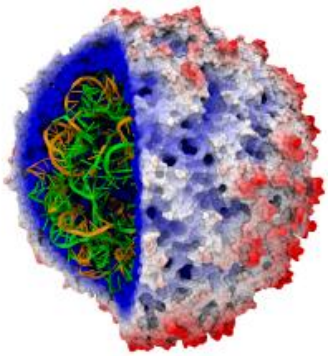
MDWeb

MDWeb is one of NBD's core structure-based drug design technologies. It has been developed in one of the most highly reputed simulation groups in Europe (M. Orozco group, Institute of Research in Biomedicine, Barcelona). It is a bundle of workflows for molecular dynamics simulations that streamline the build-up and analysis of trajectories, allowing the implementation of MD simulations in the high throughput regime.

Features & Advantages

- It automates many of the most tedious procedures for building molecular dynamics systems.
- It not only handles macromolecules but also ligand-receptor complexes requiring the parametrization of small molecules.
- It can build macromolecular systems solvated in explicit water or in mixtures of water plus different co-solvent molecules.
- It is being currently fine-tuned to also handle membrane-embedded proteins.



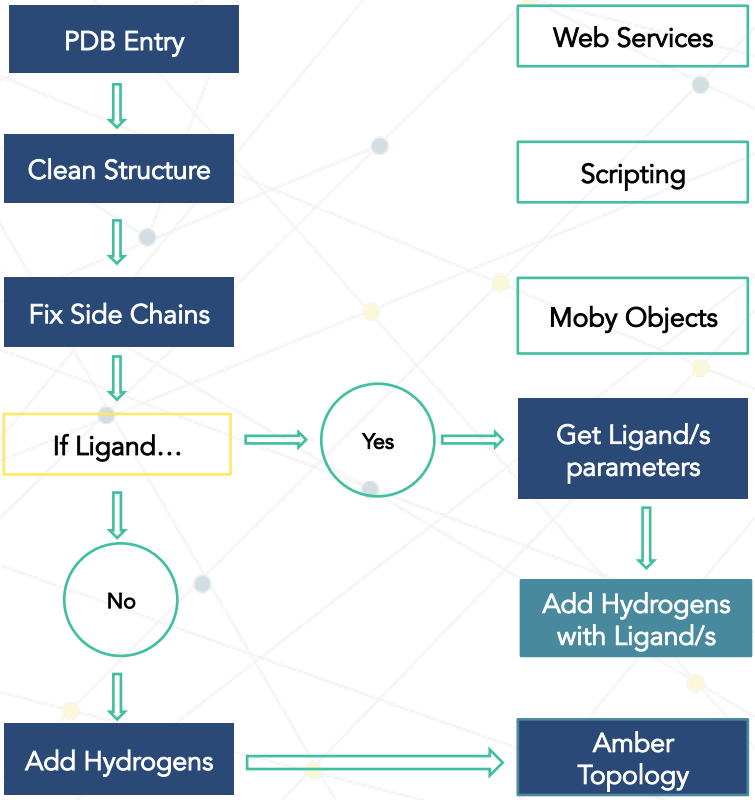
Applications

- Extend the conformational landscape of experimentally determined structures of your target and enrich it with a computationally generated ensemble
- Easily carry out molecular dynamics simulations of a whole protein family and find out differences between all its members
- Find out similarities and dissimilarities in terms of flexibility between your target and structurally related proteins to steer the design of selective compounds
- Study differences in flexibility, molecular recognition and binding site geometries and volumes between targets and anti-targets

Scientific References

- MDWeb and MDMoby: an integrated web based platform for molecular dynamics simulations. Bioinformatics (2012).

How MDWeb works?



MDWeb provides a friendly environment to setup new systems, run test simulations and perform analysis within a guided interface. Setup files can be prepared for Amber, NAMD, and Gromacs (other formats will be incorporated in the future) and analysis can be carried out using any standard trajectory format. Additionally, the platform is interfaced to our flexibility analysis software FlexServ, so providing coarse-grained simulation, and advanced flexibility analysis tools. Since the first simulation of biomacromolecules in 1977, molecular dynamics (MD) has experienced a long evolution and, at present, it is a mature technique that can be used to obtain an accurate picture of the dynamics of complex systems with atomistic detail.

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