Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Extracting multivalent detachment rates from heterogeneous nanoparticle populations

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Methods

Measuring $k_{r,1,1}$ and k_{diff} using single bond NAD simulations. Simplified NAD simulations in which nanoparticles (NPs) were initially tethered via a single bond, but no additional bonds were not allowed to form, were used to determine the rupture rate from 1 to 0 bonds ($k_{r,1,1}$) and the diffusion rate of unbound NPs at least 2.5 diameters away from the initial position (k_{diff}). This was accomplished by separately tracking the times to rupture and diffusion for an ensemble of 200 NPs, resulting in the profiles shown in Fig. S1. The time distributions were then fit using an exponential decay to obtain the respective rates. This resulted in k_{diff} = 66 s^{-1}, which was the same for all parameter conditions. For the base case bond properties (k_f^0 = 1.5x10^5 s^{-1}, k_r^0 = 1.1x10^{-4} s^{-1}, σ = 0.8 N/m, and γ = 0.274 nm), we obtained $k_{r,1,1}$ = 3.8 s^{-1}. For the new bond property conditions γ = 0.29 nm, γ = 0.3 nm, k_r^0 = 5x10^{-4} s^{-1}, and k_r^0 = 1.1x10^{-3} s^{-1}, we obtained $k_{r,1,1}$ values of 8.9, 17.7, 14.8, and 19.8 s^{-1}, respectively.

Bond formation and rupture rate estimates from simulation pause times. For each forward and reverse bond state transition, we will define the waiting time, τ, and assume that the distribution of waiting times for an ensemble of transitions follows an exponential distribution:

$$P(\tau) = k\exp(-k\tau) \quad \text{S1.}$$

where k is the transition rate, which can describe either bond formation (k_f) or rupture (k_r). We can then estimate k as the inverse of mean pause time:

$$k = 1/\bar{\tau} \quad \text{S2.}$$

Univariate fitting was implemented using maximum-likelihood estimation in R's MASS library. Alternatively, we assumed the distribution of waiting times followed a mixture of two sub-components:

$$P(\tau) = \alpha k_1 \exp(-k_1\tau) + (1-\alpha)k_2 \exp(-k_2\tau) \quad \text{S3.}$$

where α is the relative number of NPs in component 1, and k_1 and k_2 are the component rates. Bivariate fitting was implemented using the expectation-maximization (EM) algorithm in R's RENEXT library.

Transition matrix. We constructed a transition matrix for each BP, $\boldsymbol{K_i}$, by writing the bond number state master equation (eq 10) in vector form, as follows:

$$\mathrm{K}_i = \begin{bmatrix} -k_{r,i,0} - k_{f,i,1}, & k_{r,i,1}, & 0, & 0, & 0, & \\ k_{f,i,1}, & -k_{r,i,1} - k_{f,i,2}, & k_{r,i,2}, & 0, & 0, & \cdots, \\ 0, & k_{f,i,2}, & -k_{r,i,2} - k_{f,i,3}, & k_{r,i,3}, & 0, & \\ 0, & 0, & k_{f,i,3}, & -k_{r,i,3} - k_{f,i,4}, & k_{r,i,4}, & \cdots, \\ \cdots, & \cdots, & \cdots, & \cdots, & \cdots, & \\ k_{r,i,0}, & 0, & 0, & 0, & 0, & \cdots, \end{bmatrix} \quad \text{S4.}$$

$$\mathrm{S}_i = [S_{i,0}, S_{i,1}, S_{i,2}, S_{i,3}, \ldots, S_{i,N}, S_d]^T$$

$$\mathrm{T}_i = [T_{i,0}, T_{i,1}, T_{i,2}, T_{i,3}, \ldots, T_{i,N}]^T$$

We then parameterized $\boldsymbol{K_i}$ using the transition rates determined from fitting the NAD simulation data and determined the average time to detachment ($\boldsymbol{T_i}$) using eq 12. The vector $\boldsymbol{T_i}$ contained elements that were all very similar in value. For example, $\boldsymbol{T_1}$ of the base case (medium ICAM-1 and medium antibody, ICAM-1 monomers) had values of 1.47 and 1.76 s for bond states 0 and 1, respectively, and $\boldsymbol{T_2}$ values were 54.06, 54.06, 54.11, 54.11, and 54.12 s for bond states 0-4, respectively. Clearly, state 0 of BPs 1 and 2 should not have such disparate detachment times, as both involve unbound NPs simply diffusing away. Thus, $\boldsymbol{T_i}$ must be thought of as the time to detachment from the average state for each BP system. Thus, we averaged all elements of $\boldsymbol{T_i}$ to obtain a single detachment time, which we then inverted to determine $k^{(M)}_{D,i}$ (eq 13).

Similarly, if we allow for the possibility of two hidden sub-components within each BP, the transition matrix for each BP ($\boldsymbol{K_i}$) can be modified as follows:

$$K_i = \begin{bmatrix} -k_{r,i,0}^{(1)} - k_{f,i,1}^{(1)} & 0 & P_{r,i,1}k_{r,i,1}^{(1)} & P_{r,i,1}k_{r,i,1}^{(2)} & 0 & 0 & ... \\ 0 & -k_{r,i,0}^{(2)} - k_{f,i,1}^{(2)} & (1-P_{r,i,1})k_{r,i,1}^{(1)} & (1-P_{r,i,1})k_{r,i,1}^{(2)} & 0 & 0 & ... \\ P_{f,i,1}k_{f,i,1}^{(1)} & P_{f,i,1}k_{f,i,1}^{(2)} & -k_{r,i,1}^{(1)} - k_{f,i,2}^{(1)} & 0 & P_{r,i,2}k_{r,i,2}^{(1)} & P_{r,i,2}k_{r,i,2}^{(2)} & ... \\ (1-P_{f,i,1})k_{f,i,1}^{(1)} & (1-P_{f,i,1})k_{f,i,1}^{(2)} & 0 & -k_{r,i,1}^{(2)} - k_{f,i,2}^{(2)} & (1-P_{r,i,2})k_{r,i,2}^{(1)} & (1-P_{r,i,2})k_{r,i,2}^{(2)} & ... \\ ... & & & & & & \\ ... & & & & & & \\ k_{r,i,0}^{(1)} & k_{r,i,0}^{(2)} & 0 & 0 & 0 & 0 & ... \end{bmatrix} \quad \text{S5.}$$

$$S_i = \begin{bmatrix} S_{i,0}^{(1)} & S_{i,0}^{(2)} & S_{i,1}^{(1)} & S_{i,1}^{(2)} & ... & S_{i,n}^{(1)} & S_{i,n}^{(2)} & S_d \end{bmatrix}^T$$

$$T_i = \begin{bmatrix} T_{i,0}^{(1)} & T_{i,0}^{(2)} & T_{i,1}^{(1)} & T_{i,1}^{(2)} & ... & T_{i,n}^{(1)} & T_{i,n}^{(2)} \end{bmatrix}^T$$

The vector $\boldsymbol{T_i}$ contains elements that were still all very similar in value. For example, $\boldsymbol{T_2}$ values were 20.50, 19.15, 21.15, 20.45, 20.95, 21.19, 20.59, 20.60, 20.52, 20.60s for bond states 0-4 (2 sub-components per state).

