Advanced Molecular Modelling: biomolecules and drug design

Edition 2021: from July 5th to July 8th

Institut de Química Teòrica i Computacional
UNIVERSITAT DE BARCELONA

EXCELENCIA MARÍA DE MAEZTU

Simulation of macromolecular systems

Practice session with *EspressoMD*

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Simulation of macromolecular systems

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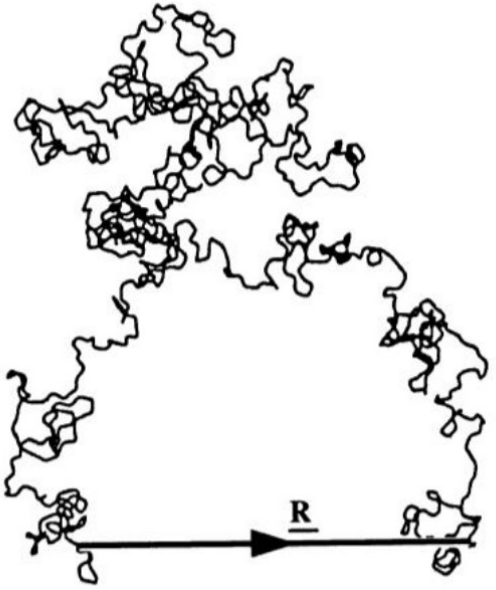
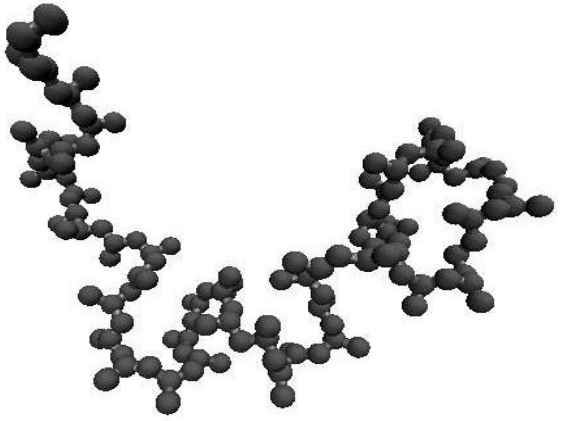
coarse-grained simulation models for polymers

Motivation: Structure, Properties?

