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Faculty of Engineering

Research Interests

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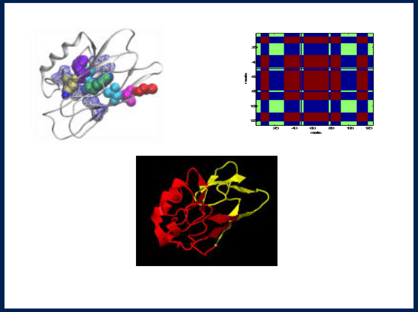
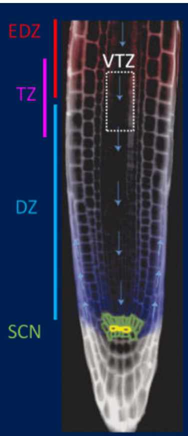


MOLECULAR scale: Protein Contact Network: an emerging paradigm in protein chemistry

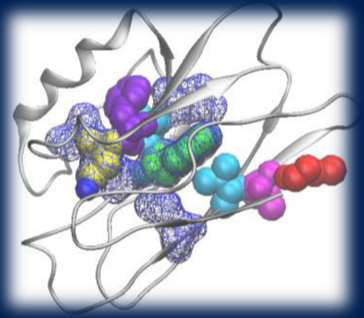


TISSUE & CELL scale: hormones diffusion and growth in root meristems

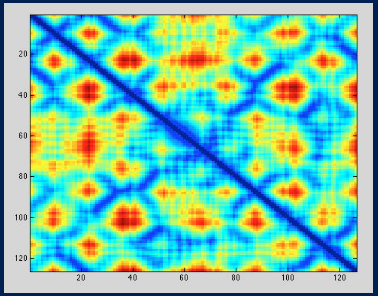
INDUSTRIAL PROCESSSING: biofuels production from products and wastes of the bioagricultural production chain

My Physical Chemistry background allows me to travel in the biotechnology research realm, from structural biology to bioprocessing for sustainable development.

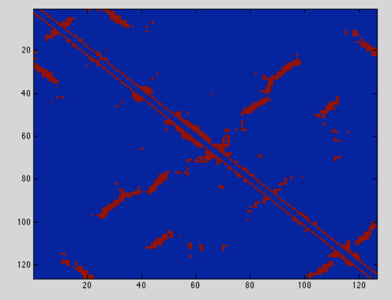
PROTEIN CONTACT NETWORKS



3D structure



Distance Matrix

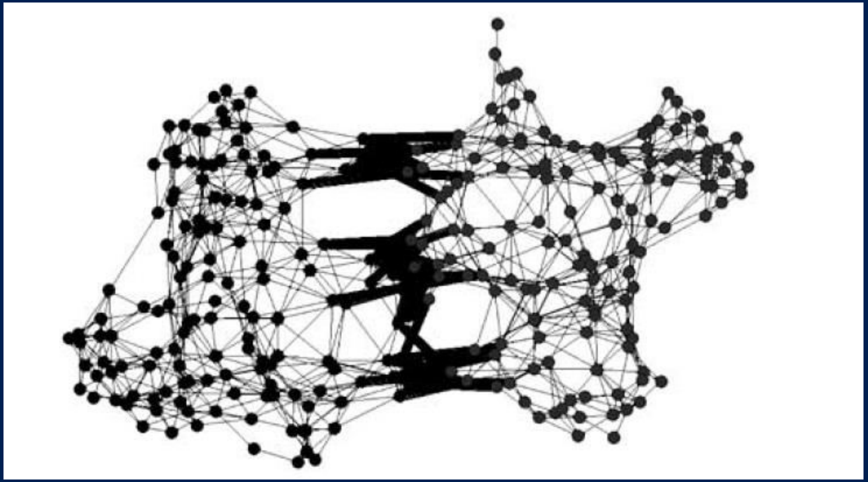


Adjacency Matrix

The identification of a simplified representation of protein structures helps elucidating the structure – function relationship at the basis of the biological activity of proteins

L. Di Paola, M. De Ruvo, P. Paci, D. Santoni, A. Giuliani (2013) “Protein Contact Networks: An Emerging Paradigm in Chemistry” *Chem Rev* , 113: 1598-1613