Results and Discussion

Population heterogeneity model fitting using two sub-components. As discussed in the main text, fits for individual BPs obtained using eq 6 were poor. This led us to conclude that bonding heterogeneity was still present in each BP, which we hypothesized could be captured using hidden sub-components, as described by eq 7. Fitting results using two sub-components are shown in Fig. S2 for the base case, and generally matched NAD simulation data well. Fitting parameters, including $k_{D,i}$ values for both sub-components and the relative number of sub-component 1 (α_i), are listed in Table S2. Upon inspection, $k_{D,i}$ values for sub-component 2 were much lower, and in most cases were 0. Thus, we chose to simplify the two sub-component scenario by assuming that the second sub-component did not detach at all ($k_{D,i}$ = 0). As shown in Fig. S2, this simplification led to similar fitting accuracy.

Estimating bond number state transition rates from NAD simulation pause times. Forward and reverse bond state transition rates were estimated using the waiting times between bond state transition observed from NAD simulations. Results are shown for the base case,

BP5, and transitioning from bond number state 4 to 5 assuming one sub-component (Fig. S1C) or two sub-components (Fig. S1D). The two sub-component result exhibited better alignment with the pause time data, which again confirmed the presence of bonding heterogeneity even within BPs. However, for simplicity, we still chose to use single exponential fits as initial values for solving the system of ODEs in eqs 10 or 11.

Table S1. Population heterogeneity model parameters for one sub-component fits.

Case	$k_{D,1}$ (s^{-1})	$k_{D,2}$ (s^{-1})	$k_{D,3}$ (s^{-1})	$k_{D,4}$ (s^{-1})	$k_{D,5}$ (s^{-1})
1. Base	0.57	0.02	1.5×10^{-4}		
2. Low Antibody	3.17	0.02	3.1×10^{-3}		
3. Low ICAM-1	0.57	1.2×10^{-2}			
4. ICAM-1 dimer	0.81	0.01	2.3×10^{-3}		
5. Clustered dimer	0.82	8.0×10^{-3}			
6. γ = 0.29 nm	2.18	0.03	1.7×10^{-3}	3.3×10^{-3}	2.0×10^{-3}
7. γ = 0.3 nm	8.48	0.06	7.2×10^{-3}	2.2×10^{-3}	
8. $k_r^0 = 5 \times 10^{-4}\ s^{-1}$	7.10	0.03	5.5×10^{-3}	3.1×10^{-3}	7.3×10^{-4}
9. $k_r^0 = 1 \times 10^{-3}\ s^{-1}$	18.22	0.05	1.3×10^{-2}		

Table S2. Population heterogeneity model parameters for two sub-component fits using 2 and 3 degrees of freedom. Two degrees of freedom assumes that one sub-component does not detach, while three degrees of freedom assumes that both can detach.

Case	Degrees of freedom	$k^{(1)}_{D,i}$, (s^{-1}), $k^{(2)}_{D,i}$, (s^{-1}), α_i								
		BP 1			BP 2			BP 3		
1. Base	2	0.57		1.00	0.23	0	0.30	$1.5x10^{-4}$	0	1.00
	3	0.57		1.00	0.23	0	0.30	$1.5x10^{-4}$	$1.5x10^{-4}$	0.00
2. Low ICAM-1	2	3.17		1.00	0.12	0	0.32	$5.2x10^{-2}$	0	0.10
	3	3.17		1.00	0.12	0	0.32	$5.2x10^{-2}$	0	0.10
3. Low Antibody	2	0.57		1.00	0.03	0	0.53			
	3	0.57		1.00	0.44	$1.0x10^{-2}$	0.03			
4. ICAM-1 Dimer	2	0.81		1.00	0.12	0	0.20	$2.3x10^{-3}$	0	1.00
	3	0.81		1.00	0.15	$1.4x10^{-3}$	0.17	$2.3x10^{-3}$	$2.3x10^{-3}$	0.00
5. Clustered Dimer	2	0.82		1.00	0.07	0	0.20			
	3	0.82		1.00	0.10	$1.9x10^{-3}$	0.14			

Table S3. Pause time fitting results used to estimate bond number transition rates.

Case 1: Base

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	3.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	3.8	0.1	9.3	6.8	255.1	0.0
	3	66.0	0.8	11.4	13.7	24.5	48.5	0.0
	4	66.0	3.5	15.1	21.5	24.9	46.4	74.8
	5	66.0	3.8	12.0	18.2	36.4	54.7	78.6
	6	66.0	0.0	0.0	1101.9	49.6	60.8	62.3
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	3.1	0.0	0.0	0.0	0.0	0.0
	2	66.0	3.8	10.5	25.5	76.7	267.3	0.0
	3	66.0	290.8	357.6	27.6	57.0	159.0	0.0
	4	66.0	3.8	597.6	748.3	58.3	132.0	192.6
	5	66.0	3.8	12.1	655.6	846.5	206.4	322.8
	6	66.0	0.0	0.0	1101.9	1800.2	254.2	223.9
$P_{r,i,j}$	1	1.0	0.5	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.1	1.0	0.6	0.0	1.0
	3	1.0	0.1	0.9	0.4	0.6	0.6	1.0
	4	1.0	0.9	0.8	0.9	0.5	0.6	0.7
	5	1.0	1.0	0.5	0.9	0.9	0.7	0.6
	6	1.0	1.0	1.0	1.0	0.8	0.6	0.5
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	6650.9	0.0	0.0	0.0	0.0	0.0
	2	0.0	53.0	2197.1	14.3	5.7	15474.6	1.0
	3	0.0	94.9	251.0	160.0	98.5	408.3	0.0
	4	0.0	692.5	125.1	136.2	192.7	187.9	211.7
	5	0.0	52.5	413.7	37.8	232.7	488.1	731.0
	6	0.0	0.0	547.8	1305.0	520.5	516.7	952.0
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	204551.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	20969.5	6759.6	7403.3	6450.7	8305.5	0.0
	3	0.0	9505.3	7517.9	7284.2	7381.6	8695.6	0.0
	4	0.0	8739.7	5990.6	7053.9	7568.0	7981.7	8273.3
	5	0.0	52.5	6354.8	5691.6	7099.7	8729.7	12429.9
	6	0.0	0.0	547.8	174609.0	11749.6	11841.9	13491.8
$P_{f,i,j}$	1	1.0	0.7	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.9	0.1	0.9	0.8	0.8	1.0
	3	1.0	0.1	0.2	0.2	0.1	0.1	1.0
	4	1.0	0.6	0.2	0.1	0.1	0.1	0.1
	5	1.0	1.0	0.2	0.1	0.1	0.1	0.1
	6	1.0	1.0	1.0	0.9	0.1	0.1	0.1