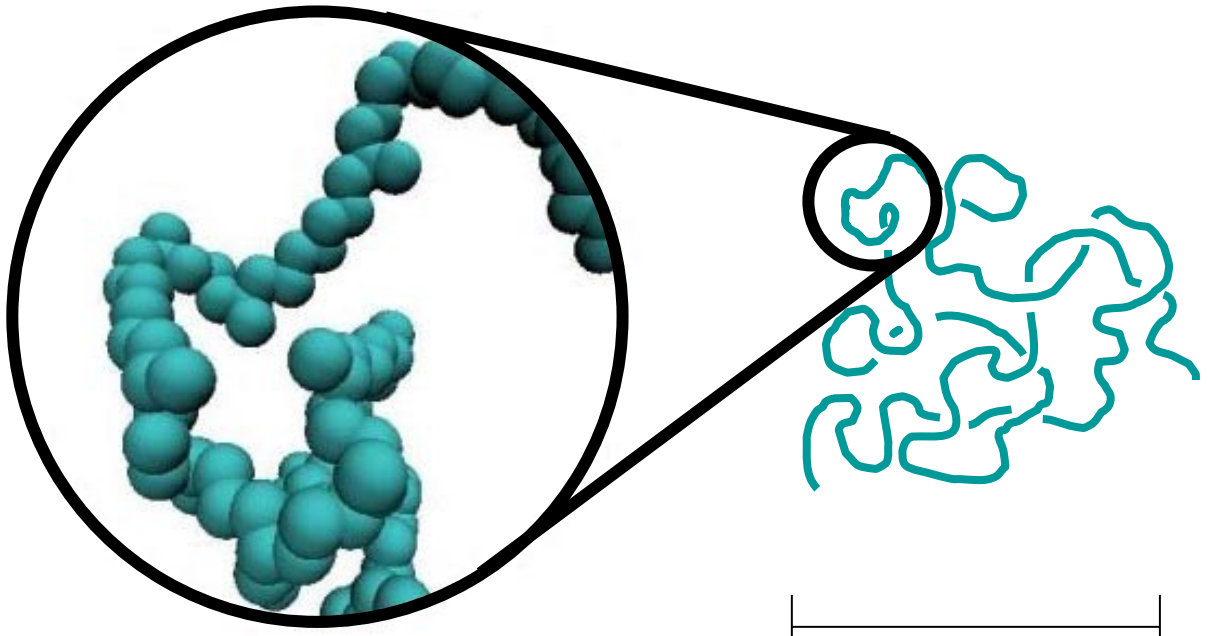
polyethylene



atactic-polypropylene

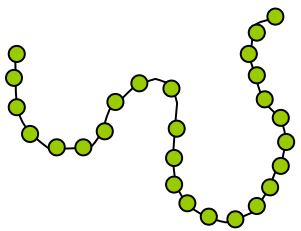


Hierarchy of Length and Time Scales

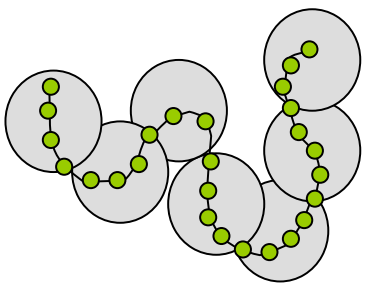


Coarse-graining of Polymer Simulations

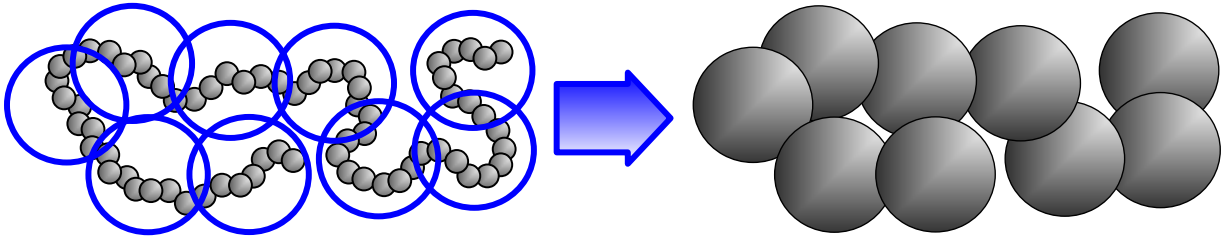
- Goal: To develop coarse-grained descriptions to access longer length and timescales