PCN & LETHAL MUTATIONS

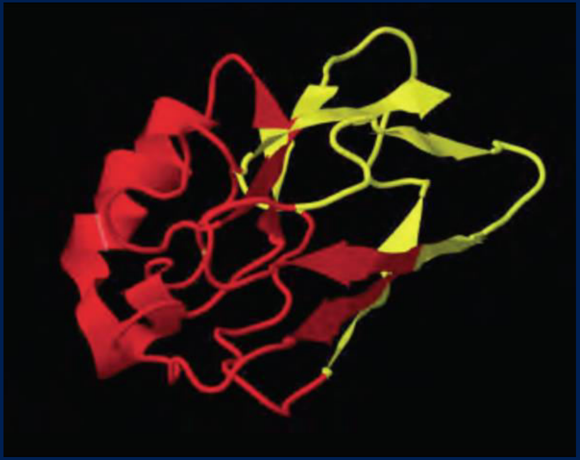


Hemoglobin structure as contact network

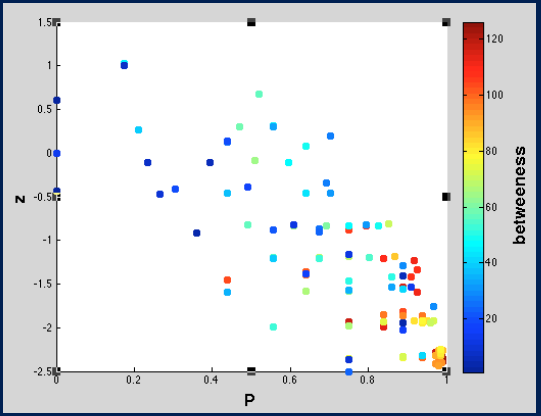
The topology of PCN varies strongly for lethal mutations, remaining almost unchanged for non-lethal mutations (comparison with native structures).

A. Giuliani, **L. Di Paola**, R. Setola (2009) “Proteins as Networks: A Mesoscopic Approach Using Haemoglobin Molecule as Case Study” *Curr Proteomics* 6: 235-245

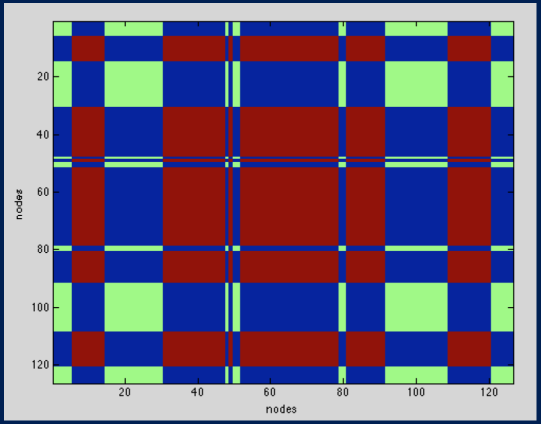
MODULE IDENTIFICATION



Azurin structure parted into two modules



Guimerà-Amaral Cartography



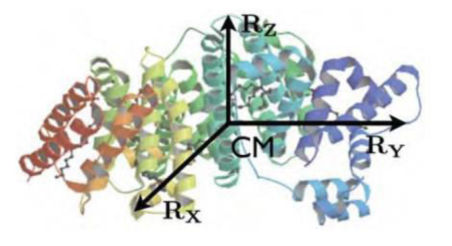
Color map of modules partition

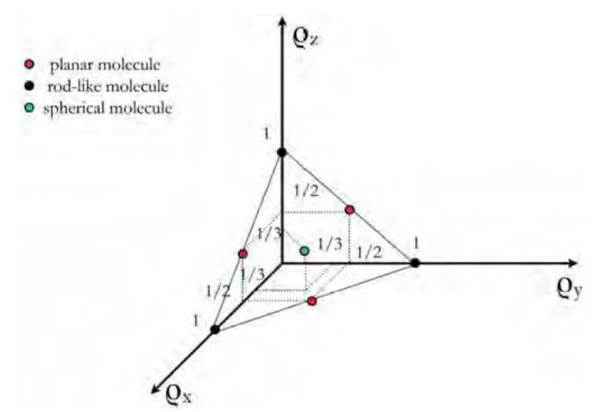
The detection of functional modules in protein structures is a key step in the topological decoding of protein function.

