



# Course on Simulation of Biological Systems

## Theory Lectures 14:00 – 17:00 GMT+1:00 Madrid

- Day 1. 1<sup>st</sup> Feb 2022. **Molecular Dynamics, Equations of Motion and Force Fields** <https://youtu.be/bSnwWyzOP4c>
- Day 2. 4<sup>th</sup> Feb 2022. **Periodic Boundary Conditions. Introduction to Enhanced-Sampling Approaches** [https://youtu.be/g\\_wrYUKNyc4](https://youtu.be/g_wrYUKNyc4)
- Day 3. 8<sup>th</sup> Feb 2022. **Umbrella Sampling and Replica Exchange** <https://youtu.be/A3SxYkoKlnM>
- Day 4. 11<sup>th</sup> Feb 2022. **QM/MM and Research Examples** <https://youtu.be/lgezhl719no>

## Computer Exercises 13:00 – 17:00 GMT+1:00 Madrid, Software: AmberTools, Orca, VMD

- Day 5. 15<sup>th</sup> Feb 2022. **Classical Molecular Dynamics** <https://youtu.be/cHpqEkMru3A>
- Day 6. 18<sup>th</sup> Feb 2022. **Umbrella Sampling** <https://youtu.be/dvo6noErrbc>
- Day 7. 22<sup>nd</sup> Feb 2022. **Computation of Redox Potentials** <https://youtu.be/NRpnKUJXA7E>
- Day 8. 25<sup>th</sup> Feb 2022. **Computation of Absorption Spectra** <https://youtu.be/lsR5i8Na1wg>