The Boltzmann Distribution

class - 13 (19.9.24)

LS2103 (Autumn 2024)

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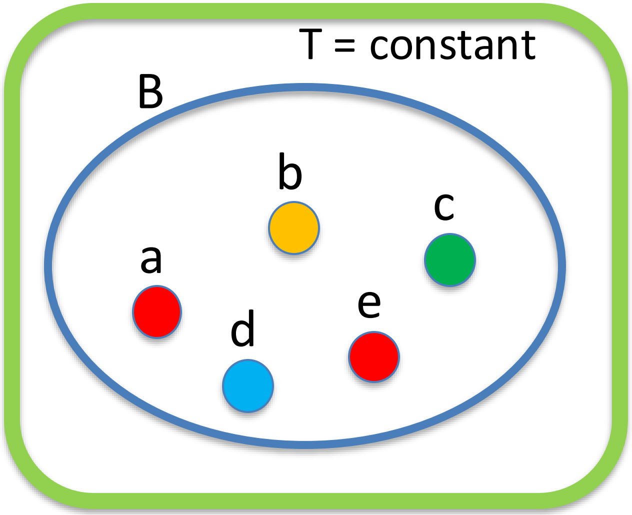
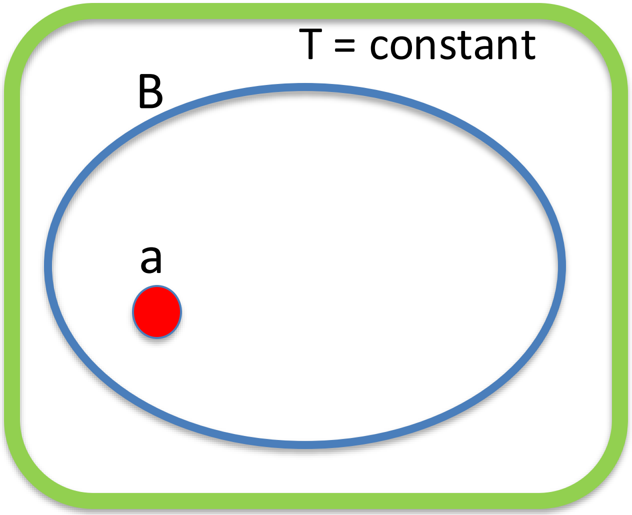
The Boltzmann Distribution



The probability for a small subsystem of energy E_a in thermal equilibrium with a macroscopic state at temperature 'T' is proportional to $\exp(-E_a/k_BT)$

The Boltzmann Distribution



Probability of occupancy of state 'a'

Consider a microscopic subsystem ('a') in contact with a much larger system ('B') at temperature 'T', such that the overall system is in equilibrium:

Eg: 'B' is a body at constant 'T', 'a' is an enclosed protein molecule

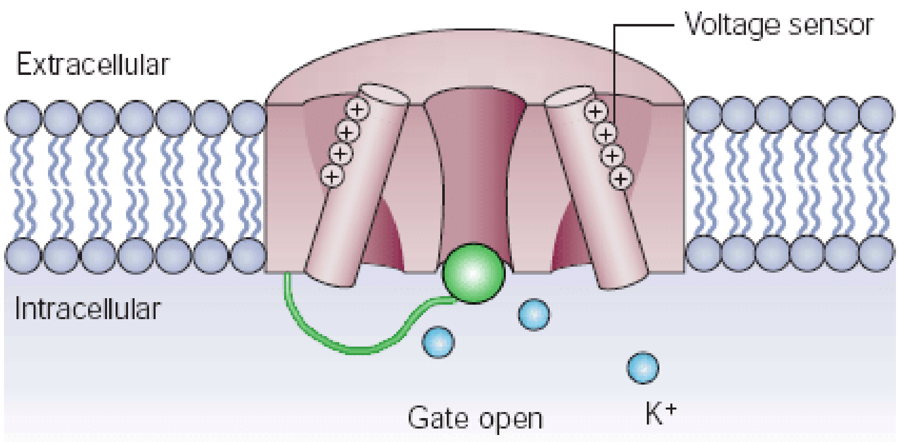
$E_a + E_B = E_{tot}$ (= constant)

