Table 1| Dimerization Network

Reaction Network	Kinetic Constants	Opened Network	Kinetic Constants
R --> 2A	k_1=1	R --> 2A	k_1=1
A --> R_2	k_2=1	A --> R_2	k_2=1
R_2 --> B	k_3=1	R_2 --> 0	k_3=1
B --> 2R	k_4=1	0 --> 2R	k_4*RT=-50
	R_T=50	R --> 3R	-k_4=-1
		A --> 2R + A	-k_4=-1
		R_2 --> 2R + R_2	-k_4=-1
Reference: Goss, P. J. E. & Peccoud, J. 1998 Quantitative modeling of stochastic systems in molecular biology by using stochastic Petri nets. http://www.pnas.org/content/95/12/6750.full			

The original reaction network considered is a dimerization reaction. The mass balance on the system is:

$$R_T = R + R_2 + A + B \tag{1}$$

The mass balance is then solved for B. This opens up the reaction network as displayed in Table 1, by eliminating component B from the reaction. The reaction constants for the four updated reactions are k_4R_T, $-k_4$, $-k_4$, and $-k_4$ with respect to the order they are displayed in Table 1. Once the network is opened up, steady state balances are derived for each component.

$$\frac{dR}{dt} = 0 = -k_1R + 2k_4R_T - 2k_4R - 2k_4A - 2k_4R_2 \tag{2}$$

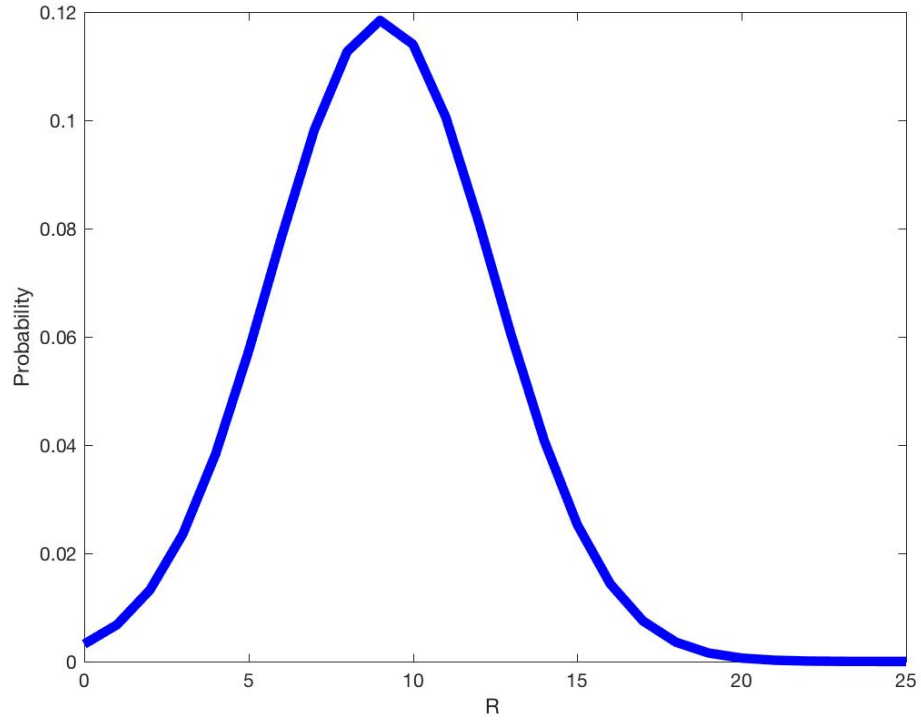
$$\frac{dA}{dt} = 0 = 2k_1R - k_2A \tag{3}$$

