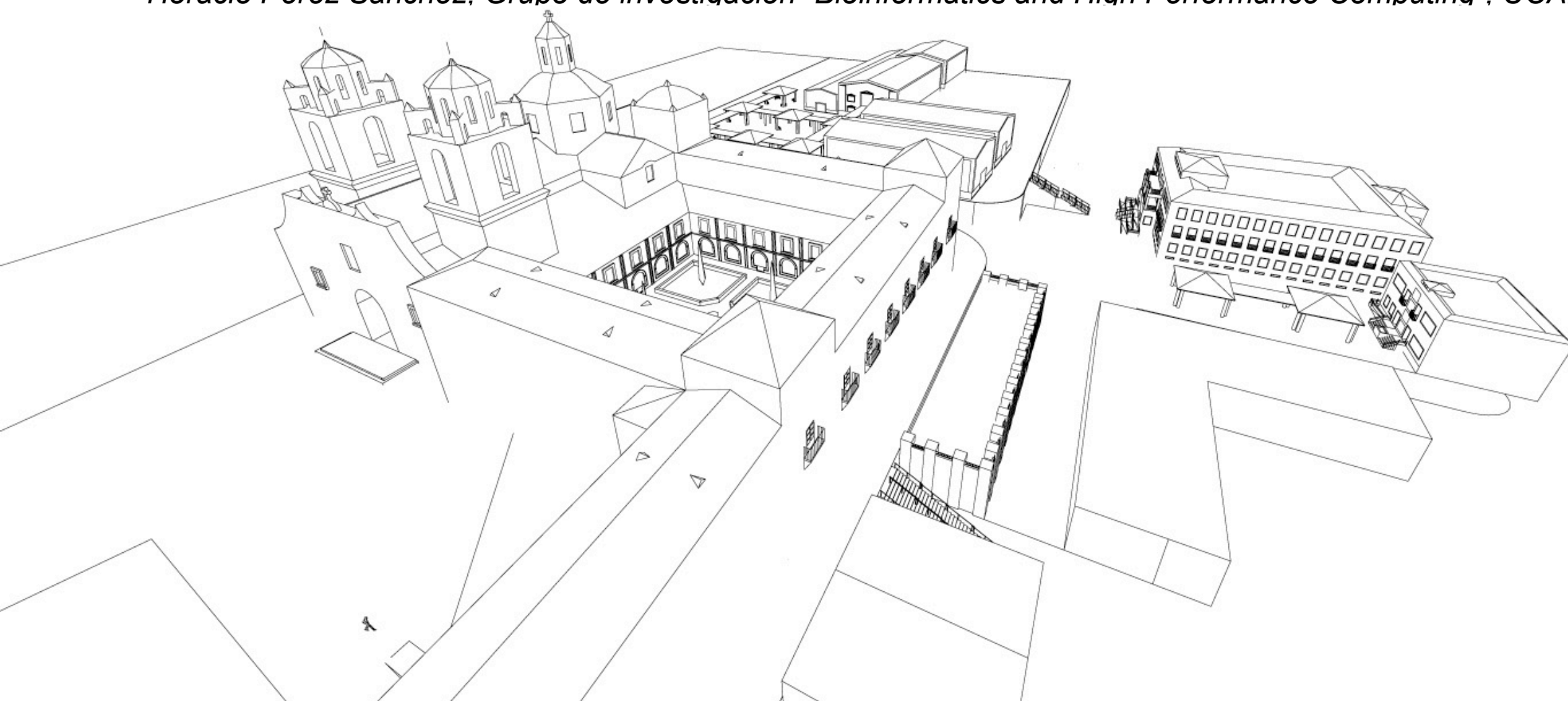




Transferencia de tecnología en el contexto del descubrimiento de compuestos bioactivos; ¿Cómo vender servicios de modelado molecular?

Horacio Pérez Sánchez, Grupo de investigación "Bioinformatics and High Performance Computing", UCAM



Lunes, 4 de mayo de 2015

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Universidad Católica San Antonio de Murcia - Tlf: (+34) 968 27 88 00 info@ucam.edu - www.ucam.edu

Bioinformatics and High Performance Computing Research Group

BIO-HPC Website



Welcome to the website of the Bioinformatics and High Performance Computing Research Group (BIO-HPC). Our multidisciplinary research group is based at the [Catholic University of Murcia](#) (UCAM, South East Spain). We work in the exploitation of High Performance Computing Architectures (Supercomputers, GPUs) for the development, acceleration and application of bioinformatics applications. We deliver and apply an improved integrated computational-experimental strategy for the discovery of bioactive (drugs, fungicides, cosmetics, food technology, etc) compounds with

Schrödinger equation

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\vec{r}) \right] \Psi(\vec{r}, t)$$

Second Series

December, 1926

Vol. 28, No. 6

THE PHYSICAL REVIEW

AN UNDULATORY THEORY OF THE MECHANICS OF ATOMS AND MOLECULES

BY E. SCHRÖDINGER

ABSTRACT

The paper gives an account of the author's work on a new form of quantum theory. §1. The Hamiltonian analogy between mechanics and optics. §2. The analogy is to be extended to include real "physical" or "undulatory" mechanics instead of mere geometrical mechanics. §3. The significance of wave-length;



The Nobel Prize in Physics 1933
Erwin Schrödinger, Paul A.M. Dirac

The Nobel Prize in Physics 1933 was awarded jointly to Erwin Schrödinger and Paul Adrien Maurice Dirac "for the discovery of new productive forms of atomic theory."




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Nobel Prizes and Laureates

Chemistry Prizes
 < 2013 >

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[All Nobel Prizes in 2013](#)


