BioVirtual

4-dimensional computational analysis of molecular interactions between biological entities (proteins, antibodies, nucleic acids and lipids) and small ligands (inhibitors, substrates, cofactors) with atomic and temporal resolution. Based on solid physical principles and incorporate environmental effects (solvents, ionic strength, temperature), we deliver high-quality graphs and attractive pictures/videos illustrating these interactions. Our computer simulations provide detailed insights on biomolecular recognition and activity events.

EKIPO ETA OSAGAI GARRANTZITSUENAK

- **Computational Chemistry Laboratory**

  Computational Chemistry is a cross-disciplinary area devoted to the accurate atomistic simulation of chemical and biochemical phenomena, from small-molecule reactions and metal-catalyzed processes to protein folding, dynamics and function. It is at the core of the structure-activity relationship and uses cutting edge technology based on state-of-the art supercomputing, nearly-exact quantum mechanics and multiscale molecular mechanics and dynamics simulations, with strong validation and feedback from experiments.

bdih

basqueindustry.eus

GRUPO spri TALDEA

EUSKO JAURLARITZA GOBIERNO VASCO

AKTIBOAK ESKAINTZEN DITUEN ZERBITZUAK

Bioinformatics and machine learning-based analysis of large databases of protein sequences

Crucial for understanding biological phenomena and designing new molecules, processes and therapies. Our high-resolution virtualization tool provides rigorous descriptions and powerful images for the valorization. The only way to interpret biological phenomena, particularly when experimental structural information is not available.

Calculation of high-quality binding energies for hit-to-lead optimization

Crucial for understanding biological phenomena and designing new molecules, processes and therapies. Our high-resolution virtualization tool provides rigorous descriptions and powerful images for the valorization. The only way to interpret biological phenomena, particularly when experimental structural information is not available.

Design of chemical reactions and linkers for protein and antibody conjugation

Crucial for understanding biological phenomena and designing new molecules, processes and therapies. Our high-resolution virtualization tool provides rigorous descriptions and powerful images for the valorization. The only way to interpret biological phenomena, particularly when experimental structural information is not available.

High-throughput virtual screening for hit identification in drug discovery

Crucial for understanding biological phenomena and designing new molecules, processes and therapies. Our high-resolution virtualization tool provides rigorous descriptions and powerful images for the valorization. The only way to interpret biological phenomena, particularly when experimental structural information is not available.

Modeling of unknow (glyco)protein and glycans and interactions between them

Crucial for understanding biological phenomena and designing new molecules, processes and therapies. Our high-resolution virtualization tool provides rigorous descriptions and powerful images for the valorization. The only way to interpret biological phenomena, particularly when experimental structural

information is not available

Molecular dynamics simulations of biological entities in water and/or cellular membranes.

Crucial for understanding biological phenomena and designing new molecules, processes and therapies. Our high-resolution virtualization tool provides rigorous descriptions and powerful images for the valorization. The only way to interpret biological phenomena, particularly when experimental structural information is not available.

Protein engineering virtual optimization with emphasis in enzymatic catalysis and thermostability.

Crucial for understanding biological phenomena and designing new molecules, processes and therapies. Our high-resolution virtualization tool provides rigorous descriptions and powerful images for the valorization. The only way to interpret biological phenomena, particularly when experimental structural information is not available.

Refinement of crystallographic and cryo-EM structures

Crucial for understanding biological phenomena and designing new molecules, processes and therapies. Our high-resolution virtualization tool provides rigorous descriptions and powerful images for the valorization. The only way to interpret biological phenomena, particularly when experimental structural information is not available.

Refinement of crystallographic and cryo-EM structures

Crucial for understanding biological phenomena and designing new molecules, processes and therapies. Our high-resolution virtualization tool provides rigorous descriptions and powerful images for the valorization. The only way to interpret biological phenomena, particularly when experimental structural information is not available

---

AKTIBOA KUDEATZEN DUEN ERAKUNDEA

Image not found or type unknown

ASOCIACIÓN CENTRO DE INVESTIGACIÓN COOPERATIVA EN BIOCIENCIAS - CIC bioGU

Harremanetarako pertsona:

Donatello Castellana