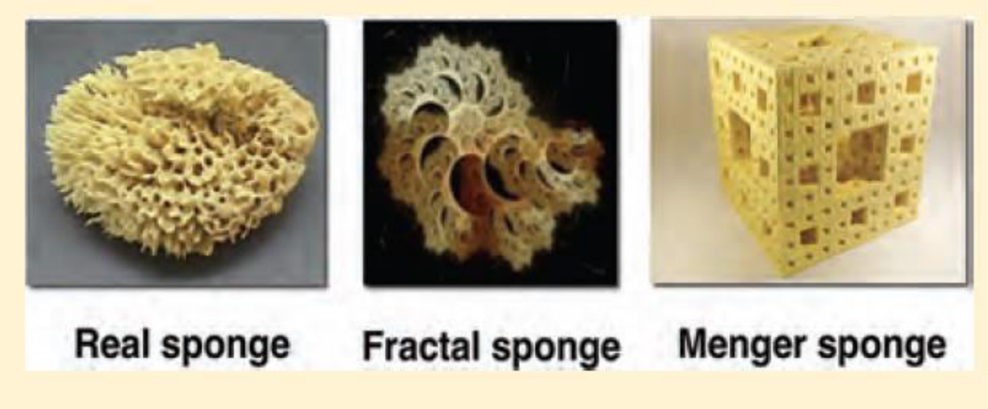
The Guimerà – Amaral cartography (middle picture) assigns a topological role to residues.

S. Tasdighian, **L. Di Paola**, M. De Ruvo, P. Paci, D. Santoni, P. Palumbo, G. Mei, A. Di Venere, A. Giuliani (2013) “Modules identification in protein structures: the topological and geometrical solutions” J Chem Inf Model, 54(1): 159-168

PCN + STRUCTURAL ANALYSIS






Real sponge
Fractal sponge
Menger sponge

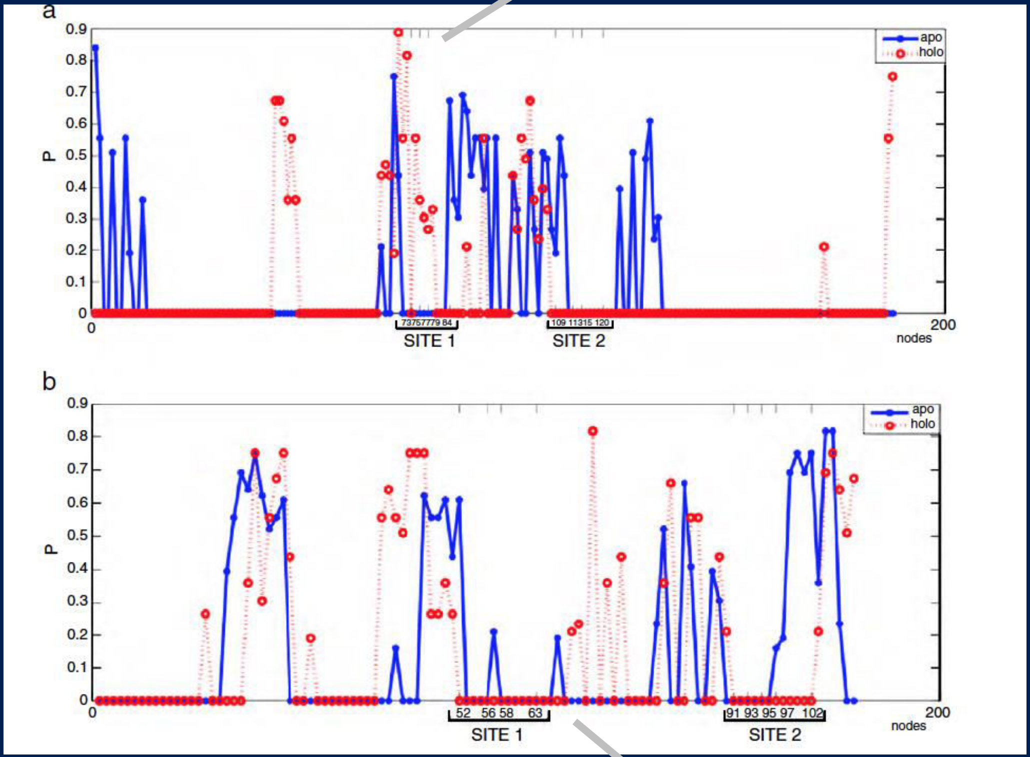
The structural analysis of PCN complements the protein contact network perspective, providing a deep insight of the protein structure interaction with environment in terms of solvent accessibility and structure shape.

