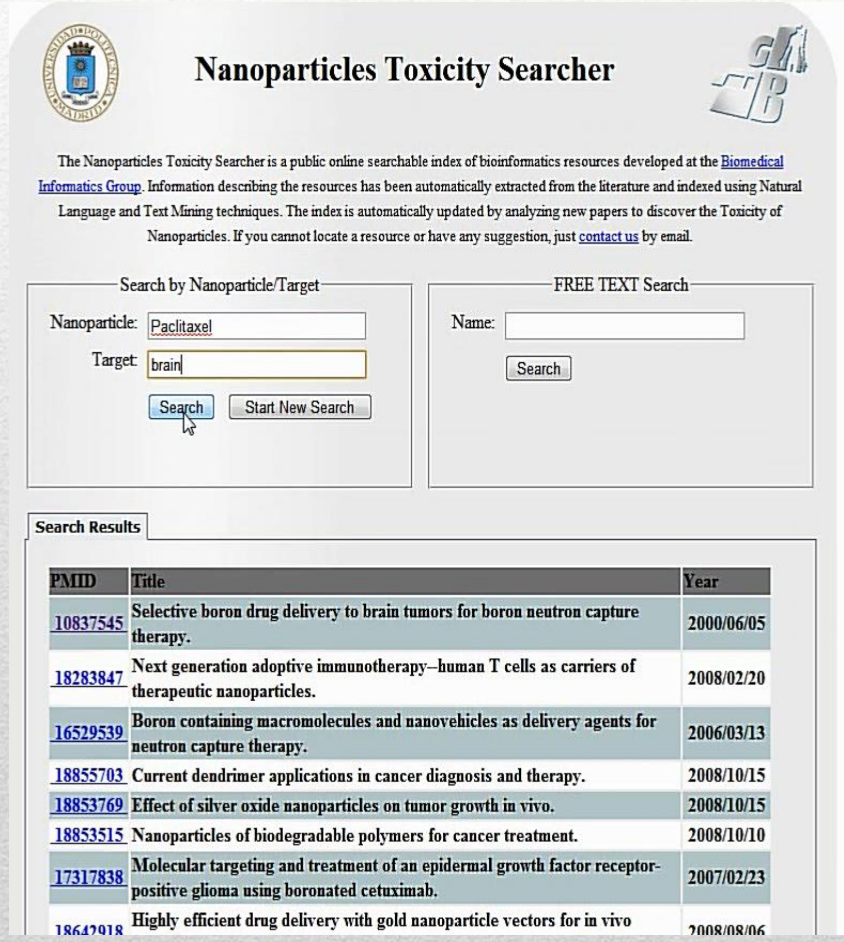


The Nanoparticle Ontology (NPO)

Developing a nanotoxicity searcher

Genexol-PM (Samyang), consists of nanoscale micelles containing Paclitaxel, the chemotherapeutic mitotic inhibitor. These micelles were given to patients with advanced tumors that were refractory to other typical drugs. In 42% of the patients the cancer was stabilized and all patients tolerated a higher drug dose by using nanoparticles

(Example from Kim et al, 2010, NEJM)



A corpus for nanotoxicity, with text mining purposes

The purpose of this study was to review published dose-response data on acute lung inflammation in rats and mice after instillation of titanium dioxide particles or six types of carbon nanoparticles.

The purpose of this study was to review published dose-response data on acute <TARGET>**lung**</TARGET> <TOXIC>**inflammation**</TOXIC> in <TARGET>**rats and mice**</TARGET> after <EXPO>**instillation**</EXPO> of <NANO>**titanium dioxide particles**</NANO> or six types of <NANO>**carbon nanoparticles**</NANO>

It extracts nanotoxicology-related entities from the scientific literature, in four different categories. We created a corpus of 300 sentences manually selected from PubMed-indexed papers and annotated with relevant nanotoxicology entities

García-Remesal M, García-Ruiz A, Pérez-Rey D, de la Iglesia D, Maojo V. Using nanoinformatics methods for automatically identifying relevant nanotoxicology entities from the literature. Biomed Res Int. 2013;2013:410294.


Research Article

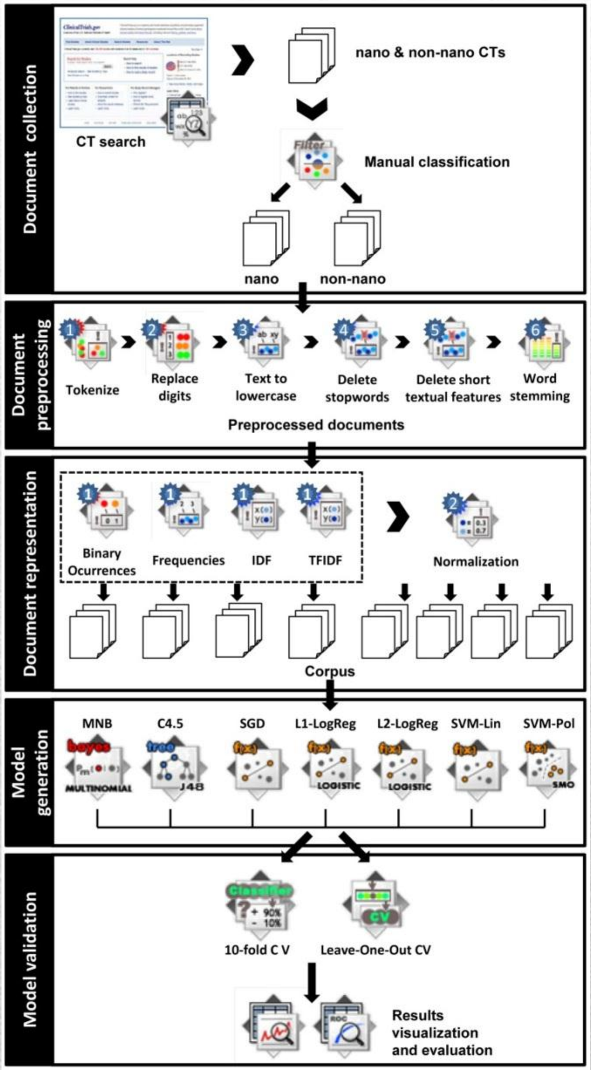
Using Nanoinformatics Methods for Automatically Identifying Relevant Nanotoxicology Entities from the Literature

Miguel García-Remesal,[1,2] Alejandro García-Ruiz,[2] David Pérez-Rey,[1,2] Diana de la Iglesia,[2] and Victor Maojo[1,2]

Received 8 May 2012; Revised 3 July 2012; Accepted 10 July 2012

Victor Maojo, UPM, June 2, 2016

Automated classification of Nanomedical Clinical Trials



- A framework to identify clinical trials from clinicaltrials.gov involving nanodrugs, nanodevices and/or nanomaterials.
- Based on supervised machine learning techniques.
- High accuracy (over 0.95)

Nanoinformatics: Developing a nanotoxicity searcher

Genexol-PM (Samyang), consists of nanoscale micelles containing Paclitaxel, the chemotherapeutic mitotic inhibitor. These micelles were given to patients with advanced tumors that were refractory to other typical drugs. In 42% of the patients the cancer was stabilized and all patients tolerated a higher drug dose by using nanoparticles

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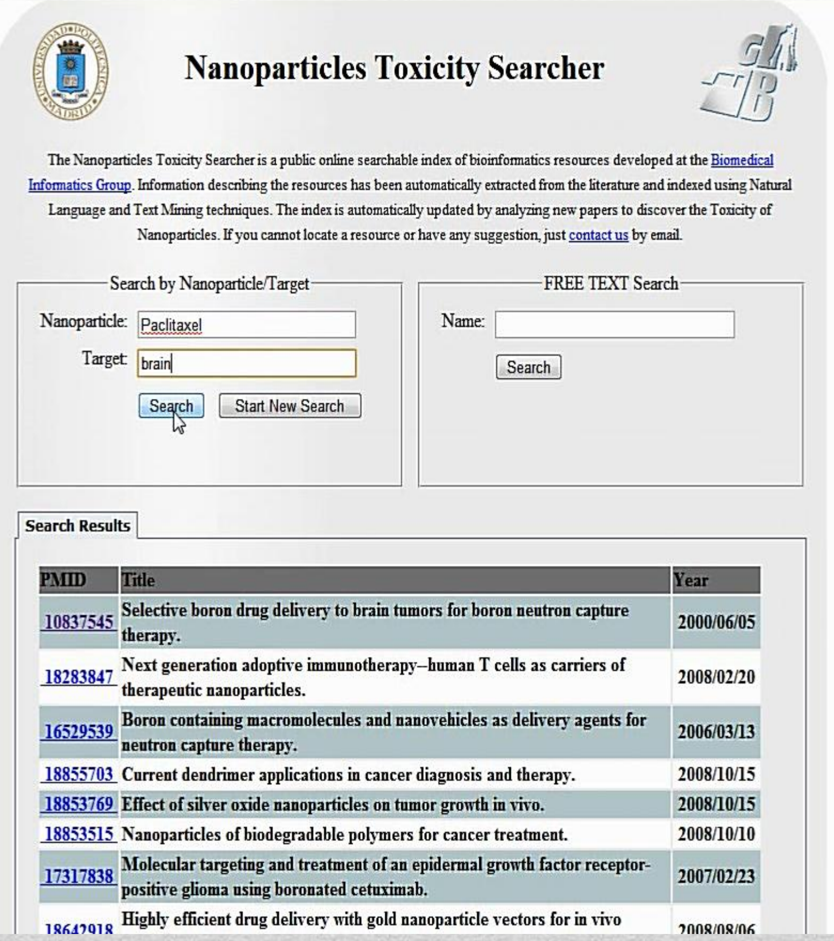

Nanoparticles Toxicity Searcher

The Nanoparticles Toxicity Searcher is a public online searchable index of bioinformatics resources developed at the Biomedical Informatics Group. Information describing the resources has been automatically extracted from the literature and indexed using Natural Language and Text Mining techniques. The index is automatically updated by analyzing new papers to discover the Toxicity of Nanoparticles. If you cannot locate a resource or have any suggestion, just contact us by email.

Search by Nanoparticle/Target

Nanoparticle: Paclitaxel

Target: brain

Search | Start New Search

FREE TEXT Search

Name:

Search

Search Results

PMID	Title	Year
10837545	Selective boron drug delivery to brain tumors for boron neutron capture therapy.	2000/06/05
18283847	Next generation adoptive immunotherapy–human T cells as carriers of therapeutic nanoparticles.	2008/02/20
16529539	Boron containing macromolecules and nanovehicles as delivery agents for neutron capture therapy.	2006/03/13
18855703	Current dendrimer applications in cancer diagnosis and therapy.	2008/10/15
18853769	Effect of silver oxide nanoparticles on tumor growth in vivo.	2008/10/15
18853515	Nanoparticles of biodegradable polymers for cancer treatment.	2008/10/10
17317838	Molecular targeting and treatment of an epidermal growth factor receptor-positive glioma using boronated cetuximab.	2007/02/23
18642918	Highly efficient drug delivery with gold nanoparticle vectors for in vivo	2008/08/06

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Hindawi Publishing Corporation
BioMed Research International
Volume 2013, Article ID 410294, 9 pages
http://dx.doi.org/10.1155/2013/410294

Research Article

Using Nanoinformatics Methods for Automatically Identifying Relevant Nanotoxicology Entities from the Literature

Miguel García-Remesal,[1,2] Alejandro García-Ruiz,[2] David Pérez-Rey,[1,2] Diana de la Iglesia,[2] and Victor Maojo[1,2]

[1] *Departamento de Inteligencia Artificial, Facultad de Informática, Universidad Politécnica de Madrid, Boadilla del Monte, 28660 Madrid, Spain*
[2] *Biomedical Informatics Group, Facultad de Informática, Universidad Politécnica de Madrid, Boadilla del Monte, 28660 Madrid, Spain*

Received 8 May 2012; Revised 3 July 2012; Accepted 10 July 2012

Academic Editor: Raffaele Calogero

1. Introduction

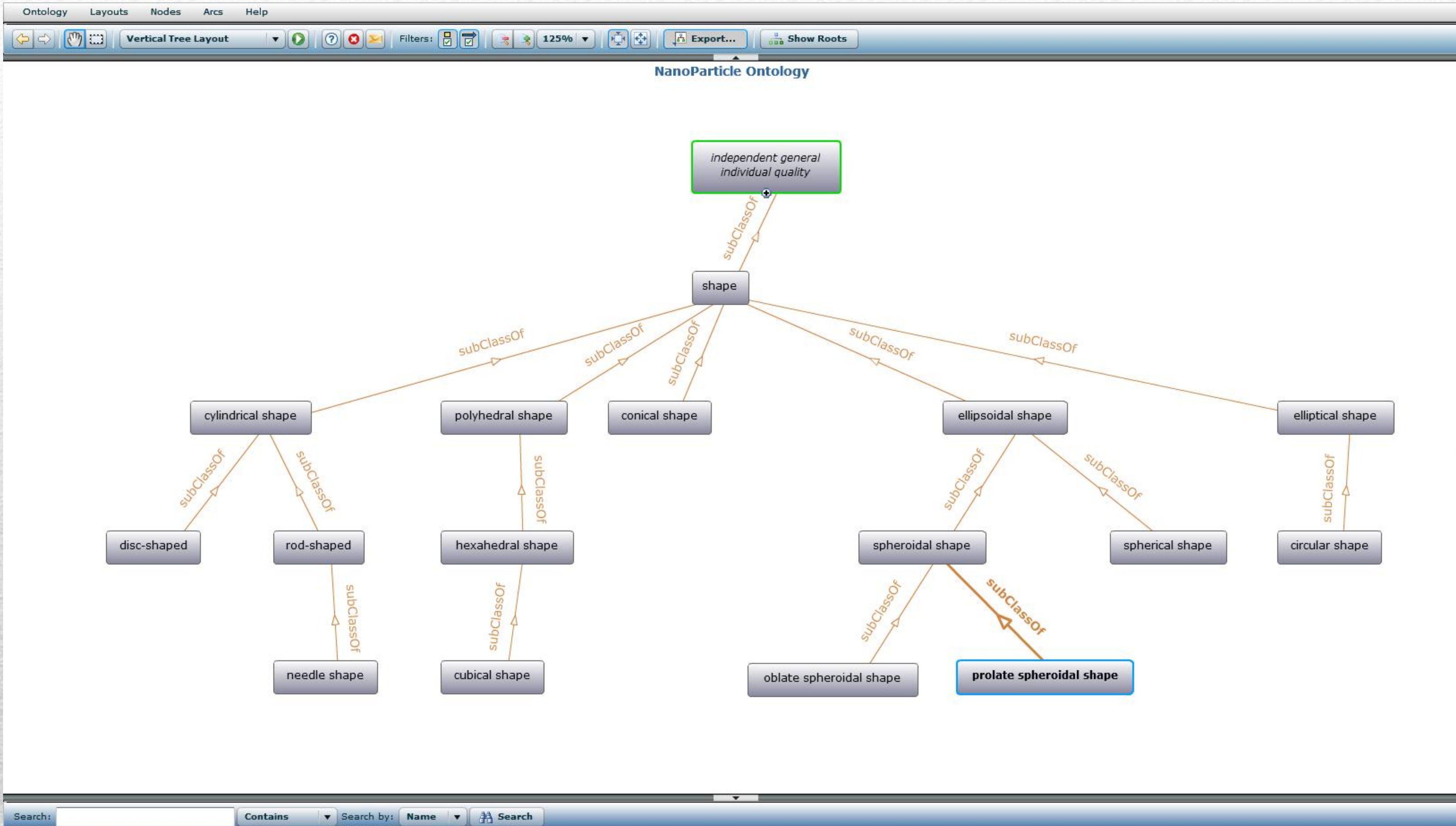
Nanoparticle ontology for cancer (Thomas, Baker et al)