One CG particle describes *n* carbons of the detailed polymer

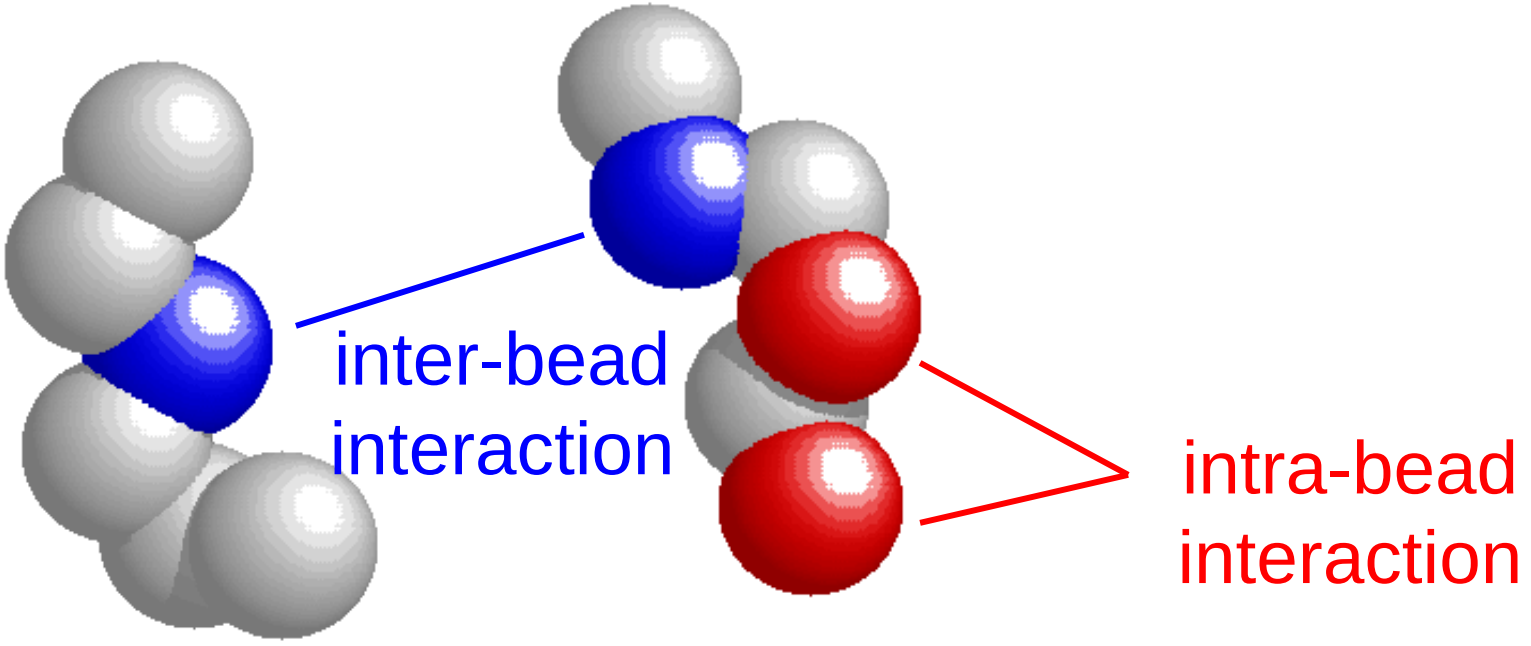


Coarse-graining method



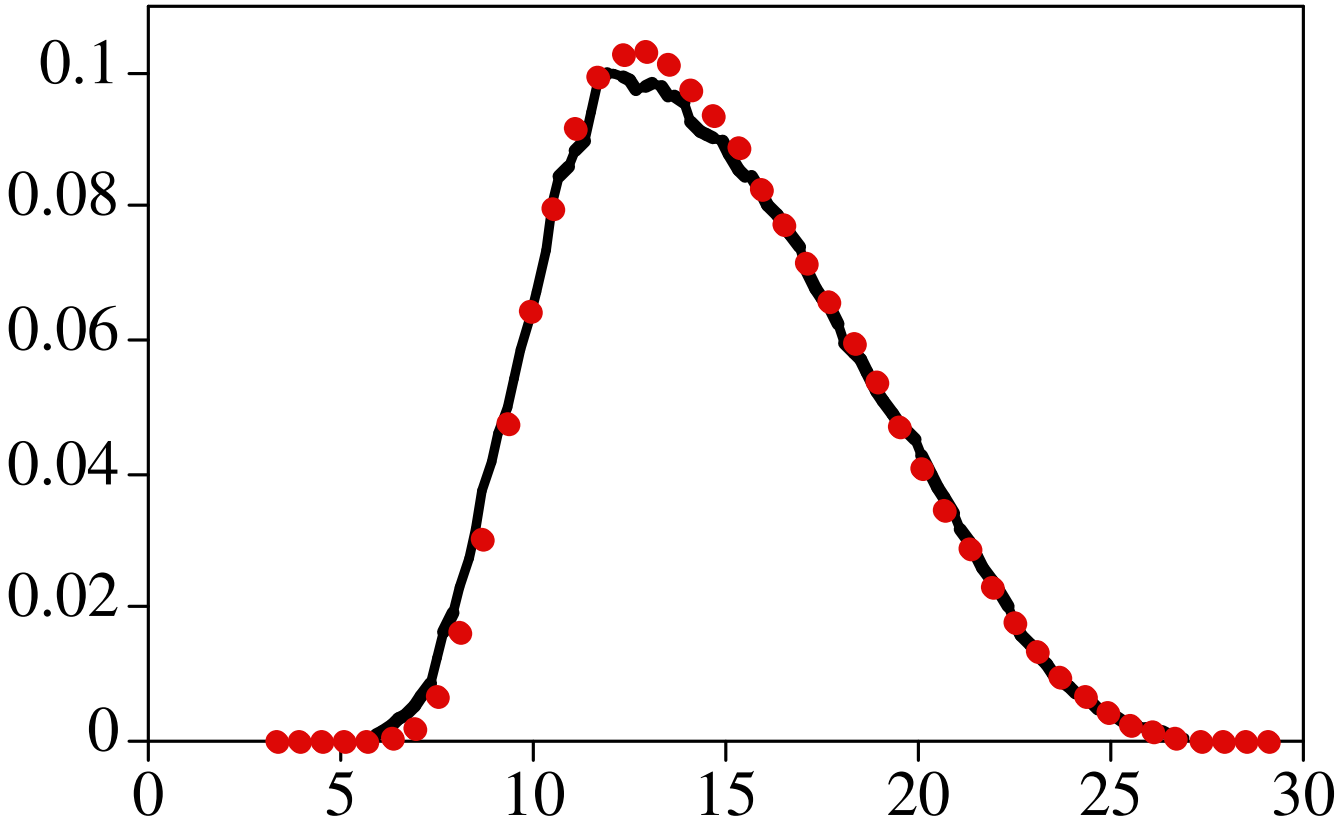
- Perform molecularly detailed simulations of polymers
- Define coarse-grained beads by grouping backbone monomers
- Calculate structural correlations between coarse-grained beads
- Determine effective bead-bead interactions that reproduce coarse-grained correlations of all-atom force-fields or experimental correlations.