Case 2: Low antibody

Parameter	BP	Bond Number State								
		0	1	2	3	4	5	6	7	8
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	8.3	10.3	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	65.6	8.1	14.5	30.4	49.8	0.0	0.0	0.0
	3	66.0	34.5	11.2	16.5	23.7	57.4	86.8	0.0	0.0
	4	66.0	5.6	11.6	26.5	32.2	52.9	141.9	0.0	0.0
	5	66.0	392.3	7.9	16.3	39.5	57.3	149.9	0.0	0.0
	6	66.0	0.0	0.0	18.2	50.4	76.7	147.4	1942.1	30376.8
	7	66.0	233.7	9.6	126.6	312.5	84.6	114.3	240.1	0.0
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	8.3	10.3	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	5913.3	13.8	28.4	85.2	140.8	0.0	0.0	0.0
	3	66.0	932.1	194.1	33.5	54.3	178.1	87.9	0.0	0.0
	4	66.0	1522.8	2042.7	569.4	104.9	207.2	892.8	0.0	0.0
	5	66.0	392.3	70.2	353.8	422.5	372.1	2341.6	0.0	0.0
	6	66.0	0.0	0.0	3324.9	764.1	591.3	2863.4	33169.8	520853.0
	7	66.0	233.7	74.1	126.6	318.0	1384.5	368.7	926.2	0.0
$P_{r,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.8	0.3	0.7	0.6	0.6	1.0	1.0	1.0
	3	1.0	0.5	0.8	0.5	0.5	0.6	0.5	1.0	1.0
	4	1.0	0.9	1.0	0.8	0.7	0.6	0.4	1.0	1.0
	5	1.0	1.0	0.8	0.8	0.8	0.7	0.5	1.0	1.0
	6	1.0	1.0	1.0	0.8	0.6	0.8	0.7	0.3	1.0
	7	1.0	1.0	0.9	1.0	0.2	0.6	0.4	0.5	1.0
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	775.1	31.1	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	762.2	180.6	51.8	146.5	289.6	0.0	0.0	0.0
	3	0.0	654.2	153.4	159.7	133.2	134.2	5525.1	0.0	0.0
	4	0.0	166.5	205.7	155.2	265.0	307.7	206.1	0.0	0.0
	5	0.0	367.5	111.4	118.9	282.4	517.6	924.3	0.0	0.0
	6	0.0	0.0	1204.5	126.0	879.6	571.2	715.9	1000.3	12274.8
	7	0.0	2374.3	244.9	1449.4	1988.0	599.8	1254.8	2723.0	0.0
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	775.1	31.1	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	21341.0	3738.8	3554.2	3018.6	4861.6	0.0	0.0	0.0
	3	0.0	7992.4	4010.7	4188.4	4173.6	4733.2	49814.5	0.0	0.0
	4	0.0	5127.9	2895.0	4422.7	4733.0	5024.6	3678.6	0.0	0.0
	5	0.0	367.5	2276.5	5002.3	5108.7	6342.1	14928.4	0.0	0.0
	6	0.0	0.0	1204.5	3361.2	9055.8	9024.4	13113.0	34148.3	47994.9
	7	0.0	2374.3	6152.8	1449.4	22320.5	7266.9	15198.6	34249.5	0.0
$P_{f,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.5	0.2	0.3	0.2	0.2	1.0	1.0	1.0
	3	1.0	0.7	0.3	0.2	0.2	0.2	0.6	1.0	1.0
	4	1.0	0.3	0.3	0.2	0.2	0.2	0.0	1.0	1.0
	5	1.0	1.0	0.3	0.2	0.2	0.2	0.5	1.0	1.0
	6	1.0	1.0	1.0	0.2	0.4	0.3	0.2	0.1	0.7
	7	1.0	1.0	0.5	1.0	0.4	0.2	0.4	0.1	1.0

Case 3: Low ICAM-1

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	3.2	3.7	0.0	0.0	0.0	0.0
	2	66.0	17.7	7.9	11.8	14.9	0.0	0.0
	3	66.0	2.8	13.7	14.4	22.3	28.3	0.0
	4	66.0	4.3	419.4	23.0	25.3	43.5	0.0
	5	66.0	9.3	0.0	0.0	61.8	61.8	38.8
	6	66.0	0.0	4.8	0.0	75.1	63.9	53.9
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	25.3	9.9	0.0	0.0	0.0	0.0
	2	66.0	486.2	13.2	20.4	26.9	0.0	0.0
	3	66.0	92.6	426.9	29.1	52.9	28.4	0.0
	4	66.0	4.3	3797.8	216.0	62.1	112.4	0.0
	5	66.0	9.3	0.0	0.0	1857.5	234.4	112.2
	6	66.0	0.0	4.8	0.0	169.6	2378.1	179.5
$P_{r,i,j}$	1	1.0	0.8	0.1	1.0	1.0	1.0	1.0
	2	1.0	0.5	0.4	0.4	1.0	1.0	1.0
	3	1.0	0.4	0.9	0.4	0.5	0.5	1.0
	4	1.0	1.0	0.6	0.7	0.5	0.6	1.0
	5	1.0	1.0	1.0	1.0	0.6	0.6	0.0
	6	1.0	1.0	1.0	1.0	0.7	0.7	0.6
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	291.2	31.5	0.0	0.0	0.0	0.0
	2	0.0	261.7	164.3	56.2	119.8	0.0	0.0
	3	0.0	842.5	81.7	111.0	100.4	58.7	0.0
	4	0.0	675.7	48.0	272.6	230.9	180.6	0.0
	5	0.0	254.8	4296.3	2128.4	903.4	757.0	232.1
	6	0.0	0.0	271.2	81.0	2389.0	1819.0	1258.8
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	6458.8	4297.7	0.0	0.0	0.0	0.0
	2	0.0	9863.9	6872.8	7417.2	6617.6	0.0	0.0
	3	0.0	65455.0	5949.0	6964.9	7924.2	9001.7	0.0
	4	0.0	675.7	3009.2	7611.6	8048.2	8200.3	0.0
	5	0.0	254.8	4296.3	2128.4	12195.8	10675.6	14430.4
	6	0.0	0.0	698919.0	81.0	287045.0	13450.5	14458.1
$P_{f,i,j}$	1	1.0	0.2	0.2	1.0	1.0	1.0	1.0
	2	1.0	0.4	0.2	0.3	0.3	1.0	1.0
	3	1.0	0.6	0.1	0.1	0.2	0.3	1.0
	4	1.0	1.0	0.2	0.1	0.1	0.1	1.0
	5	1.0	1.0	1.0	1.0	0.2	0.2	0.1
	6	1.0	1.0	0.8	1.0	0.9	0.3	0.3

