Pisa group – Biophys

Activity

The activity of the Pisa group is focused on the developments and applications of numerical simulation methods of complex systems of biological interest.

Members (FTE: 5.0)

Name -- Position -- INFN Position

Giuseppe Brancato – Professore Associato 100%

Vincenzo Barone -- Professore Ordinario 100%

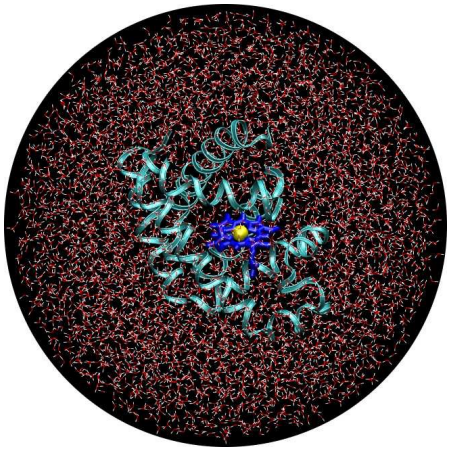
Giordano Mancini -- Tecnico 100%

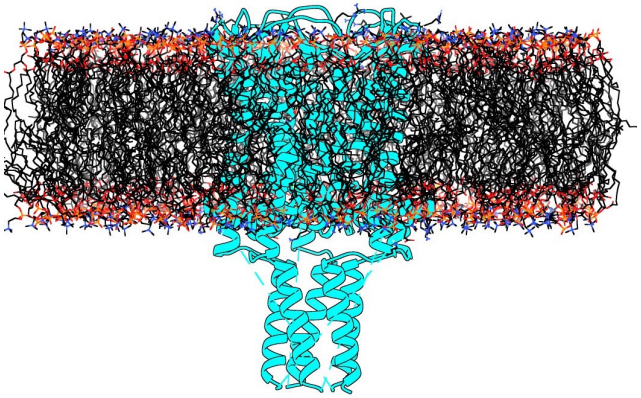
Luca Sagresti – Dottorando 100%

Alfonso Ferretti – Dottorando 100%

Mario Nicodemi INFN section: Napoli
Sebastiano Stramaglia INFN section: Bari
Guido Tiana INFN section: Milano
Giuseppe Brancato INFN section: Pisa
Silvia Morante INFN section: Roma II
Silvia Scarpetta INFN section: Salerno
Michele Caselle INFN section: Torino
Pietro Faccioli INFN section: Trento

Molecular Dynamics (MD) Simulations





Size: >100,000 atoms

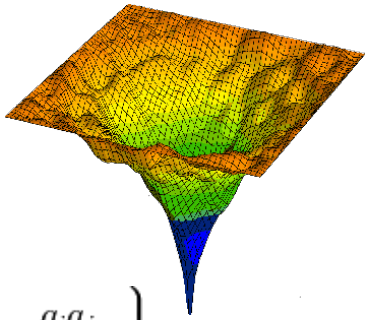
Time scale: 100 ns – 1 μs

Molecular dynamics is a computational method that allows to follow the time evolution of a molecular system on the basis of a known potential

Simulation with full atomistic details:
Protein
Environment (Solvent + Lipid Membrane)

Molecular mechanics force fields

$$V(r^N) = \sum_{\text{bonds}} \frac{1}{2} k_b (l - l_0)^2 + \sum_{\text{angles}} k_a (\theta - \theta_0)^2 + \sum_{\text{torsions}} \frac{1}{2} V_n [1 + \cos(n\omega - \gamma)] + \sum_{j=1}^{N-1} \sum_{i=j+1}^{N} \left\{ \epsilon_{i,j} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - 2 \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \right\}$$