OWL object property	No. of times used in class-level associations
has_relation_to	(0)
bearer_of	(2)
has_function	(54)
has_property	(32)
has_quality	(97)
has_role	(93)
contained_in	(5)
contains	(4)
derives_from	(41)
has_component_part	(47)
has_conjugated_component_part	(1)
has_encapsulated_component_part	(1)
has_entrapped_component_part	(2)
determines_property	(5)
has_application	(7)
has_bond_with	(2)
has_double_bond_with	(2)
has_single_bond_with	(2)
has_triple_bond_with	(0)
has_identification_type	(8)
has_part	(276)
has_participant	(14)
has_agent	(4)
has_output_participant	(7)
has_technique	(1)
has_unit_of_measure	(39)
inheres_in	(3)
function_of	(0)
quality_of	(24)
role_of	(8)
is_integral_part_of	(223)
is_realized_in	(101)
negatively_regulates	(20)
part_of	(110)
participates_in	(18)
agent_in	(2)
positively_regulates	(8)
property_determined_from	(1)
parameter_determined_from	(8)
realizes	(11)
regulates	(3)
stimulus_causes_response	(3)
technique_used_for	(1)
unit_of	(31)
uses_instrument	(12)

Challenges:

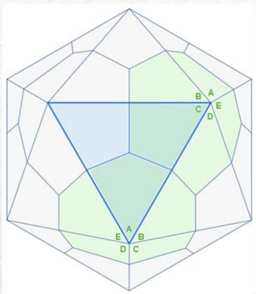
- Useful for cancer applications
- But to create an useful taxonomy/ontology for nanoparticles themselves?

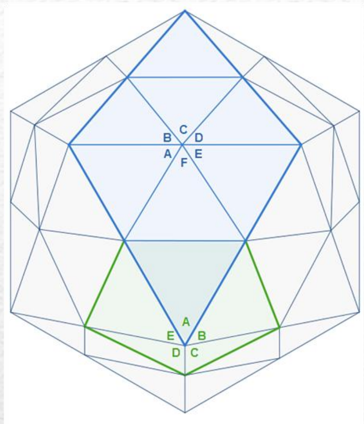
From the NPO

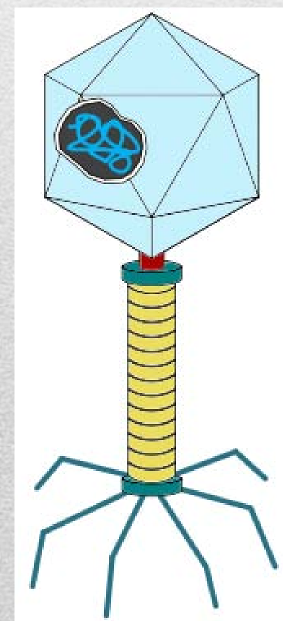


Ontology
Layouts
Nodes
Arcs
Help
Vertical Tree Layout
Filters:
125%
Export...
Show Roots
NanoParticle Ontology
independent general individual quality
subClassOf
shape
cylindrical shape
polyhedral shape
conical shape
ellipsoidal shape
elliptical shape
disc-shaped
rod-shaped
hexahedral shape
spheroidal shape
spherical shape
circular shape
needle shape
cubical shape
oblate spheroidal shape
prolate spheroidal shape
Search:
Contains
Search by:
Name
Search

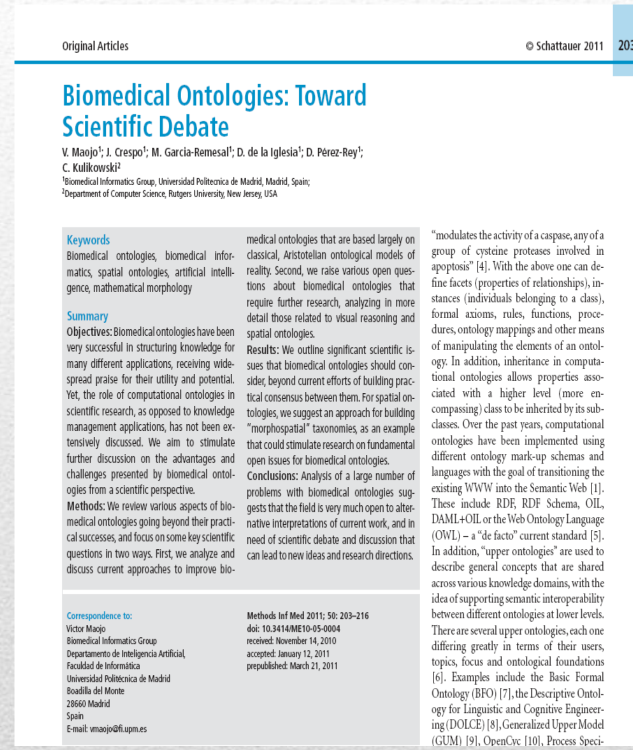
Work on pattern classification and ontologies: Taxonomies of shapes and forms







Shapes
- •1-D Shapes
- •2-D Shapes
  - — 2-D Geometrical shapes
    - o2-D Geometrical shapes with genus 0
      - ▪Circles
      - ▪Polygons
        - •Convex polygons
        - oSquares
        - oTriangles
        - o…
      - ▪Non-convex polygons
    - o2-D Geometrical shapes with genus 1
  - —2-D Non-geometrical shapes
- •3-D Shapes



Original Articles © Schattauer 2011 203

Biomedical Ontologies: Toward Scientific Debate

V. Maojo[1]; J. Crespo[1]; M. Garcia-Remesal[1]; D. de la Iglesia[1]; D. Pérez-Rey[1]; C. Kulikowski[2]

[1]Biomedical Informatics Group, Universidad Politecnica de Madrid, Madrid, Spain;
[2]Department of Computer Science, Rutgers University, New Jersey, USA

Keywords
Biomedical ontologies, biomedical informatics, spatial ontologies, artificial intelligence, mathematical morphology

Summary
Objectives: Biomedical ontologies have been very successful in structuring knowledge for many different applications, receiving widespread praise for their utility and potential. Yet, the role of computational ontologies in scientific research, as opposed to knowledge management applications, has not been extensively discussed. We aim to stimulate further discussion on the advantages and challenges presented by biomedical ontologies from a scientific perspective.
Methods: We review various aspects of biomedical ontologies going beyond their practical successes, and focus on some key scientific questions in two ways. First, we analyze and discuss current approaches to improve biomedical ontologies that are based largely on classical, Aristotelian ontological models of reality. Second, we raise various open questions about biomedical ontologies that require further research, analyzing in more detail those related to visual reasoning and spatial ontologies.
Results: We outline significant scientific issues that biomedical ontologies should consider, beyond current efforts of building practical consensus between them. For spatial ontologies, we suggest an approach for building "morphospatial" taxonomies, as an example that could stimulate research on fundamental open issues for biomedical ontologies.
Conclusions: Analysis of a large number of problems with biomedical ontologies suggests that the field is very much open to alternative interpretations of current work, and in need of scientific debate and discussion that can lead to new ideas and research directions.

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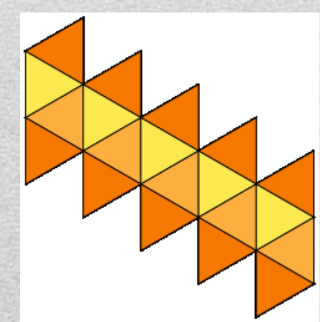
accepted: January 12, 2011
prepublished: March 21, 2011

"modulates the activity of a caspase, any of a group of cysteine proteases involved in apoptosis" [4]. With the above one can define facets (properties of relationships), instances (individuals belonging to a class), formal axioms, rules, functions, procedures, ontology mappings and other means of manipulating the elements of an ontology. In addition, inheritance in computational ontologies allows properties associated with a higher level (more encompassing) class to be inherited by its subclasses. Over the past years, computational ontologies have been implemented using different ontology mark-up schemas and languages with the goal of transitioning the existing WWW into the Semantic Web [1]. These include RDF, RDF Schema, OIL, DAML+OIL or the Web Ontology Language (OWL) – a "de facto" current standard [5]. In addition, "upper ontologies" are used to describe general concepts that are shared across various knowledge domains, with the idea of supporting semantic interoperability between different ontologies at lower levels. There are several upper ontologies, each one differing greatly in terms of their users, topics, focus and ontological foundations [6]. Examples include the Basic Formal Ontology (BFO) [7], the Descriptive Ontology for Linguistic and Cognitive Engineering (DOLCE) [8], Generalized Upper Model (GUM) [9], OpenCyc [10], Process Speci-



Victor Maojo, UPM, June 2, 2016

What is reality?
How to represent it through semantics in a computer?

積分蛋白

糖蛋白

磷脂

側鏈

疏水區

親水區

親水

流動鑲嵌膜模型

跨膜蛋白

Gene ontology

Integral protein
積分蛋白

Glycoprotein
糖蛋白

Phospholipid
磷脂

Carbohidrate side chain
側鏈

Hydrophobic region
疏水區

Components of a cellular membrane, represented as concepts/classes in Gene Ontology

