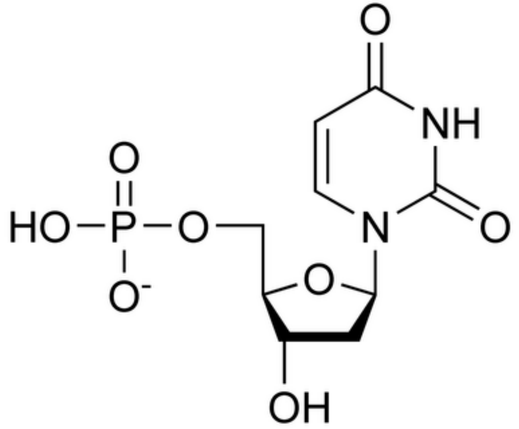
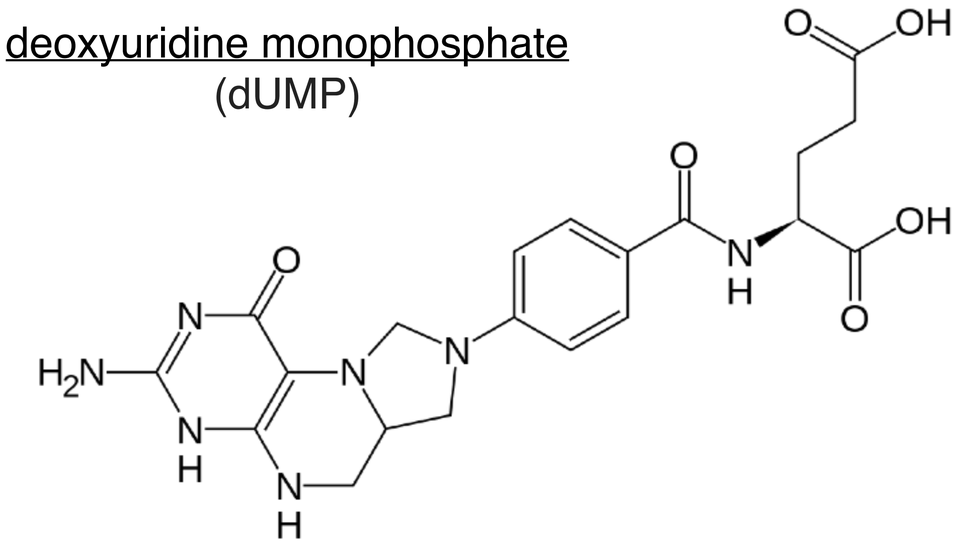
Modeling Electrostatics

- In biological macromolecules, the electrostatic potential is usually calculated based on the Poisson-Boltzmann equation
  - The Poisson equation describes the potential field due to a given charge distribution. Atoms in the biomolecule are assumed to have a fixed charge.
  - The Poisson-Boltzmann equation assumes that (infinitely small) ions surround a biomolecule in accordance with the Boltzmann distribution
- The PB equation is a partial differential equation that is solved numerically
- The equation is often linearized to be more numerically stable
- Chun Liu in Applied Math has worked on versions
  - that are time-dependent
  - account for the finite size of ions

Thymidylate Synthase Catalyzes

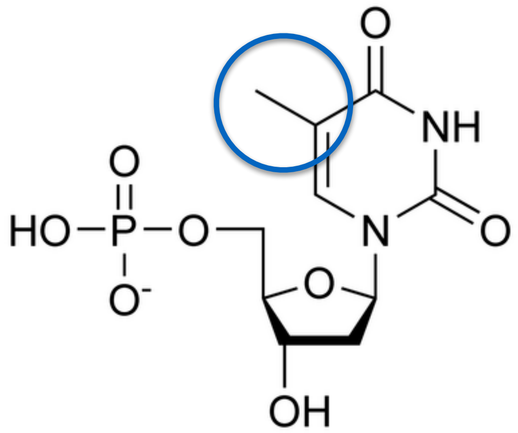


deoxyuridine monophosphate
(dUMP)

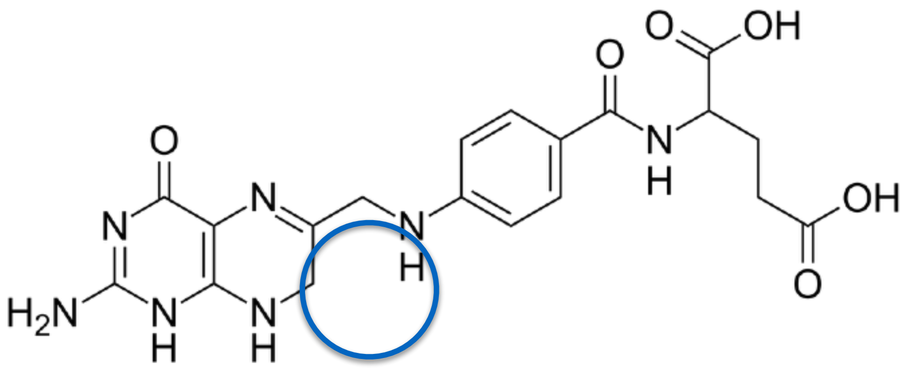


N5,N10-methylene tetrahydrofolate

to



deoxythymidine monophosphate
(dTMP)



dihydrofolate