

Date:	07/09/2015
Type:	Research group in Cheminformatics & Nutrition (2014 SGR1217)
Size:	5 senior lecturer + 4 pre-doc + 0.5 technician
Country:	SPAIN
Keywords:	Natural products Functional foods Bioactivity prediction of small molecules Cheminformatics Bioinformatics By-products valorization
Description of activities / other details:	<p>Activity: the research group in Cheminformatics & Nutrition activity focuses on using computational tools to: (1) predict which <u>natural molecules</u> have one specific bioactivity; (2) find new uses for specific molecules (e.g., valorization of by-products by finding new uses for molecules that are present on them). Our results can be used either to design functional foods/nutraceuticals for specific risk population's groups (e.g., people that have the risk to become diabetic) or to develop new molecular cosmetics products or to find/design/improve drugs. Moreover, our group is able to experimentally confirm the predicted bioactivity by means of in vitro, in vivo and ex vivo experiments. These experiments are performed at the self group facilities.</p> <p>Working topics:</p> <p>(1) Finding natural molecules with anti-inflammatory activity</p> <p><i>Identification of human IKK-2 inhibitors of natural origin (part I): modeling of the IKK-2 kinase domain, virtual screening and activity assays. Sala E, Guasch L, Iwaszkiewicz J, Mulero M, Salvadó MJ, Pinent M, Zoete V, Grosdidier A, Garcia-Vallvé S, Michielin O, Pujadas G. PLoS One. 2011 Feb 24;6(2):e16903</i></p> <p><i>Identification of human IKK-2 inhibitors of natural origin (Part II): in Silico prediction of IKK-2 inhibitors in natural extracts with known anti-inflammatory activity. Sala E, Guasch L, Iwaszkiewicz J, Mulero M, Salvadó MJ, Bladé C, Ceballos M, Valls C, Zoete V, Grosdidier A, Garcia-Vallvé S, Michielin O, Pujadas G. Eur J Med Chem. 2011 Dec;46(12):6098-103</i></p> <p>(2) Finding natural molecules with anti-diabetic activity</p> <p><i>Identification of novel human dipeptidyl peptidase-IV inhibitors of natural origin (part I): virtual screening and activity assays. Guasch L, Ojeda MJ, González-Abuín N, Sala E, Cereto-Massagué A, Mulero M, Valls C, Pinent M, Ardévol A, Garcia-Vallvé S, Pujadas G. PLoS One. 2012;7(9):e44971</i></p> <p><i>Identification of novel human dipeptidyl peptidase-IV inhibitors of natural origin (Part II): in silico prediction in antidiabetic extracts. Guasch L, Sala E, Ojeda MJ, Valls C, Bladé C, Mulero M, Blay M, Ardévol A, Garcia-Vallvé S, Pujadas G. PLoS One. 2012;7(9):e44972</i></p> <p><i>Identification of PPARgamma partial agonists of natural origin (I): development of a virtual screening procedure and in vitro validation. Guasch L, Sala E, Castell-Auví A, Cedó L, Liedl KR, Wolber G, Muehlbacher M, Mulero M, Pinent M, Ardévol A, Valls C, Pujadas G, Garcia-Vallvé S. PLoS One. 2012;7(11):e50816</i></p> <p><i>Identification of PPARgamma partial agonists of natural origin (II): in silico prediction in natural extracts with known antidiabetic activity. Guasch L, Sala E, Mulero M, Valls C, Salvadó MJ, Pujadas G, Garcia-Vallvé S. PLoS One. 2013;8(2):e55889.</i></p> <p><i>Discovery of Natural Products that Modulate the Activity of PPARgamma: A Source for New Antidiabetics. Garcia-Vallve S, Guasch L, Mulero M. Foodinformatics Applications of Chemical Information to Food Chemistry, 151-176. Editors: Karina Martinez-Mayorga and José Luis Medina-Franco. Springer 2014</i></p> <p><i>DPP-IV, An Important Target for Antidiabetic Functional Food Design. Ojeda MJ, Cereto-Massagué A, Valls C, Pujadas G. Foodinformatics Applications of Chemical Information to Food Chemistry, 177-212. Editors: Karina Martinez-Mayorga and José Luis Medina-Franco. Springer 2014</i></p> <p>(3) Finding natural molecules with anti-obesity activity</p>

(4) Development of methodologies/computational tools for improving the prediction of the bioactivity of small molecules

DecoyFinder: an easy-to-use python GUI application for building target-specific decoy sets. Cereto-Massagué A, Guasch L, Valls C, Mulero M, Pujadas G, Garcia-Vallvé S. *Bioinformatics.* 2012 Jun 15;28(12):1661-2

The good, the bad and the dubious: VHELIBS, a validation helper for ligands and binding sites. Cereto-Massagué A, Ojeda MJ, Joosten RP, Valls C, Mulero M, Salvado MJ, Arola-Arnal A, Arola L, Garcia-Vallvé S, Pujadas G. *J Cheminform.* 2013 Jul 29;5(1):36. doi: 10.1186/1758-2946-5-36.

(5) Development of methodologies/computational tools for predicting new uses for existing drugs or molecules that are abundant in by-products of natural origin

Molecular fingerprint similarity search in virtual screening. Cereto-Massagué A, Ojeda MJ, Valls C, Mulero M, Garcia-Vallvé S, Pujadas G. *Methods.* 2015 Jan;71:58-63.

Tools for in silico target fishing. Cereto-Massagué A, Ojeda MJ, Valls C, Mulero M, Pujadas G, Garcia-Vallvé S. *Methods.* 2015 Jan;71:98-103.