$$\frac{dR_2}{dt} = 0 = k_2A - k_3R_2 \tag{4}$$

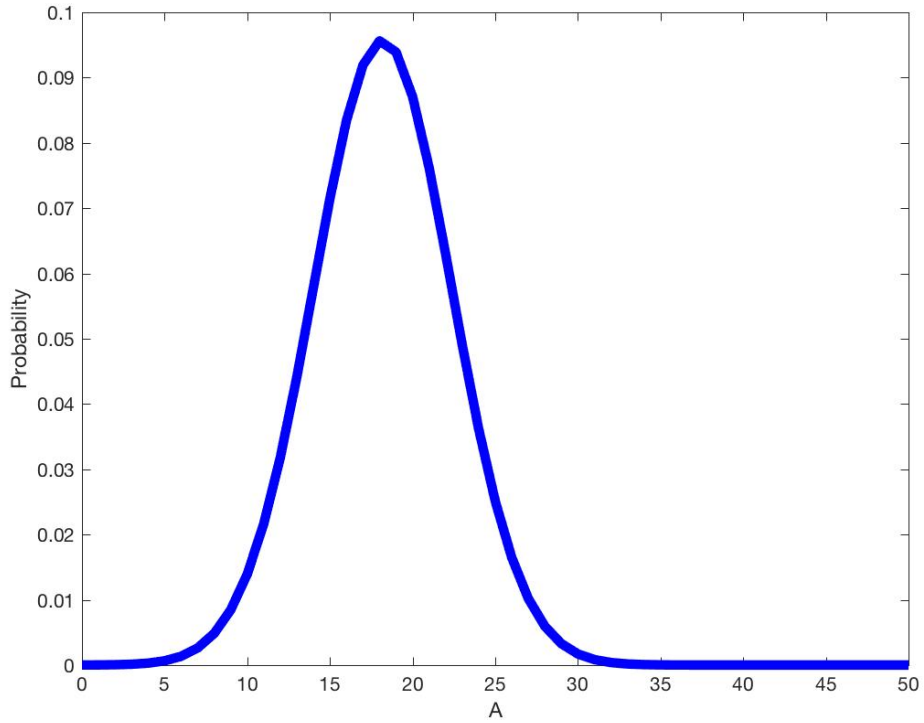
With three equations and eight variables, five of the variables have to be set. In this case the kinetic constants are set to 1 and the total amount is set to 50 molecules. From there the average concentrations of components R, A, and R_2 are solved as 9.09, 18.2, and 18.2 molecules. To run the simulation the minimum values for all components are set to zero. The maximum value for component R is set to 25, and the maximum value for components A and R_2 are set to 50. The maximum number of moments is set to 2, and all of the initial guesses for the Lagrange Multipliers are set to zero. The results of the simulation are displayed in Figure 1. The plots display the proper steady state values as calculated from the mass balances.

Table 2| Simulation Parameters

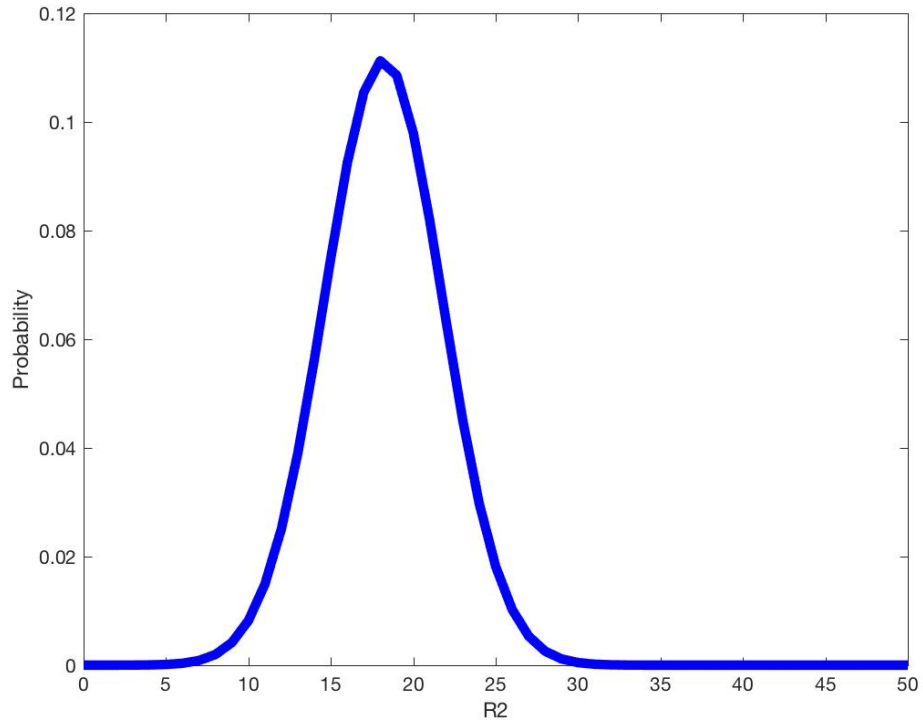
Minimum Values (A, R, R_2)	Maximum Value (R)	Maximum Value (A)	Maximum Value (R_2)	Maximum Number of Moments	LaGrange Multipliers (Initial Guess)
0	25	50	50	2	0


0.12
0.1
0.08
0.06
0.04
0.02
0
Probability
0
5
10
15
20
25
R

(A)


0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
Probability
0
5
10
15
20
25
30
35
40
45
50
A

(B)



(C)

Figure 1| Results from Simulation. A. Component R **B.** Component A **C.** Component R_2