The Nobel Prize in Chemistry 2013
 Martin Karplus, Michael Levitt, Arieh Warshel

The Nobel Prize in Chemistry 2013



© Harvard University
Martin Karplus



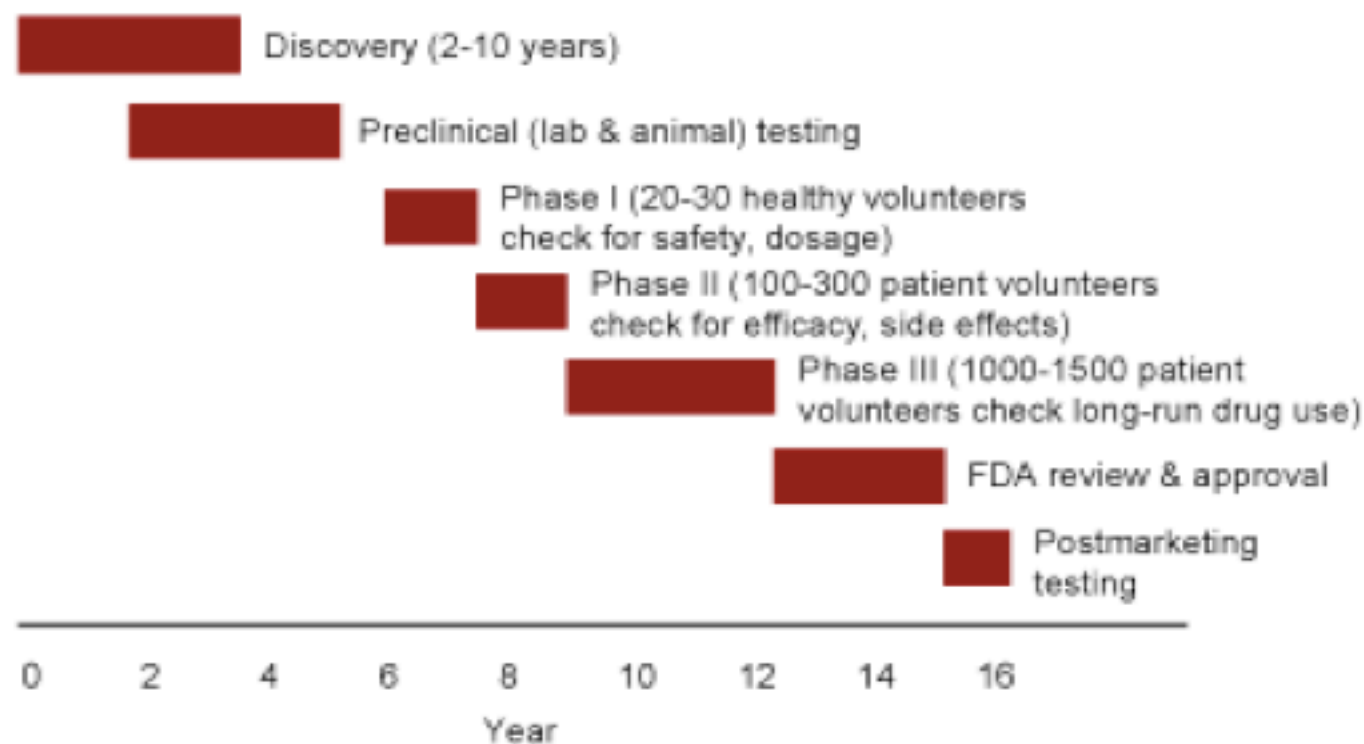
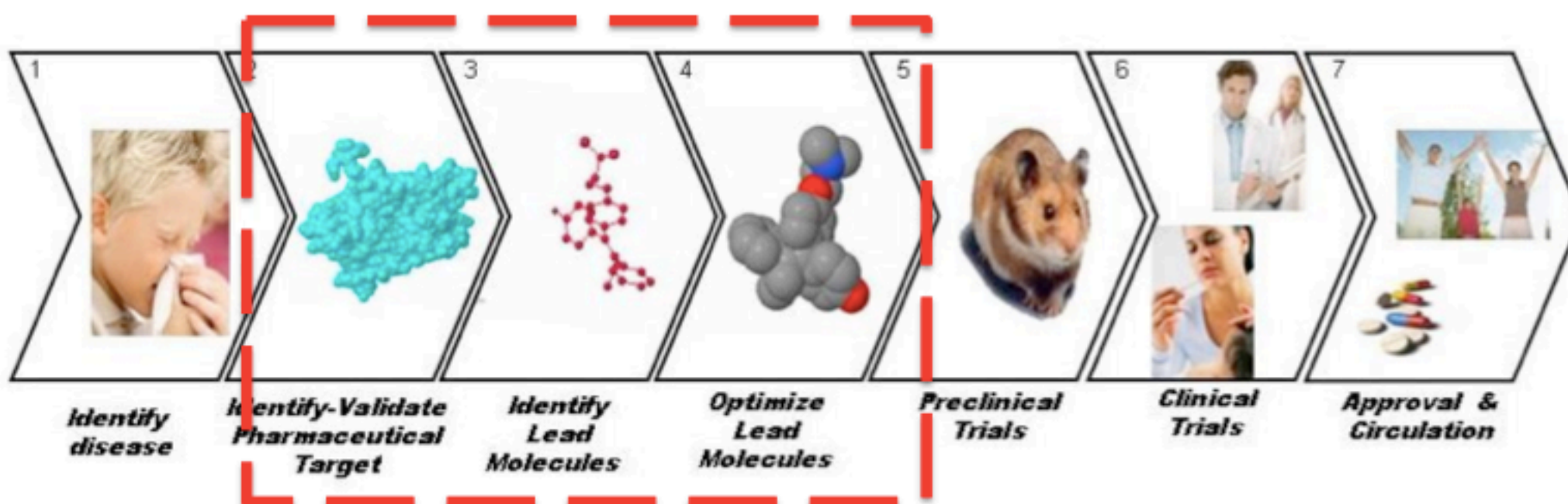
Photo: © S. Fisch
Michael Levitt



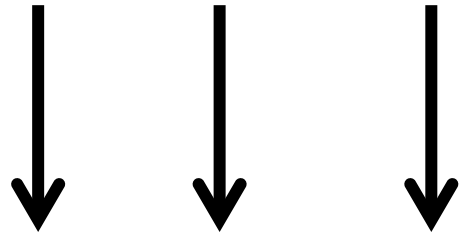
Photo: Wikimedia Commons
Arieh Warshel

The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*.

DRUG DISCOVERY PROCESS



€€€, RESEARCH FUNDS (UCAM)



BIOINFORMATICS AND HIGH PERFORMANCE COMPUTING RESEARCH GROUP

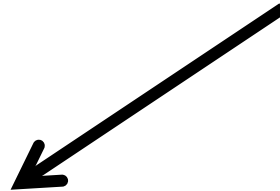


The Schrödinger Equation

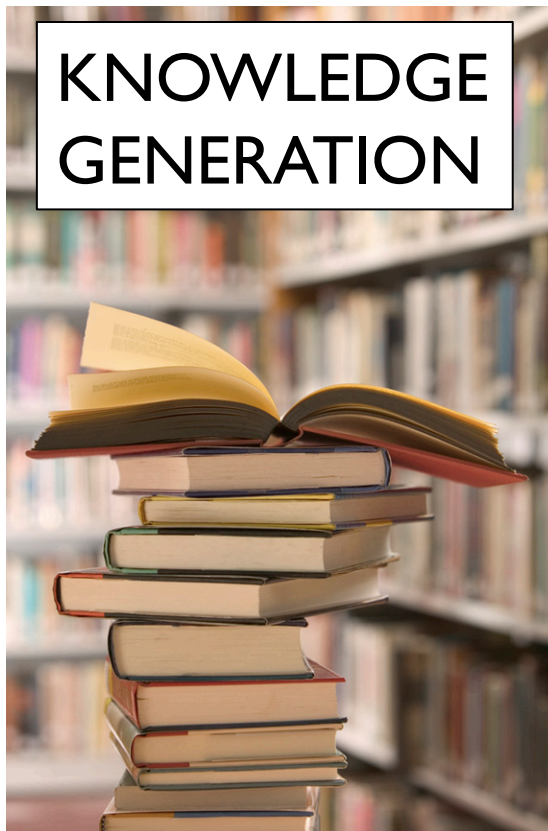
$$\left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E \psi(x)$$

