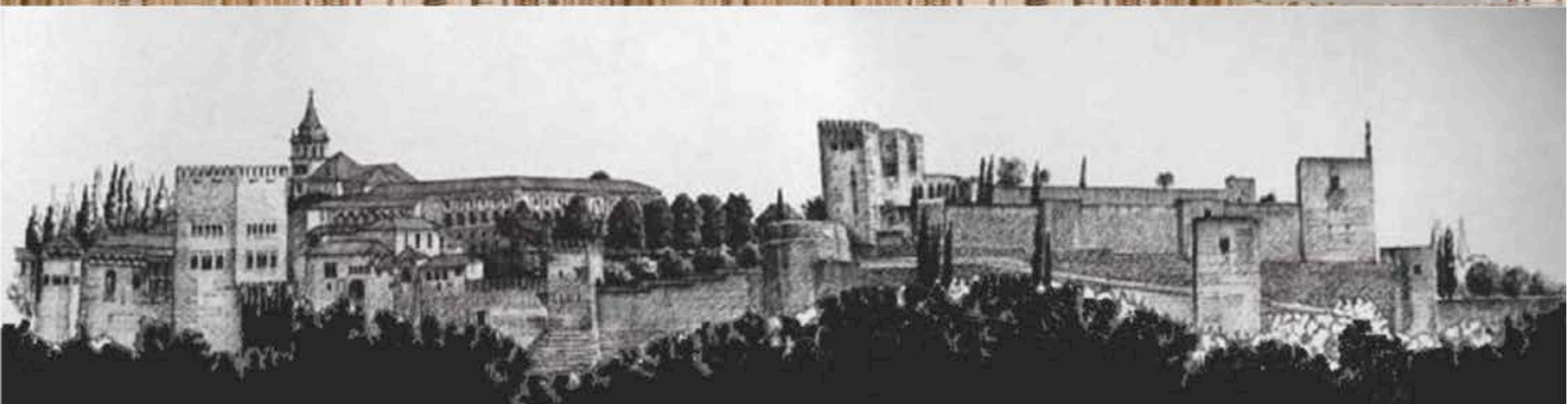




*XV<sup>th</sup> CONGRESS OF THE  
SPANISH BIOPHYSICAL SOCIETY*



*Granada, 10-12 June, 2015*

*Facultad de Ciencias. Campus Fuentenueva*

**S B E**

**S B E**

**BOOK**

**OF**

**ABSTRACTS**



## Presentation

On behalf of the Organising Committee, it is a great honour to invite you to the 15<sup>th</sup> Congress of the Spanish Biophysical Society in Granada, a world heritage city by UNESCO.

The congress will be held at the "Facultad de Ciencias", an excellent facility in the centre of the city, as a part of the University of Granada, which will allow for an easy access to all scientific sessions.

The University of Granada (UGR), founded in 1531, continues a long teaching tradition, the roots of which can be traced back to the madrasahs of the last Nasrid Kingdom. The University is a vibrant presence in the city of Granada, benefiting from the distinctive beauty of its environment and a privileged geographical location due to its proximity to the Sierra Nevada and the Mediterranean coast.

The commitment to high-quality research has placed the UGR in a prominent position in terms of national rankings. The Postgraduate School offers 68 master's and 116 doctorate programmes. For many years, the UGR has promoted a significant international activity. It is the leading European university in terms of receiving students and the second Spanish university in terms of the mobility of its own students.



*Dra. Ana Isabel Azuaga Fortes  
(in the name of the Organizing Committee)*

The congress will be structured in parallel symposiums/symposia with several plenary lectures, conducted by outstanding scientists in their areas. All participants will be able to attend the scientific program, which has been carefully designed to promote debating and enriching discussions, with especial "care" given to the poster sessions. The wide variety of areas within Biophysics to be discussed during the conference will provide to the participants with a unique vision of the state-of-the-art at an international level in this attractive and highly developing field.

Any important news regarding to the organization as well as registration, accommodation, etc., will be conveniently posted and periodically updated on the website of the Conference ([www.sbe.es/granada2015](http://www.sbe.es/granada2015)), as well as useful tourist/social information about the City of Granada, which may be of participants' interest.

We specially encourage young scientists to participate in the 15<sup>th</sup> Spanish Biophysical Congress, where they should expect not only an enriching scientific training during the Congress but also a wonderful personal experience in the city.

## Organizing Committees

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Francisco Conejero Lara

## STEROID MOLECULAR PROPERTIES INFLUENCE THE BIOPHYSICAL STATE OF STEROID-CONTAINING MEMBRANES

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The effects of steroids on the biophysical state of membranes were investigated by analyzing the ordering, rigidifying, condensing and/or raft promoting activity on membranes of a library of 82 steroids. Based on the documented membrane activity, steroids were classified by means of a categorical variable [1] into three possible categories: disrupters, neutrals or promoters of such activity. All steroids were subjected to geometry optimization using the semi-empirical procedure AM1 and 245 molecular descriptors were next computed [2] on the low energy conformations. After the removal of the invariant descriptors, the remaining 93 were correlated with membrane activity through principal component analysis (PCA) [3] and mean contrasting.

Employing three principal components (71 % of explained variance), the PCA score plot showed two well-defined clusters of steroids reflecting similarities in their molecular properties. After the identification and counting of cluster's members (Table) it was found that disrupter steroids represent around 94 % of the population of cluster 1. On the other hand, the 100 % of the promoter and the 95 % of the neutral steroids were located in cluster 2.

*Distribution of steroids in clusters according to their activity on membranes.*

Category of membrane activity	% in cluster		% in category		
	cluster 1	cluster 2	cluster 1	cluster 2	
Disrupter steroids	93.8	13.6	62.5	37.5	100
Neutral steroids	6.2	28.8	5.0	95.0	100
Promoter steroids	0	57.6	0	100	100
	100	100			

Collectively, these findings indicate that steroids having similarities in some molecular properties have similar activity on membranes, and that some of steroid molecular properties influence the biophysical state of steroid-containing membranes. By means of a thorough analysis of the PCA scores and loading it was found that the area, log P, volume, mass, refractivity, number of rotatable bonds and polarizability are the most relevant properties in determining the effect of steroids on membranes. A mean contrasting test revealed significant differences ( $p < 0.001$ ) in all of these properties among the promoter and the disrupter populations, agreeing and reinforcing the preceding conclusions.

### References:

- [1] J.J. Wenz, *Predicting the effect of steroids on membrane biophysical properties based on the molecular structure*, Biochim.Biophys.Acta, 1818, 896-906, (2012).
- [2] Dragon, Talete SRL, Milano Chemometrics and QSAR Research Group, Milano, Italy, (2007).
- [3] The Unscrambler, Camo Process As, Oslo, Norway. <http://www.camo.no>, (2007).