Case 4: ICAM-1 dimer

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	4.2	6.6	0.0	0.0	0.0	66.0
	2	66.0	7.4	6.5	9.2	30.9	0.0	66.0
	3	66.0	7.4	10.9	13.3	19.9	0.0	66.0
	4	66.0	5.7	3.8	20.1	28.5	41.2	66.0
	5	66.0	0.0	11.9	4561.4	79.5	70.2	66.0
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	13.5	6.7	0.0	0.0	0.0	66.0
	2	66.0	74.1	11.7	17.9	135.8	0.0	66.0
	3	66.0	198.6	420.0	25.7	49.7	0.0	66.0
	4	66.0	161.3	14.2	153.3	74.1	105.5	66.0
	5	66.0	0.0	11.9	4561.4	1822.9	195.9	66.0
$P_{r,i,j}$	1	1.0	0.9	0.5	1.0	1.0	1.0	1.0
	2	1.0	0.4	0.2	0.2	0.8	1.0	1.0
	3	1.0	0.7	0.9	0.4	0.5	1.0	1.0
	4	1.0	0.8	0.1	0.8	0.6	0.6	1.0
	5	1.0	1.0	1.0	1.0	0.3	0.6	1.0
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	276.1	31.6	0.0	0.0	0.0	0.0
	2	0.0	360.1	123.0	52.5	369.4	0.0	0.0
	3	0.0	185.5	136.1	97.9	124.3	0.0	0.0
	4	0.0	277.5	69.2	198.2	231.1	245.6	0.0
	5	0.0	0.0	147.3	11536.0	2084.6	924.0	0.0
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	8798.5	10702.3	0.0	0.0	0.0	0.0
	2	0.0	26690.7	10475.3	14689.1	14522.3	0.0	0.0
	3	0.0	7503.1	9902.6	11909.5	15083.1	0.0	0.0
	4	0.0	3568.4	9088.9	13286.9	13753.9	15140.6	0.0
	5	0.0	0.0	5747130.0	11536.0	18997.5	13763.9	0.0
$P_{f,i,j}$	1	1.0	0.2	0.5	1.0	1.0	1.0	1.0
	2	1.0	0.3	0.2	0.3	0.1	1.0	1.0
	3	1.0	0.2	0.2	0.1	0.1	1.0	1.0
	4	1.0	0.4	0.2	0.1	0.1	0.1	1.0
	5	1.0	1.0	0.9	1.0	0.2	0.1	1.0

Case 5: Clustered ICAM-1 dimer

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	3.8	0.1	0.0	0.0	0.0	0.0
	2	66.0	3.8	2.1	0.3	41.4	0.0	0.0
	3	66.0	3.6	10.6	13.8	22.3	44.1	0.0
	4	66.0	0.0	10.6	23.5	30.4	50.0	0.0
	5	66.0	2.3	8.4	63.5	50.1	58.9	75.5
	6	66.0	0.0	0.0	0.0	0.0	161.4	92.2
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	1.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	2.7	1.5	0.2	29.7	0.0	0.0
	3	66.0	150.4	191.7	26.9	69.8	149.2	0.0
	4	66.0	0.0	583.8	247.0	86.9	194.5	0.0
	5	66.0	2.3	8.4	1000000000.0	3067.5	260.0	221.5
	6	66.0	0.0	0.0	0.0	0.0	2408.6	853.3
$P_{r,i,j}$	1	1.0	1.0	0.7	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.9	0.5	0.4	1.0	1.0
	3	1.0	0.9	0.7	0.3	0.5	0.8	1.0
	4	1.0	1.0	0.9	0.8	0.6	0.5	1.0
	5	1.0	1.0	1.0	0.9	0.9	0.6	0.5
	6	1.0	1.0	1.0	1.0	1.0	0.2	0.7
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	94.1	0.2	0.0	0.0	0.0	0.0
	2	0.0	264.9	781.2	0.1	189.7	0.0	0.0
	3	0.0	498.2	91.2	189.0	107.5	507.1	42.5
	4	0.0	0.0	88.4	93.2	286.1	321.4	0.0
	5	0.0	181.7	693.1	1844.2	780.5	1129.8	920.2
	6	0.0	0.0	6226.3	39377.8	506.4	3677.7	2828.4
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	18.8	0.0	0.0	0.0	0.0	0.0
	2	0.0	4.8	14.3	0.0	3.5	0.0	0.0
	3	0.0	142679.0	10954.7	12479.4	18129.1	17681.0	42.5
	4	0.0	0.0	6585.1	12203.1	13536.3	16470.3	0.0
	5	0.0	181.7	132742.0	19392.0	13687.8	18459.4	23556.6
	6	0.0	0.0	6226.3	39377.8	506.4	39605.0	28111.1
$P_{f,i,j}$	1	1.0	1.0	0.7	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.9	0.5	0.4	1.0	1.0
	3	1.0	0.8	0.2	0.1	0.1	0.1	1.0
	4	1.0	1.0	0.2	0.1	0.1	0.1	1.0
	5	1.0	1.0	0.8	0.4	0.1	0.2	0.1
	6	1.0	1.0	1.0	1.0	1.0	0.3	0.3