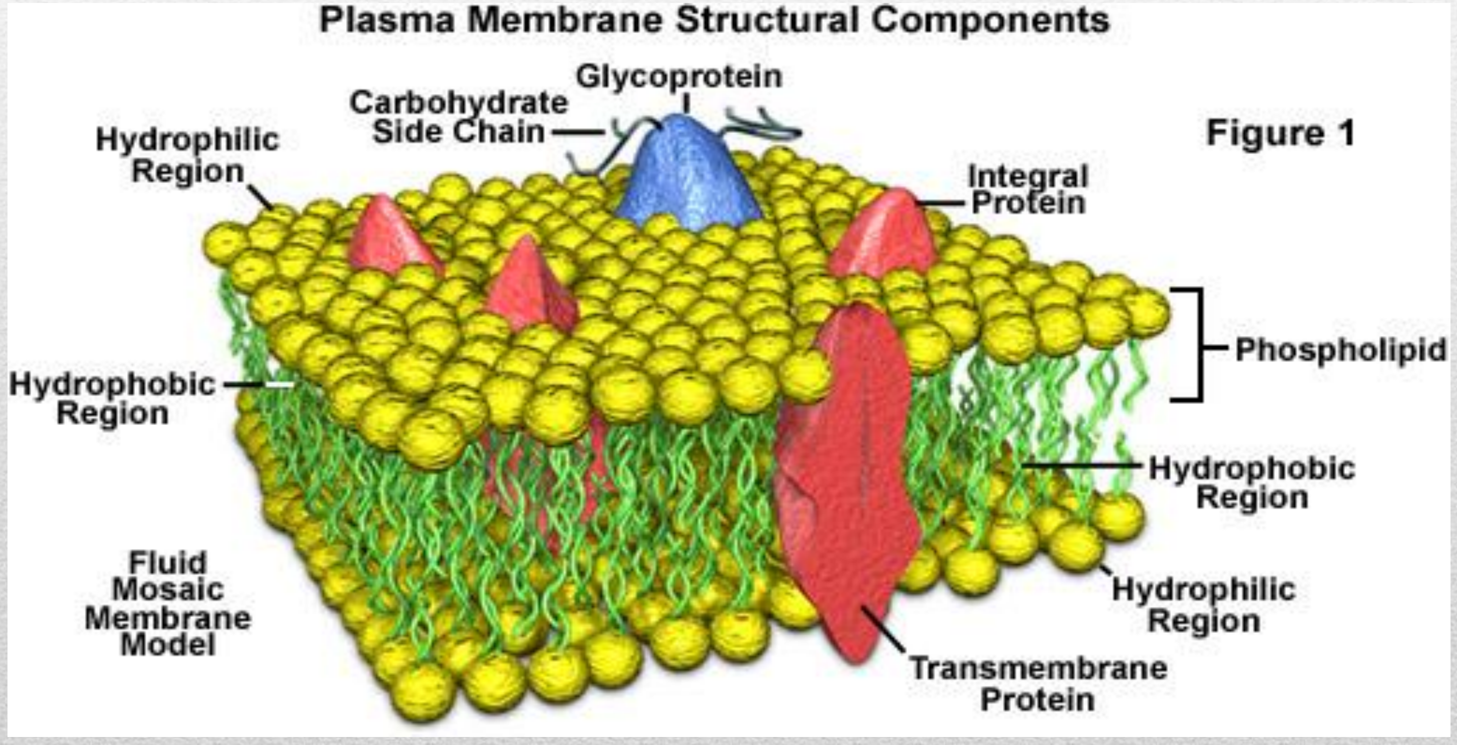
Hydrophilic region
親水區

Hydrophillic
親水

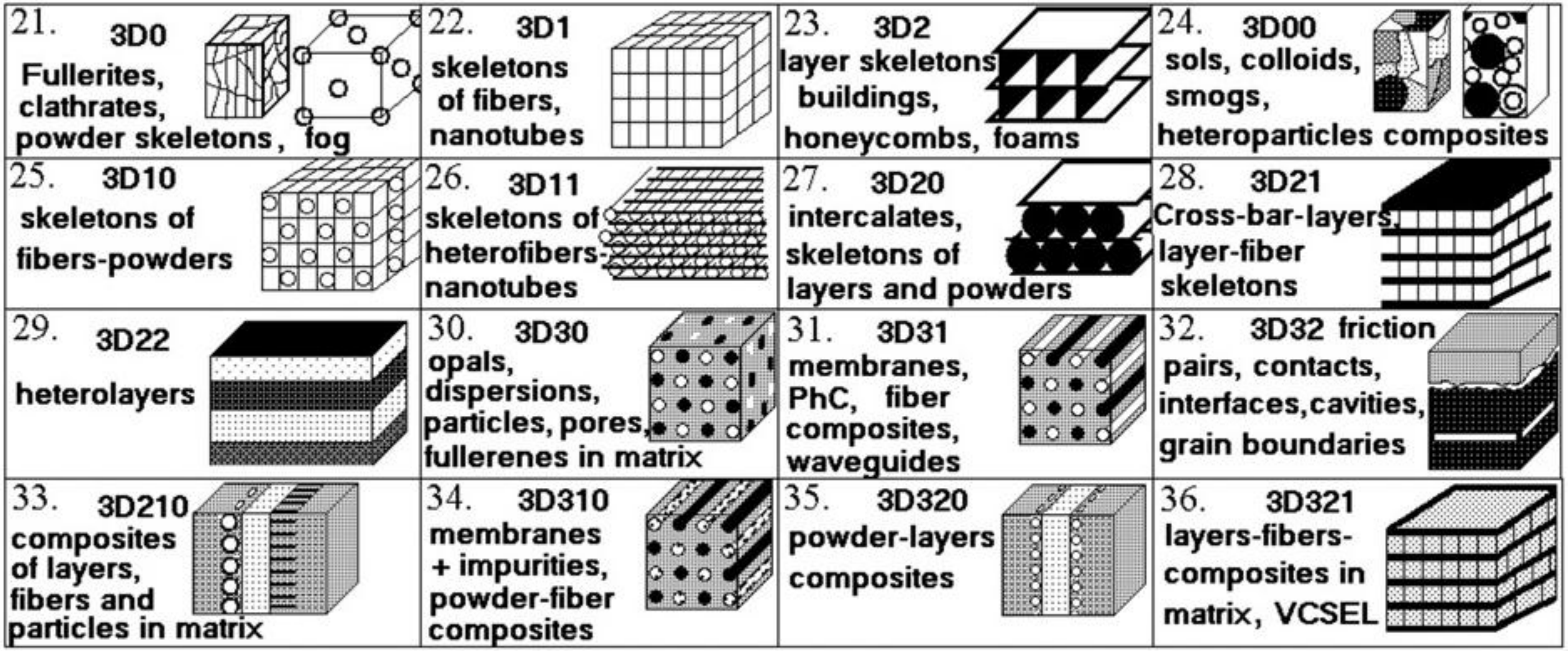
Fluid mosaic membrane model
流動鑲嵌膜模型

Transmembrane Protein
跨膜蛋白

What a scientist (or anyone) must consider here as reality?



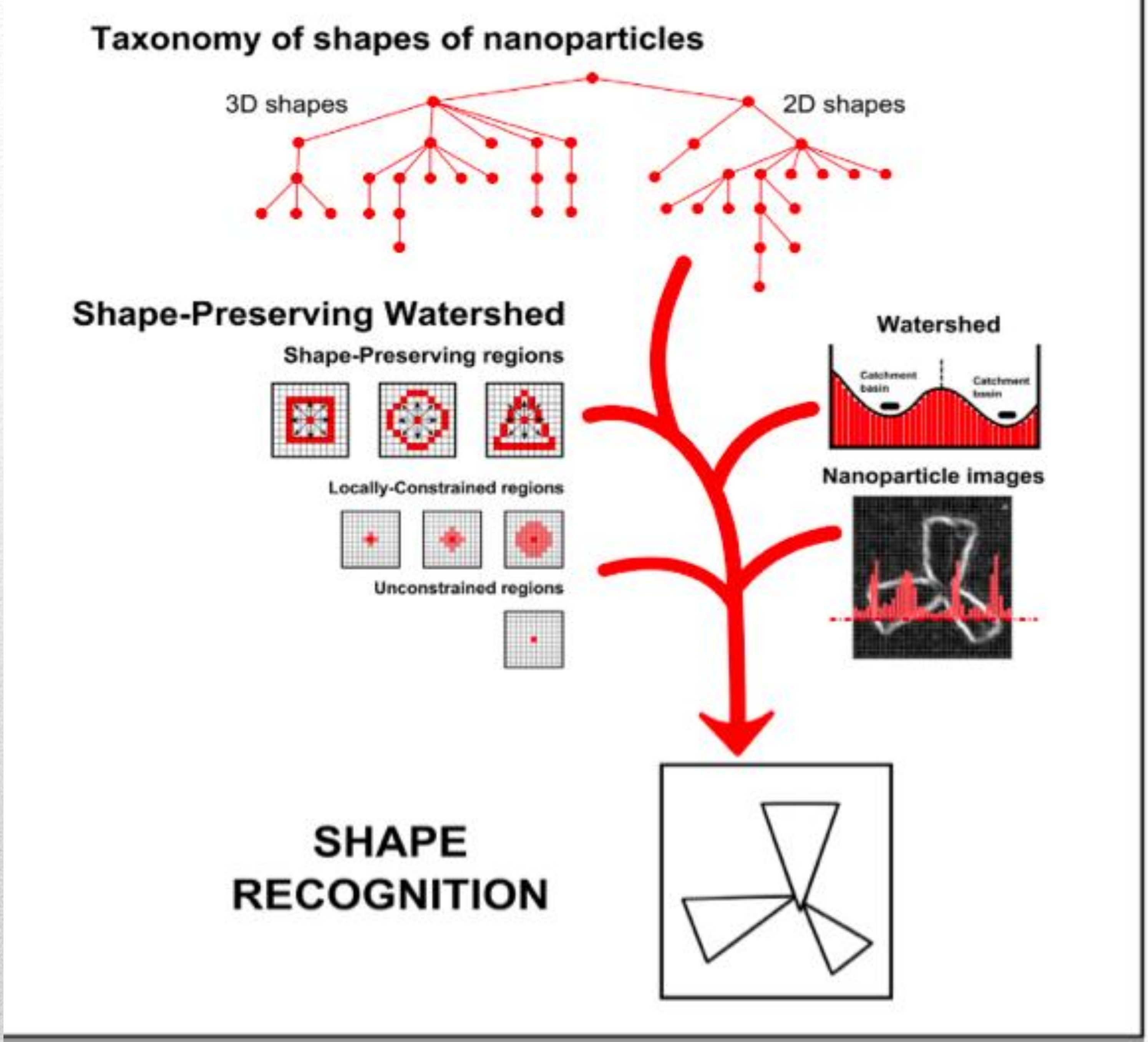
Work on pattern classification and nano-ontologies



From Pokropivny and Skorokhod

Classifications of nanoparticles

- Pending: categorization and nomenclature of nanoparticles
- Descriptions of morphological and spatial properties are consistently reported in the nanotechnology literature (observed and measured using various microscopy techniques).
- Knowing the shapes and forms of nanoparticles can be a necessary component of future classifications of nanoparticles


Taxonomy of shapes of nanoparticles
3D shapes
2D shapes
Shape-Preserving Watershed
Shape-Preserving regions
Locally-Constrained regions
Unconstrained regions
Watershed
Catchment basin
Catchment basin
Nanoparticle images
SHAPE
RECOGNITION

Approach

- We examined representative nanotechnology papers to make an initial listing of the terms used to describe shapes of nanoparticles and nanomaterials composites

- Most common terms in 2D and 3D shapes: rings or graphene patterns (hexagon), elliptical compounds and cells (ellipse, circle, plate), and the projections of crystals in the form of polygonal shapes (rectangles, squares, triangles) or similarly for spheres, rings, cubes, column, wires, rods, etc.

Table S1 – List of 2D shape terms extracted from the analyzed nanotechnology literature.

Shape	Terms	Dim	ASP	% ASP	TA	% TA
Hexagon	hexagon, hexagonal	2D	13	37,14%	55	20,15%
Ellipse	ellipse, elliptical, elliptic, ellipses	2D	7	20,00%	50	18,32%
Circle	circle, circular, circles	2D	15	42,86%	35	12,82%
Rectangle	rectangle, rectangular, rectangles	2D	5	14,29%	29	10,62%
Square	square, squared, squares	2D	8	22,86%	22	8,06%
Plate	nanoplate, nanoplates, plates	2D	3	8,57%	20	7,33%
Triangle	triangle, triangular, triangles	2D	8	22,86%	18	6,59%
Platelet	platelet, platelets	2D	7	20,00%	15	5,49%
Pentagon	pentagon, pentagonal, pentagons	2D	2	5,71%	8	2,93%
Spiral	spiral	2D	5	14,29%	8	2,93%
Ribbon	ribbon	2D	3	8,57%	6	2,20%
Rhombus	rhombus, rhombic, rhombuses	2D	2	5,71%	4	1,47%
Octagon	octagon, octagonal	2D	1	2,86%	1	0,37%
Polygon	polygon, polygonal	2D	1	2,86%	1	0,37%
Quadrilateral	quadrilateral	2D	1	2,86%	1	0,37%
TOTAL					**273**	

ASP: Appearances in studied papers; **TA**: Total appearances.

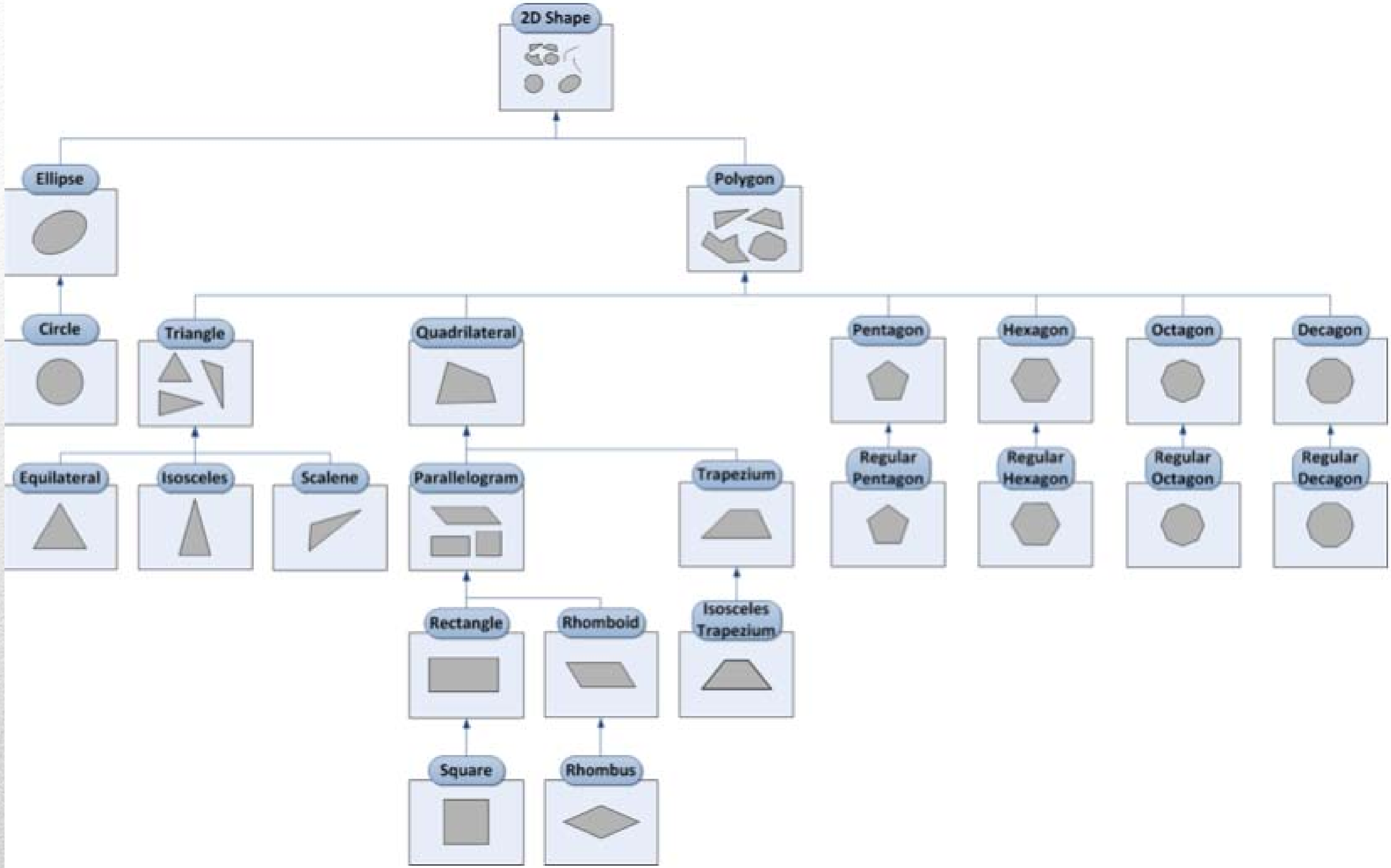


Figure S1 – Taxonomic hierarchy of 2D shapes. Both Ellipse and Polygon subclasses are derived from the general 2D Shape class. As a particularization of Ellipses, the Circle is derived. Under Polygon class we have considered three, four, five, six, eight, and ten-sided polygons (respectively as Triangle, Quadrilateral,

Table S2 – List of 3D shape terms extracted from the analyzed nanotechnology literature.

Shape	Terms	Dim	ASP	% ASP	TA	% TA
Sphere	sphere, spherical, spheres	3D	28	80,00%	356	25,59%
Tube	tube, tubular	3D	25	71.43%	259	18,62%
Helix	helix, helical, helices, helixes	3D	8	22,86%	98	7,05%
Ring	ring, rings, ringlike	3D	12	34,29%	85	6,11%
Cube	cube, cubic, cubes	3D	14	40,00%	81	5,82%
Column	column, columnar, columns	3D	3	8,57%	73	5,25%
Cylinder	cylinder, cylindric, cylindrical	3D	11	31,43%	67	4,82%
Ellipsoid	ellipsoid, ellipsoidal, ellipsoids	3D	9	25,71%	62	4,46%
Rod	rod, rods, rodlike	3D	12	34,29%	61	4,39%
Cage	cage, cages	3D	7	20,00%	34	2,44%
Disk	disk, disks, discoidal	2D	8	22,86%	31	2,23%
Octahedron	octahedron, octahedral	3D	5	14,29%	28	2,01%
Pyramid	pyramid, pyramidal, pyramids	3D	5	14,29%	25	1,80%
Spheroid	spheroid, spheroidal, spheroids	3D	7	20,00%	24	1,73%
Tetrahedron	tetrahedron, tetrahedral	3D	7	20,00%	21	1,51%
Icosahedron	icosahedron, icosahedral	3D	6	17,14%	16	1,15%
Oblate	oblate	3D	5	14,29%	15	1,08%
Polyhedron	polyhedron, polyhedral	3D	5	14,29%	10	0,72%
Backbone	backbone, backbones	3D	4	11,43%	9	0,65%
Cone	cone, conical, conic, cones	3D	5	14,29%	7	0,50%
Needle	needle, needles	3D	3	8,57%	6	0,43%
Dodecahedron	dodecahedron, dodecahedral	3D	3	8,57%	5	0,36%
Prolate	prolate	3D	3	8,57%	5	0,36%
Barb	barbed	3D	2	5,71%	4	0,29%
Flake	flake	3D	1	2,86%	3	0,22%
Parallelepiped	parallelepiped, parallelepipeds	3D	1	2,86%	2	0,14%
Torus	torus, tori	3D	1	2,86%	1	0,07%
Prickle	prickle, prickles	3D	1	2,86%	1	0,07%
Spike	spike	3D	1	2,86%	1	0,07%
Spindle	spindle	3D	1	2,86%	1	0,07%
TOTAL					**1391**	

ASP: Appearances in studied papers; **TA**: Total appearances.