Available technology

We have a license for using the Small-Molecule Drug Discovery Suite from Schrödinger for commercial (*i.e.*, profit) uses. Moreover, we have access to the drug discovery suites from OpenEye and Cresset (although the use of these two suites is restricted to non-commercial research). We have also an in-house database with around 225.000 natural molecules where each one is labeled with the natural sources from where they can be obtained and, therefore, we can easily make smallest databases with natural molecules obtained from particular ecosystems (*e.g.*, marine, mediterranean, etc.).

Successful stories of our research

Our work for the cosmetic company Provital S.A. leads to the development of two cosmetic ingredients: **(1) MELAVOID™** (a depigmentant which prevents spots and treats uneven skin tone); and **(2) AQUAXTREM™** (that stimulates the hydration mechanisms of the skin). Both ingredients are already at the market as part of different cosmetic products. Moreover, MELAVOID™ was awarded with the 1st prize in the category “Most innovative raw material” during the BSB Innovation Prize ceremonies (In-Cosmetics Paris 2013).

Former PhD students in our group are currently working in several drug-discovery companies (*e.g.* Intelligent Pharma) and at the National Cancer Institute at U.S.A.

Experience in R+D projects/contracts:

Project/contract title: Grup de recerca consolidat en “Quimioinformàtica i Nutrició”. **Project call:** Convocatòria de suport als grups de recerca de Catalunya. **Company/Government Funding Agency:** Agència de Gestió d'Ajuts Universitaris i de Recerca (Generalitat de Catalunya). **Project/contract ID:** 2014 SGR1217 **Amount:** 0€ **From:** 2014 **to:** 2016. **Project/contract leader:** Gerard Pujadas Anguiano

Project/contract title: Identificació de ingredients alimentarios

para la prevención del síndrome metabólico. **Project call:** ATAL - Área ANEP de ciencia y tecnología de los alimentos. **Company/Government Funding Agency:** MCIN - Ministerio de Ciencia e Innovación. **Project/contract ID:** AGL2011-25831 **Amount:** 90.000,00€ **From:** 2012 **to:** 2014. **Project/contract leader:** Santiago Garcia Vallvé

Project/contract title: Efectos sinérgicos de los polifenoles y los omega-3 PUFA sobre la obesidad y patologías relacionadas. **Project call:** ATAL - Área ANEP de ciencia y tecnología de los alimentos. **Company/Government Funding Agency:** MEDU - Ministerio de Educación y Ciencia. **Project/contract ID:** AGL2008-00387 **Amount:** 355.000,00€ **From:** 2009 **to:** 2013. **Project/contract leader:** Luis Maria Arola Ferrer

Project/contract title: Valorització de bolets autòctons per usos gastronòmic i saludables. **Project call:** No applicable. **Company/Government Funding Agency:** AC10 - Agència de Suport a l'Empresa Catalana (ACC1Ó). **Project/contract ID:** TECCOL11-1-0017-00 **Amount:** 38.907,99 **From:** 2011 **to:** 2012. **Project/contract leader:** Luis Maria Arola Ferrer

Project/contract title: Predicción in silico de nuevos compuestos activos de origen natural para su uso cosmético. **Project call:** No applicable. **Company/Government Funding Agency:** Provital, SA. **Project/contract ID:** No applicable **Amount:** 32.400,00€ **From:** 2009 **to:** 2009. **Project/contract leader:** Gerard Pujadas Anguiano

Project/contract title: APLICACIONES DE BIOINFORMATICA A LA GENERACION D'ALIMENTOS FUNCIONALES. **Project call:** No applicable. **Company/Government Funding Agency:** SHIR - Shirota Functional Foods. **Project/contract ID:** T08197S **Amount:** 26.720,00€ **From:** 2008 **to:** 2009. **Project/contract leader:** Gerard Pujadas Anguiano

Project/contract title: Descubrimiento, valoración y comercialización de nuevas moléculas de aplicación industrial basándose en métodos bioinformáticos y quimioinformáticos. **Project call:** No applicable. **Company/Government Funding Agency:** CTNS - Centre Tecnològic de Nutrició i Salut. **Amount:** --- **From:** 2011 **to:** 2013. **Project/contract leader:** Gerard Pujadas Anguiano

Project/contract title: Validación de la eficacia in silico e in vitro de varios extractos naturales. Posada a punto de nuevas técnicas de target fishing. **Project call:** No applicable. **Company/Government Funding Agency:** CTNS - Centre Tecnològic de Nutrició i Salut. **Amount:** 9.500,00€ **From:** 2012 **to:** 2012. **Project/contract leader:** Gerard Pujadas Anguiano

Experience in international cooperation:

Peroxisome proliferator-activated receptor gamma (PPAR γ) and ligand choreography: newcomers take the stage. Garcia-Vallvé S, Guasch L, Tomas-Hernández S, Del Bas JM, Ollendorff V, Arola L, Pujadas G, Mulero Abellan M. J Med Chem. 2015 Jul 23;58(14):5381-94

The good, the bad and the dubious: VHELIBS, a validation helper

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Qualified group members with technological and R&D capabilities:

Gerard Pujadas
Santiago Garcia-Vallvé
Miquel Mulero
Cristina Valls
Raúl Beltran

Innovative elements in our research:

We have been pionnering in the use of the technology for drug discovery and design to the find natural products with one specific bioactivity in order to use them for functional food, nutraceutic or molecular cosmetic applications.

Agreements with research entities:

We have a collaboration agreement with the Technological Center for Health & Nutrition (<http://www.ctns.cat/>) for offering our technology/services to functional food, nutraceutic or molecular cosmetics companies.

Contact person

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