L. Di Paola, P. Paci, D. Santoni, M. De Ruvo, A. Giuliani (2012) *J Chem Inf Modell* 52(2): 474-482
N. Arrigo, P. Paci, **L. Di Paola**, D. Santoni, M. De Ruvo, A. Giuliani, and F. Castiglione (2012) *Open Bioinf J* , 6:1–8

ALLOSTERY

The topological role of residues in active sites helps discriminates between allosteric and non allosteric protein structures.

Sensor (recoverin)



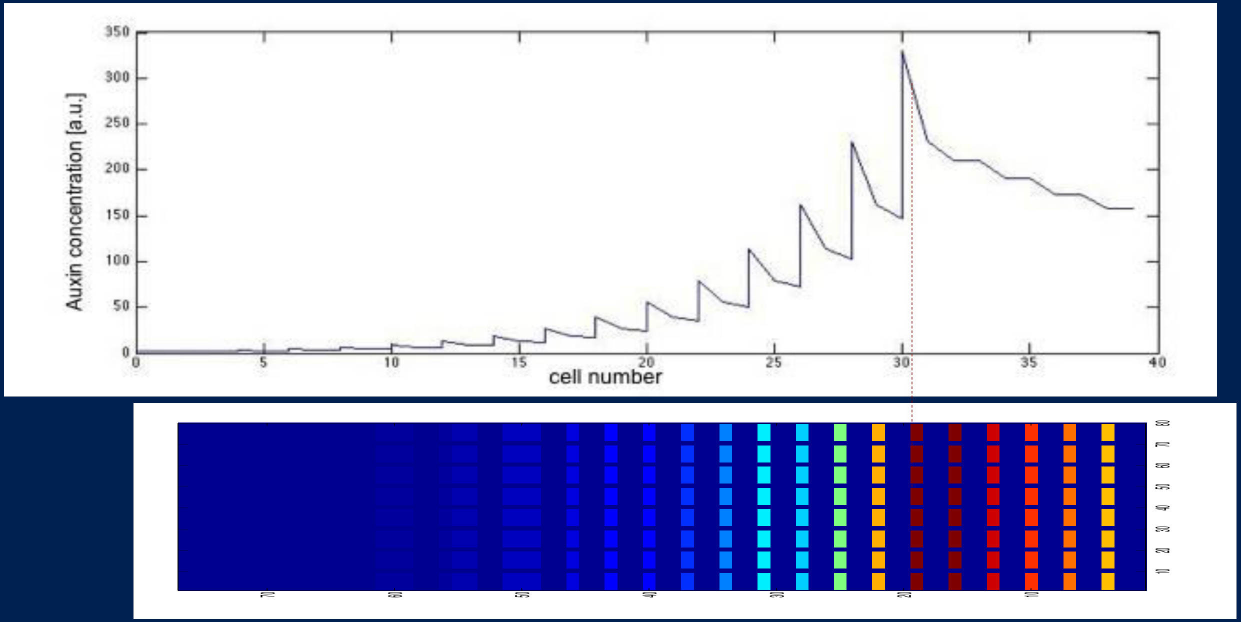
buffer (parvalbumin)

S. Tasdighian, **L. Di Paola**, M. De Ruvo, P. Paci, D. Santoni, P. Palumbo, G. Mei, A. Di Venere, A. Giuliani (2013) “Modules identification in protein structures: the topological and geometrical solutions” J Chem Inf Model, in press

DISCRETE MODEL FOR AUXIN MAPS IN ROOTS

Necessary condition for the maximum in the QC (red):

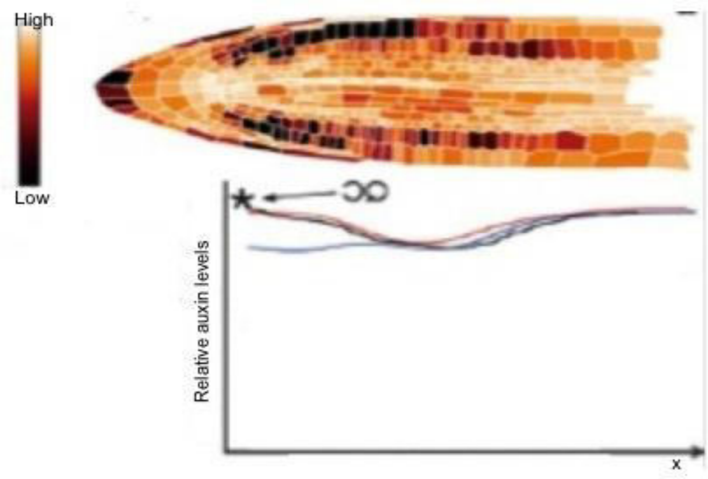
$$J_0 < P \cdot c_0 \cdot \frac{P_{PIN} - P_{BG}}{P_{PIN} \cdot \left(1 + \frac{P_{BG}}{P_C}\right)}$$