Hamiltonian operator Wave function Energy

SUPERCOMPUTER

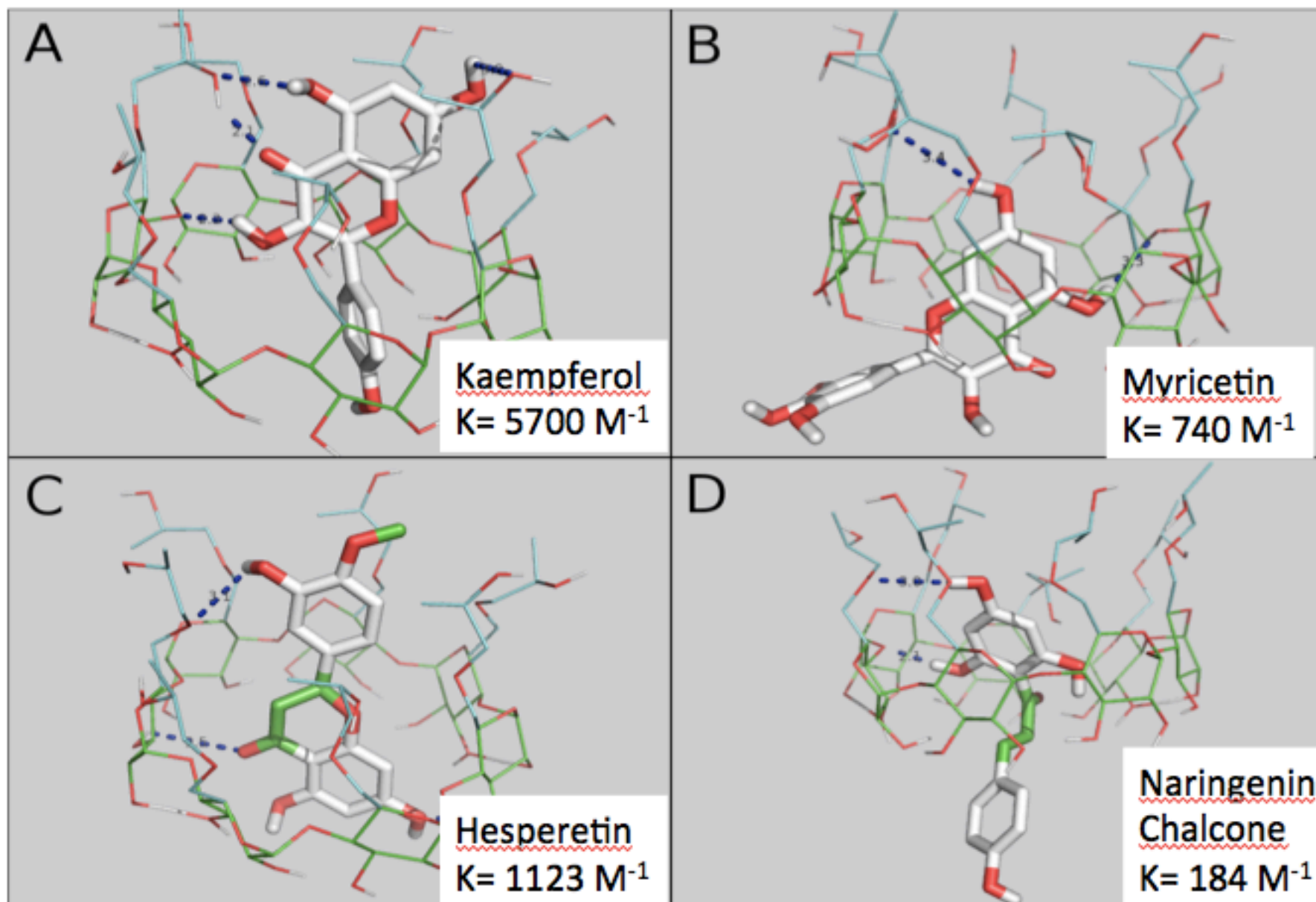


KNOWLEDGE GENERATION



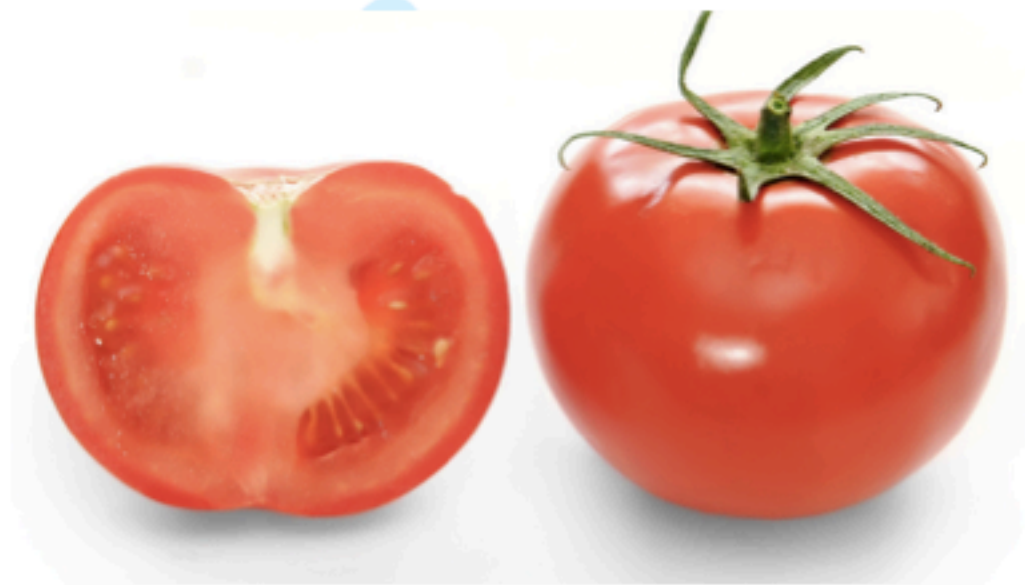
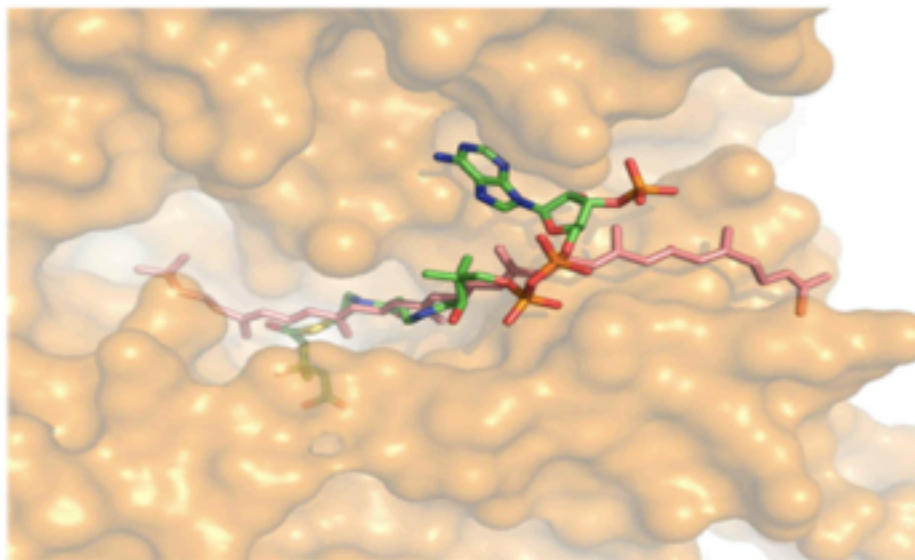
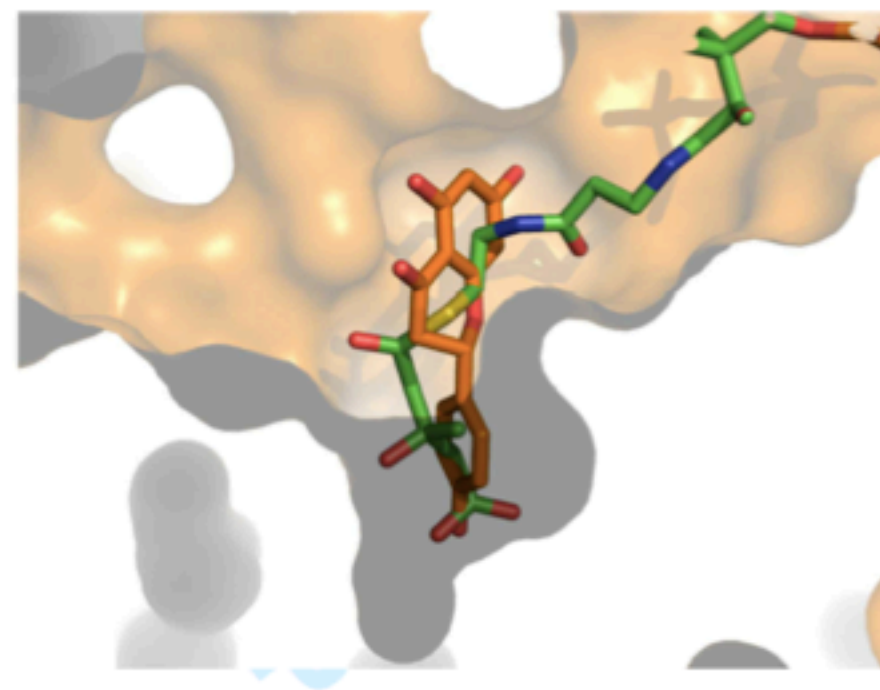
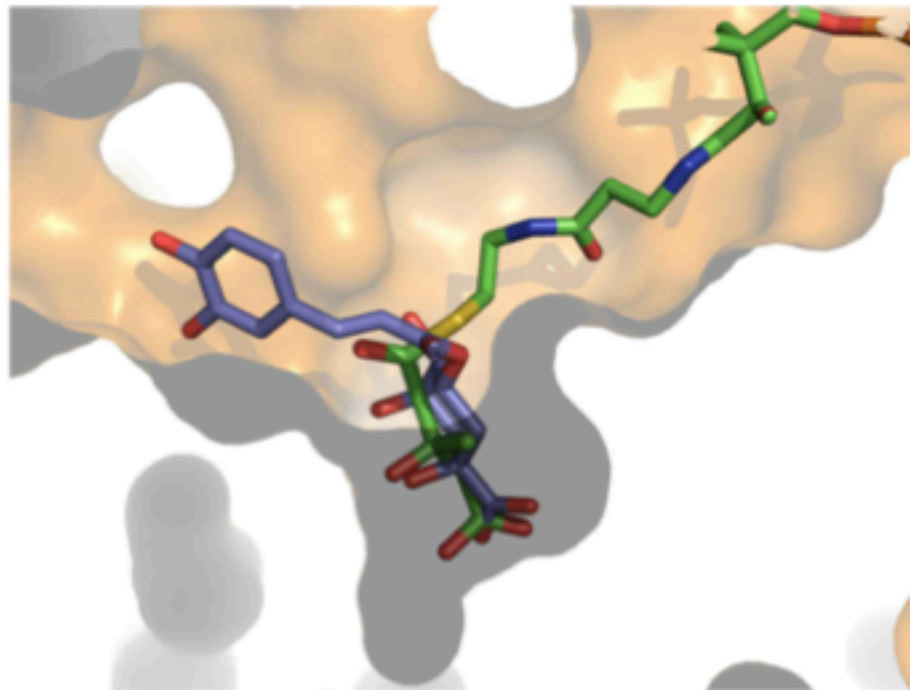
FUNDAMENTAL RESEARCH

