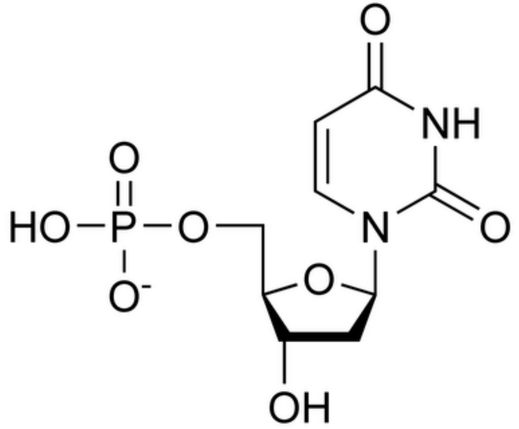
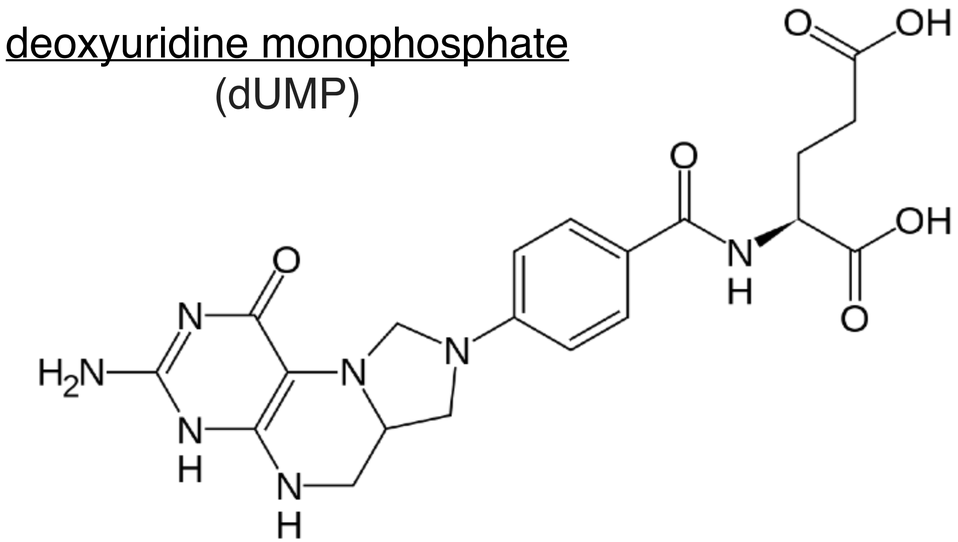
Thymidylate Synthase Catalyzes

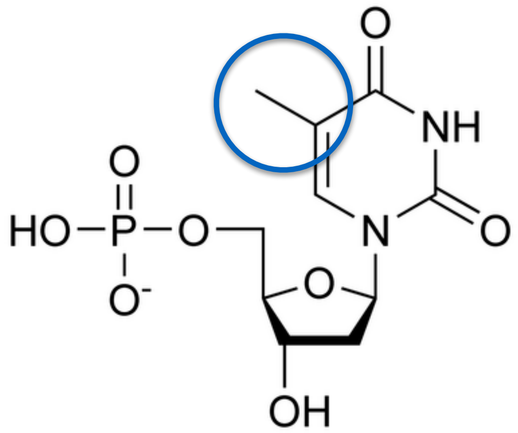


deoxyuridine monophosphate
(dUMP)