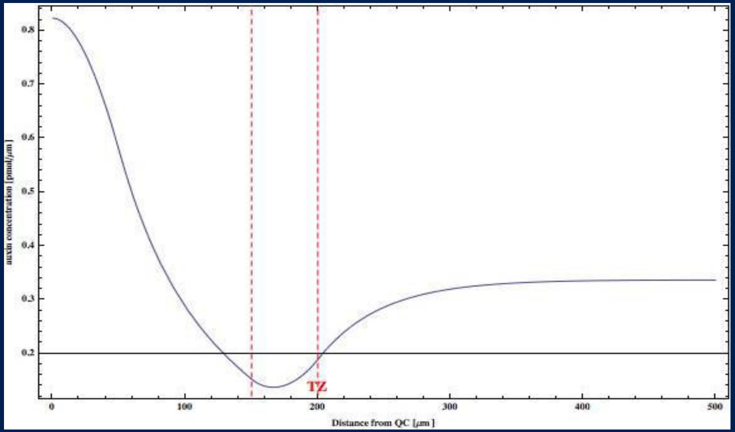
I applied the transport phenomena principles to the analyse auxin maps in root meristems: the discrete model, at cell scale, describes biological constraints that are observed in natural systems.

CONTINUOUS MODEL

(experimental data by S. Sabatini)