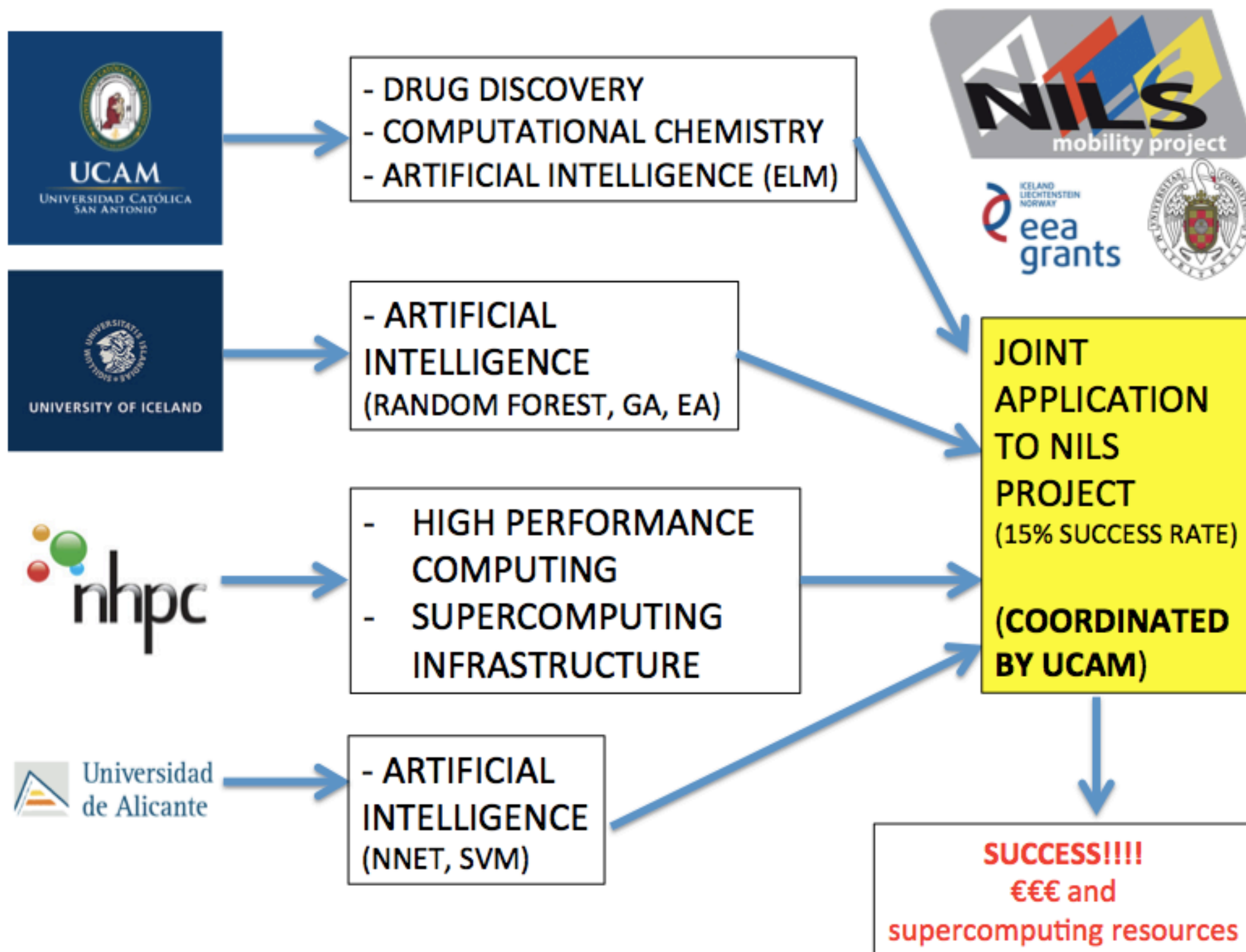
Molecular encapsulation of flavonoids with cyclodextrins (Collaboration with Estrella Núñez, UCAM)



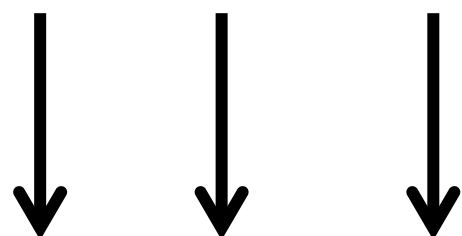
- Molecular modeling for the understanding interactions and encapsulation phenomena
- Efficient identification of new, high affinity guest molecules of cyclodextrin
- Modeling of modifications of cyclodextrins

FOOD SCIENCE: The inhibitor effects of bioactive compounds binding to hepatic HMGCR: in vivo study and molecular modelling





€€€, RESEARCH FUNDS (UCAM)



BIOINFORMATICS AND HIGH PERFORMANCE COMPUTING RESEARCH GROUP

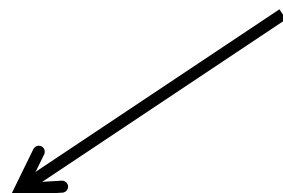


The Schrödinger Equation

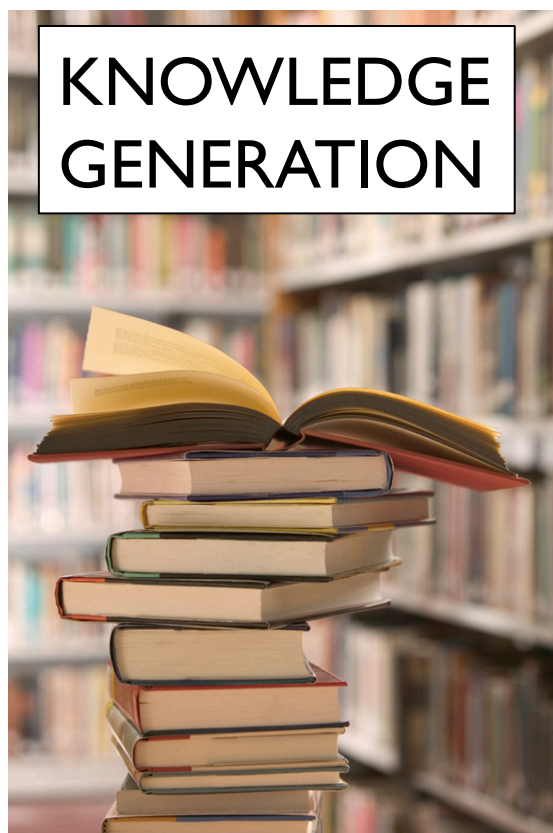
$$\left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E \psi(x)$$