Coarse Grained Potential



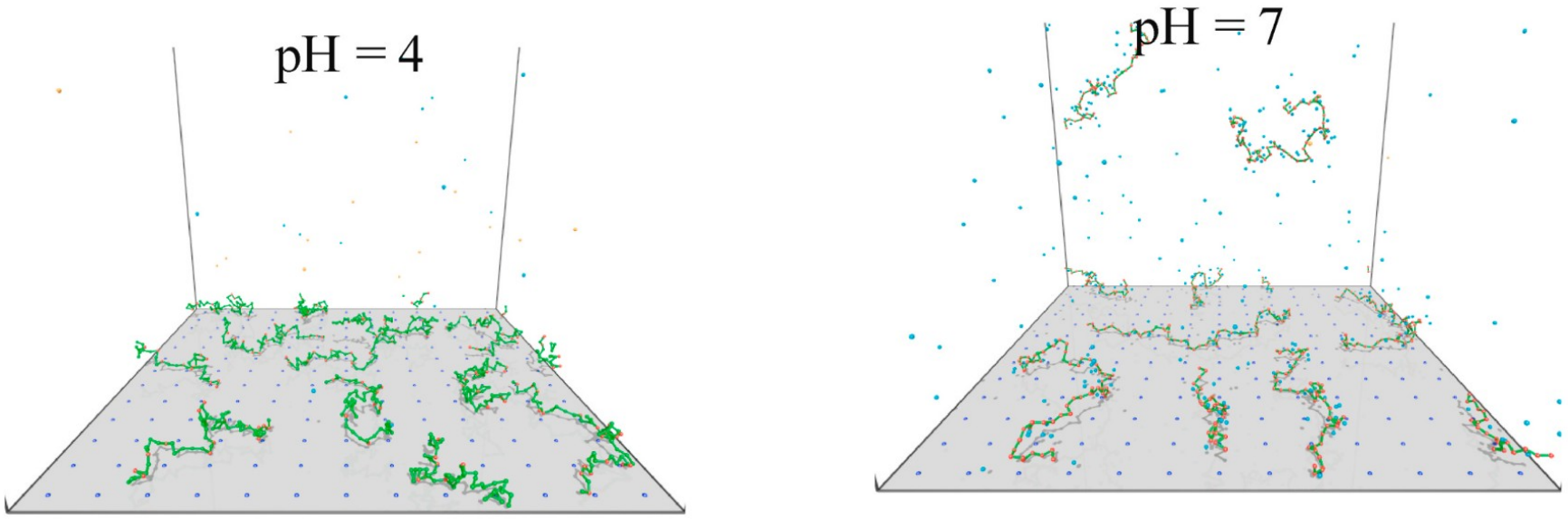
$$E_{\text{total}} = E_{\text{inter}} + E_{\text{intra}}$$

Oligomer conformation distribution



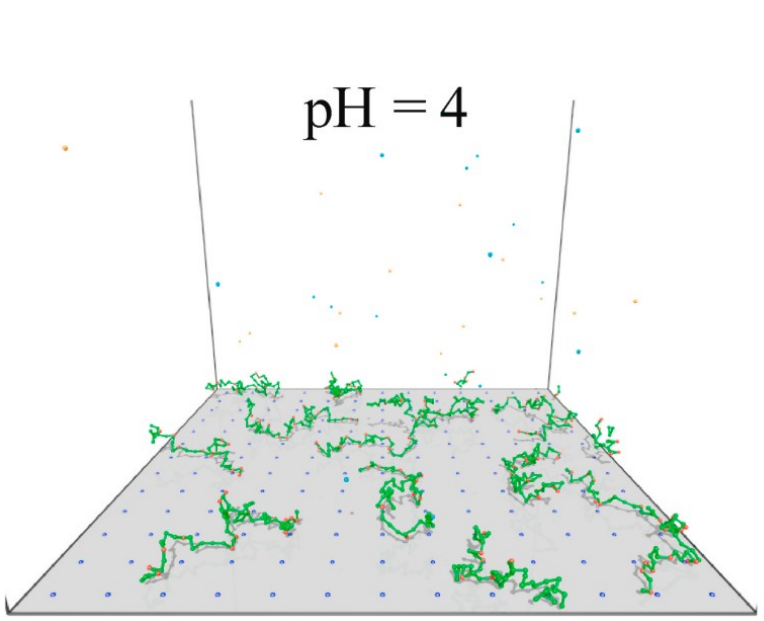
CG method reproduces conformational statistics of molecular oligomers