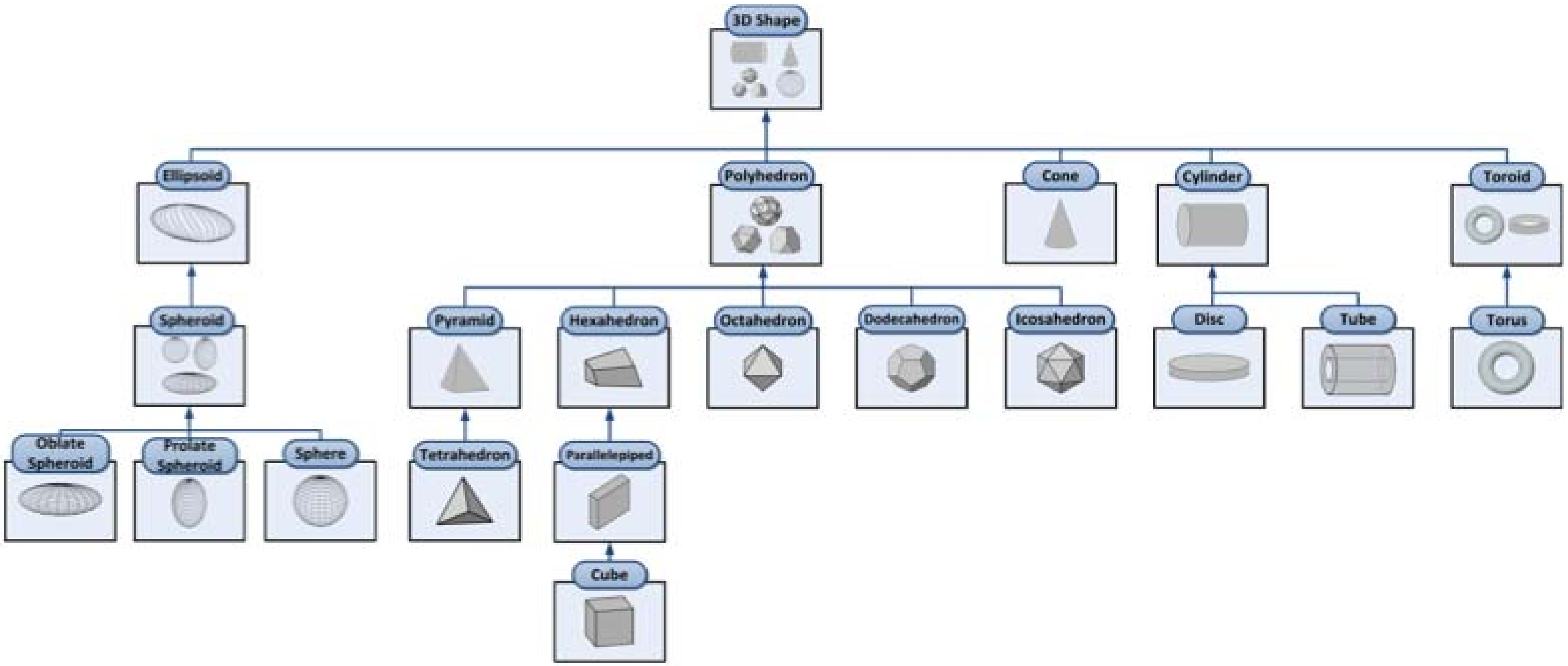
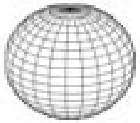
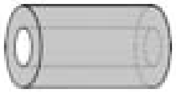
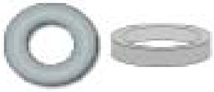
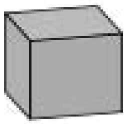


Figure S2 – Taxonomic hierarchy of 3D shapes. In this case, the most general 3D Shape class derives in five main subclasses: Cone, Cylinder, Ellipsoid, Polyhedron, and Toroid. Under Ellipsoid subclass

Table S4. Example of the classification of nanometer scaled elements according to their shapes

Nanometer scaled element	Shape	Visual class	Description
Zinc oxide (1) Gold Nanoparticles (2, 3) Fullerenes (4) Lipid Nanospheres (5) Al/Fe oxide Nanospheres (6) Oligosaccaridepolypeptide dendrimers (7) Alkanethiolate (8) Rhodium nanoparticle (9) ...	Sphere		3D shape whose boundaries are equidistant to a center in all directions. Also, a 3D shape generated by rotating a circle around its diameter
Carbon nanotubes (2-8, 10-25) Silica nanotubes (6, 13) Lipid nanotubes (5) Peptide nanotubes (3, 7) Au/TiO2/ZnO nanotubes (2) Boron nitride nanotubes (7) ...	Tube		3D shape formed by a cylinder hollowed along its axis.
Mesoporous silica nanoparticles (13) Metal nanoparticle-block copolymers (6) Si nanowires (6, 11, 14, 25) SiO2 / ZnS / CdS / Ni nanowires (11) Ultra-thin alumina mask nano-patterned cylinders (2) ...	Cylinder		3D shape enclosed by two parallel coaxial circles and the surface that joins both circles
Polystirene nanoparticles (13, 26) Dendrimers (27) Ag nanoparticles (9) Pt nanoparticles (9) ...	Ellipse		Regular oval shape, traced by a point moving in a plane so that the sum of its distances from two other points (foci) is constant, or resulting when a cone is cut by an oblique plane that does not intersect the base. (Oxford Dict.)
Gold Nanoparticles (2, 6) Si, Ni nanoparticles (2) InGaN (2) ...	Ring (Toroid)		3D shape generated by any planar closed surface rotated around an axis that does not intersect it
Nanometer-sized DNA structure (15) MgO (16) NaCl (16) Ag nanoparticles (16) Pt nanoparticles (9) Mo nanoparticles (25) ...	Cube		Parallelepiped whose faces are all squares

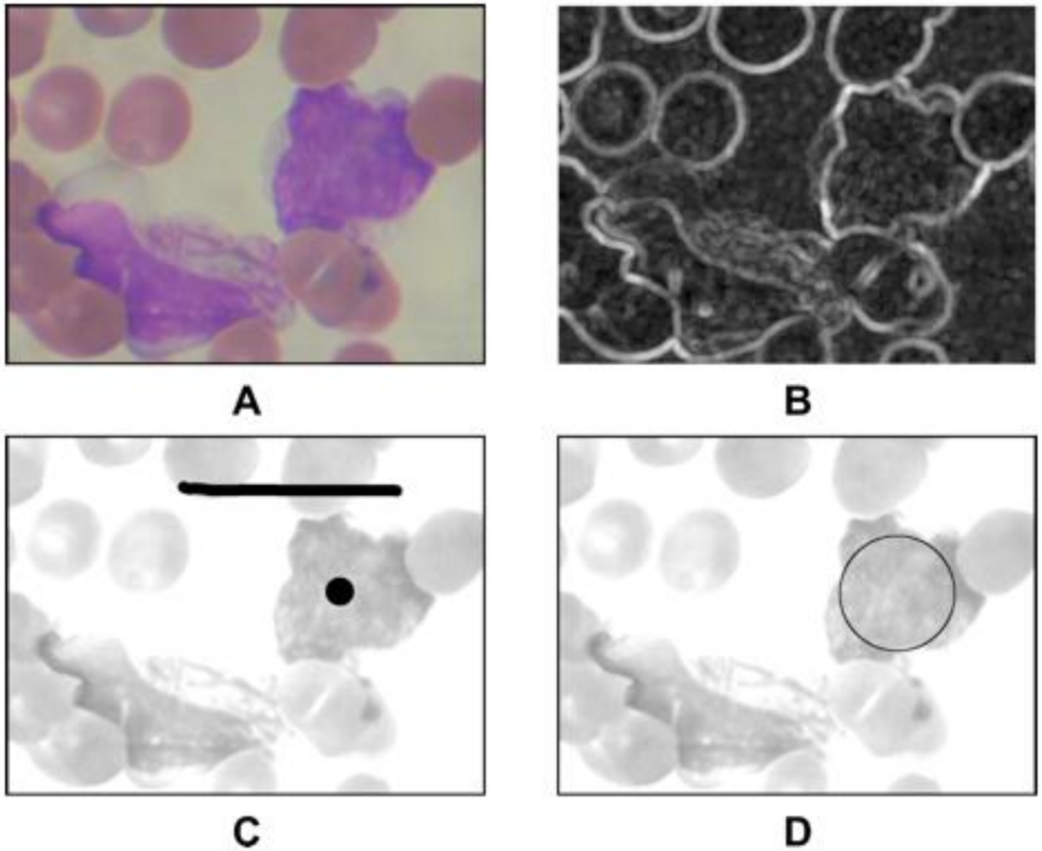


Figure S5 – SPW applied to a natural image of blood cells. **A.** Original image; **B**. Image gradient; **C.** Markers on the original image (original image has been lighten for a better understanding); **D.** Recognized inner circle.

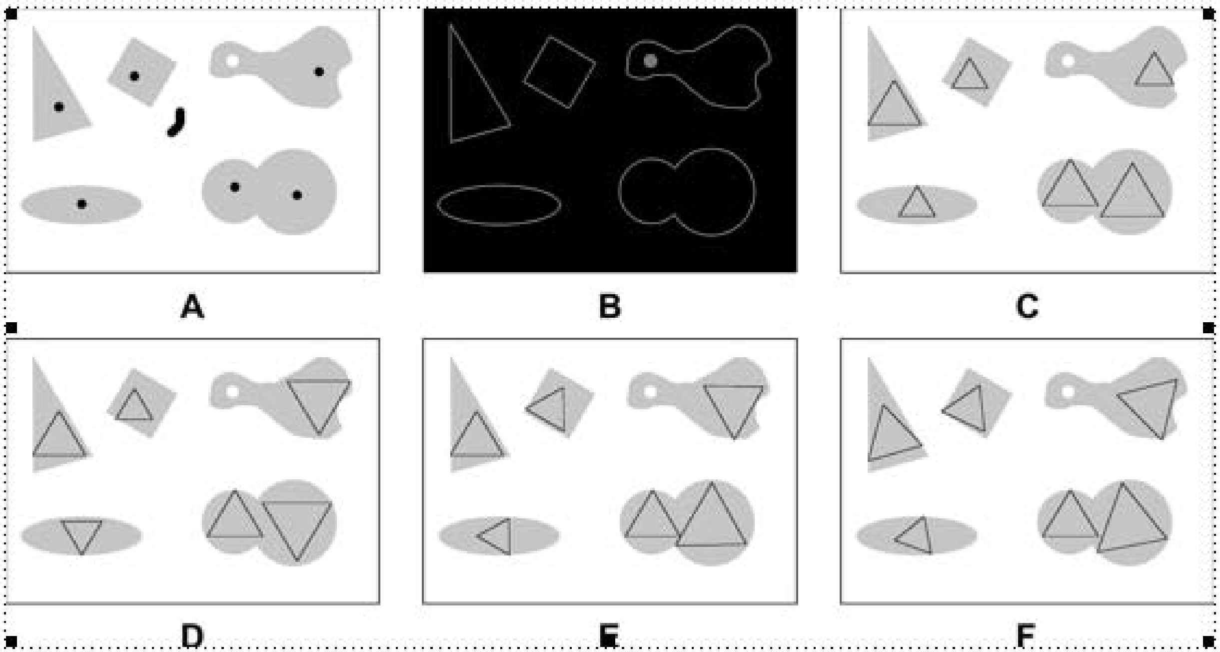


Figure S6 – SPW applied to a set of synthetic images with equilateral triangles as constraining regions. **A.** Original image with markers; **B.** image gradient (normalized); **C.** SPW without allowing rotations to constraining regions; **D-F.** SPW allowing rotations to constraining regions.

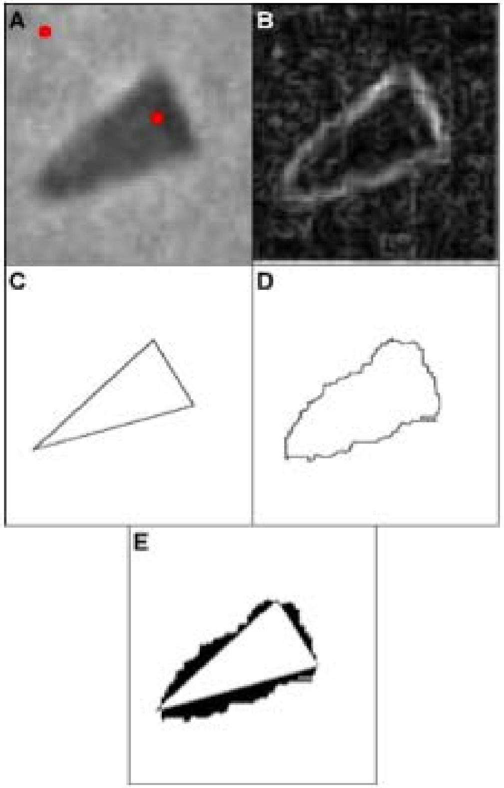


Figure S9 – SPW method applied to a single ZnO nanostructure. **A.** Original image with markers. Reprinted (adapted) with permission from (46). Copyright (2006) American Chemical Society; **B.** Image gradient (normalized); **C.** Results of the SPW method; **D.** Results of a standard watershed method; **E.** Area differences (in black).