Hamiltonian operator Wave function Energy

SUPERCOMPUTER



KNOWLEDGE GENERATION



FUNDAMENTAL RESEARCH

DISCOVERY OF DRUGS



APPLIED RESEARCH



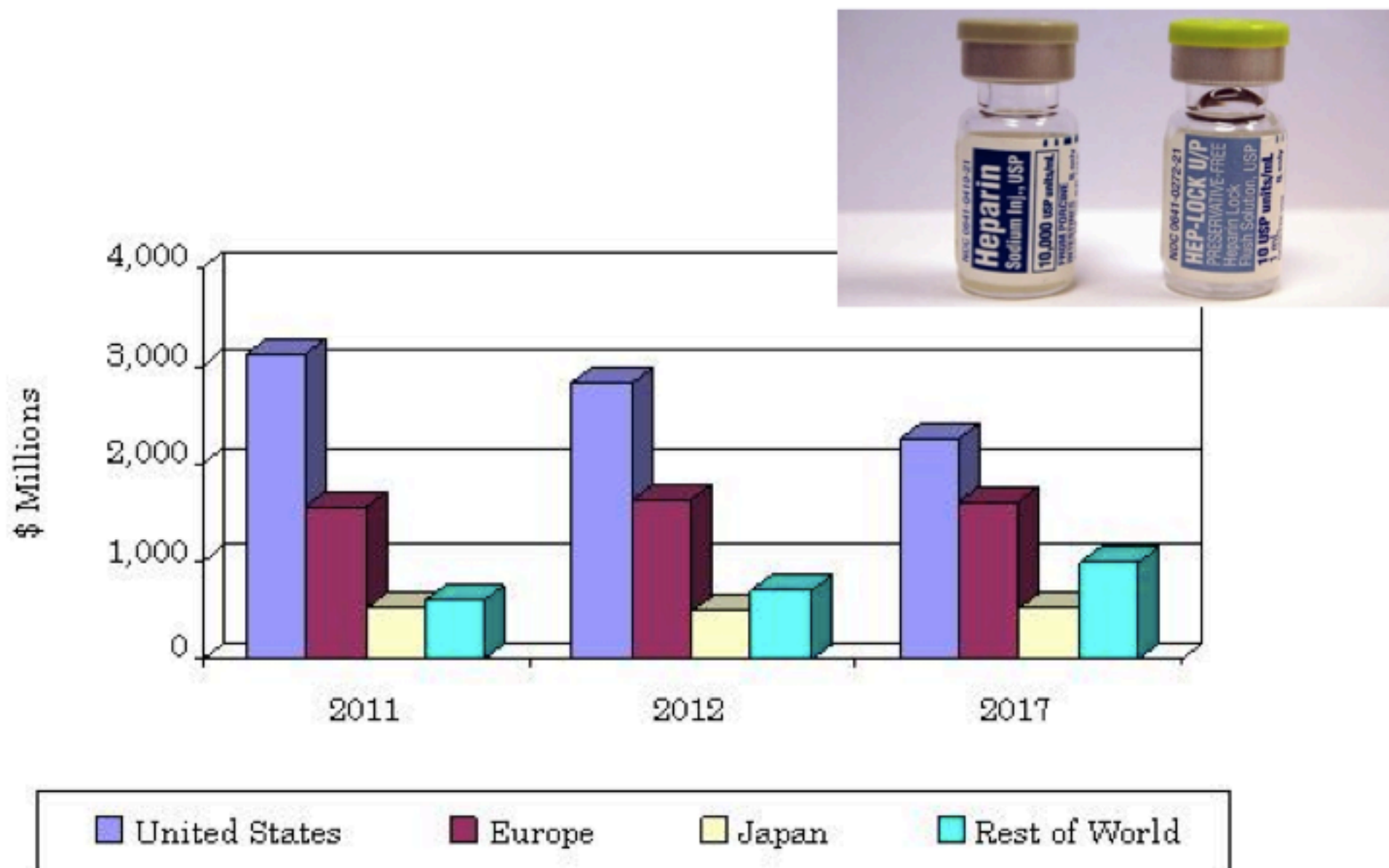
biología en el contexto del de

oactivos; ¿Cómo vender servicios de modelado molecular?