Case 6: γ = 0.29 nm

Parameter	BP	Bond Number State								
		0	1	2	3	4	5	6	7	8
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	9.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	26.1	33.1	39.5	106.7	110.9	0.0	0.0	0.0
	3	66.0	137.7	39.3	53.3	74.2	152.6	308.5	0.0	0.0
	4	66.0	12.7	34.9	78.8	100.7	152.3	209.2	0.0	0.0
	5	66.0	0.0	55.1	51.1	116.8	183.7	311.0	188.4	0.0
	6	66.0	79.9	73.6	51.1	134.8	233.6	324.7	350.6	0.0
	7	66.0	0.0	0.0	0.0	250.3	237.9	296.0	287.1	0.0
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	9.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	533.8	86.6	80.4	3342.3	258.9	0.0	0.0	0.0
	3	66.0	6549.5	519.2	129.6	184.4	630.3	1530.8	0.0	0.0
	4	66.0	106.9	887.8	2306.2	298.0	474.4	383.3	0.0	0.0
	5	66.0	0.0	1170.1	1758.2	2794.2	1223.6	1495.8	574.8	0.0
	6	66.0	79.9	3456.1	1189.4	3132.8	1470.6	2000.3	2657.8	0.0
	7	66.0	0.0	0.0	0.0	3959.8	4409.6	1508.4	2736.4	0.0
$P_{r,i,j}$	1	1.0	0.5	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.3	0.8	0.5	0.8	0.2	1.0	1.0	1.0
	3	1.0	0.7	0.6	0.6	0.5	0.6	0.6	1.0	1.0
	4	1.0	0.4	0.6	0.9	0.6	0.6	0.9	1.0	1.0
	5	1.0	1.0	0.8	0.9	0.8	0.7	0.6	0.2	1.0
	6	1.0	1.0	0.8	0.8	0.8	0.7	0.6	0.6	1.0
	7	1.0	1.0	1.0	1.0	0.4	0.6	0.6	0.6	1.0
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	143.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	575.8	348.3	174.8	532.5	942.2	0.0	0.0	0.0
	3	0.0	292.2	332.1	305.8	251.0	445.8	2276.2	0.0	0.0
	4	0.0	351.9	238.3	429.7	543.1	659.6	771.4	0.0	0.0
	5	0.0	0.0	704.3	215.0	529.3	1162.4	2017.2	601.7	0.0
	6	0.0	9364.1	262.1	178.6	617.4	1693.9	2330.9	3765.0	0.0
	7	0.0	0.0	4832.3	707.7	1285.9	1047.8	2322.0	3244.1	633.6
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	13928.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	14002.5	7143.3	7592.8	8401.6	10974.8	0.0	0.0	0.0
	3	0.0	5768.5	7839.6	8263.1	8596.7	10094.4	20055.4	0.0	0.0
	4	0.0	49334.6	6516.2	9063.1	9114.6	9869.6	13800.0	0.0	0.0
	5	0.0	0.0	7764.5	7361.5	9335.9	12449.1	18350.1	34439.1	0.0
	6	0.0	9364.1	14980.5	7169.1	9279.0	14652.4	20669.2	32670.2	0.0
	7	0.0	0.0	4832.3	707.7	9642.1	12840.1	19803.0	33471.0	633.6
$P_{f,i,j}$	1	1.0	0.1	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.5	0.2	0.2	0.1	0.1	1.0	1.0	1.0
	3	1.0	0.2	0.2	0.1	0.1	0.1	0.3	1.0	1.0
	4	1.0	0.7	0.2	0.1	0.1	0.1	0.2	1.0	1.0
	5	1.0	1.0	0.3	0.2	0.1	0.2	0.3	0.1	1.0
	6	1.0	1.0	0.5	0.2	0.1	0.2	0.3	0.2	1.0
	7	1.0	1.0	1.0	1.0	0.2	0.2	0.3	0.1	1.0

Case 7: γ = 0.3 nm

Parameter	BP	Bond Number State								
		0	1	2	3	4	5	6	7	8
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	29.1	31.8	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	94.9	80.3	86.3	153.4	0.0	0.0	0.0	0.0
	3	66.0	57.2	140.3	125.1	174.8	347.5	579.4	0.0	0.0
	4	66.0	50.1	106.2	137.7	239.2	343.7	516.3	667.8	0.0
	5	66.0	83.6	64.6	165.7	256.9	397.3	652.4	740.4	0.0
	6	66.0	0.0	4633.8	152.1	392.1	472.5	645.9	955.4	0.0
	7	66.0	0.0	0.0	126.1	309.3	476.4	600.6	744.4	0.0
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	29.2	31.9	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	1753.3	904.2	165.0	315.9	0.0	0.0	0.0	0.0
	3	66.0	847.6	2210.4	317.6	397.4	1437.3	2176.4	0.0	0.0
	4	66.0	6261.4	1537.8	3032.6	1620.4	1267.1	2212.5	862813.0	0.0
	5	66.0	5022.2	430.5	3393.0	2677.1	3261.9	3088.2	4855.3	0.0
	6	66.0	0.0	4633.8	8009.1	4398.1	2229.4	4249.5	7355.8	0.0
	7	66.0	0.0	0.0	590.3	9143.1	5607.2	3828.0	5847.9	0.0
$P_{r,i,j}$	1	1.0	0.7	0.5	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.5	0.9	0.4	0.5	1.0	1.0	1.0	1.0
	3	1.0	0.3	0.5	0.6	0.5	0.7	0.6	1.0	1.0
	4	1.0	0.5	0.8	0.8	0.7	0.6	0.6	1.0	1.0
	5	1.0	0.6	0.8	0.8	0.8	0.7	0.6	0.7	1.0
	6	1.0	1.0	1.0	0.6	0.4	0.7	0.7	0.6	1.0
	7	1.0	1.0	1.0	0.1	0.9	0.4	0.7	0.6	1.0
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	146.1	26.8	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	704.5	340.4	281.1	405.8	0.0	0.0	0.0	0.0
	3	0.0	531.8	635.0	648.3	545.9	829.3	2614.3	0.0	0.0
	4	0.0	820.9	889.6	399.2	828.7	1424.0	2176.6	592.9	0.0
	5	0.0	1467.1	367.1	467.4	974.1	996.5	2860.9	1682.3	0.0
	6	0.0	0.0	307.2	1707.9	2127.3	2187.9	2536.5	5348.2	0.0
	7	0.0	0.0	5526.6	796.5	1860.5	2389.7	3331.9	4454.0	170823.0
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	14031.5	141.3	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	11388.3	7277.5	8155.0	8876.6	0.0	0.0	0.0	0.0
	3	0.0	36017.2	10269.6	8947.4	9308.5	11994.2	19260.1	0.0	0.0
	4	0.0	8936.1	9404.1	9126.5	10590.3	12740.6	17689.1	10482.4	0.0
	5	0.0	4662.6	8237.3	9625.2	10907.7	12435.4	22771.2	29979.5	0.0
	6	0.0	0.0	6133.0	23138.7	15906.6	16063.6	20100.7	35698.6	0.0
	7	0.0	0.0	5526.6	8464.8	18210.3	18931.6	23042.0	33404.5	170823.0
$P_{f,i,j}$	1	1.0	0.4	0.3	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.4	0.2	0.2	0.1	1.0	1.0	1.0	1.0
	3	1.0	0.6	0.2	0.2	0.2	0.1	0.2	1.0	1.0
	4	1.0	0.4	0.2	0.2	0.1	0.2	0.3	0.0	1.0
	5	1.0	0.4	0.2	0.1	0.2	0.1	0.3	0.1	1.0
	6	1.0	1.0	0.1	0.3	0.2	0.3	0.2	0.2	1.0
	7	1.0	1.0	1.0	0.3	0.4	0.2	0.3	0.2	1.0

