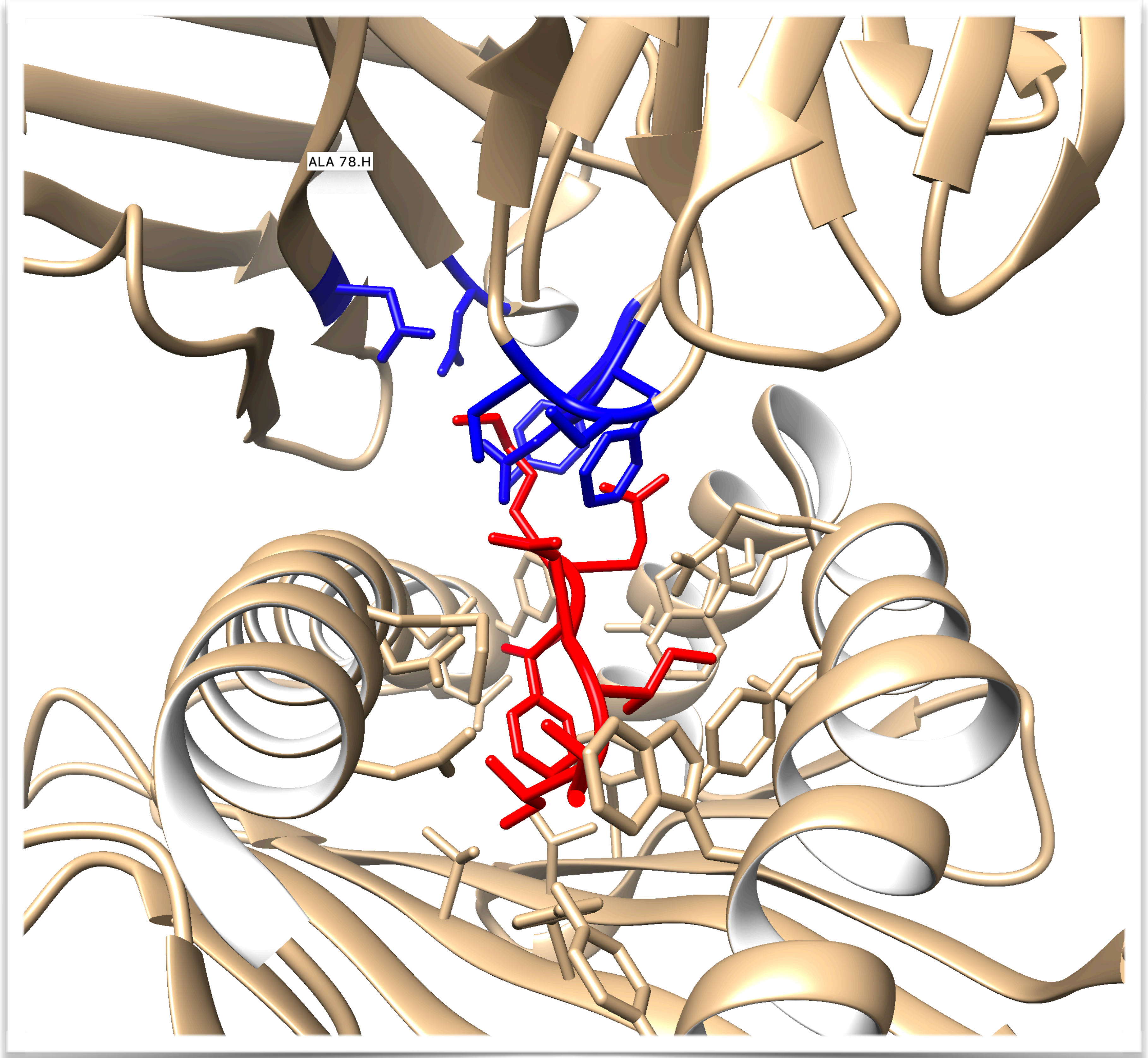

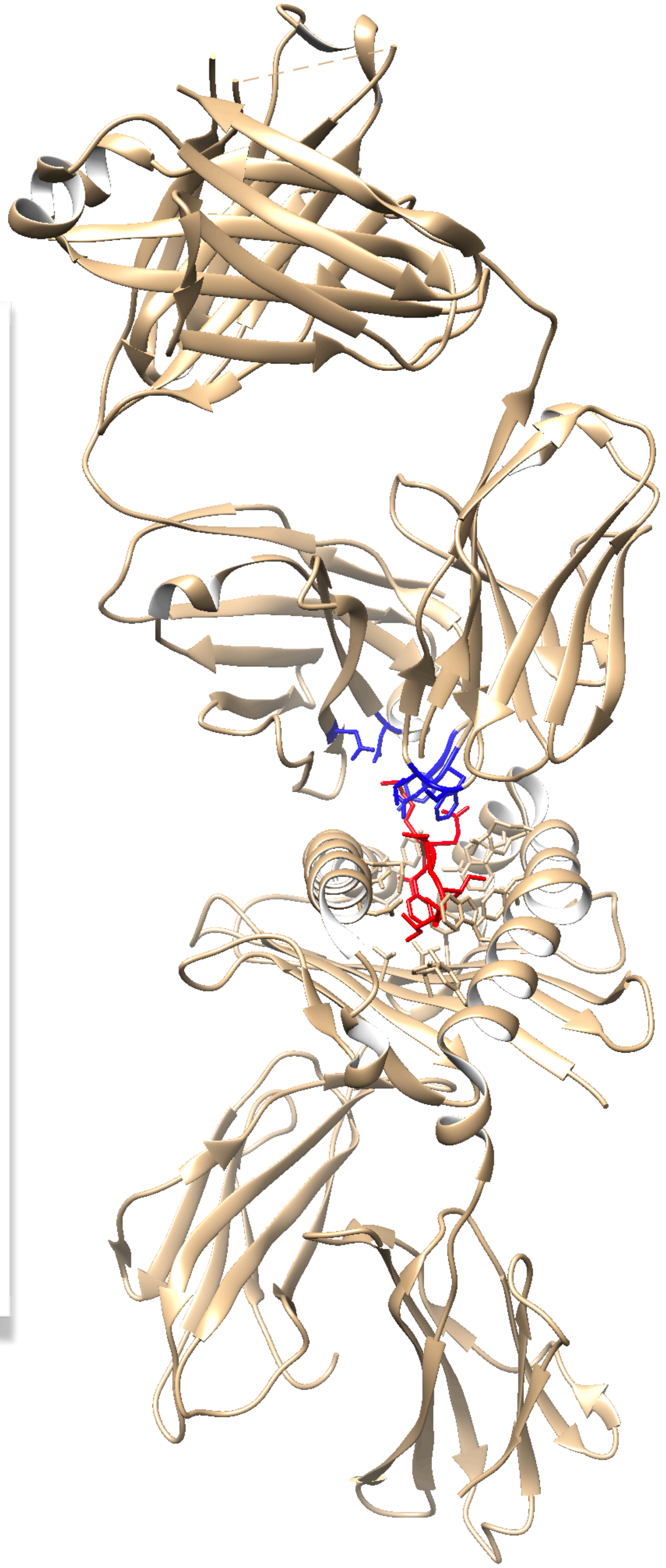

LECTURE 5

MODELING **REACTIONS**

Idealized model
Molecular collisions
Maxwell-Boltzman distribution (1860)
Positions (dv/V)
Velocities (~m/T)^1.5 exp(~-mv^2/T)
Probability formulation (collision x energy)
Propensity function (k x1 x2)
Diffusion (dc/dt = D d2c/dx2 c)
Stokes-Einstein equation (D=kBT/6pi eta r)
Diffusion limited k/(1+a/D) x1x2
Markov chain formulation
Chemical master equation
SSA algorithms
Mass action law
ODE model
Gene expression
Explicit solution
Rise time calculation
Degradation dependence

BIONUMBERS
(https://bionumbers.hms.harvard.edu/)
Transcription rate (20-40nt/sec)
mRNA export time (1-10min)
Translation rate (5-10 codons/sec)
Folding time (10-30min/protein)
Diffusion time yeast (0.5sec)
Diffusion distance sqrt(Dt)
Diffusion rate in cytoplasm (8um^2/sec)
Diffusion rate in water (100um^2/sec)
ER flux yeast (460molecules/sec)
Secretion time (~20min)

Time scale separation
Fast dynamics
Slow dynamics
Enzyme reactions
Gene regulation
Positive regulation
Negative regulation
Transcription regulatory networks

EXERCISE
Create a CRR schematic for gene expression
Formulate ODE model using mass action law
Parametrize the model
Simulate the model for different degradation rates
Compute the 50% rise time