



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_092

**ARTIFICIAL INTELLIGENCE AND MULTIOBJECTIVE OPTIMIZATION
FOR THE DE NOVO DESIGN OF TARGETED CHEMICAL LIBRARIES**



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Artificial intelligence and multiobjective optimization represent powerful strategies to bridge chemical and pharmacological sides for the automated generation of new bioactive compounds. The talk will focus on a novel pair-based multiobjective approach implemented in an adapted SMILES generative algorithm for the humanlike de novo design of targeted chemical libraries whose overall features are optimized by finding the best trade-offs among relevant physicochemical properties (MW, logP, HBA, HBD) and additional similarity-based constraints biasing specific pharmacological targets. In this respect, a number practical examples concerned with the de novo design of chemical libraries targeting neuraminidase, acetylcholinesterase, and the main protease of severe acute respiratory syndrome coronavirus 2 will be discussed.

Reference:

Alberga D., Gambacorta N., Trisciuzzi D., Ciriaco F., Amoroso N., Nicolotti O. De novo drug design of targeted chemical libraries based on artificial intelligence and pair based multiobjective optimization (2020) Journal of Chemical Information and Modeling, 60 (10), pp. 4582-4593
ISSN: 15499596; DOI:10.1021/acs.jcim.0c00517

WEBINAR [HTTPS://MEET.GOOGLE.COM/HCI-HITD-KJP](https://meet.google.com/hci-hitd-kjp)
14 LUGLIO 2021, ORE 9:00

HOST: STEFANO ALCARO alcaro@unicz.it

SEMINARIO APERTO A DOTTORANDI, SPECIALIZZANDI E STUDENTI CDL IN FARMACIA, STPA, BIOTECNOLOGIE TRIENNALE E MAGISTRALE.