

**Project MSCA-ITN**  
**“PROTECTION against Endocrine Disruptors;  
detection, mixtures, health effects, risk  
assessment and communication (PROTECTED)”**

**ProtoQSAR**

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Cheminformatics and modeling solutions  
to optimize your chemicals



**Early Stage Researcher (ESR) offer**  
**December 2016**



# ProtoQSAR

Cheminformatics and modeling solutions  
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## Introduction

ProtoQSAR is offering a unique opportunity for an Early Stage Researcher (ESR) to undertake research in the framework of the project "PROTECTED" (PROTECTION against Endocrine Disruptors; detection, mixtures, health effects, risk assessment and communication). The ESR will be funded for 3 years through the prestigious Marie Skłodowska-Curie Actions (MSCA) Innovative Training Network (ITN) programme, an initiative by the European Commission (EC) to foster academic-industrial collaboration in the frame of an innovative and entrepreneurial PhD training program.

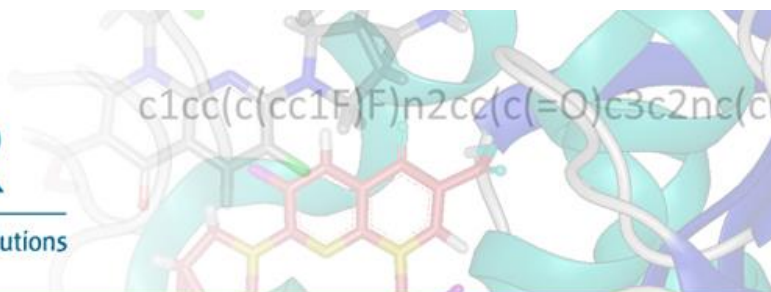


**MARIE CURIE ACTIONS**

PROTECTED aims to develop expertise and protective capabilities against Endocrine Disruptors (EDs). EDs and their mixtures are a modern day health concern leading to failing ecological systems, poor agricultural production and health effects such as obesity, cancer and infertility. While analytical methods have advanced enormously, focus has been mainly on synthetic chemicals, overlooking emerging EDs and real-life multiple substance exposure. A new generation of creative, entrepreneurial and innovative early-stage researchers equipped with skills to assess and understand the real-life risk of complex mixtures of EDs and trained to convert resulting knowledge and ideas into accessible tools and services for the long-term control of potential ED risk is urgently needed.

The PROTECTED Innovative Training Network proposes a holistic approach by providing 15 individual, personalised research projects with exposure to scientific, innovative and entrepreneurial training mobility across the ITN. The intersectorial network is comprised of 12 training sites at academia, research centres, a bioassay technology SME, a QSAR technology SME, water provider, and animal feed supplier. Together they cover multiple disciplines including analytical science of food, feed, and environment, epidemiology, risk assessment, social science and toxicology. This combined expertise enables a highly focused program for developing novel tools and concepts and training for the detection, analysis and improved risk assessment of EDs, especially mixture effects. Methodology will include emerging technologies; multiplexed analysis, mixture modelling, mechanistic and exposure studies, explants and cell or whole organism bioassays.

The project will provide a unique and high level of training for a new generation of specialists with transferable skills and enhanced career perspectives. In total, 15 Early Stage Researchers (ESRs) will be appointed by the PROTECTED consortium for 36 months each. These specialists will ultimately aid the efficient development of future control strategies for improved health.



## Job description

The aim of the ESR at ProtoQSAR will be to develop computational predictive models for the effects of EDs and their mixtures. Predicting the ED effects of specific groups of chemicals (POPs, plasticisers, PAHs, mycotoxins and algal toxins) and their mixtures will be achieved through the use of advanced *in silico* techniques, mainly predictive quantitative structure-activity relationships (QSAR) models.

Databases of chemicals with ED effects will be completed by the ESR, a crucial step, since chemical structure information and experimental end-points have a strong influence on QSAR model reliability. Information on chemicals in epidemiology studies, natural hormones levels during foetal development will be provided by other partners of the ITN, for predictive computational development and validation purposes, and real life mixtures will also be generated with the same objective. Once all the necessary information is compiled, the ESR will apply different chemo-informatics approaches to produce models for EDs and their mixtures. Experimental validation of the robustness and predictive ability of the models will also be performed. Finally, virtual screening (VS) tools will be applied for searching alternatives to chemicals with ED concern.