Case 8: $k_r^0 = 5x10^{-4}\ s^{-1}$

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}\ (s^{-1})$	1	66.0	18.7	52.1	0.0	0.0	0.0	0.0
	2	66.0	115.7	51.4	66.2	77.5	182.2	0.0
	3	66.0	77.9	61.5	75.9	104.8	176.1	277.8
	4	66.0	38.9	63.5	95.4	131.1	204.8	303.0
	5	66.0	0.0	137.5	142.4	158.7	222.8	370.9
	6	66.0	69.5	31.2	75.8	165.5	292.9	440.9
$k^{(2)}_{r,i,j}\ (s^{-1})$	1	66.0	36.0	52.1	0.0	0.0	0.0	0.0
	2	66.0	4311.7	342.3	130.5	169.4	182.9	0.0
	3	66.0	2695.9	2201.3	177.8	222.8	767.9	963.7
	4	66.0	2518.6	1693.7	2458.0	405.7	645.9	851.1
	5	66.0	0.0	2050.9	3134.7	3889.8	1128.0	1700.3
	6	66.0	69.5	92.2	388.0	3317.3	3158.2	3264.0
$P_{r,i,j}$	1	1.0	0.6	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.7	0.9	0.7	0.5	0.5	1.0
	3	1.0	0.5	0.9	0.5	0.5	0.7	0.6
	4	1.0	0.7	0.7	0.9	0.6	0.6	0.5
	5	1.0	1.0	0.2	0.7	0.9	0.7	0.7
	6	1.0	1.0	0.1	0.9	0.8	0.8	0.7
$k^{(1)}_{f,i,j}\ (s^{-1})$	1	0.0	17112.2	108.8	0.0	0.0	0.0	0.0
	2	0.0	726.4	336.4	222.1	210.4	369.9	0.0
	3	0.0	259.5	628.8	375.6	336.5	657.7	2706.5
	4	0.0	673.0	412.3	458.7	497.3	907.7	925.8
	5	0.0	0.0	484.0	771.1	535.4	871.0	2281.6
	6	0.0	5415.3	1091.7	317.1	558.0	1713.6	2144.2
$k^{(2)}_{f,i,j}\ (s^{-1})$	1	0.0	17112.2	165317.0	0.0	0.0	0.0	0.0
	2	0.0	15060.9	7137.5	7940.5	7321.2	7954.4	0.0
	3	0.0	17147.7	8146.4	8462.0	8600.3	8943.4	21847.2
	4	0.0	11244.1	8030.7	9063.7	9206.1	11542.7	11654.8
	5	0.0	0.0	6529.1	9583.1	9965.3	12025.0	19913.9
	6	0.0	5415.3	8931.5	9286.3	11281.1	14144.4	18959.9
$P_{f,i,j}$	1	1.0	1.0	0.9	1.0	1.0	1.0	1.0
	2	1.0	0.4	0.1	0.2	0.2	0.1	1.0
	3	1.0	0.3	0.1	0.1	0.2	0.2	0.3
	4	1.0	0.4	0.2	0.2	0.1	0.2	0.1
	5	1.0	1.0	0.2	0.1	0.1	0.1	0.3
	6	1.0	1.0	0.2	0.2	0.1	0.2	0.2

Case 9: $k_r^0 = 10^{-3}$ s^{-1}

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	136.9	104.5	0.0	0.0	0.0	0.0
	2	66.0	133.1	113.6	131.2	222.6	0.0	0.0
	3	66.0	61.5	142.4	201.0	232.0	372.2	0.0
	4	66.0	70.3	157.2	226.2	324.0	457.9	676.5
	5	66.0	208.8	164.5	174.2	318.0	492.9	863.7
	6	66.0	4249.1	98.0	170.0	481.0	476.5	687.1
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	136.9	104.5	0.0	0.0	0.0	0.0
	2	66.0	2978.2	1665.5	225.8	551.6	0.0	0.0
	3	66.0	1092.2	2725.0	2508.7	522.0	865.8	0.0
	4	66.0	1076.9	3487.9	4021.6	2910.9	1630.1	2684.4
	5	66.0	210.1	4864.4	2697.0	1546.2	4036.2	4593.6
	6	66.0	4249.1	417.7	3974.9	3923.0	2670.7	3626.4
$P_{r,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.6	0.8	0.4	0.8	1.0	1.0
	3	1.0	0.3	0.6	0.8	0.5	0.5	1.0
	4	1.0	0.3	0.5	0.8	0.8	0.6	0.6
	5	1.0	0.5	0.9	0.6	0.8	0.7	0.6
	6	1.0	1.0	0.8	0.7	0.4	0.7	0.6
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	1614.6	58.2	0.0	0.0	0.0	0.0
	2	0.0	359.4	489.7	395.0	515.3	0.0	0.0
	3	0.0	396.5	551.7	616.1	739.7	717.2	0.0
	4	0.0	448.5	363.3	667.3	988.2	1714.2	2598.7
	5	0.0	689.7	709.1	396.1	1221.7	1058.9	3563.0
	6	0.0	8879.7	1401.8	238.1	1165.5	2361.1	2894.6
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	1614.6	58.2	0.0	0.0	0.0	0.0
	2	0.0	9744.5	8310.9	8598.7	10111.7	0.0	0.0
	3	0.0	13342.6	9286.4	9394.8	9968.2	10235.2	0.0
	4	0.0	9621.0	9428.5	9382.5	11100.8	14133.9	20962.2
	5	0.0	14124.3	10470.3	9803.5	11140.8	12928.3	27177.9
	6	0.0	8879.7	15486.3	10082.2	12669.5	15937.7	21784.7
$P_{f,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	0.2	0.2	0.2	0.2	1.0	1.0
	3	1.0	0.4	0.2	0.2	0.2	0.2	1.0
	4	1.0	0.2	0.1	0.1	0.2	0.2	0.3
	5	1.0	0.2	0.2	0.1	0.2	0.2	0.3
	6	1.0	1.0	0.4	0.2	0.1	0.3	0.3

Table S4. Bond transition rates from ODE model.