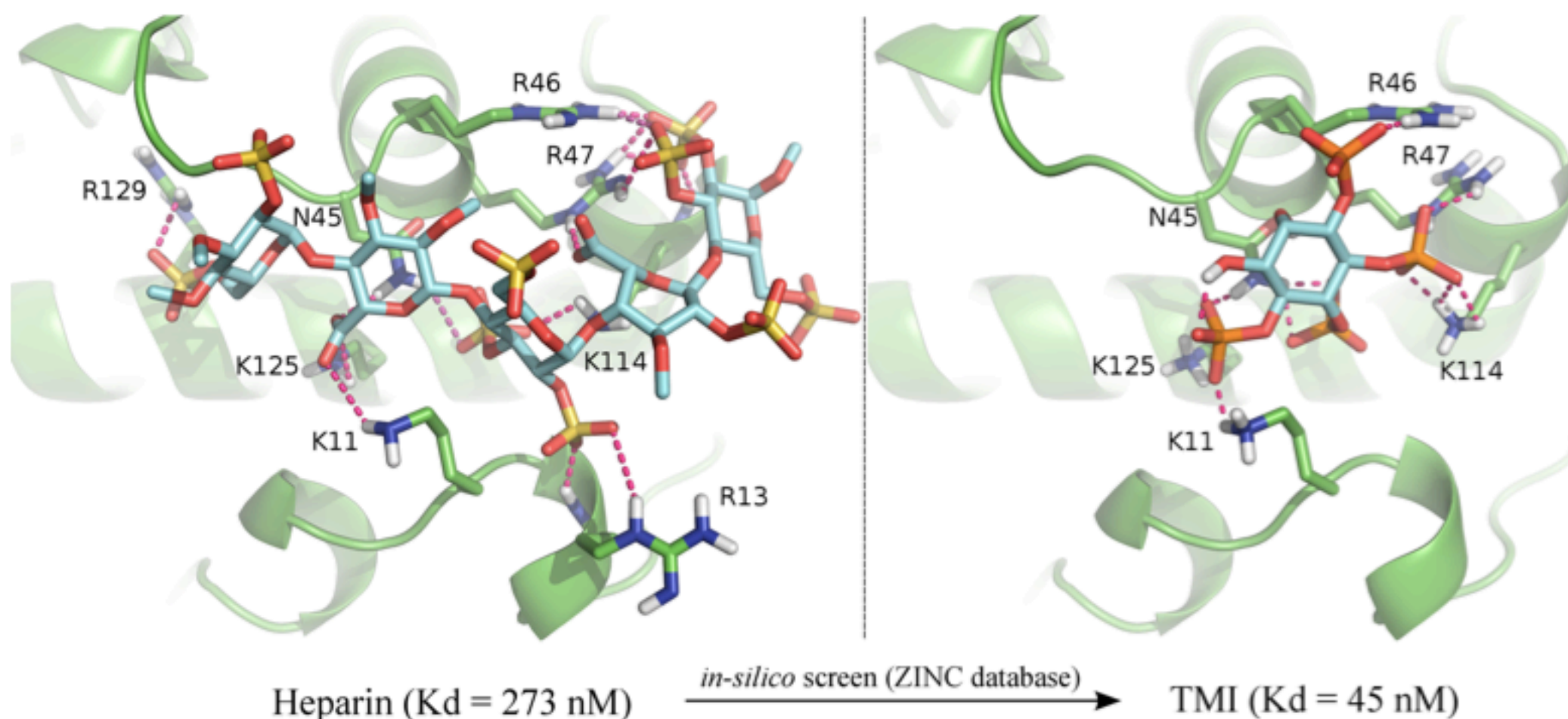
Prof. Dr. Horacio Pérez Sánchez -

Tlf: (+34) 968 27 88 19 – hperez@ucam.edu

GLOBAL MARKET FOR ANTICOAGULANT DRUGS



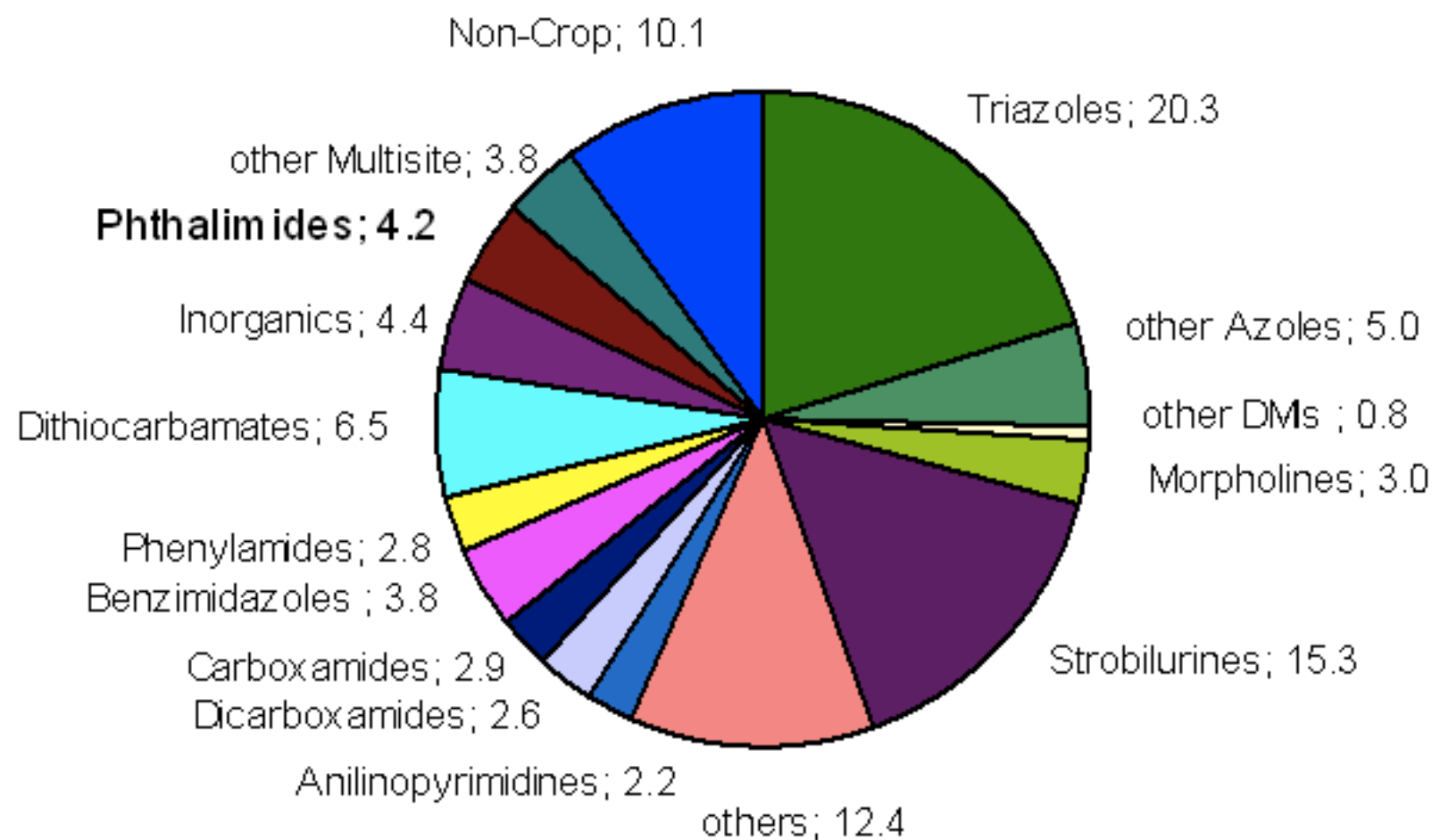
PREDICTED INTERACTIONS AFTER VIRTUAL SCREENING FOR HIT COMPOUNDS



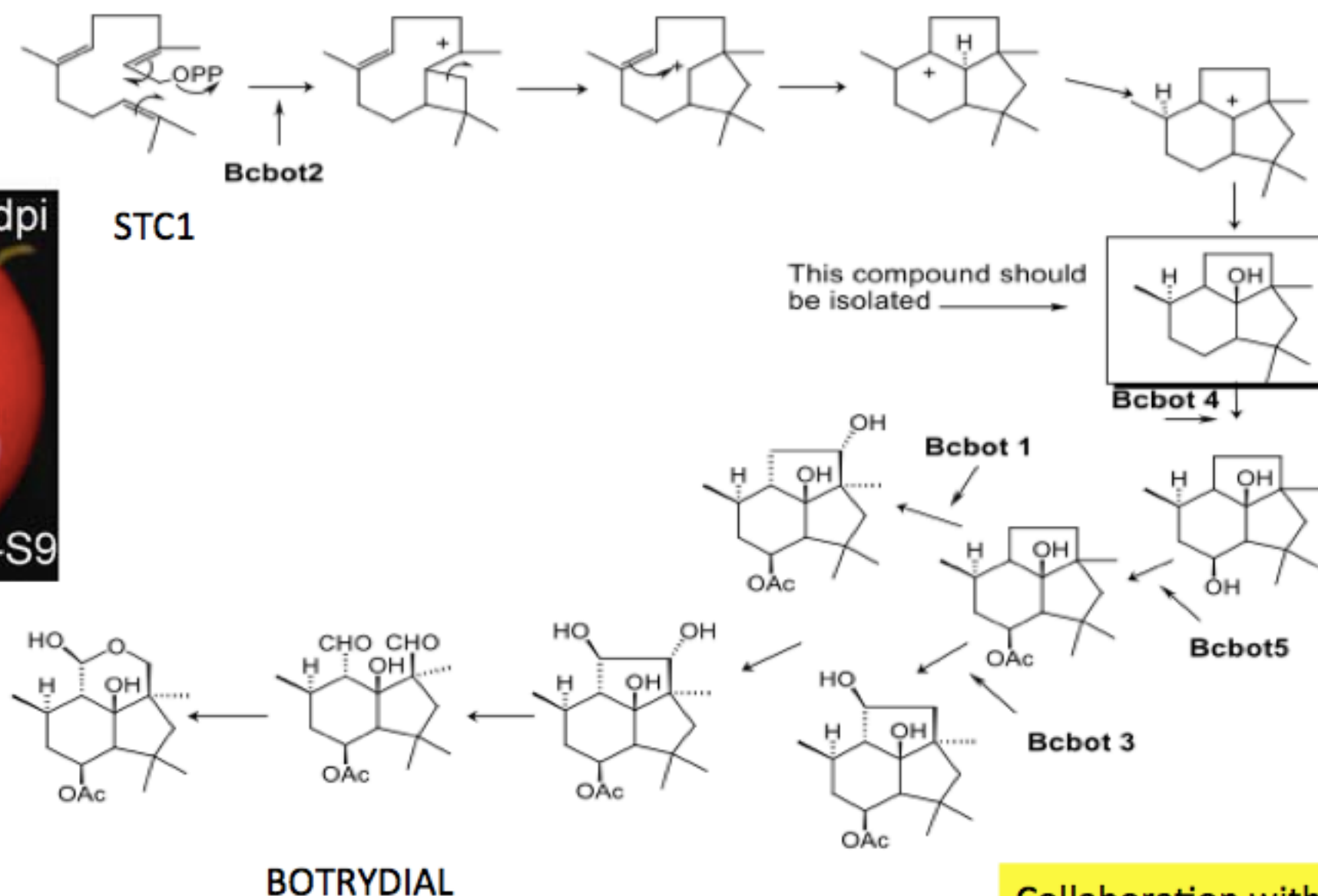
J. Navarro-Fernández, H. Pérez-Sánchez, I. Martínez-Martínez, I. Meliciani, J.A. Guerrero, V. Vicente, J. Corral, W. Wenzel, (2012) "In-silico discovery of a compound with nanomolar affinity to antithrombin causing partial activation and increased heparin affinity", *Journal of Medicinal Chemistry* (in press). DOI: 10.1021/jm300621j