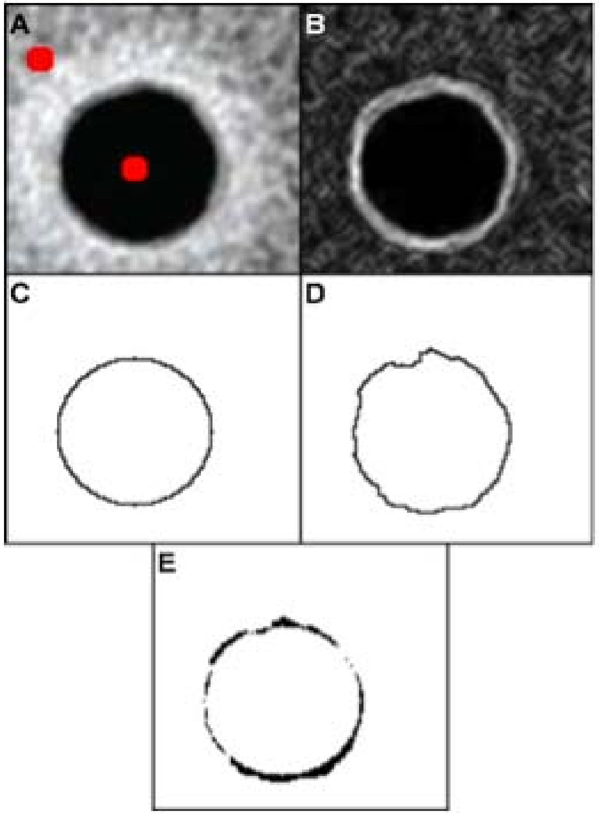


Figure S10 – SPW method applied to a gold nanosphere. **A.** Original image with markers. Reprinted (adapted) with permission from (29). Copyright (2006) American Chemical Society. **B.** Image gradient (normalized); **C.** Results of the SPW method; **D.** Results of a standard watershed method; **E.** Area differences (in black).

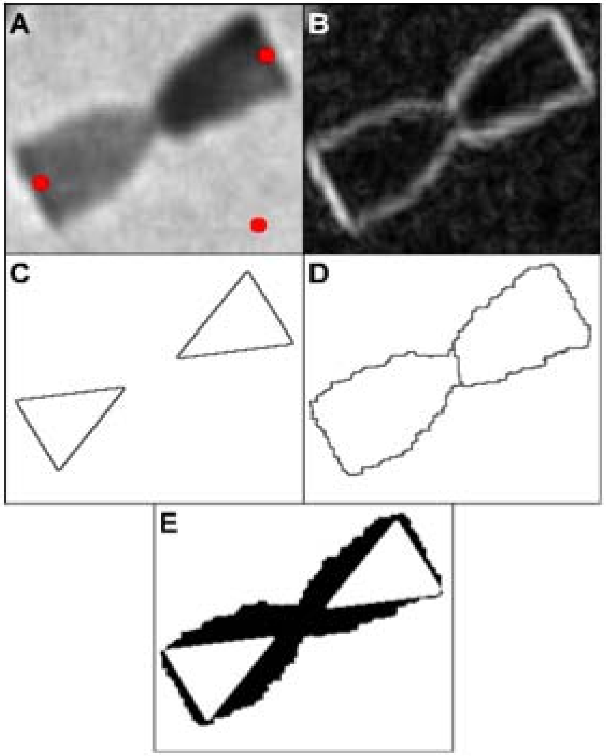


Figure S11 – SPW method applied to a double ZnO nanostructure. **A.** Original image with markers. Reprinted (adapted) with permission from (46). Copyright (2006) American Chemical Society; **B.** Image gradient (normalized); **C.** Results of the SPW method; **D.** Results of a standard watershed method; **E.** Area differences (in black).

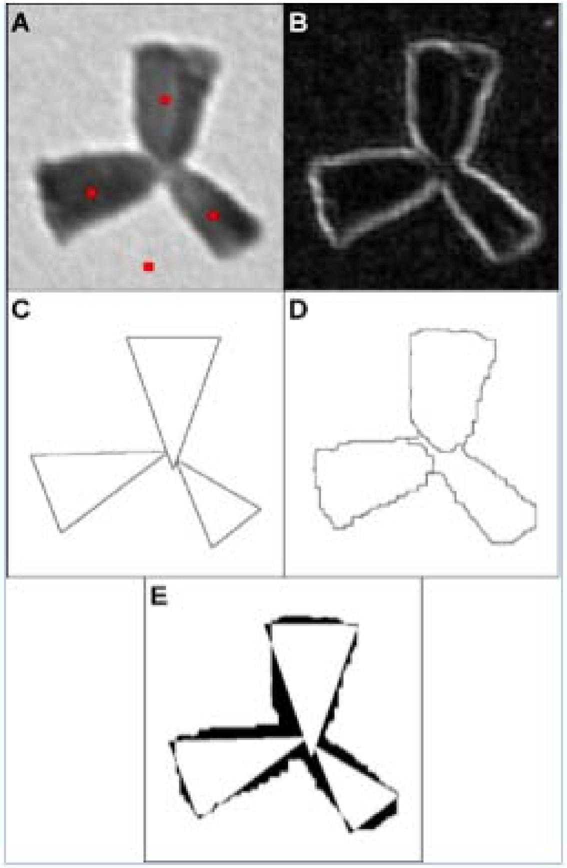


Figure S12 – SPW method applied to a triple ZnO nanostructure. **A.** Original image with markers. Reprinted (adapted) with permission from (46). Copyright (2006) American Chemical Society; **B.** Image gradient (normalized); **C.** Results of the SPW method; **D.** Results of a standard watershed method; **E.** Area differences (in black).

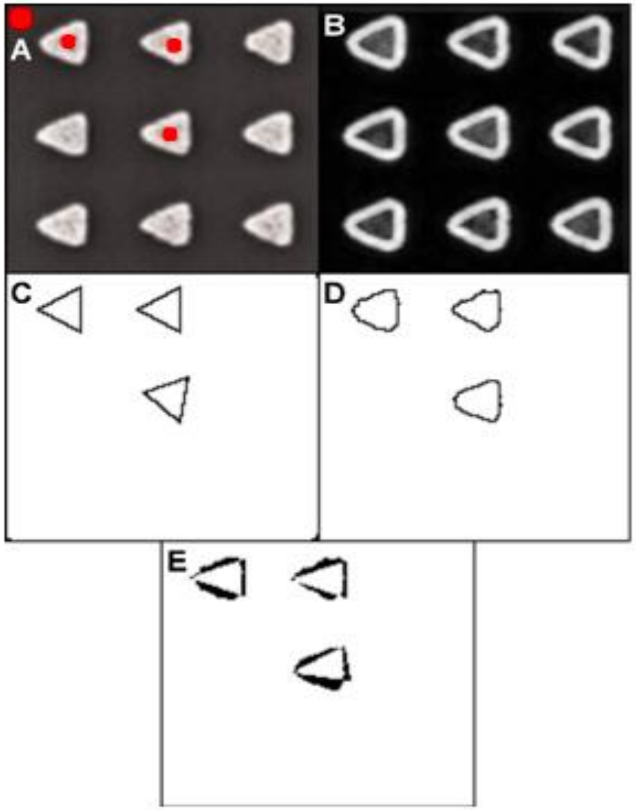


Figure S13 – SPW method applied to S-FIL PEGDA particles arranged as 200 nm triangles. Reprinted (adapted) with permission from (47) Copyright (2008) Elsevier. **A.** Original image with markers; **B.** Image gradient (normalized); **C.** Results of the SPW method; **D.** Results of a standard watershed method; **E.** Area differences (in black).

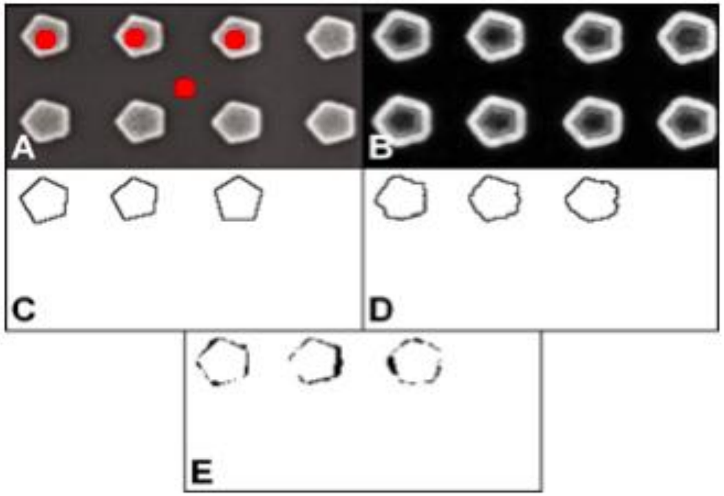


Figure S14 - SPW method applied to S-FIL PEGDA particles arranged as 400 nm pentagons. Reprinted (adapted) with permission from (47) Copyright (2008) Elsevier. **A.** Original image with markers; **B.** Image gradient (normalized); **C.** Results of the SPW method; **D.** Results of a standard watershed method; **E.** Area differences (in black).

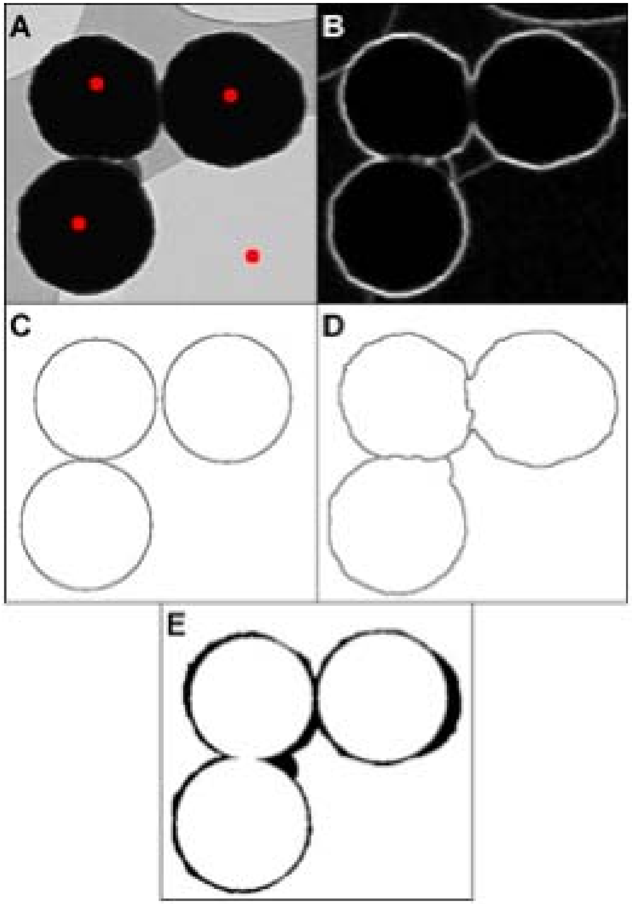


Figure S15 – SPW method applied to three carbon nanospheres. Reprinted (adapted) with permission from (48) Copyright (2005) Elsevier. **A.** Original