Case 1: Base

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	3.8	0.0	0.0	0.0	0.0	0.0
	2	66.0	3.8	0.2	2.9	2.6	255.2	0.0
	3	66.0	3.8	3.4	8.2	4.7	167.2	0.0
	4	66.0	3.5	15.1	21.5	24.9	46.4	74.8
	5	66.0	3.8	12.0	18.2	36.4	54.7	78.6
	6	66.0	0.0	0.0	1,101.9	49.6	60.8	62.3
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	1.1	0.0	0.0	0.0	0.0	0.0
	2	66.0	22.1	1.0	16.6	15.3	1,483.3	0.0
	3	66.0	0.2	0.1	0.3	0.2	7.0	0.0
	4	66.0	3.8	597.6	748.3	58.3	132.0	192.6
	5	66.0	3.8	12.1	655.6	846.5	206.4	322.8
	6	66.0	0.0	0.0	1,101.9	1,800.2	254.2	223.9
$P_{r,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.1	1.0	0.6	0.1	1.0
	3	1.0	1.0	0.9	0.4	0.6	0.7	1.0
	4	1.0	0.9	0.8	0.9	0.5	0.6	0.7
	5	1.0	1.0	0.5	0.9	0.9	0.7	0.6
	6	1.0	1.0	1.0	1.0	0.8	0.6	0.5
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	283.2	0.0	0.0	0.0	0.0	0.0
	2	0.0	53.5	1,746.1	3.4	4.4	10,239.3	1.0
	3	0.0	55.3	6,828.6	358.4	2.8	82.3	0.0
	4	0.0	692.5	125.1	136.2	192.7	187.9	211.7
	5	0.0	52.5	413.7	37.8	232.7	488.1	731.0
	6	0.0	0.0	547.8	1,305.0	520.5	516.7	952.0
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	176.8	0.0	0.0	0.0	0.0	0.0
	2	0.0	4.9	160.8	0.3	0.4	943.0	0.0
	3	0.0	0.6	75.1	3.9	0.0	0.9	0.0
	4	0.0	8,739.7	5,990.6	7,053.9	7,568.0	7,981.7	8,273.3
	5	0.0	52.5	6,354.8	5,691.6	7,099.7	8,729.7	12,429.9
	6	0.0	0.0	547.8	174,609.0	11,749.6	11,841.9	13,491.8
$P_{f,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.1	1.0	0.6	0.1	1.0
	3	1.0	1.0	0.9	0.4	0.6	0.7	1.0
	4	1.0	0.6	0.2	0.1	0.1	0.1	0.1
	5	1.0	1.0	0.2	0.1	0.1	0.1	0.1
	6	1.0	1.0	1.0	0.9	0.1	0.1	0.1

Case 2: Low antibody

Parameter	BP	Bond Number State								
		0	1	2	3	4	5	6	7	8
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	3.7	27.3	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	3.8	0.2	0.6	77.1	60.4	0.0	0.0	0.0
	3	66.0	3.8	42.3	6.2	1.4	39.6	182.9	0.0	0.0
	4	66.0	3.6	11.6	26.5	32.2	52.9	141.9	0.0	0.0
	5	66.0	3.9	7.9	16.3	39.5	57.3	149.9	0.0	0.0
	6	66.0	0.0	0.0	18.2	50.4	76.7	147.4	1,942.1	30,376.8
	7	66.0	233.7	9.6	126.6	312.5	84.6	114.3	240.1	0.0
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	26.7	194.4	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	7.5	0.3	1.1	152.3	119.3	0.0	0.0	0.0
	3	66.0	0.3	3.2	0.5	0.1	3.0	13.7	0.0	0.0
	4	66.0	1.5	2,042.7	569.4	104.9	207.2	892.8	0.0	0.0
	5	66.0	3.9	70.2	353.8	422.5	372.1	2,341.6	0.0	0.0
	6	66.0	0.0	0.0	3,324.9	764.1	591.3	2,863.4	33,169.8	520,853.0
	7	66.0	233.7	74.1	126.6	318.0	1,384.5	368.7	926.2	0.0
$P_{r,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.3	1.0	0.6	0.5	1.0	1.0	1.0
	3	1.0	1.0	0.8	0.5	0.5	0.6	0.5	1.0	1.0
	4	1.0	0.9	1.0	0.8	0.7	0.6	0.4	1.0	1.0
	5	1.0	1.0	0.8	0.8	0.8	0.7	0.5	1.0	1.0
	6	1.0	1.0	1.0	0.8	0.6	0.8	0.7	0.3	1.0
	7	1.0	1.0	0.9	1.0	0.2	0.6	0.4	0.5	1.0
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	23.8	14.2	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	54.4	1,014.0	1.7	283.3	85.3	0.0	0.0	0.0
	3	0.0	0.0	1,212.0	50.1	1.2	0.1	5,880.3	0.0	0.0
	4	0.0	16,652.2	2,056.9	155.2	265.0	307.7	206.1	0.0	0.0
	5	0.0	367.5	111.4	118.9	282.4	517.6	924.3	0.0	0.0
	6	0.0	0.0	1,204.5	126.0	879.6	571.2	715.9	1,000.3	12,274.8
	7	0.0	2,374.3	244.9	1,449.4	1,988.0	599.8	1,254.8	2,723.0	0.0
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	1.2	0.7	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	1.3	23.3	0.0	6.5	2.0	0.0	0.0	0.0
	3	0.0	0.0	39.7	1.6	0.0	0.0	192.7	0.0	0.0
	4	0.0	5,127.9	2,895.0	4,422.7	4,733.0	5,024.6	3,678.6	0.0	0.0
	5	0.0	367.5	2,276.5	5,002.3	5,108.7	6,342.1	14,928.4	0.0	0.0
	6	0.0	0.0	1,204.5	3,361.2	9,055.8	9,024.4	13,113.0	34,148.3	47,994.9
	7	0.0	2,374.3	6,152.8	1,449.4	22,320.5	7,266.9	15,198.6	34,249.5	0.0
$P_{f,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.3	1.0	0.6	0.5	1.0	1.0	1.0
	3	1.0	1.0	0.8	0.5	0.5	0.6	0.5	1.0	1.0
	4	1.0	0.3	0.3	0.2	0.2	0.2	0.0	1.0	1.0
	5	1.0	1.0	0.3	0.2	0.2	0.2	0.5	1.0	1.0
	6	1.0	1.0	1.0	0.2	0.4	0.3	0.2	0.1	0.7
	7	1.0	1.0	0.5	1.0	0.4	0.2	0.4	0.1	1.0