and

$E_B >> E_a$

A model ion channel

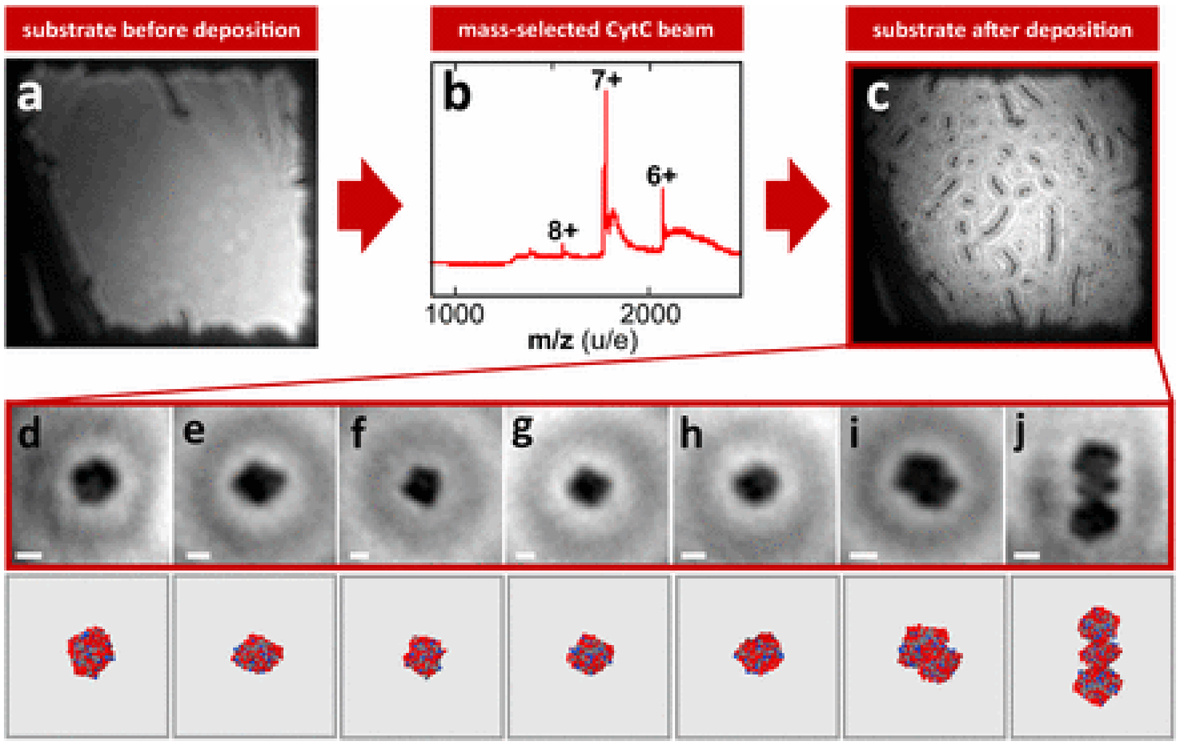
Find the **free energy difference (ΔG)** between the open and closed states