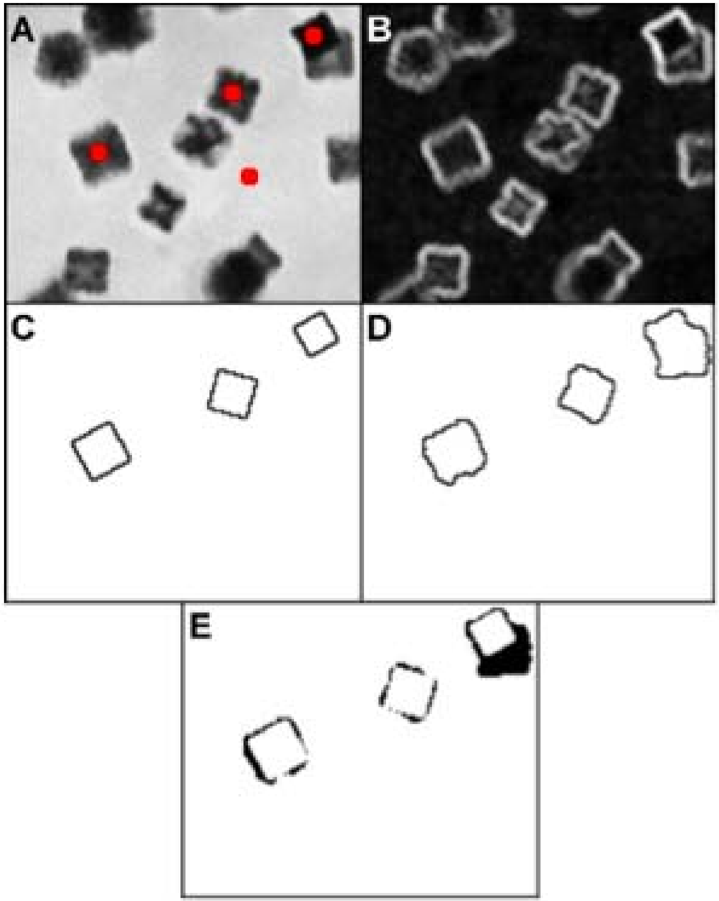
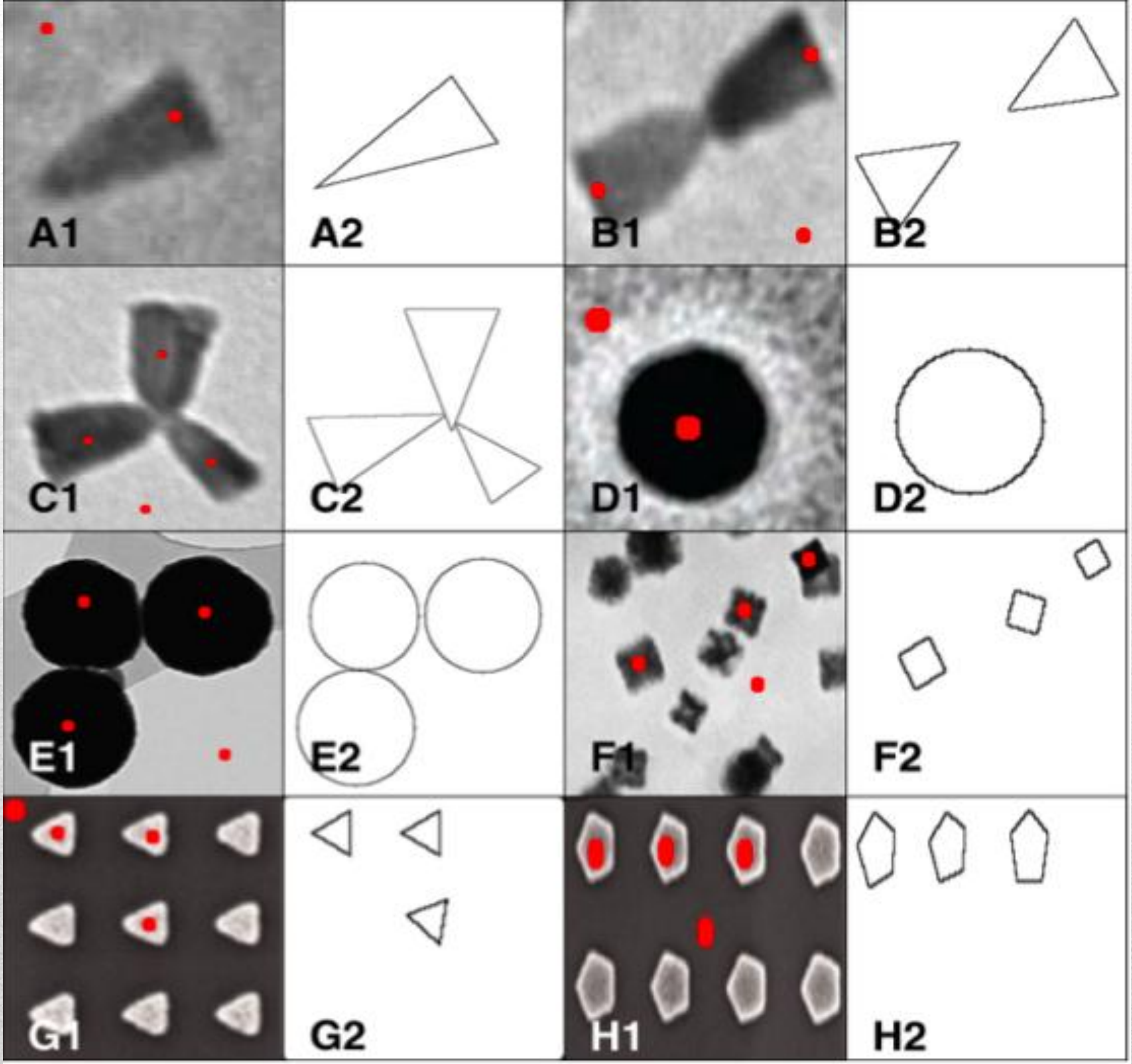
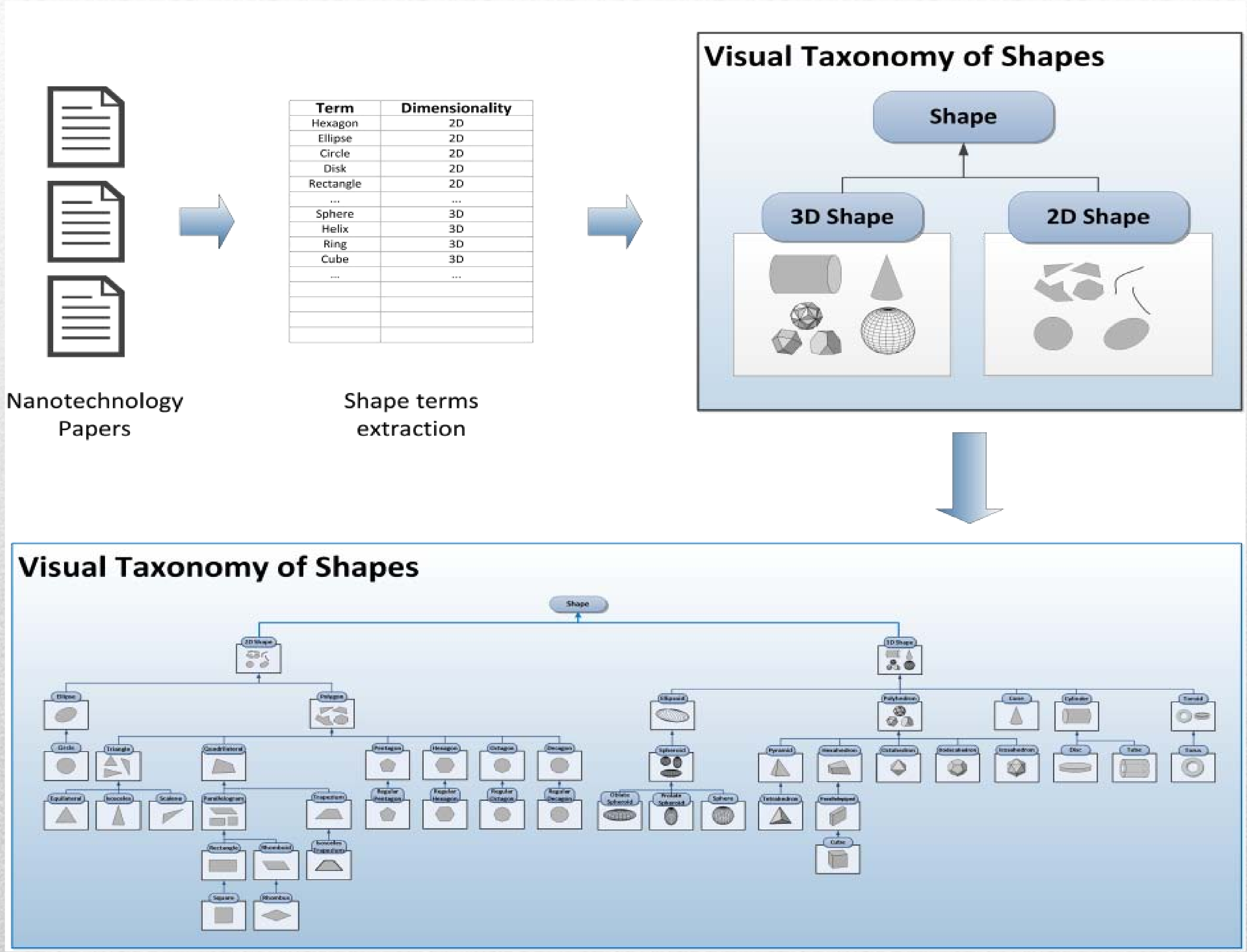


Figure S16 – SPW method applied to well-separated 50 nm Mo nanoparticles. Reprinted (adapted) with permission from (49)(49)(49)(merged) Copyright


A1
A2
B1
B2
C1
C2
D1
D2
E1
E2
F1
F2
G1
G2
H1
H2

Visual Taxonomy of shapes



Nanomedicine journal

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xx (2014) xxx – xxx

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Towards the Taxonomic Categorization and Recognition of Nanoparticle Shapes

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Abstract

The shape of nanoparticles and nanomaterials is a fundamental characteristic that has been shown to influence a number of their properties and effects, particularly for nanomedical applications. The information related with this feature of nanoparticles and nanomaterials is, therefore, crucial to exploit and foster in existing and future research in this area. We have found that descriptions of morphological and spatial properties are consistently reported in the nanotechnology literature, and in general, these morphological properties can be observed and measured using various microscopy techniques. In this paper, we outline a taxonomy of nanoparticle shapes constructed according to nanotechnologists' descriptions and formal geometric concepts that can be used to address the problem of nanomaterial categorization. We employ an image segmentation technique, belonging to the mathematical morphology field, which is capable of identifying shapes in images that can be used to (semi-) automatically annotate nanoparticle images.

Key words: Nanoparticle shapes; Taxonomic categorization; Nanoinformatics; Image processing; Watershed segmentation

Shape is a fundamental characteristic of components of living beings and entities such as viruses, cells, bacteria, organs, and, from an atomic perspective, of molecules and macromolecules, which includes nanoparticles. Regarding the latter, important characteristics of nanoparticles to medical applications such as drug delivery capabilities, adsorption, or the effectiveness of "nanodrugs" have shown to be influenced by the shape they present.[1–6]

A fundamental and pending problem in nanotechnology is the categorization and nomenclature of nanoparticles. To address this problem, two essential criteria have been identified[7]: uniqueness -so we can know exactly what materials we are talking about- and equivalence -to indicate if two materials are essentially the same one.

One of the first attempts for classifying nanostructured materials was made by Gleiter,[8] who considered the heterogeneousness of nanocompounds and the dimensionality of nanocomponents. This approach was extended by Pokropivny and Skorokhod,[9] combining the dimensionality of the nanocompounds. Similarly, Tomalia[10] proposed the development of a "periodic table" of nanoparticles and nanomaterials, including "shape" and "size" as two characteristics. Given the variability of these morphospatial characteristics of nanoparticles and nanomaterials,[11] knowing the shapes and forms of nanoparticles can be a necessary component of future classifications of nanoparticles and an aid in discerning mechanisms for their interactions in different environments.

The development of new nanomaterials by design requires categorizations of candidate materials based on their mechanisms of action. These mechanisms of action depend on a range of particle properties such as size, shape, crystal structure, reactivity, electronic band structure, toxicity, or affinity to biomolecules, etc., in addition to the properties of the media in which they are dispersed. Consequently, any categorization effort should accommodate annotation and mappings with respect to additional properties. Moreover, there is a growing need for the research

The authors of this work declare that there is not any competing commercial interest regarding the contents of this article.

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2nd part

Around various thoughts and topics for discussion about nanoinformatics, partially based on a comparison with other informatics disciplines

Elsevier book (*Nanoinformatics: Principles and Practices*)

- *Chapter 2 Nanoinformatics Program Essentials (Victor Maojo and others)*
- *Genesis of informatics in education (Victor Maojo and others)*
- *Model curricula for informaticians (Victor Maojo and others)*

-> Marty Fritts and Casimir Kulikowski (IEEE, ACMI, AAAS Fellow, NAM member)

Failed survey in ACMI (American College of Medical Informatics)

Nanoinformatics

- It cannot be considered just as the development of informatics applications for nanotechnology or nanomedicine
- Nanoinformaticians:
    - People who reason and solve problems at the intersection between nano areas and informatics –but reasoning is quite different at both sides
    - «Brokers» between informaticians and nanotechnologists
    - Emphasis should be centered on deep scientific issues, not just applications (e.g., ontologies, databases)

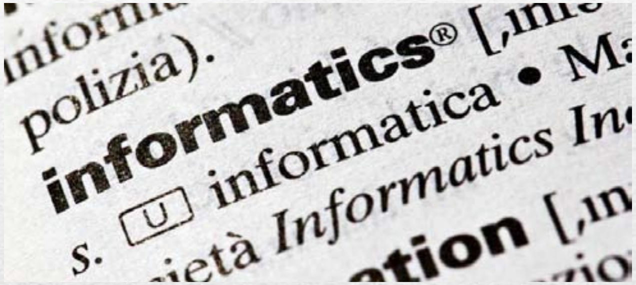
Nanoinformatics: possible topics (after Chapter 1 of the Elsevier book)

"(Biomedical) nanoinformatics refers to the use of informatics techniques for analyzing and processing information about the structure and physico-chemical characteristics of nanoparticles and nanomaterials, their interaction with their environments, and their applications for nanomedicine" (adapted from a Marty Fritts paper or presentation)

Topics

- Terminologies and Standards
- Ontologies and semantic search
- Data Integration and Exchange
- Systems' interoperability
- Data and text mining for nanotechnological research
- Linking nano-information to computerized medical records
- Basic and translational research
- Modeling and Simulation
- Imaging Informatics
- Nanoparticle characterization
- Networks of international researchers, projects and labs
- Nanoinformatics Education
- Ethical Issues

Definition of Nano - informatics



Informatics: what is?

Definition is not really so important, but to define the components, objectives, challenges, training, etc of the area

Three main components: Science + Engineering + Art (too early for nano?)

Informatics

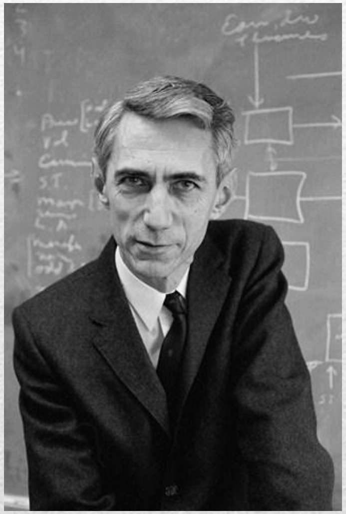
"Informatics" derives from the German "Informatik", the Russian "Informatika" and the French "informatique" —which combines "information" + "automatique". One concept lies at its core: *information*. is meant by information is not so obvious: it can convey a wide range of meanings:

- The concept of information as originally proposed by Szilard to provide an answer to the famous "Maxwell's demon" thought experiment in physics.
- The engineering or communications and coding theory sense that Shannon used to defined the term, where "information" is associated with the concept of entropy — also from physics.
- Other meanings of scientific information, such as, for instance, the information that is associated with molecules —e.g., binding—, with particles and sub-particles — quantum information— or with other biological entities like cells, tissues, organs, etc. This can refer to how DNA codes biological information—which is basically known— or how this information is translated and transmitted to higher levels of biological aggregation and function through living cells such as human neurons — which is as yet unknown. As Shannon himself realized and stated, his (syntactical) theory was not relevant to capture the characteristics of biological information·
- Broad societal and colloquial uses of the concept *information*, such as referring to the news, signals, stimuli, data + meaning, etc, seen from different social, economic, historical, or political or technological perspectives, defined, usually, quite vaguely.

Maojo V, Kulikowski CA. Note on Friedman's 'what informatics is and isn't'. Journal of the American Medical Informatics Association. 2013 Dec;20(e2):e365-6.

Information in computers and nature

Communication (Information) theory cannot be applied to biology as to engineering (Shannon, who knew a bit about this issue)



Claude Shannon

Focus?

MI: focus is the patient (simple and broad, but a convincing statement)

Bioinformatics: focus around genes (people and living beings)

Focus of nanoinformatics? Nanoparticles' physics, enginnering, interactions, toxicity, delivery, dynamics, applications…

Grand challenges

Advantages: no shortage of costumers (potential target equal to the world's population)

Focused on medicine and biology, whereas nanoinformatics addresses various fields

Medical informatics: grand challenges

There were many (extract knowledge from data and texts, modeling medical reasoning, creating unified terminologies, medical decision making, standards for interoperability, point-of care devices, etc)

MI Pioneers at the ACMI dinner, 2015, SF

Maybe the most relevant one is to build a personalized, universal Electronic Health Record (but this is mostly a Engineering and social challenge, not purely scientific)

Biology fundamentals (of bioinformatics)

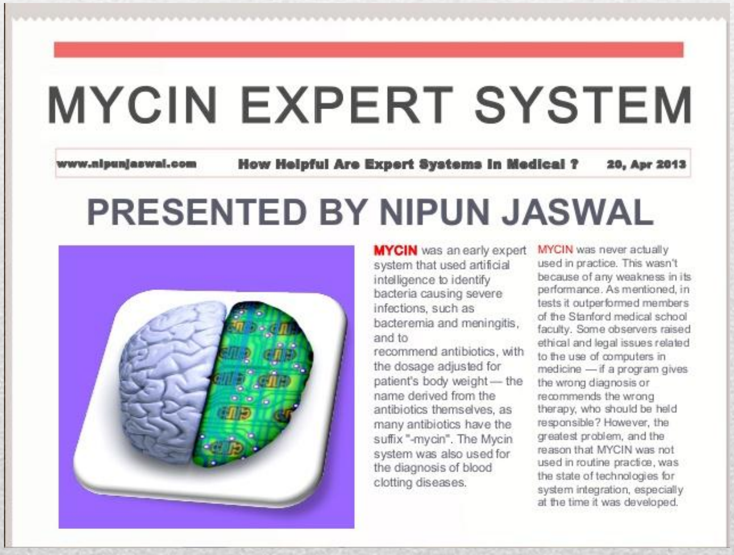
DNA → RNA → Protein

Crick's dogma of biology (under scrutiny in the last decade) made genomic research affordable when technology was ready and led later to establish the basis of the Human Genome Project

The Buck and the Big Bang

As stated by Bruce Blum, a software engineer and medical informatics pioneer, at an early stage medical informaticians decided not to pursue grand scientific challenges (the ones that could lead to Nobel prices) but systems that could lead to recover large investments (e.g., medical records, laboratory and hospital information systems)

Academic problems?



