

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.



basqueindustry.eus



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

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Design of chemical reactions and linkers for protein and antibody conjugation

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High-throughput virtual screening for hit identification in drug discovery

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

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

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

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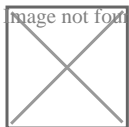
Refinement of crystallographic and cryo-EM structures

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AKTIBOA KUDEATZEN DUEN ERAKUNDEA



ASOCIACIÓN CENTRO DE INVESTIGACIÓN COOPERATIVA EN BIOCENCIAS - CIC bioGU

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