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Bio-modeling @SNS

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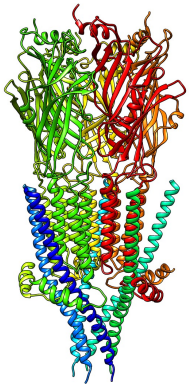
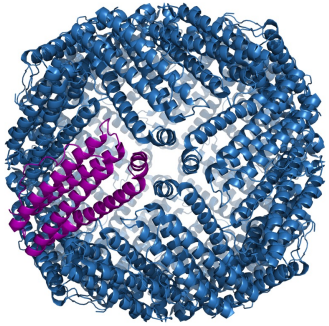
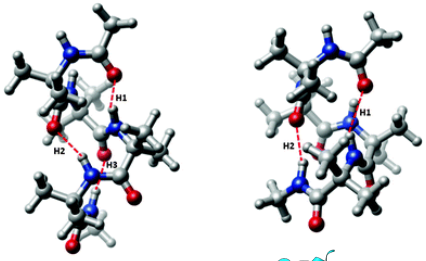
5HT3 Serotonin Receptor



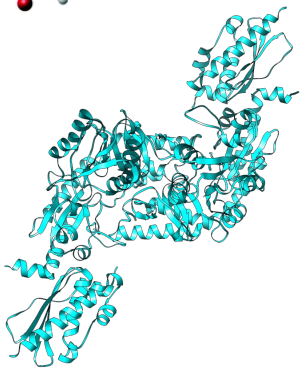
Ferritin



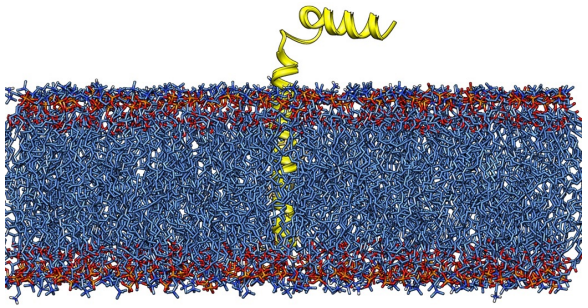
Aib-based peptides



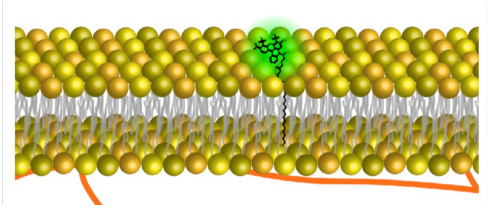
Fe-S cluster biosynthesis (IscS-IscU system)



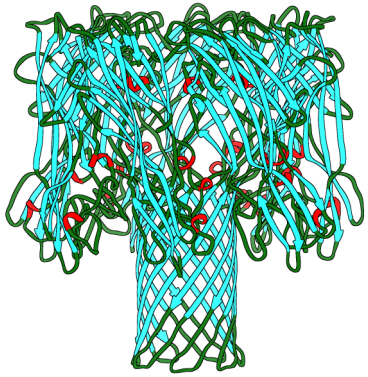
Phospholamban

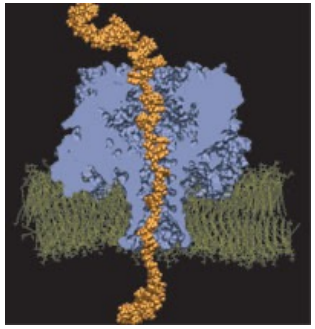


Lipid Membranes

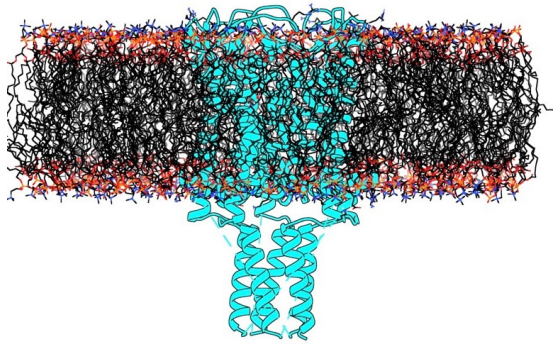


Hemolysin





MscL channel



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PUBS

INFN Istituto Nazionale di Fisica Nucleare SEZIONE DI PISA

Mateo L. M.; Sagresti L.; Luo Y.; Guldi D. M.; Torres T.; **Brancato G.(*)**; Bottari G., *Expanding the Chemical Space of Tetracyanobuta-1,3-Diene (TCBD) through a Cyano-Diels-Alder Reaction: Synthesis, Structure, and Physicochemical Properties of an Anthryl-Fused-TCBD Derivative*, Chemistry – A European Journal **27**, 16049–55 (2021). DOI: 10.1002/chem.202103079.

