

PANACHE NEWSLETTER

ISSUE
#5



editorial

Dear Reader,

Welcome to the fifth issue of the PANACHE newsletter!

The PANACHE consortium begins this new year with the same enthusiasm to continue working on the production and testing of different connexin and pannexin (hemi)channel inhibitors for the treatment of liver, cardiovascular and inflammatory joint disease.

This issue introduces ProtoQSAR, a company which applies computational approaches for the selection of molecules, elucidation of the mechanism of action, and screening of connexin and pannexin (hemi)channel inhibitors. Also, this issue will cover the latest online events and provide a summary of our first face-to-face conference since the start of the pandemic.

We hope you enjoy this new issue of the newsletter!

In the meantime, stay tuned by visiting our [website](#), and follow us on [Twitter](#), [Instagram](#), [Facebook](#) or [LinkedIn](#).

The PANACHE consortium.

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PARTNER in the spotlight

ProtoQSAR

ProtoQSAR is a SME based at the European Centre of Innovative Companies (CEEI) in the Technological Park of Paterna, Valencia (Spain).

The company applies computational techniques in different fields like toxicology, pharmacology, nanotechnology, nutraceuticals, etc. ProtoQSAR employees apply and develop *in silico* techniques such as QSAR, homology modelling, molecular docking and molecular dynamic

simulations. Their overarching goal is to help in the research process by developing tools that save time and costs, and minimize the need for animal testing.

The ProtoQSAR team has co-authored many publications in international peer-reviewed journals, and they have developed several software tools to predict important properties of interest (endpoints) in regulatory toxicology. They currently work on a dozen of projects funded by the EU, the Spanish Government, and other public agencies.



Rafael Gozalbes, Ph.D., CEO & Founder

Rafael Gozalbes is the founder and CEO of ProtoQSAR. He obtained his doctoral degree in Pharmacy at the University of Valencia (Spain) in 1998. He spent three years as a postdoctoral researcher at the Université Paris VII – CNRS. In 2001 he joined the French biotech CEREP as a senior scientist in the molecular modelling group, and in 2007 he worked as a scientist in the Lab of Structural Biochemistry, Príncipe Felipe Research Centre (CIPF), Spain. Rafael founded ProtoQSAR in 2012, and he is currently leading the PANACHE work package 3.



Eva Serrano Candelas, Ph.D.

Chief technical officer at ProtoQSAR. She coordinates the technical aspects in PANACHE.



Laureano E. Carpio, M.Sc.

Predoctoral researcher, he performs molecular modelling studies to elucidate the mode of action of the PANACHE molecules.



Pravin Ambure, Ph.D.

Senior scientist, he develops QSAR models to predict physicochemical and pharmacokinetic features of molecules.



José Vicente Tarazona, Ph.D.

Administrative project manager at ProtoQSAR. He leads the company's administrative aspects within PANACHE.

ProtoQSAR has a diverse team that includes senior scientists, postdoctoral researchers and Ph.D. students, who are experts in varied domains, from bioinformatics to biotechnology and chemistry.



To learn more about the group and its members please visit <https://www.protoqsar.com/>

ROLE in PANACHE

The ProtoQSAR team is leading the *in silico* work package of the project.

The team is responsible for developing QSAR models to predict different properties of the connexin and pannexin (hemi)channel inhibitors, such as solubility and CPP (cell-penetrating peptide) behaviour.

In addition, the team works on molecular modelling approaches to elucidate the mode of action of these molecules upon interaction with different (hemi)channels of pannexin and connexin proteins. These molecular modelling techniques, in combination with the QSAR models, will facilitate the selection of the inhibitors for further *in vivo* studies.

LATEST event

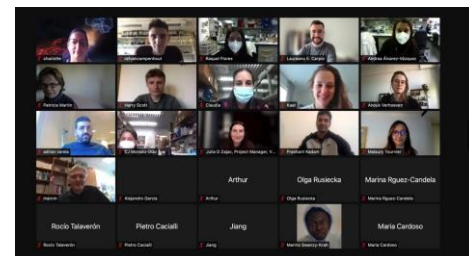
Second PANACHE workshop

This one-day international event took place online on November 22nd 2021, and was organized by Brenda Kwak, UNIGE.

The morning session of this workshop focused on topics that demand particular attention when designing biomedical studies, with interesting talks from renowned speakers such as Christoph Scheieman from the University of Geneva, Hester den Rujiter from the University Medical Center Utrecht, Simone Becattini from the University of Geneva and Paul C. Evans from the University of Sheffield.

This was followed by presentations of recent results from experts in the connexin and pannexin research field, including Arantxa Tabernero from the University of Salamanca and Brant Isakson from the University of Virginia School of Medicine.

Additionally, young researchers participated as well with flash presentations of their work in the connexin and pannexin field, illustrating the interesting potential of these studies.



For more information about the workshop please visit: www.panache-project.eu

UPCOMING event



THE INTERNATIONAL GAP JUNCTION CONFERENCE (IGJC)

When: 16-20th July 2022

Where: La Coruña, Spain

Organizer: María Mayán. INIBIC. Spain

Abstract deadline: 14th May 2022

Deadline for early registration: 14th May 2022

The International Gap Junction Conference (IGJC) has been held every two years since 1974, alternating primarily between Europe and North America. The meeting brings together a diverse international community of basic science researchers who focus on connexins and pannexins.

The IGJC topics include the channel structure and function/biophysics of connexins and pannexins and their role in cancer, inflammation, tissue regeneration, cardiovascular function, development/reproduction, inherited diseases, etc.

Please, [click here to register](#)

STAY tuned



For all of you who want to know more about connexin and pannexin (hemi)channels, this is your section! You will find a selection of relevant recent publications, including those published by the PANACHE consortium.

CONSORTIUM publications

Leroy K. *et al.* (IVTD)

Expression and Functionality of Connexin-Based Channels in Human Liver Cancer Cell Lines

[Click here to read more](#)

Kwak B. *et al.* (UNIGE)

Connexins and Pannexins in cardiovascular disease

[Click here to read more](#)

Leroy K. *et al.* (IVTD)

Connexin-Based Channel Activity Is Not Specifically Altered by Hepatocarcinogenic Chemicals

[Click here to read more](#)

Carpintero-Fernández P *et al.* (INIBIC)

Genome wide CRISPR/Cas9 screen identifies the coagulation factor IX (F9) as a regulator of senescence

[Click here to read more](#)

RELEVANT publications selected from PubMed

Wakefield B. *et al.*

Pannexin 3 deletion reduces fat accumulation and inflammation in a sex-specific manner

[Click here to read more](#)

Yang K. *et al.*

Mechanisms of Pannexin 1 (PANX1) Channel Mechanosensitivity and Its Pathological Roles

[Click here to read more](#)

Peng B *et al.*

The role of connexin hemichannels in inflammatory diseases

[Click here to read more](#)

Sellitto C. *et al.*

Connexin hemichannel inhibition ameliorates epidermal pathology in a mouse model of keratitis ichthyosis deafness syndrome

[Click here to read more](#)



KEEPING UP WITH PANACHE!

Stay tuned to our latest news, results and activities



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