DIPARTIMENTO DI FARMACIA E BIOTECNOLOGIE

AVVISO DI SEMINARIO

Il giorno martedì **20/09/2022**
alle ore **14.30**

in presenza:

Aula 1 – FaBiT, via Belmeloro 6, Bologna BO

oppure *in streaming:*

https://teams.microsoft.com/l/meetup-join/19%3aN09c0NIyEssBnF7ObCyDOQwkgDWm1qdd9f7F2nJV9fw1%40thread.tacv2/1631519544944?context=%7b%22Tid%22%3a%22e99647dc-1b08-454a-bf8c-699181b389ab%22%2c%22Oid%22%3a%225a941351-ef41-4aa4-8771-fa50a6d62ca1%22%7d

Dott. Bartocci Alessio

Università di Strasburgo, Strasburgo, Francia
(ospite Prof. Musiani Francesco)

terrà un seminario dal titolo:

FROM PROTEIN-LIGAND INTERACTIONS TO PROTEIN REGULATION: INSIGHTS FROM MOLECULAR DYNAMICS SIMULATIONS

Colleghi e studenti sono cordialmente invitati

Commissione Ricerca e Attività Correlate - FaBiT

ABSTRACT

Molecular dynamics (MD) simulations are one of possible methods to investigate supramolecular and biological systems. Among these systems, the study of protein-ligand complexes attracts particular interest, with possible applications ranging from protein crystallization [1,2] to understanding the molecular mechanisms behind drug binding [3]. For example, atomistic MD simulations were used to characterize the experimentally detected calixarene binding sites on the cytochrome-C surface [4], to highlight key residues implicated in the interaction process and to provide a possible explanation of the enhanced protein-protein contacts mechanism [4]. The search and characterization of ligand binding sites, on the other hand, in the pentameric ligand gated ion channels (pLGICs) transmembrane domain (TMD) [5] is difficult at this resolution, but may be achieved by using Coarse-Grained (CG) representations through millisecond time-scale simulation lengths [6]. By combining a "multiscale approach" with CG [7,8] MD simulations and a "backmapping" process to all-atom representation, it is possible not only to characterize binding sites of specific molecules, but also their specific binding modes at atomic resolution, proposing a characteristic fingerprint.

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[2] S. Engilberge, M.L. Rennie, E. Dumont, P.B. Crowley, *ACS NANO*, **13** (2019) 10343-10350
[3] G. Heinzelmann, N.M. Henriksen, M.K. Gilson, *JCTC*, **13** (2017) 3260-3275
[4] A. Bartocci, G.P. Pereira, M. Cecchini, E. Dumont, *JCIM*, (2022), **accepted**
[5] A.H. Cerdan, M. Sisquellas, G.P. Pereira, D.E. Barreto Gomes, J.P. Changeaux, M. Cecchini, *Bioinformatics*, **36** (2020) 3379
[6] S.J. Marrink, H.J. Risselada, S. Yefimov, D.P. Tieleman, A.H. de Vries, *J. Phys. Chem. B,* **111** (2007) 7812-7824
[7] P.C.T. Souza, S. Thallmair, P. Conflitti, C. Ramírez-Palacios, R. Alessandri, S. Raniolo, V. Limongelli, S. J. Marrink, *Nature Communication*, **11** (2020), 1-11
[8] P.C.T. Souza, R. Alessandri, J. Barnoud, S. Thallmair, I. Faustino, F. Grunewald, F. Patmanidis, H. Abdizadeh, B.M. Bruininks, T.A. Wassenaar et al., *Nature Methods*, **18** (2021), 382-388

BIOGRAPHICAL SKETCH

November 2012 – November 2015, University of Perugia (Department of Chemistry), Italy, **Ph.D. in Theoretical Chemistry** (Prof. Fernando Pirani) *"Characterization of the weak hydrogen and halogen bonds by molecular beam scattering experiments and ab-initio calculations*";

October 2016–December 2018, University of Genoa (Department of Physics), Italy, **Post-Doc in Computational Biophysics** (Prof. Giulia Rossi);

January 2019-January 2021, École Normale Supérieure de Lyon (Department of Chemistry), France, **Post-Doc in Theoretical Chemistry** (Prof. Elise Dumont);

From February 2021, University of Strasbourg (Department of Chemistry), France, **Post-Doc in Theoretical Chemistry** (Prof. Marco Cecchini).