

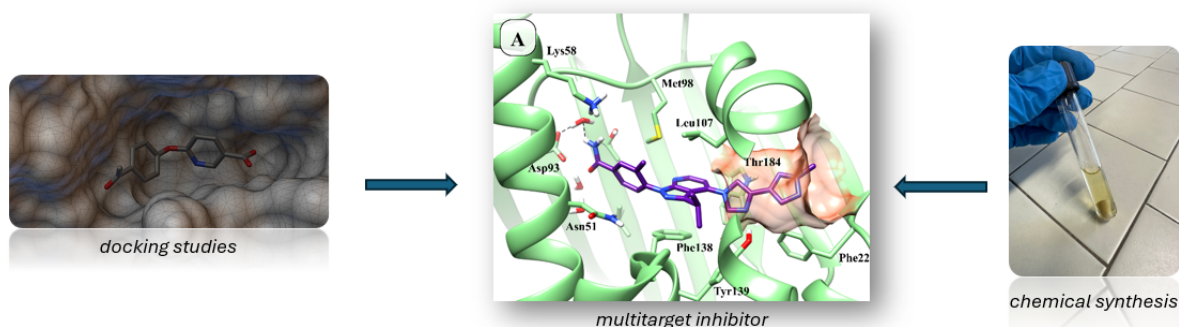


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Molecular hybridization as a tool for designing multitarget-directed ligands for complex diseases

Multi-target enzyme inhibitors offer comprehensive therapeutic strategies by simultaneously targeting multiple disease-related pathways, thus enhancing biological efficacy [1]. The ability of a multitarget inhibitor to mitigate drug resistance, improve selectivity and provide beneficial synergistic effects makes them promising candidates for the treatment of complex diseases. Additionally, the versatility of these inhibitors allows for a more personalized cure, addressing the multifactorial origins of various medical conditions. For instance, the development of a molecule capable of inhibiting two biological pathways begins with a thorough analysis of the pharmacophores through docking studies (Figure 1) [2]. Subsequently, two molecules (or parts of them) are combined in a new, single entity by chemical synthesis. Some examples of validated multitarget enzyme inhibitors will be described, which demonstrate the potential of the molecular hybridization as a promising and effective tool in medicinal chemistry.



Dr. Andrea Citarella is a Postdoc researcher (assegnista tipo A) at the Department of Chemistry of the University of Milan working at the interface of synthetic organic chemistry, structural and computational biology. During his post-doctoral studies Dr. Citarella was involved in a project financed by AIRC, in collaboration with the University of Modena and Reggio-Emilia, focusing on the design, synthesis and biological evaluation of HDAC6/Hsp90 dual inhibitors for the treatment of prostate cancer. Now, in collaboration with the Department of Biosciences at the University of Milan, he is involved in a project aimed at studying the biochemical modulation of D-Aspartate oxidase in brain by means of synthetic inhibitors.

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Ospite: Prof. Paolo Bergese