Electrophysiology experimental data: time scan

Population Ratio of States: Free Energy Interpretation

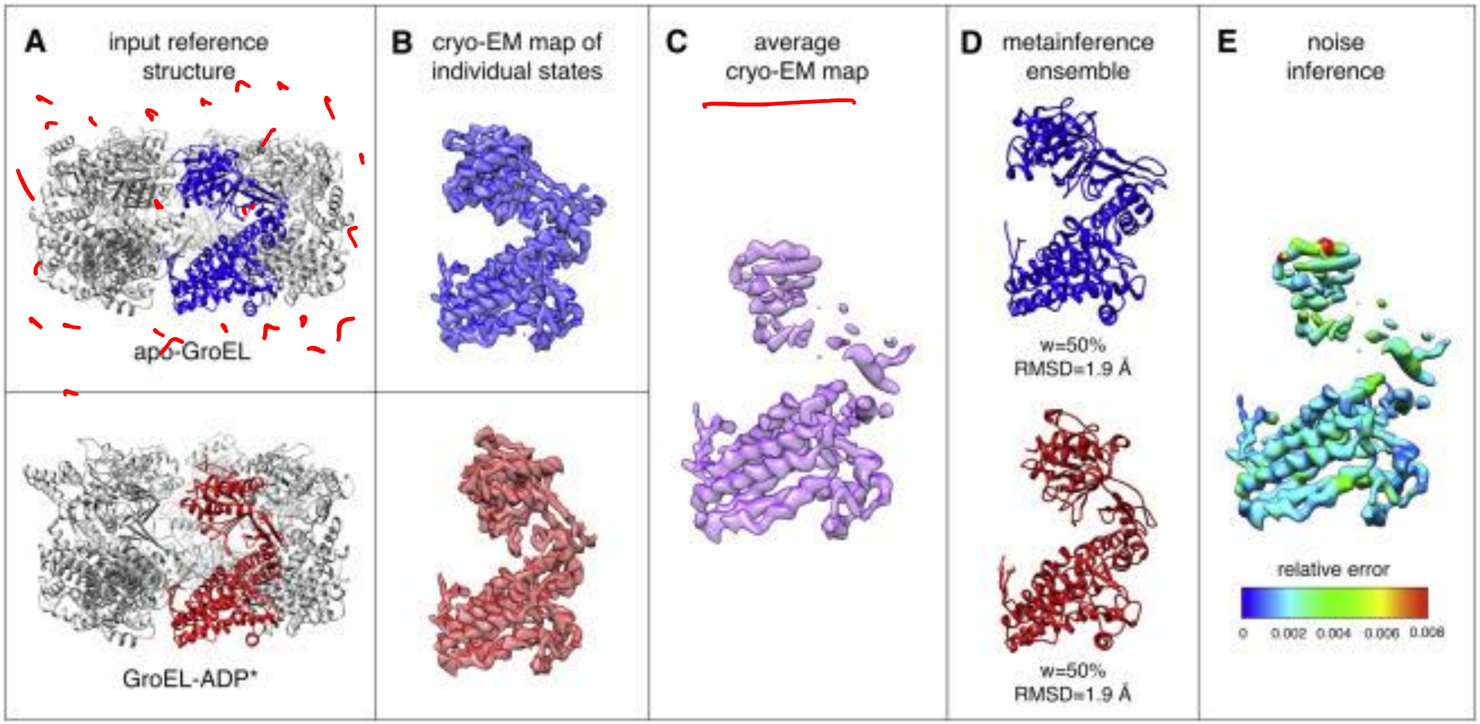
Ensemble of Substates: Single molecule imaging experiments



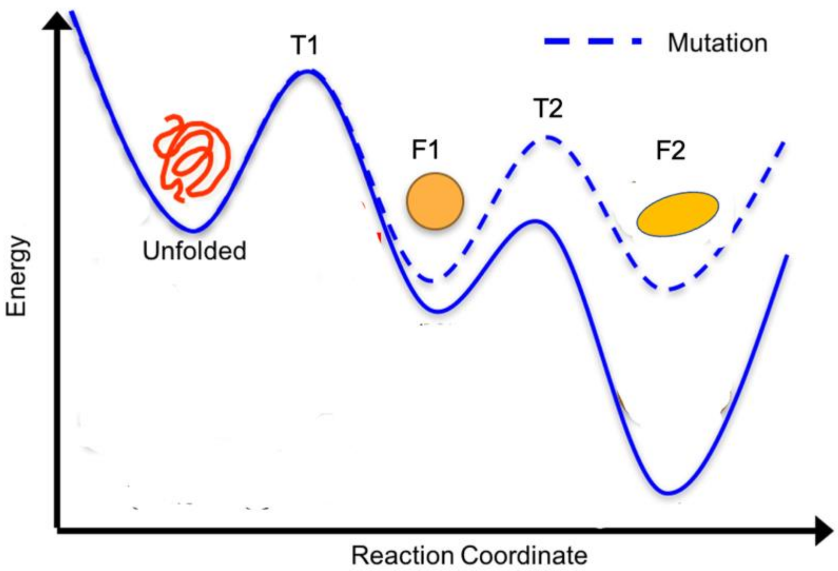
Longchamp et al., PNAS 2017, 114, 1474-147

Population Ratio of States: Free Energy Interpretation

Ensemble of Substates: CryoEM studies



Bonomi et al., Biophys. J., 2018, 114, 1604-1613



- The unfolded state has an energy of -20.0 kCal/mol.
- The F1 and F2 of the mutant have the same energy level of -21.5 kCal/mol.
- The magnitude of stability enhancement of the F1 and F2 states in the wild-type (over mutant) are 1.5 kCal/mol and 7.0 kCal/mol, respectively.

- The state T1 lies 5.0 kCal/mol above the Unfolded state
- In the mutant, the state T2 lies 4.5 kCal/mol above the F1 state.
- The state T2 for the wild-type lies 2.0 kCal/mol above the F1 state.
- Re-draw the Energy Landscape with correct energy values labelled
- Find the *ratio* of the rate of transition from state F2 to state F1, in the wild-type and mutant.
- Find the population ratios (Unfolded: F1: F2) for native and mutant