Speaker information

General Information

Name	Antonio Lupia	
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Affiliation	University of Cagliari (UNICA) – Italy, Department of Life and Environmental Sciences (DiSVA)	
Education Background	Degree in Pharmacy, PhD in Life Science	
Professional Appointment	Researcher (RTDA)	
Research Interest	The scientific interests concern the application of computational methods, including Pharmacophore, Molecular Docking, 3D-QSAR, Molecular Dynamics and Virtual Screening techniques, as well as a great interest in the study and application of processes based on Machine Learning (ML) to investigate the drug-receptor interactions, design and lead-optimization of potential drugs. To date, the main research interest is focused on the *Flaviviridae* family (DENV 1-2-3-4), ZIKA, WNV, YFV, and, in particular, NS3pro/hel complexes, which have been established as valuable targets for drug design to treat all flavivirus infections.	
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Speaker information

Recent Publications

1. **Bile acids serve as endogenous antagonists of the Leukemia inhibitory factor (LIF) receptor in oncogenesis**
   Di Giorgio, C., Morretta, E., Lupia, A., ...Zampella, A., Fiorucci, S.
   Biochemical Pharmacology, **2024**, 223, 116134
2. **The leukemia inhibitory factor regulates fibroblast growth factor receptor 4 transcription in gastric cancer**
   Di Giorgio, C., Bellini, R., Lupia, A., ...Zampella, A., Fiorucci, S.
   Cellular Oncology, **2024**, 47(2), pp. 695–710
3. **Exploring the DNA_2-PNA heterotriplex formation in targeting the Bcl-2 gene promoter: A structural insight by physico-chemical and microsecond-scale MD investigation**
   Falanga, A.P., Lupia, A., Tripodi, L., ...Oliviero, G., Borbone, N.
   Heliyon, **2024**, 10(3), e24599
4. **Molecular and Structural Aspects of Clinically Relevant Mutations of SARS-CoV-2 RNA-Dependent RNA Polymerase in Remdesivir-Treated Patients**
   Gratteri, C., Ambrosio, F.A., Lupia, A., ...Artese, A., Alcaro, S.
   Pharmaceuticals, 2023, 16(8), 1143
5. **Development of Cyclic Peptides Targeting the Epidermal Growth Factor Receptor in Mesenchymal Triple-Negative Breast Cancer Subtype**
   Nisticò, N., Aloisio, A., Lupia, A., ...Quinto, I., Iaccino, E.
   Cells, 2023, 12(7), 1078
6. **Discovery of BAR502, as potent steroidal antagonist of leukemia inhibitory factor receptor for the treatment of pancreatic adenocarcinoma**
   Di Giorgio, C., Bellini, R., Lupia, A., ...Zampella, A., Fiorucci, S.
   Frontiers in Oncology, 2023, 13, 1140730
7. **Molecular Basis for Non-Covalent, Non-Competitive FAAH Inhibition**
   Morgillo, C.M., Lupia, A., Deplano, A., ...Moraca, F., Catalanotti, B.
   International Journal of Molecular Sciences, 2022, 23(24), 15502
8. **Repositioning Mifepristone as a Leukaemia Inhibitory Factor Receptor Antagonist for the Treatment of Pancreatic Adenocarcinoma**
   Di Giorgio, C., Lupia, A., Marchianò, S., ...Zampella, A., Fiorucci, S.
   Cells, 2022, 11(21), 3482
9. **Ligand-based drug repurposing strategy identified SARS-CoV-2 RNA G-quadruplex binders**
   Moraca, F., Marzano, S., D'Amico, F., ...Pagano, B., Amato, J.
   Chemical Communications, 2022, 58(85), pp. 11913–11916
10. **Peptide platform as a powerful tool in the fight against covid-19**
    Murdocca, M., Citro, G., Romeo, I., ...Sangiuolo, F.C., Novelli, G.
    Viruses, 2021, 13(8), 1667

Speaker information

Speech Topic and Abstract

Title:

In-silico approaches applied to studying potential Flavivirus NS3 protease/helicase binders.

Abstract:

The *Flaviviridae* family members comprise many enveloped viruses, including Dengue (DENV, isoforms 1-4), West Nile, and Zika. These small spherical particles incorporate a single genomic RNA of positive-sense polarity encoding three structural and seven non-structural proteins (NS). The numerous crystal structures of the enzymatic NS proteins available in the Protein Data Bank (PDB) allow us to accelerate further molecular understanding and improve the structure-guided drug discovery process. In this panorama, the NS3 complex (protease and helicase) is essential for viral replication and represents a valid druggable target. Combining classical and advanced computational methods, such as Structure- and Ligand-based, Virtual Screening (VS), conventional and accelerated Molecular Dynamics simulations (MDs), and Dynophore, we aim to identify new drug candidates able to bind different sites (catalytic or allosteric), thus altering the conformational equilibrium of the protein function. This approach may prove worthwhile in developing new broad-spectrum inhibitors for DENV, WNV, and ZIK viruses.