## Key responsibilities of the ESR

- ✓ To manage and carry out an independent research project in close collaboration with the ProtoQSAR staff and collaborators.
- ✓ To actively participate in research and training activities within the ProtoQSAR's group.
- ✓ To contribute to preparation of reports.
- ✓ To contribute to writing articles for scientific journals.
- ✓ To disseminate research results in the scientific community (via international conferences) and in the non-scientific community (via outreach and public engagement).
- ✓ To engage in additional training events and secondments within the PROTECTED network.
- ✓ Optionally, the ESR can follow in parallel a PhD program related to the PROTECTED work at ProtoQSAR, financed by the company with the project budget allocated for research activities.

## Candidate background

- ✓ 1st class or 2.1 Honours Degree or equivalent in Chemistry, Pharmacology, Toxicology or a related discipline.
- ✓ Demonstrable knowledge or basic background on chemoinformatics and molecular modelling.
- ✓ Demonstrable knowledge and interest in medicinal chemistry and drug discovery.
- ✓ Be in the first 4 years (full-time equivalent) of his/her research career and not yet have been awarded a doctorate. This 4-year period is measured from the date of obtaining the degree which would formally entitle to embark on a doctorate.

- ✓ Be a national of any country and must not have resided or carried out their main activity in Spain for more than 12 months in the 3 years immediately prior to the selection for this position.
- ✓ Be willing and able to perform secondments or participate in training programs at the facilities of other consortium members such as The Netherlands, Norway, France, Chile, Belgium and the United Kingdom.
- ✓ For candidates wishing to follow a PhD programme in parallel, they have to be eligible and qualified for enrolment in the PhD programme at the University of their choice (preferably at the University of Valencia, Spain, which is located close to the ProtoQSAR offices).
- ✓ For more information on MSCA-ITN, please visit: <http://ec.europa.eu/research/mariecurieactions/>

## Terms of appointment

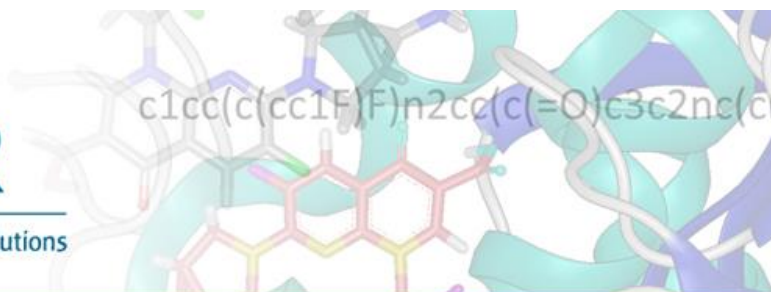
MSCA-ITN offers an attractive salary and working conditions. A unique feature of MSCA-ITN is that during the PhD research, ESR PhD students will be given the opportunity to perform secondments at the facilities of other consortium members. ESR PhD students will benefit from a dedicated training program in the various fields of expertise of the consortium partners. Salary is complemented with a mobility allowance.

## Person specifications and qualities

- ✓ Strong analytical and problem solving skills
- ✓ Ability to logically conceptualize and summarize the research findings
- ✓ Advanced analytical skills
- ✓ Excellent verbal and writing communication skills
- ✓ Ability to interact with colleagues and staff
- ✓ Demonstrable intellectual ability.
- ✓ Ability to communicate complex information clearly.
- ✓ Ability to organise resources, manage time and meet deadlines

## How to apply

If interested, please send Curriculum Vitae, a letter of motivation and two-three recommendation letters to [info@protoqsar.com](mailto:info@protoqsar.com) before the closing application deadline Monday 16th January 2017.



## The company

**ProtoQSAR** is a company founded in 2012 and located in the Science Park of University of Valencia (Spain).

- **Objective:** application of computational methods to the prediction of physico-chemical, biological and/or toxicological properties of chemicals.
- **Competences:** cheminformatics (QSAR, grouping, Read-across, etc.), management and analysis of chemical data, computational toxicology, molecular modelling (docking, pharmacophores, virtual screening).
- **Main working areas:** pharmaceuticals, cosmetics, biocides, detergents, nanomaterials (nanoQSAR), functional food.
- **Services:** contracted research, consulting services, *in silico* predictions, training activities.
- **Team:** currently four people with more than 15 years in academic and industrial environment, around 80 scientific peer-reviewed publications, several chapters in specialized books, more than 50 participations in international professional meetings.
- **Network:** we collaborate with several academic groups and companies specialized in different areas (medicinal chemistry, pharmacokinetics, ecotoxicology, etc.), in order to propose more complete solutions to our customers.

