Review Questions

- What is molecular mechanics and why do people use it instead of quantum mechanics?
- Generally speaking, how does a molecular dynamics simulation work?

References

• Durrant, J. D.; McCammon, J. A. Molecular Dynamics Simulations and Drug Discovery. BMC Biol 2011, 9 (1), 71. https://doi.org/10.1186/1741-7007-9-71, adapted under the CC BY 2.0 license.