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Università degli Studi *Magna Græcia* di Catanzaro
- Dipartimento di Scienze della Salute -

SEMINARIO

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"DOCKING AND POST-DOCKING IN DRUG DISCOVERY: THE "BEAR" EXAMPLE"

Virtual screening (VS) has emerged as a straightforward computational tool for the rapid identification of bioactive compounds from large collections of chemicals. Typically, VS is performed with molecular docking, which is able to virtually screen and rank a large number of molecules into the active site of a target structure in a reasonable amount of time. This technique is powerful and cost-effective, and allows to prioritise and select best-hit compounds for biological assays. However, the inherent limitations in the accuracy of these methods often lead to false positives or false negatives and reduce VS success rates. For this reason, post-docking methods are emerging as a way to improve docking results.
We have developed Binding Estimation After Refinement (BEAR), an automated post-docking procedure for the conformational refinement of docking poses through molecular dynamics followed by more accurate prediction of binding free energies using MM-PBSA. The main achievements obtained with the validation and application of BEAR in drug discovery will be illustrated.

Venerdì 19 luglio 2013, ore 11.00

Aula R, livello 1, corpo H

Ed. Bioscienze, Campus universitario "*S. Venuta*", Catanzaro

Host: Stefano Alcaro – Dipartimento di Scienze della Salute - UMG