MYCIN EXPERT SYSTEM

www.nipunjaswal.com How Helpful Are Expert Systems In Medical ? 20, Apr 2013

PRESENTED BY NIPUN JASWAL

MYCIN was an early expert system that used artificial intelligence to identify bacteria causing severe infections, such as bacteremia and meningitis, and to recommend antibiotics, with the dosage adjusted for patient's body weight — the name derived from the antibiotics themselves, as many antibiotics have the suffix "-mycin". The Mycin system was also used for the diagnosis of blood clotting diseases.

MYCIN was never actually used in practice. This wasn't because of any weakness in its performance. As mentioned, in tests it outperformed members of the Stanford medical school faculty. Some observers raised ethical and legal issues related to the use of computers in medicine — if a program gives the wrong diagnosis or recommends the wrong therapy, who should be held responsible? However, the greatest problem, and the reason that MYCIN was not used in routine practice, was the state of technologies for system integration, especially at the time it was developed.

Some classical research, very (academically) succesful, were not focused on real (clinical) problems

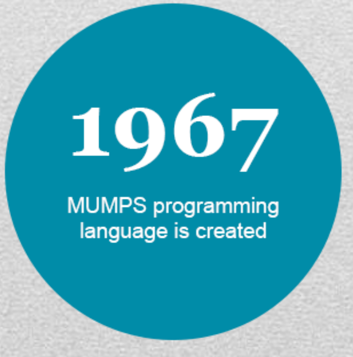
Up-to-date in technology?

BMI has been (usually) behind the state of the art regarding computer science/informatics methods and tools

Industry prefers a conservative approach

Example with MUMPS, a fourth generation language, only used by a few banks, companies and (many) hospitals

Many ancillary systems (and particularly data) must be preserved



From knowledge to data

Emphasis in bio and medical informatics was placed from the 1960s to 1980s in knowledge-based systems

Shift to data-centered systems after 1980s

	1950s	1960s	1970s	1980s
Data applications	Research	Prototype	Mature	Refined
Information applications	Concepts	Research	Prototype	Mature
Knowledge applications	Concepts	Concepts	Research	Prototype

Scope of medical computing (Blum)

From knowledge to data

And Nanoinformatics???

Supporting organizations behind

European Commission

NCBI National Center for Biotechnology Information

Large infrastructures (NCBI for bioinformatics, IAMIS centers for biomedical informatics)

Programs began around 1980

NATIONAL LIBRARY OF MEDICINE

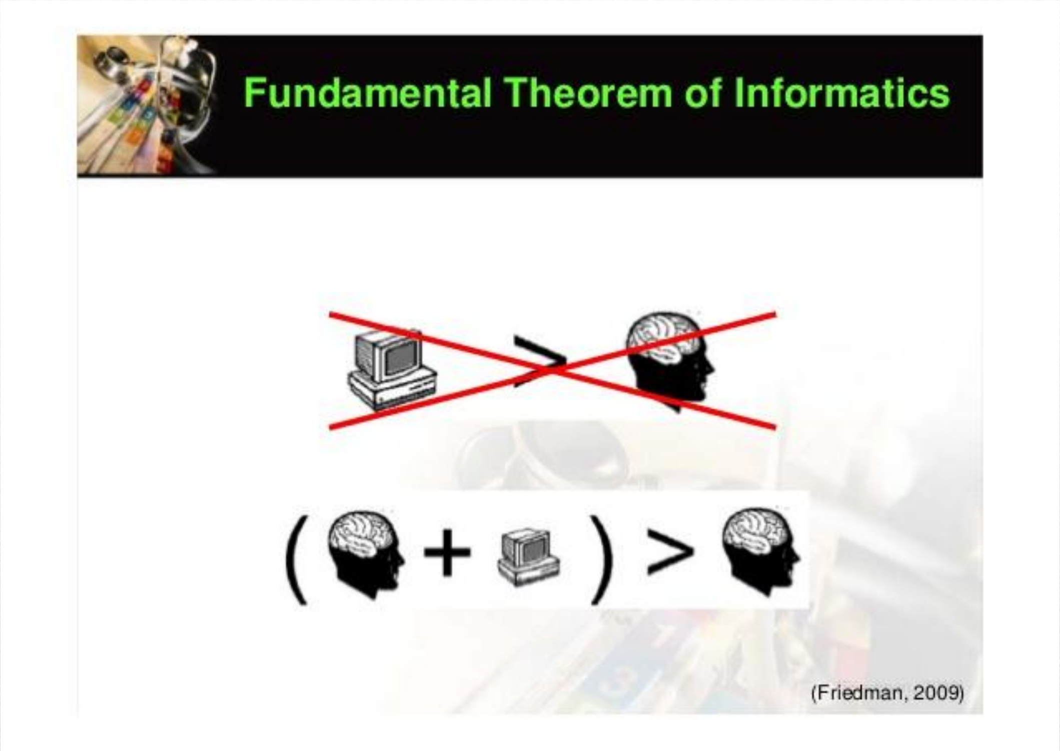
- A catalyzer of –informatics disciplines
- Training programs since 1970
- Thousands of trained people
- Many positions available now everywhere

Initiatives: example (NLM)
Pilot study grants for Integrated Advanced Information Management Systems (IAIMS)

From one Call:

- The National Library of Medicine provides IAIMS grants to health-related institutions and organizations that seek assistance for projects to plan, design, test and deploy systems and techniques for integrating data, information and knowledge resources into a comprehensive networked information management system that serves the organizations clinical, research, educational and administrative needs
- The long-term goal of NLMs IAIMS program is a comprehensive and convenient information management system, one that brings useful, usable knowledge to action settings in health care, education and research. Particular emphasis is placed on organization-wide and trans-organizational mechanisms that enable the easy flow of information between arenas of action, such as between health care and education, or between health-related organizations, such as from a community clinic to a hospital or public health department.
- Since 1984, NLM has provided IAIMS grants to academic health sciences centers to build networks and organizational mechanisms for information management. In its first two decades, the emphasis of IAIMS was building organizational mechanisms and infrastructure that were largely internal to academic centers. Technological advances and widespread access to the Internet make it possible now to shift the emphasis of IAIMS from building these capabilities to using them. The IAIMS challenge for the 21st century is to involve all kinds of health-related organizations in using local and national networks to acquire, manage, and deliver knowledge in a way that binds it to effective action.

Search for central theories of informatics



It cannot easily resist a serious scientific analysis, but it was quite succesful at some time

Note on Friedman's 'what informatics is and isn't'

Friedman's article 'What informatics is and isn't',[1] presents a necessary and timely analysis of the field of informatics. After defining some of its characteristics, training needs and also examples of what it isn't, the author re-introduces what he has called 'the fundamental theorem of informatics'[1]—originally formulated for biomedical informatics—'that persons supported by information technology will be better than the same persons performing the same task unassisted'. Figure 1 shows it graphically.

Both the theorem and the picture have become well known in the biomedical informatics field. However, while an interesting, thought-provoking exercise, this proposal about 'what informatics is and isn't' faces several scientific vulnerabilities, as noted below.

THE TERM 'INFORMATICS'

The term 'informatics' derives from the German 'Informatik', the Russian 'Informatika' and the French 'informatique', which combines 'information' with 'automatique'. One concept lies at its core: information. While it is clear how 'informatics' is semantically linked to 'information', what is meant by information is not so obvious: it can convey a wide range of meanings:

- The concept of information as originally proposed by Szilard to provide an answer to the famous 'Maxwell's demon' thought experiment in physics.
- The engineering or communication and coding theory sense that Shannon used to defined the term, in which 'information' is associated with the concept of entropy—also from physics.
- Other meanings of scientific information, such as, for instance, the information that is associated with molecules, for example, binding, with particles and sub-particles—quantum information—or with other biological entities such as cells, tissues, organs, etc. This can refer to how DNA codes biological information, which is basically known, or how this information is translated and transmitted to higher levels of biological aggregation and function through living cells such as human neurons, which is as yet unknown. As Shannon himself realized and stated, his (syntactical) theory was not relevant to capture the characteristics of biological information.[2]
- Broad societal and colloquial uses of the concept information, such as referring to the news, signals, stimuli, data plus meaning, etc, seen from different social, economic, historical, or political or technological perspectives, defined, usually, quite vaguely.

Without a standard meaning of information, it is difficult—or impossible—to establish a definition of informatics that can cover the scope of its uses from such an informational perspective.

VULNERABILITIES OF THE 'FUNDAMENTAL THEOREM OF INFORMATICS'

The fundamental theorem faces a number of vulnerabilities:

- It is not really about a fundamental scientific issue, nor does it provide a formal foundation for scientific inquiry. This contrasts with examples such as Shannon's information theory—including its theorems—which, using entropy to quantify channel capacity, provided the formal foundations for signal coding and communication.
- It is not a theorem, as in mathematics or logic, which Merriam–Webster online defines as: '(a) a formula, proposition, or statement in mathematics or logic deduced or to be deduced from other formulas or propositions, (b) an idea accepted or proposed as a demonstrable truth, often as a part of a general theory.' Friedman's is a challenging, intuitive hypothesis, but not really a theorem, as it can be neither deduced nor demonstrated –nor falsified.
- It is not about informatics itself. If it were, it would address and explain an intrinsic concept related to informatics, such as logic, processing, communication, storage, etc, which could help develop new theories, methods or products specific to informatics, but is here instead focused on the operational use of informatics by people.
- The proposed 'fundamental theorem' implies some kind of Turing-like test, including conditions for its applicability, and experimentally measurable outcomes to demonstrate its validity. It can be considered too general, and subject to refutation in practice.
- Computer interaction is hardly as unambiguous as the 'fundamental theorem' suggests. Harvard's Shoshana Zuboff,[3] presciently described how computers introduced by organizations lacking good information models, and socially well-adapted management structures (often by persons lacking adequate skills or understanding of information processes) can hurt, rather than improve work process efficiency and effectiveness.
- Computers relying on imprecise or inappropriate models of economic, technological and sociological conditions frequently detract from intelligent human performance. For creative artistic endeavors, such as writing, the value added by computers can be questionable, as per Nobelist Vargas Llosa: 'the more intelligent our computer is, the dumber we will be'.[4]

THE 'FUNDAMENTAL THEOREM' PICTURE

Figure 1, obviously metaphorical in 'adding together' very different entities like a human brain and a computer, brings to mind the strictures from John Von Neumann himself,[5] on the fundamental

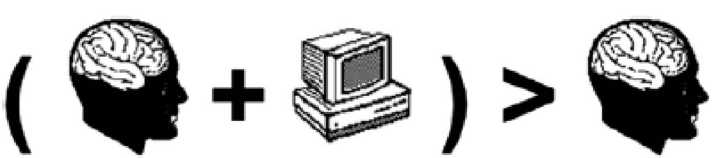


Figure 1 Friedman's 'fundamental theorem of informatics'.[1]

Maojo V, Kulikowski CA. Note on Friedman's 'what informatics is and isn't'. J Am Med Inform Assoc. 2013 Dec;20(e2):e365-6.

Victor Maojo, UPM, June 2, 2016

Problematic examples

Some philosophers entered the area of biomedical ontologies stating that these should follow Aristotelian assumptions (since ontology is an area of classical philosophy!)

The argument (or phallacy, for some) suceed, and many ontologies follow such direction

Biomedical Ontologies: Toward Scientific Debate

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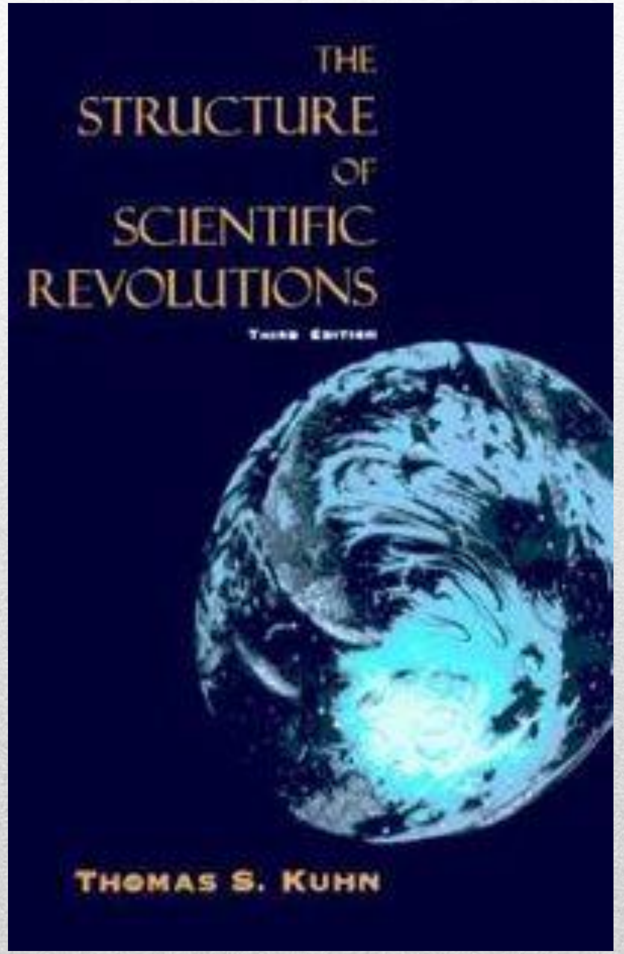
Keywords
Biomedical ontologies, biomedical informatics, spatial ontologies, artificial intelligence, mathematical morphology

Summary
Objectives: Biomedical ontologies have been very successful in structuring knowledge for many different applications, receiving widespread praise for their utility and potential. Yet, the role of computational ontologies in medical ontologies that are based largely on classical, Aristotelian ontological models of reality. Second, we raise various open questions about biomedical ontologies that require further research, analyzing in more detail those related to visual reasoning and spatial ontologies.
Results: We outline significant scientific issues that biomedical ontologies should consider, beyond current efforts of building practical consensus between them. For spatial on-

"modulates the activity of a caspase, any of a group of cysteine proteases involved in apoptosis" [4]. With the above one can define facets (properties of relationships), instances (individuals belonging to a class), formal axioms, rules, functions, procedures, ontology mappings and other means of manipulating the elements of an ontology. In addition, inheritance in computational ontologies allows properties associated with a higher level (more en-

Something new? No…



"It is, I think, particularly in periods of acknowledged crisis that scientists have turned to philosophical analysis as a device for unlocking the riddles of their field. Scientists have not generally needed or wanted to be philosophers. Indeed, normal science usually holds creative philosophy at arm's length, and probably for good reasons.". (**Thomas S. Kuhn,** 1962)

Without paradigms (i.e. central theories, exemplars, solid objectives, clear vision, scientific debate), will be absorbed by other areas (BMI for nanomedicine) or just technical staff for nanotechnologists

Medical Informatics and Bioinformatics: Integration or Evolution through Scientific Crises?