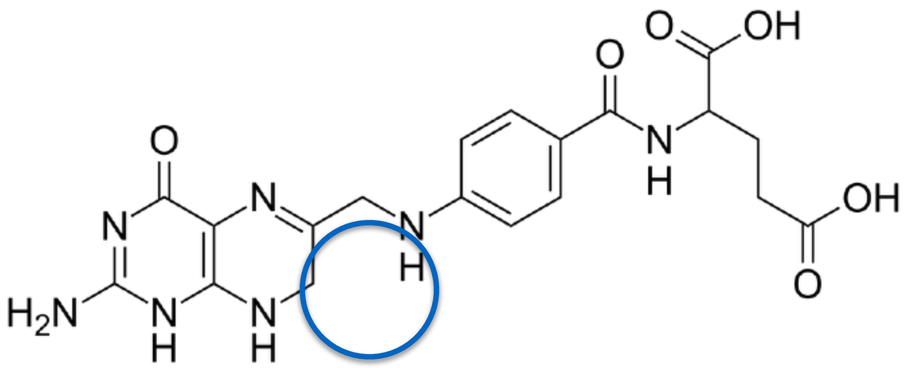


N5,N10-methylene tetrahydrofolate

to



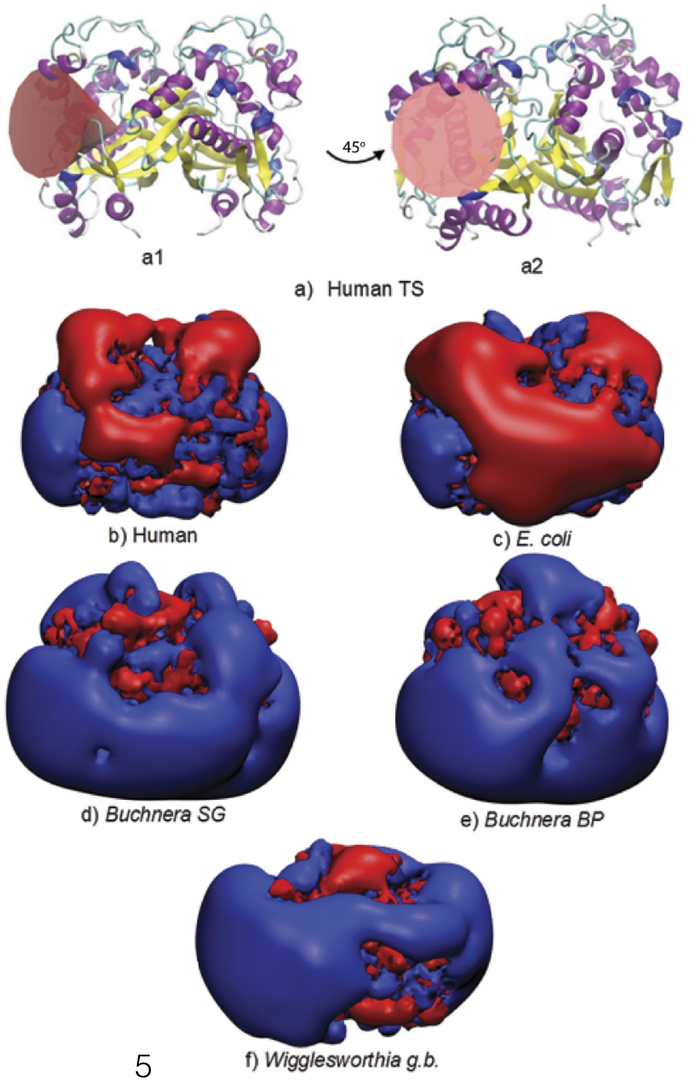
deoxythymidine monophosphate
(dTMP)

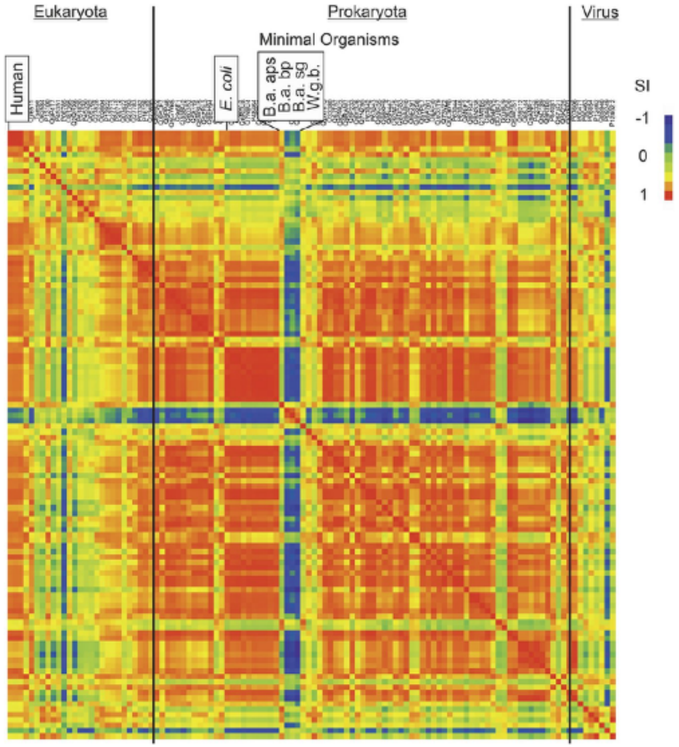


dihydrofolate

Summary of “Conservation and Role of Electrostatics in Thymidylate Synthase”

- Built 110 homology models
- Calculated and compared electrostatic potential of the enzyme across species
- Found minimal organisms, including Wigglesworthia glossinidias brevipalpis (W.g.b.), to have divergent potential
- Rationalized W.g.b. TS to be functional and unsuccessfully tried to express and purify it
- Mutated E. coli TS to be more like W.g.b. TS and found the enzyme to be less active





Left: Figure 1 of Garg *et al.* (2015) Electrostatic potentials and definition of region for comparative analysis. Above: Figure 2 of Garg *et al.* (2015). Heat map of pairwise similarity index