Barbosa N.; Sagresti L.; **Brancato G.(*)**, *Photoinduced Azobenzene-Modified DNA Dehybridization: Insights into Local and Cooperativity Effects from a Molecular Dynamics Study*, Physical Chemistry Chemical Physics **23**, 25170–79 (2021). DOI: 10.1039/D1CP04032D.

Barbosa N.; Pagliai M.; Sinha S.; Barone V.; Alfè D.; **Brancato G.(*)**, *Enhancing the Accuracy of Ab Initio Molecular Dynamics by Fine Tuning of Effective Two-Body Interactions: Acetonitrile as a Test Case*, The Journal of Physical Chemistry A **48**, 10475–10484 (2021). DOI: 10.1021/acs.jpca.1c07576.

Del Frate G.; Macchiagodena M.; Akhunzada M. J.; D'Autilia F.; Catte A.; Bhattacharjee N.; Barone V.; Cardarelli F.; **Brancato G.(*)**, *Probing liquid-ordered and disordered phases in lipid model membranes: a combined theoretical and spectroscopic study of a fluorescent molecular rotor*, The Journal of Physical Chemistry B **2**, 480-491 (2021). DOI: 10.1021/acs.jpcb.1c08324.

Ferretti A.; Sourab S.; Sagresti L.; Araya-Hermosilla E.; Prato M.; Mattoli V.; Pucci A.; **Brancato G.(*)**, One-step Functionalization of Mildly and Strongly Reduced Graphene Oxide with Maleimide: An Experimental and Theoretical Investigation of the Diels-Alder [4+2] Cycloaddition Reaction, Physical Chemistry Chemical Physics **4**, 2491-2503 (2022). DOI: 10.1039/d1cp04121e.

Catte A.; Tiecher C.; Bhattacharjee N.; **Brancato G.(*)**; Kocer A., *Unravelling the molecular origin of an inherited channelopathy in the voltage-gated potassium channel Kv4.3*, submitted.

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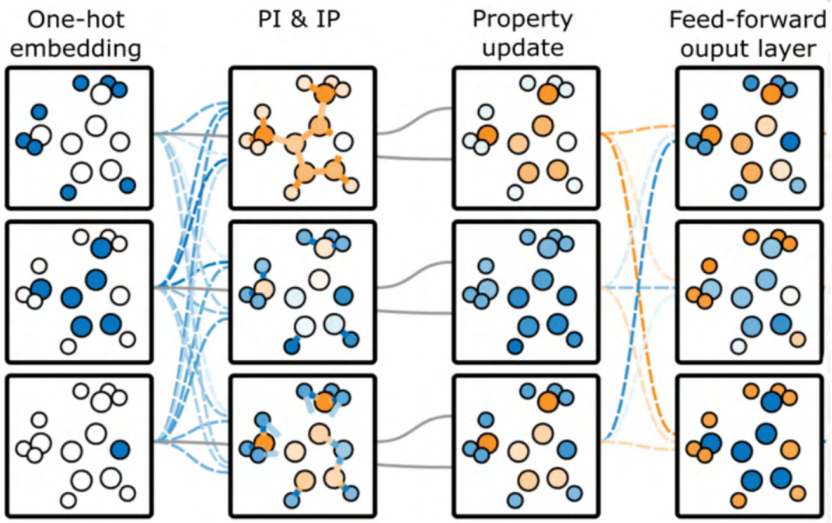

March 16-18 2022

RECENT ADVANCES IN MACHINE LEARNING ACCELERATED MOLECULAR DYNAMICS

Sala Azzurra
Palazzo della Carovana
Scuola Normale Superiore
Piazza dei Cavalieri, 7, Pisa

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Richieste 2023

Missioni Interne ed esterne: 7.5KE (5.0 FTE)

1) Prof.sa Annalisa Pastore, King's College, UK
2) Prof.sa Armagan Kocer, Univ. Groeningen, NL

Partecipazione alle seguenti conferenze

1) CECAM Workshop
2) ACS Conferences
3) ESP Conference

Inviti Ospiti Stranieri

Prof. Giovanni Bottari

Universidad Autonoma de Madrid, Spain