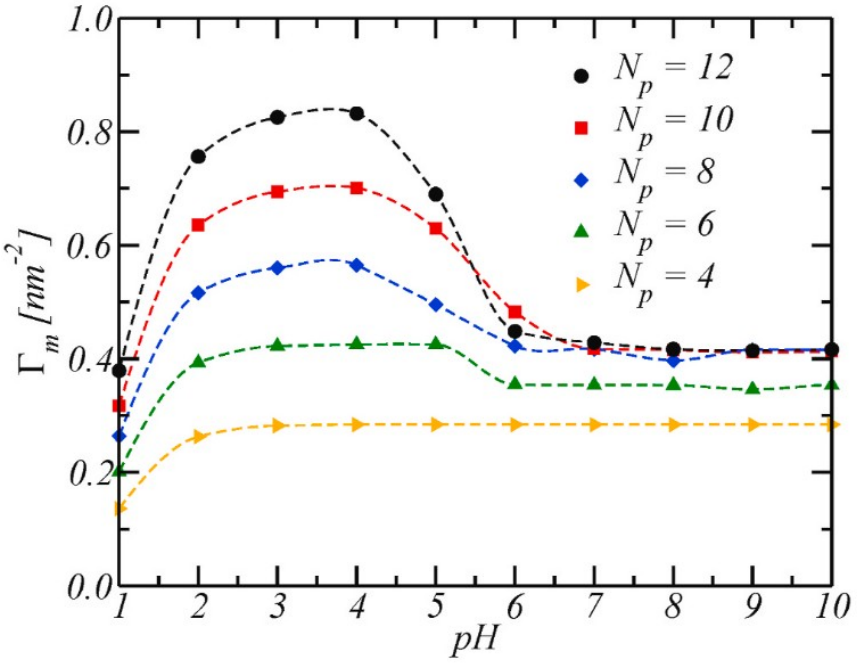
Weak-polyelectrolytes adsorption



- Narambuena, C. F., Blanco, P. M., Rodriguez, A., Rodriguez, D. E., Madurga, S., Garcés, J. L., & Mas, F. (2021). **Non-monotonic behavior of weak-polyelectrolytes adsorption on a cationic surface: A Monte Carlo simulation study.** *Polymer*, 212, 2020. https://doi.org/10.1016/j.polymer.2020.123170