GLOBAL FUNGICIDES MARKET (2005)

Total Market Value 2005 = \$ 8916 m

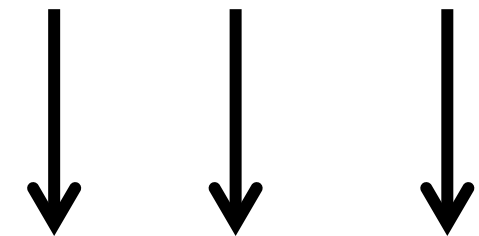


DISCOVERY OF FUNGICIDES



Collaboration with
University of Cadiz
Prof. Isidro Collado

€€€, RESEARCH FUNDS (UCAM)



BIOINFORMATICS AND HIGH PERFORMANCE COMPUTING RESEARCH GROUP

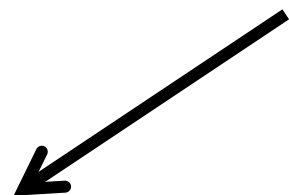


The Schrödinger Equation

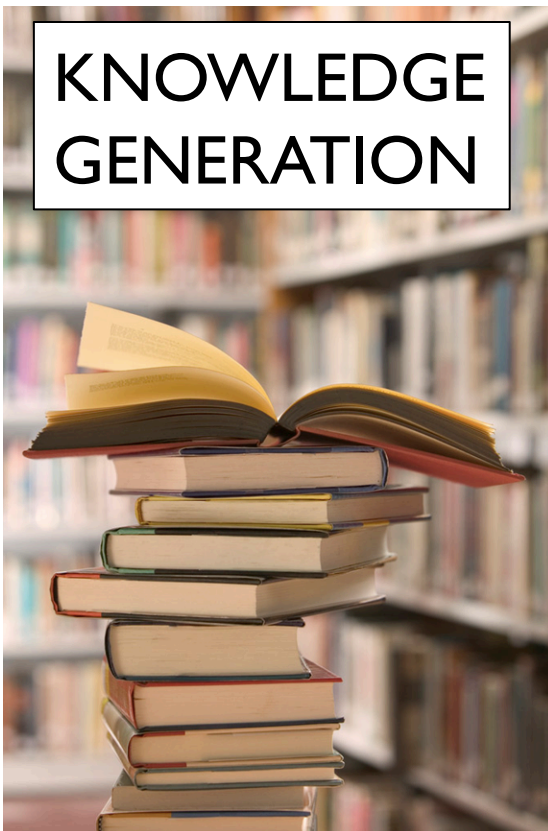
$$\left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E \psi(x)$$

Hamiltonian operator Wave function Energy

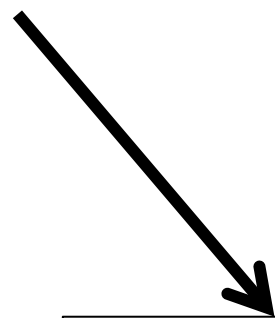
SUPERCOMPUTER



KNOWLEDGE GENERATION



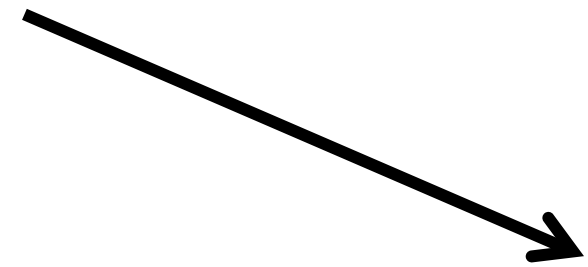
FUNDAMENTAL RESEARCH



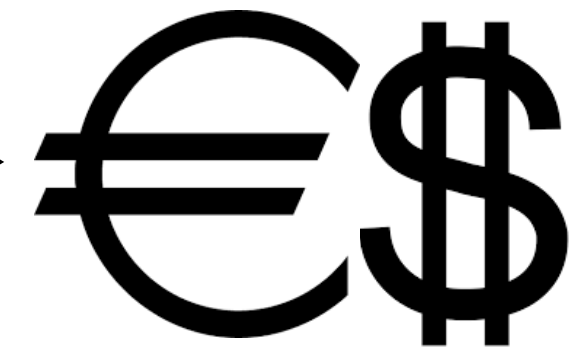
DISCOVERY OF DRUGS



APPLIED RESEARCH



CONTRACT BASED MOLECULAR MODELING SERVICES



TECHNOLOGY TRANSFER



biología en el contexto del de

oactivos; ¿Cómo vender servicios de modelado molecular?



US 20110218788A1

(19) **United States**

(12) **Patent Application Publication**
Wenzel et al.

(10) **Pub. No.: US 2011/0218788 A1**

(43) **Pub. Date: Sep. 8, 2011**

(54) **METHOD AND SYSTEM FOR DETERMINING
THE SOLVENT ACCESSIBLE SURFACE
AREA AND ITS DERIVATIVES OF A
MOLECULE**

(75) Inventors: **Wolfgang Wenzel**, Weingarten
(DE); **Horacio Emil
Perez-Sanchez**, Karlsruhe (DE);
Konstantin Klein, Stettensee (DE)

(73) Assignee: **KARLSRUHER INSTITUT
FÜR TECHNOLOGIE**,
Karlsruhe (DE)

(21) Appl. No.: **13/039,874**

(22) Filed: **Mar. 3, 2011**

(30) **Foreign Application Priority Data**

Mar. 4, 2010 (EP) 10002203.7

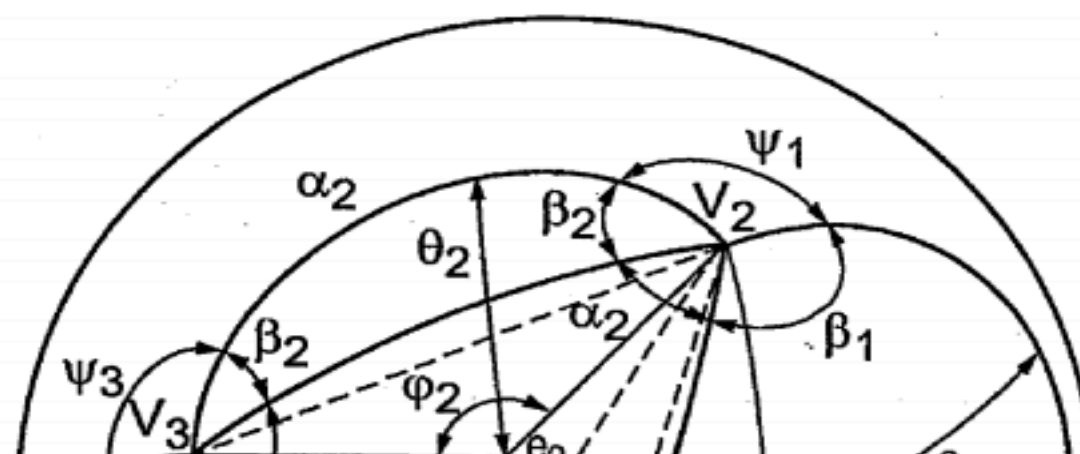
Publication Classification

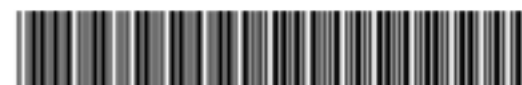
(51) **Int. Cl.**
G06G 7/58 (2006.01)

(52) **U.S. Cl.** 703/12

(57) **ABSTRACT**

A computer-readable storage medium encoded with computer-readable program code for causing a computer to perform a molecular dynamics simulation for determining the solvent accessible surface area of a molecule (M) with respect to atomic coordinates, wherein the molecule (M) comprises a plurality of atoms, a sphere (B_i) is assigned to each atom, and each sphere (B_i) comprises a radius (p_i) and a center position (r_i). The program code includes instructions for: determining for each sphere (B) all neighbouring spheres (B_j) that intersect with the sphere (B); defining a set of one or more contours (C_m), such that all intersecting circles of sphere B with spheres B_j intersect on the surface of sphere B; determining for each contour (C_m) an area enclosed by the contour (C_m), wherein the contour (C_m) includes the area on the surface of said sphere (B) that is enclosed by one or more arcs (a_1, a_2, a_3) resulting from an intersection of the surface of said sphere (B) with one of the surface of one intersecting sphere (B_j) or the surfaces of a plurality of intersecting spheres (B_j) that have an overlapping intersection area on the surface of said sphere (B); determining the solvent accessible surface (S) of said sphere (B) as the surface of said sphere (B) subtracted by the area comprised by all contours (C_m) on the surface of said sphere (B); and determining the solvent accessible surface area of the molecule (M) based on a sum of solvent accessible surface areas (S_i) of the spheres.





