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CIC biomaGUNE
Biomaterialetako Ikerkuntza Kooperatiboko Zentroa
Centro de Investigación Cooperativa en Biomateriales

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SEMINAR

Friday, 13th April, 12.00 pm, Seminar Room

Host: Dr. Aitziber L. Cortajarena

Role of conformational dynamics in the design of novel function and nanohybrid materials

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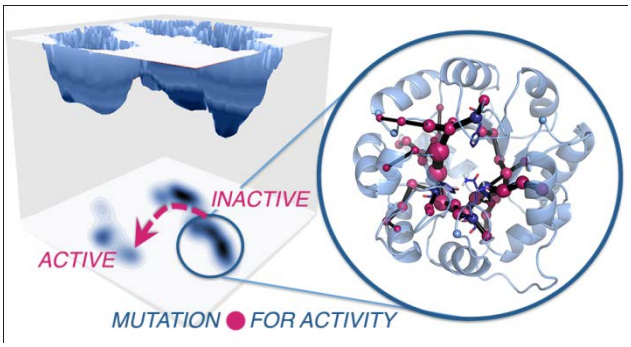
Biomolecules exist as an ensemble of conformations important for their function. By introducing mutations to the protein sequence, the populations of the different conformational states can be gradually tuned for allowing novel function. The dynamic nature of biomolecules and of processes such as assembly, or biomolecular recognition central to all biological processes makes the evaluation of the conformational dynamics of proteins highly appealing. In this talk, a dynamic view of such important biological processes will be presented with an special emphasis on the nanohybrid formation, HIV-1 maturation inhibition, and enzyme function. The importance of Molecular Dynamics (MD) simulations for unveiling the molecular basis of improved catalysis achieved by Directed Evolution, and how MD can guide the rational design of enzymes towards new synthetically relevant targets will be presented.



[1] López-Andarias, J.; H. Mejías, S.; Sakurai, T.; Matsuda, W.; Seki, S.; Feixas, F.; Osuna, S.; Atienza, C.; Martín, N.; Cortajarena, A. L. Toward bioelectronic nanomaterials: photoconductivity in protein-porphyrin hybrids wrapped around SWCNT, *Adv. Funct. Mat.* **2017**, accepted for publication.

[2] Romero-Rivera, A.; Garcia-Borràs, M.; Osuna, S. The role of conformational dynamics in the evolution of retro-aldolase activity, *ACS Catalysis* **2017**, *7*, 8524-8532.

[3] Romero-Rivera, A., Garcia-Borràs, M., Osuna, S. Computational tools for the evaluation of laboratory-engineered biocatalysts, *Chem. Commun.* **2017**, 53, 284-297.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