Weak-polyelectrolytes adsorption





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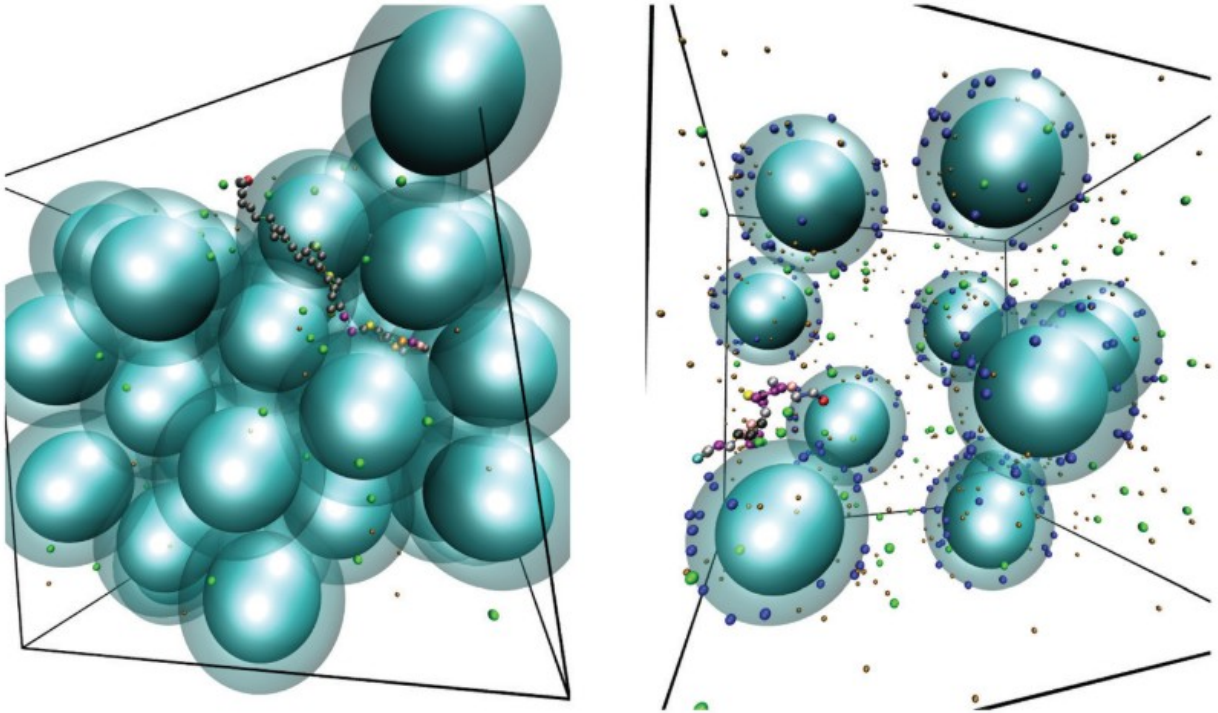
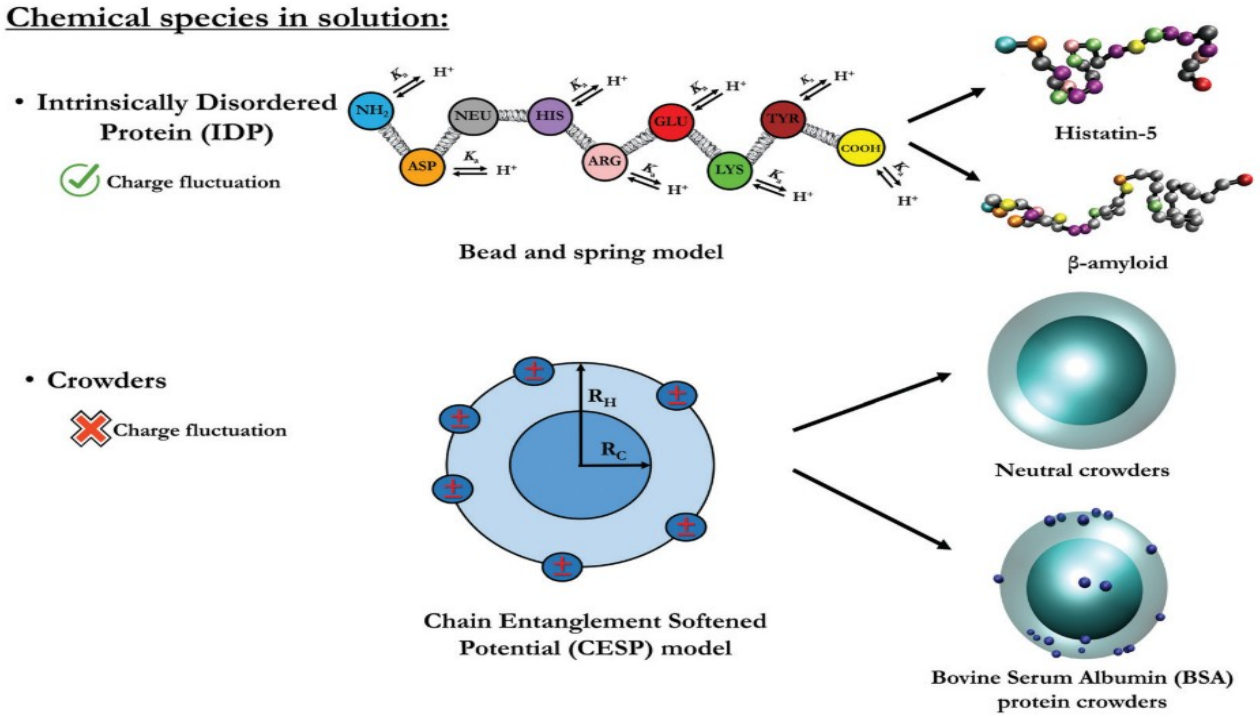
Macromolecular Crowding



- Blanco, P. M., Madurga, S., Garcés, J. L., Mas, F., & Dias, R. S. **Influence of macromolecular crowding on the charge regulation of intrinsically disordered proteins.** *Soft Matter*, 655–669, 2021. https://doi.org/10.1039/d0sm01475c

Macromolecular Crowding



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