(11) **EP 2 505 202 A1**

(12) **EUROPEAN PATENT APPLICATION**

(43) Date of publication:
03.10.2012 Bulletin 2012/40

(51) Int Cl.:
A61K 31/6615 ^(2006.01) **A61P 7/02** ^(2006.01)
A61P 9/10 ^(2006.01)

(21) Application number: **11002649.9**

(22) Date of filing: **30.03.2011**

(84) Designated Contracting States:
**AL AT BE BG CH CY CZ DE DK EE ES FI FR GB
GR HR HU IE IS IT LI LT LU LV MC MK MT NL NO
PL PT RO RS SE SI SK SM TR**
Designated Extension States:
BA ME

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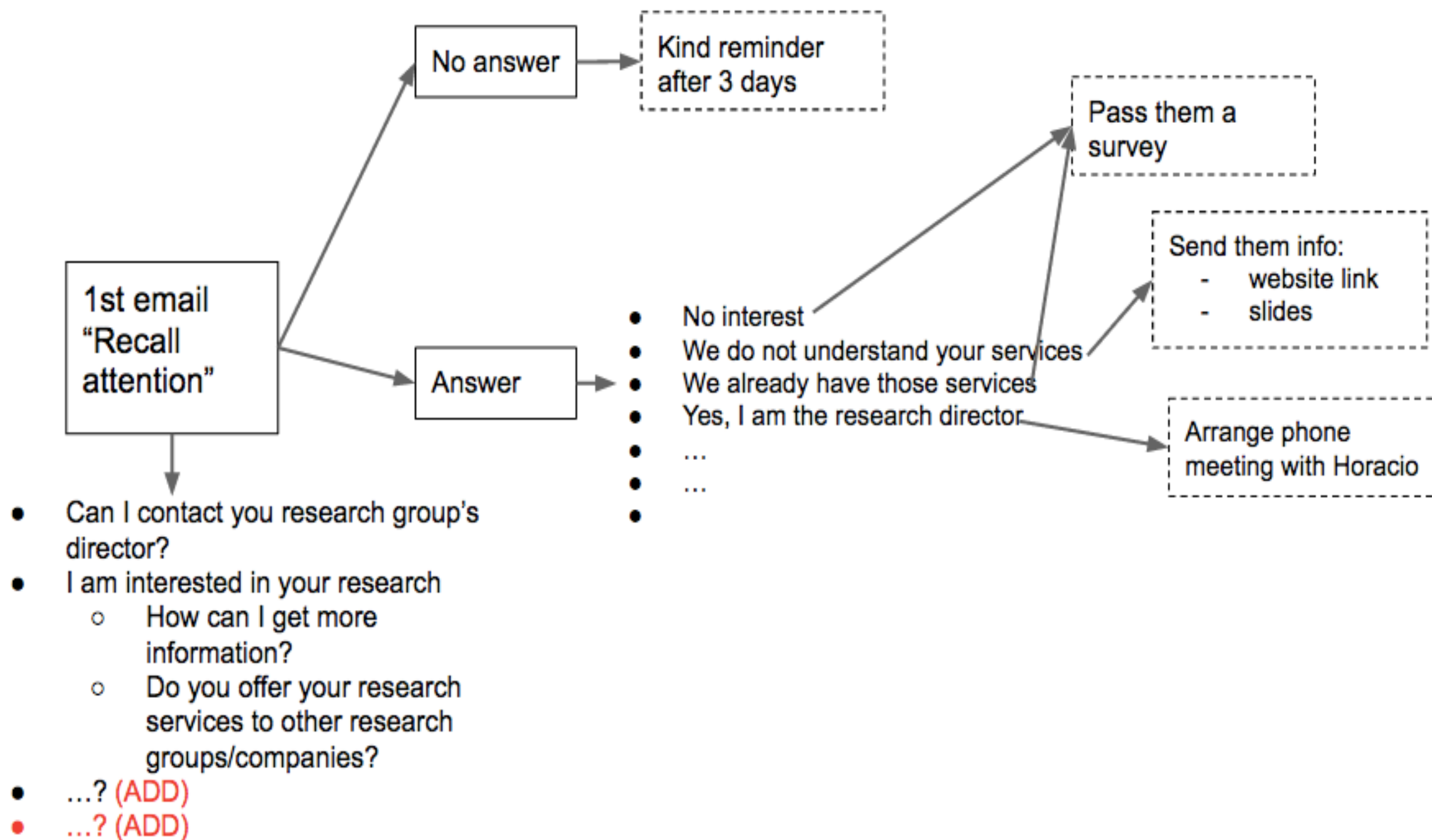
(74) Representative: **Müller-Boré & Partner**
Patentanwälte
Grafinger Straße 2
81671 München (DE)

(54) **D-myo-inositol 3,4,5,6-tetrakisphosphate to modulate thrombin/antithrombin activity by heparin binding**

(57) The present invention relates to D-myo-inositol 3,4,5,6-tetrakisphosphate for use in activating anti-thrombin in a patient as well as to a pharmaceutical composition containing D-myo-inositol 3,4,5,6-tetrakisphos-

phate for use in recovery of antithrombin activity in patients with antithrombin deficiency or in prophylaxis for a disease associated with increased blood clotting.

EMAIL CAMPAIGN V4 SCRIPT



CONTRATOS FIRMADOS COMO GRUPO DE INVESTIGACIÓN PARA PRESTACIÓN DE SERVICIOS A UNIVERSIDADES Y EMPRESAS

- COMPAÑÍA BIOTECH CALIFORNIA (USA)
 - Descubrimiento de aplicaciones terapéuticas de un compuesto de origen marino

- GRUPO DE INVESTIGACIÓN DE UNIVERSIDAD ESPAÑOLA
 - Obtención de información sobre mecanismo de acción de un nuevo compuesto en enfermedades relacionadas con la médula espinal

- SPIN-OFF PROCEDENTE DE CENTRO DE INVESTIGACIÓN ESPAÑOL
 - Análisis de resultados de encapsulación de fármacos mediante proteínas de origen vegetal

DIFICULTADES PRINCIPALES QUE TIENE UN GRUPO DE INVESTIGACIÓN PARA ACERCARSE A EMPRESAS

- DESCONOCIMIENTO DEL LENGUAJE DE LA EMPRESA
 - *NECESIDAD DE INTERMEDIARIOS CON EXPERIENCIA*

- DIFICULTAD PARA FUNCIONAR CON EL TIMING DE UNA EMPRESA
 - *NECESIDAD DE RECURSOS SUFICIENTES PARA PODER ACOMETER PROYECTOS*

- LOS GRUPOS DE INVESTIGACION NO SON TOMADOS EN SERIO POR LA MAYORÍA DE LAS EMPRESAS
 - *NECESIDAD DE CREACIÓN DE UNA SPIN-OFF*

■ **Coordination action** in EU FP7 (grant agreement no. 609491)

Technology transfer projects (TTPs)

- **TETRACOM's major new instrument**
- **TTP model:**
 - **Bilateral project** between a university partner U and a company partner C
 - Typical **duration**: 3-12 months
 - C intends to purchase or license **a particular existing technology** (e.g. a SW tool or a HW IP block) from U, normally along with some **services** (porting, training,)
 - TETRACOM provides **partial funding**