We belong to various scientific and professional associations (Spanish Society of Medicinal Chemistry, Spanish Association of Toxicology (Group of Alternative Methods), The Cheminformatics & QSAR Society, etc.) and we also have various company accreditations, such as:

- "Innovative SME" qualification, awarded by the Spanish Ministry of Economy and Competitiveness for the period 2016-2018.
- "Crédit Impôt Recherche" (French research tax credit): positive certification as a private research entity, awarded by the Ministry of Education and Research of France for the period 2014-2016.
- All our QSAR models strictly comply with the international rules for validation and acceptance established by the Organization for Economic Co-operation and Development (OECD). These rules are currently adopted for scientific and/or regulatory purposes by international bodies such as the European Chemicals Agency (ECHA), European Medicines Agency (EMA), European Food Safety Authority (EFSA) or the US Food and Drug Administration (FDA).

ProtoQSAR currently participates in other international collaborative projects:

- H2020 MSCA-RISE (EU): "Exploiting Protein complexes that Induce Cell death (EPIC)".
- Interreg SUDOE (EU): "Herramientas web avanzadas para la promoción de la aplicación de la nanotecnología y el uso seguro de nanomateriales en el sector del plástico (NANODESK).
- LIFE + (EU): "COMputational tool for the assessment and substitution of Biocidal Active substanceS of Ecotoxicological concern (COMBASE)".



## The city and the region

The Region of Valencia (Valencian Community) has made the leap to modernity without turning its back on its roots. This is one of the secrets that make this beautiful region a point of reference in global tourism. It is an area of contrasts that invites you to discover its natural beauty spots by the coast or the mountains. A special kind of light enhances colourful towns such as Játiva, Requena, Cullera, Peñíscola, Gandía and Sagunto, which will seduce you with exquisite Mediterranean cuisine. Miles and miles of beaches and magical coves where you can enjoy brilliant sunshine and an endless range of recreational activities.



*The Region of Valencia*



*Valencian paella*



*Peñíscola*

The city of Valencia offers a combination of avant-garde style, culture and Mediterranean spirit, bound to captivate any visitor. Valencia is a cosmopolitan capital that invites you to embark on a unique and surprising journey to discover:

- ✓ Its days of sunshine: a mild climate with 300 days of sunshine per year and an average temperature of 19° C make Valencia an ideal destination at any time of year.
- ✓ Its Mediterranean cuisine: a rich and varied cuisine whose key ingredient is rice prepared in a variety of ways, with paella as the signature dish.
- ✓ Its beaches: in Valencia, you have seven kilometres of beaches on which to find your perfect spot. Choose from city beaches, which you can get to by metro or tram, or more unspoilt beaches, such as El Saler in the Albufera Natural Park.



*Turia Park*



*Center of Valencia*

- ✓ Its lifestyle: thousands of people soak up the sun all year round at an outdoor bar or café, while having a few tapas and a glass of wine or cold beer. And at night, there are lots of different kinds of scene in the various nightlife areas, from the hotspots in the old town, to those by the sea or in the student areas.
- ✓ Its festivals and traditions: its most important festivals include Las Fallas, when the city is filled with gigantic sculptures that are burned to mark the arrival of springtime. Other festivals include Maritime Holy Week, the procession of Our Lady of the Forsaken, Valencian Corpus Christi and the July Fair.
- ✓ Its green spaces: Valencia converted the former bed of the River Turia, which used to run through the city, into an enormous 9 km long park. Today it is a green lung in which to walk, cycle, play sport, go to cafés, etc. Valencia also has a unique and fascinating nature area: the Albufera Natural Park.



*Fallas*



*City of Arts and Sciences*

- ✓ Its 2000 years of history: Valencia contains influences from Roman, Visigoth, Moorish and Medieval cultures. This is evident in many of its iconic monuments and buildings, such as the Lonja de la Seda (Silk Exchange, designated a UNESCO World Heritage Site), La Almoina, the Serranos and Quart Towers and the Cathedral.
- ✓ Its cutting-edge architecture: great 21st century buildings, such as the City of Arts and Sciences designed by Santiago Calatrava, The Conference Centre by Norman Foster and the Veles e Vents building by David Chipperfield, have all helped to make Valencia a landmark of architecture and a symbol of European avant-garde.

You can find more information about Valencia and the Valencian Community in different tourist specialized web pages as <http://www.visitvalencia.com/en/home>, <http://www.valenciaturisme.org/en/> or <http://en.comunitatvalenciana.com/>.