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Summary

Objectives: To contribute a new perspective on recent investigations into the scientific foundations of medical informatics (MI) and bioinformatics (BI). To support efforts that could generate synergies and new research directions.

Methods: MI and BI are compared and contrasted from a philosophy of science perspective. Historical examples from MI and BI are analyzed based on contrasting viewpoints about the evolution of scientific disciplines.

Results: Our analysis suggests that the scientific approaches of MI and BI involve different assumptions and foundations, which, together with largely non-overlapping communities of researchers for the two disciplines, have led to different courses of development. We indicate how their respective application domains, medicine, and biology may have contributed to these differences in development.

Conclusions: An analysis from the point of view of the philosophy of science is characteristic of established scientific disciplines. From a Kuhnian perspective, both disciplines may be entering a period of scientific crisis, where their foundations are questioned and where new ideas (or paradigm shifts) and a progressive research programme are needed to advance them scientifically. We discuss research directions and trends both supporting and challenging integration of the subdisciplines of MI and BI into a unified field of biomedical informatics (BMI), centered around the evolution of information cybernetics.

Keywords
Medical informatics, bioinformatics, philosophy of science, paradigm shift, scientific crisis, evolution

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1. Introduction

The rapid completion of the Human Genome Project and the many other successes in genomics and proteomics have radically changed the role of computational methods in biology over the past five years. Bioinformatics (BI) is emerging as a discipline which encompasses a wide range of informatics methodologies, essential to solving biological problems at the molecular and cellular levels. Its success is reflected by: 1) BI publications and tools being routinely cited for contributing to research results in the major biological journals; 2) funding agencies intensely supporting BI projects; 3) BI research groups dramatically expanding in industrial and academic programs; and 4) the impact of major BI scientific journals rapidly increasing. Much of the promise of BI is influenced by expectations that these computational and informatics tools will lead to deeper understanding of human health and the treatment of disease, which is expected to come from the more integrated perspectives of evolutionary, population, environmental, and systems biology [1].

Yet, how real are these expectations for BI in the near future? Some recent articles [2, 3] suggest that genetics is still far from showing which genes play significant roles in most human diseases – and whether and how they play such roles. Whereas the objectives and methods needed for the Human Genome Project were ambitious but well-focused, considerable complexity and more widely distributed research efforts are envisioned in follow-on projects and programs that attempt to map the difficult pathway from genotype to phenotype [4].

In contrast to BI, medical informatics (MI) is a more established discipline, with roots which can be traced back to the 1950s. It evolved from a myriad of computational applications in clinical and academic medicine, ranging from the very practical interfacing of advanced instrumentation and clinical information programs, to the formal computational modeling of logic and uncertainty in medical decision making [5, 6]. By the 1970s medical information systems of many types became wide-spread, and MI emerged as a discipline that integrated the diversity of research, practice, and educational software and hardware tools and methodologies which proliferated. The emergence of the Internet and the web in the 1990s completely changed the dynamics of the field, making an abundance of heterogeneous, biomedical information widely available. MI researchers have responded with an increased focus on data and knowledge standardization, interoperability and management. At the same time, problems of quality of information content, responsibility for, and security of the distributed networked medical information raises issues unique to health care. During the course of MI's development, there has been an ongoing debate about whether MI is more of a science, art, or engineering discipline [7-10]. This kind of debate is not uncommon as disciplines evolve, and the much younger field of BI has only recently begun to experience them [11, 12]. The emergence of BI has increased the debate about the directions and future research agenda for both fields, and whether they are likely to be integrated within a common framework of biomedical informatics (BMI), as an increasing number of MI professionals shift their research and academic interests towards BI.

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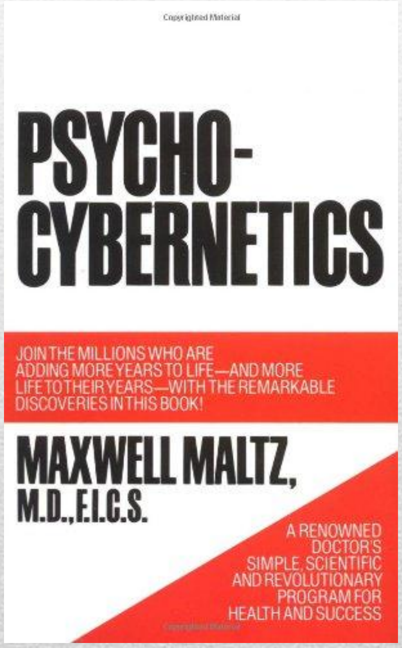
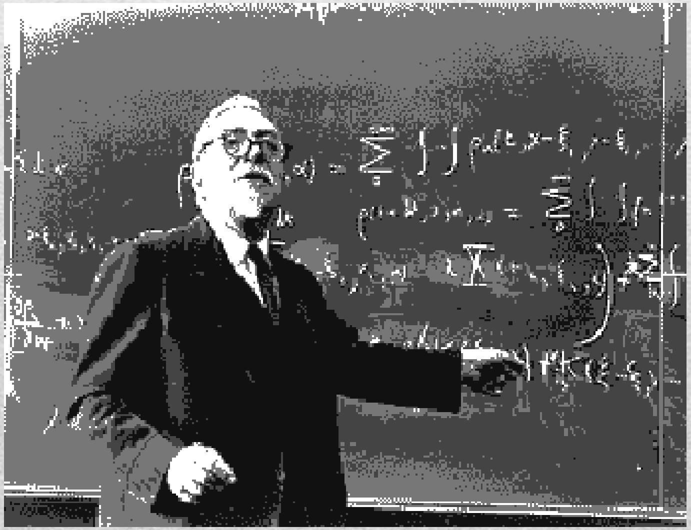
Disciplines appear, succeed…but may disappear soon, too

Cybernetics vanished because it dispersed into too many issues, some of them not scientific (e.g., psychocybernetics, social, control of the mind), and the lack of previous geniuses (von Neumann, Pitts, Shannon, Wiener…)





Name of the discipline

- (Bio)medical computing, computers in medicine, etc. in the 1950s and 60s
- Medical informatics in the 1980s
- Biomedical informatics around 2000
- Proposals now for “data science”

- Computational biology since the 1960s
- + Bioinformatics around 1995

(Note: Presented in 2009)

Hopefully, there is room for another -informatics area (or even discipline)

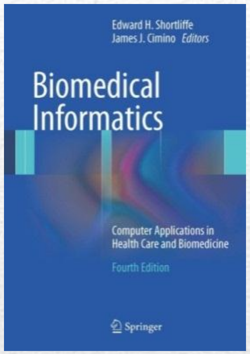
Medical Informatics, Bioinformatics, Biomedical Informatics, Health Informatics, Clinical Informatics, Clinical Bioinformatics, Translational Bioinformatics, Public Health Informatics, Genome Informatics, Dental Informatics, Nursing Informatics, Imaging Informatics, Neuroinformatics, Molecular Informatics, Chemoinformatics, Pharmainformatics

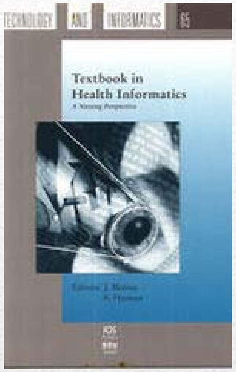
i.e., MI (a), BI, BMI, HI, CI, CBI, TBI, PHI, GI, DI,NI (a), II, NI (b), MI (b), ChI, PI…

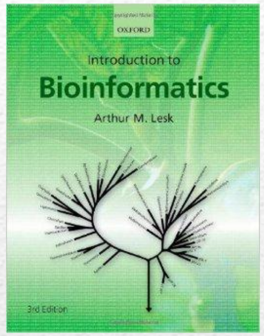
And now, Nanoinformatics, ie, NI

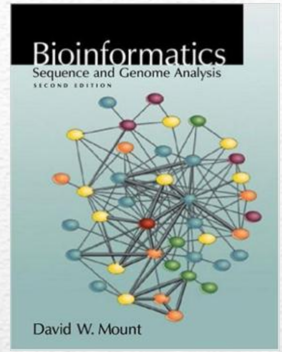
You got it???

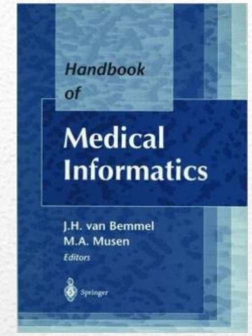
Many textbooks of Bio- and Medical Informatics published in the last 25 years

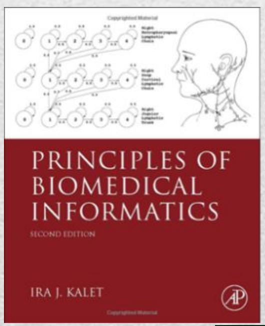


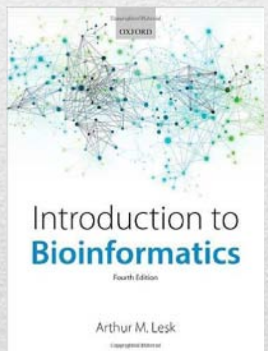


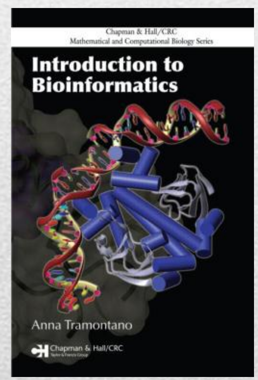


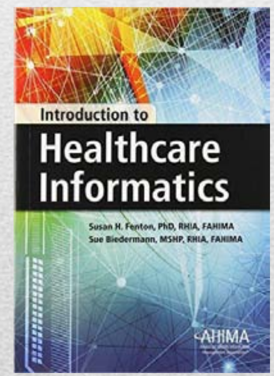


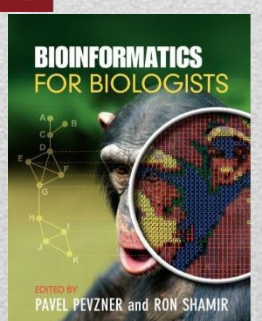


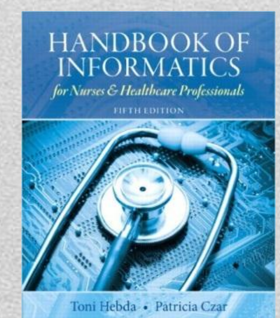












Just a few examples.
There are many more…

Victor Maojo, UPM, June 2, 2016

Societies: academic vs industry

EFMI
EUROPEAN FEDERATION for MEDICAL INFORMATICS

AMIA
INFORMATICS PROFESSIONALS. LEADING THE WAY.

IMIA

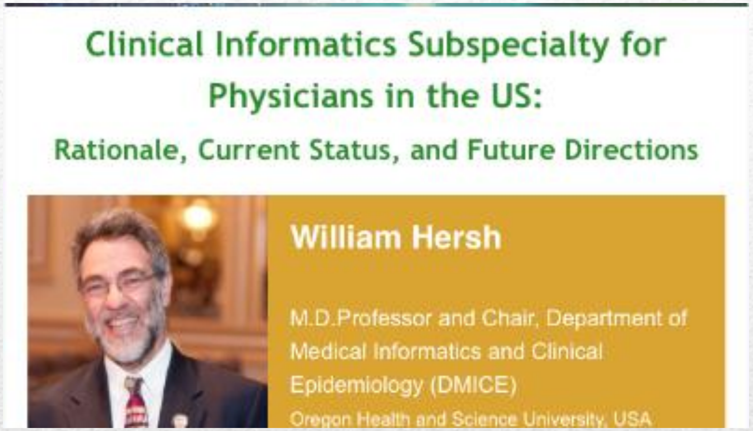
iSCB
INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY

ACMI
INFORMATICS FELLOWS. LEADING WITH DISTINCTION.

EMB
IEEE Engineering in Medicine & Biology Society

HiMSS
transforming healthcare through IT

Professional careers



In medical informatics:

1960s: logicians, mathematicians and engineers

1970s: computer scientists

1980s: physicians, nurses, pharmacists, etc

Now a medical subspeciality

In bioinformatics, a mixture of computer scientists and biologists

Terminologies

SNOMED® INTERNATIONAL

ICD-10

LOINC®
Logical Observation Identifiers Names and Codes

HGNC
HUGO Gene Nomenclature Committee

Medical Subject Headings MeSH

IEEE

DICOM℠
Digital Imaging and Communications in Medicine

HL7® INTERNATIONAL

IHE™

A service of the U.S. National Library of Medicine | National Institutes of Health

Unified Medical Language System®

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Education: directions

	Yes/No
Nanoinformatics as an independent discipline or area, with a solid future for prospective students? If yes, then:	
Graduate programs (BS, MS, PhD, joint programs in two areas)	
Training research programs	
Intensive courses (1-2 weeks)	
On-line programs (1-12 months, 1 week)	
MOOCs	

Curriculum

Areas:

- Basic nanotechnology (topics needed to be included)
- Informatics (programming, data structures, databases, algorithms, networks, artificial intelligence, Web engineering, data science, etc)
- Others: Scientific methodologies, start-up creations, study designs, manuscript writing…

Candidates:

- Nanotechnologists (physicists, engineers, biologists)
- Informaticians (computer scientists, engineers)
- Others? (in biomedical informatics, there is even a bunch of philosophers...)

Academic

Own departments or high-level units?

It took almost 50 years to top universities such as Stanford or Harvard to create specific departments (although training programs were created 30+ years ago)

Conclusions

We’ve got a long road ahead (for the area and the book), so let me avoid to extract conclusions now!

Thanks!