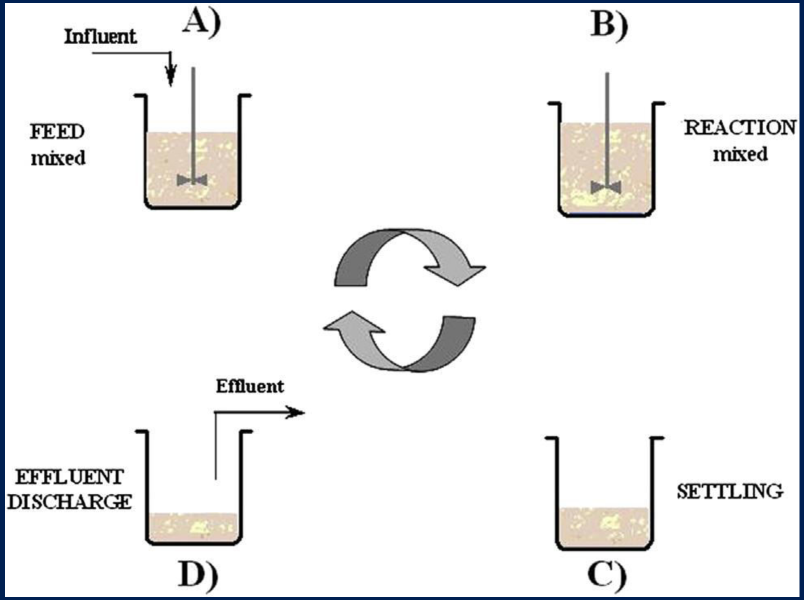


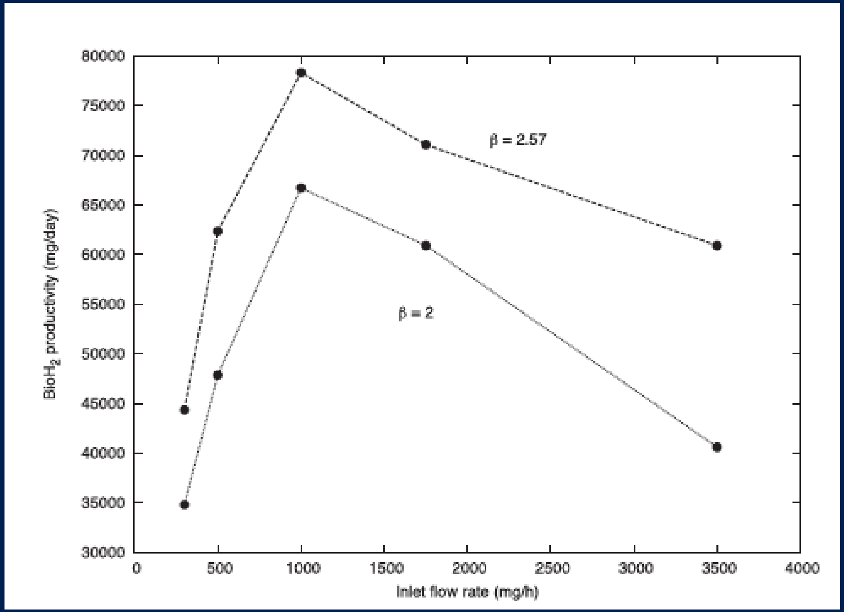
Adapted from Brunoud et al. (2012) *Nature*



The translation of the discrete model into a continuous counterpart represents a key step to validate the model and derive quantitatively the model parameters (work in progress).

Bioprocessing for sustainable development





The analysis of reactive systems for biofuels production directs the bioprocess optimization in the perspective of the industrial scale implementation.

- V. Piemonte, **L. Di Paola**, S. Chakraborty, A.o Basile, Sequencing batch reactors (SBRs) for BioH2 production: Reactor operation criteria, *Int J Hydrogen Energy*, 39 (10):4863-4869;

Recent Publications

- **L. Di Paola**, M. De Ruvo, P. Paci, D. Santoni, A. Giuliani (2013) “Protein Contact Networks: An Emerging Paradigm in Chemistry” *Chem Rev* , 113: 1598-1613;
- V. Piemonte, **L. Di Paola**, S. Chakraborty, A.o Basile, Sequencing batch reactors (SBRs) for BioH2 production: Reactor operation criteria*, Int J Hydrogen Energy*, 39 (10):4863-4869;
- S. Tasdighian, **L. Di Paola**, M. De Ruvo, P. Paci, D. Santoni, P. Palumbo, G. Mei, A. Di Venere, A. Giuliani (2014) “Modules identification in protein structures: the topological and geometrical solutions” *J Chem Inf Model*, 54(1): 159-168;
- P. Paci, **L. Di Paola**, D. Santoni, M. De Ruvo, A. Giuliani (2012) “Structural and Functional Analysis of Hemoglobin and Serum Albumin through Protein Long-Range Interaction Networks” *Curr Proteomics* 9(3): 160-166;
- M. De Ruvo, A Giuliani, P. Paci, D. Santoni, **L. Di Paola** (2012) “Shedding light on protein-ligand binding by graph theory: the topological nature of allostery” *Biophys Chem* 165-166: 21-29;
- **L. Di Paola**, P. Paci, D. Santoni, M. De Ruvo, A. Giuliani (2012) “Proteins as sponges: a statistical journey along protein structure organization principles” *J Chem Inf Model* 52(2): 474-482;
- **L. Di Paola**, A. Terrinoni, F. Vitale (2012) “Extracorporeal membrane blood oxygenators: effect of membrane wetting on gas transfer and device performance” *Asia-Pacific J Chem Eng* 7(S3): S348-S355;
- A. Giuliani**, L. Di Paola**, R. Setola (2009) “Proteins as Networks: A Mesoscopic Approach Using Haemoglobin Molecule as Case Study” *Curr Proteomics* 6: 235-245 (IF 0.828);
- N. Arrigo, P Paci, **L Di Paola**, D Santoni, M De Ruvo, A Giuliani, and F Castiglione. (2012) Characterizing protein shape by a volume distribution asymmetry index. *Open Bioinformatics J* , 6:1–8;
- Giuliani, A.**; Di Paola, L**.; Paci, P.; De Ruvo, M.; Arcangeli, C.; Santoni, D.; Celino, M. (2013) In *Advances in Protein and Peptide Science*; Dunn, B., Ed.; Bentham, 2012; Chapter Updating and revising "Proteins as Networks: Usefulness of Graph Theory in Protein Science”, 28-38;

Journal of Physical Chemistry & Biophysics Related Journals

- Journal of Electrical & Electronic Systems
- Journal of Lasers, Optics & Photonics

Gynecology & Obstetrics
Related Conferences

- 3rd International Conference and Exhibition on Lasers, Optics & Photonics

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