OMICS-BASED DISCOVERY

NBD is involved in the application of bioinformatics and simulation tools aimed at unveiling the genetic basis of disease, the pathological changes associated to mutations, the genetic variation among different sub-populations and their relationships with disease risk, patient stratification and response to therapy. The deluge of omics-based data is progressively being incorporated earlier in discovery and development projects.

2.1 Rational macromolecular design

NBD scientists have a wide experience in the macromolecular simulation field, having been engaged for decades in in silico studies of structure and flexibility of DNA, RNA and chemically modified nucleic acids, where a great effort has been devoted to the development and improvement of currently available force fields. They have also been involved in different projects of enzyme engineering, where not only the affinity but also the kinetics of binding plays a crucial role.

- **Nucleic acid structure modeling and design of chemically-modified nucleic acids.**
  Study the structure and flexibility of any natural or non-natural nucleic acid. Accurately parametrize any nucleic acid with chemically-modified backbone or base. Simulate and improve the properties nucleic acid-based research and diagnostic tools.

- **Enzyme design.**
  Accurately simulate the process of binding and unbinding of substrates and products for enzymes with known 3D structure, gain insight not only on their binding modes but crucially on their migration pathways, and rationally design new mutants with improved properties.

- **Protein-protein docking.**
  Simulate one of the most challenging problems in computational biology, the formation of protein-protein complexes and define the most important interaction points between the two partners, locate hotspots in the two protein surfaces and determine their druggability.

2.2 PRECISION MEDICINE

NBD scientists have been involved in many national and international genomics initiatives, such as the sequencing of the tomato genome, genome-wide studies of mutations associated to chronic lymphocytic leukemia, the development of in silico tools for the annotation of mutations in cancer, genome-wide prediction of promoter regions, epigenetics processes associated to the packaging of DNA in nucleosomes and others. The coupling of all the technologies of rational small molecule and macromolecular design with the information derived from NGS technologies enables NBD to tackle biomedical projects from the personalized medicine perspective. Through different strategic collaborations, NBD can tackle problems related to NGS projects, target discovery and validation, somatic mutation annotation related to pathology, and others

- **Drug design for fragmented populations.**
  Incorporate omics-based information into the structural models of receptors, enzymes and proteins to determine the link between SNPs, structural variants and response to therapy and/or phenotypic changes.

- **Prediction of pathological variants.**
  Predict the pathological character of single point aminoacid mutations in proteins of therapeutic interest.

- **SNP annotation.**
  Annotate and characterize somatic structural variants by using NGS sequencing data from tumor genomes with great sensitivity and specificity.

- **Toxicogenomics and pharmacogenomics.**
  Combine information on gene and protein activity with molecular structure tools to uncover trends in toxicogenomics and pharmacogenomics studies.

- **Target discovery.**
  Use sequence and structural information derived from the application of all tools available to NBD to generate mechanistic hypothesis of disease origin and progression.

NBD

Rethink & Accelerate

NOSTRUM BIODISCOVERY

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