UNIVERSITÀ DEGLI STUDI
MAGNA GRÆCIA DI CATANZARO

DOTTORATO DI RICERCHE
IN SCIENZE DELLA VITA

**UNIVERSITÀ DEGLI STUDI *MAGNA GRÆCIA* DI CATANZARO**
**- DIPARTIMENTO DI SCIENZE DELLA SALUTE -**
**- DOTTORATO DI RICERCHE IN SCIENZE DELLA VITA -**
**- SCUOLA DI SPECIALIZZAZIONE IN FARMACIA OSPEDALIERA -**

# SEMINARIO CORSO CV_S_053

# CLASSICAL AND ADVANCED COMPUTATIONAL STRATEGIES TO IMPROVE THE DRUG-DESIGN PROCESS


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The use of computational tools[1] in the field of drug-design has taken on a pivotal role in recent years, not only for the discovery of novel and more efficient drugs, but also for the repositioning of existing drugs (drug repurposing). Through the use of increasingly advanced and accurate simulation methods it is possible, in fact, to virtually identify molecular hits (both of synthetic and natural origin) that strongly interact with biological targets and to further improve their affinity through the lead optimization phase. This seminar is aimed to illustrate the main drug-design approaches used in the field of computational chemistry for the research and the identification of new potential drugs: from the classical methods such as Structure-based and Ligand-based Virtual Screening and Molecular Dynamics,[2] up to more advanced approaches, such as Dynophore and Metadynamics.[3] Some successful applications of these methods that led to the discovery of new bioactive molecules will also be treated.

**References:**


[1] Artese, A.; Alcaro, S.; Moraca, F. et al. *Future Med. Chem.* **2013**, *5*, 907-27.
[2] Maruca, A.; Ambrosio, F.A.; Lupia, A. et al. *Physical Sciences Reviews.* **2018**; 20180113.
[3] Lupia, A.; Moraca, F.; Bagetta, D. et al. *Physical Sciences Reviews.* **2019**; 20180114.


## COMPLESSO MONUMENTALE SAN GIOVANNI – AULA GISSING
## CORSO MAZZINI, 88100 CATANZARO – 3 MAGGIO 2019, ORE 10:00

**HOST:** STEFANO ALCARO alcaro@unicz.it
SEMINARIO APERTO A DOTTORANDI, SPECIALIZZANDI E STUDENTI CDL IN FARMACIA, STPA, BIOTECNOLOGIE TRIENNALE E MAGISTRALE.