Case 3: Low ICAM-1

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	3.4	1.1	0.0	0.0	0.0	0.0
	2	66.0	4.0	4.1	0.5	281.7	0.0	0.0
	3	66.0	2.8	13.7	14.4	22.3	28.3	0.0
	4	66.0	4.3	419.4	23.0	25.3	43.5	0.0
	5	66.0	9.3	0.0	0.0	61.8	61.8	38.8
	6	66.0	0.0	4.8	0.0	75.1	63.9	53.9
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	7.9	2.4	0.0	0.0	0.0	0.0
	2	66.0	0.9	0.9	0.1	60.4	0.0	0.0
	3	66.0	92.6	426.9	29.1	52.9	28.4	0.0
	4	66.0	4.3	3797.8	216.0	62.1	112.4	0.0
	5	66.0	9.3	0.0	0.0	1857.5	234.4	112.2
	6	66.0	0.0	4.8	0.0	169.6	2378.1	179.5
$P_{r,i,j}$	1	1.0	1.0	0.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.7	0.1	0.7	1.0	1.0
	3	1.0	0.4	0.9	0.4	0.5	0.5	1.0
	4	1.0	1.0	0.6	0.7	0.5	0.6	1.0
	5	1.0	1.0	1.0	1.0	0.6	0.6	0.0
	6	1.0	1.0	1.0	1.0	0.7	0.7	0.6
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	302.7	0.8	0.0	0.0	0.0	0.0
	2	0.0	19.4	1594.5	0.1	141.0	0.0	0.0
	3	0.0	842.5	81.7	111.0	100.4	58.7	0.0
	4	0.0	675.7	48.0	272.6	230.9	180.6	0.0
	5	0.0	254.8	4296.3	2128.4	903.4	757.0	232.1
	6	0.0	0.0	271.2	81.0	2389.0	1819.0	1258.8
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	1.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	0.4	32.0	0.0	2.8	0.0	0.0
	3	0.0	65455.0	5949.0	6964.9	7924.2	9001.7	0.0
	4	0.0	675.7	3009.2	7611.6	8048.2	8200.3	0.0
	5	0.0	254.8	4296.3	2128.4	12195.8	10675.6	14430.4
	6	0.0	0.0	698919.0	81.0	287045.0	13450.5	14458.1
$P_{f,i,j}$	1	1.0	1.0	0.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.7	0.1	0.7	1.0	1.0
	3	1.0	0.6	0.1	0.1	0.2	0.3	1.0
	4	1.0	1.0	0.2	0.1	0.1	0.1	1.0
	5	1.0	1.0	1.0	1.0	0.2	0.2	0.1
	6	1.0	1.0	0.8	1.0	0.9	0.3	0.3

Case 4: ICAM-1 dimer

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	3.8	19.9	0.0	0.0	0.0	
	2	66.0	3.4	0.1	20.5	37.9	0.0	
	3	66.0	3.8	58.6	6.1	3.0	0.0	
	4	66.0	5.7	3.8	20.1	28.5	41.2	
	5	66.0	0.0	11.9	4,561.4	79.5	70.2	
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	12.3	64.5	0.0	0.0	0.0	
	2	66.0	1.7	0.1	10.5	19.4	0.0	
	3	66.0	0.2	3.0	0.3	0.2	0.0	
	4	66.0	161.3	14.2	153.3	74.1	105.5	
	5	66.0	0.0	11.9	4,561.4	1,822.9	195.9	
$P_{r,i,j}$	1	1.0	1.0	0.5	1.0	1.0	1.0	
	2	1.0	1.0	0.2	1.0	0.8	1.0	
	3	1.0	1.0	0.8	0.5	0.4	1.0	
	4	1.0	0.8	0.1	0.8	0.6	0.6	
	5	1.0	1.0	1.0	1.0	0.3	0.6	
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	299.4	2.6	0.0	0.0	0.0	
	2	0.0	8.7	283.4	6.3	4.0	0.0	
	3	0.0	0.0	1,987.3	59.6	0.4	0.0	
	4	0.0	277.5	69.2	198.2	231.1	245.6	
	5	0.0	0.0	147.3	11,536.0	2,084.6	924.0	
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	47.8	0.4	0.0	0.0	0.0	
	2	0.0	0.4	11.6	0.3	0.2	0.0	
	3	0.0	0.0	30.8	0.9	0.0	0.0	
	4	0.0	3,568.4	9,088.9	13,286.9	13,753.9	15,140.6	
	5	0.0	0.0	5,747,130.0	11,536.0	18,997.5	13,763.9	
$P_{f,i,j}$	1	1.0	1.0	0.5	1.0	1.0	1.0	
	2	1.0	1.0	0.2	1.0	0.8	1.0	
	3	1.0	1.0	0.8	0.5	0.4	1.0	
	4	1.0	0.4	0.2	0.1	0.1	0.1	
	5	1.0	1.0	0.9	1.0	0.2	0.1	

Case 5: Clustered ICAM-1 dimer

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	3.8	6.9	0.0	0.0	0.0	0.0
	2	66.0	3.7	9.1	0.3	75.7	0.0	0.0
	3	66.0	3.6	10.6	13.8	22.3	44.1	0.0
	4	66.0	0.0	10.6	23.5	30.4	50.0	0.0
	5	66.0	2.3	8.4	63.5	50.1	58.9	75.5
	6	66.0	0.0	0.0	0.0	0.0	161.4	92.2
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	4.6	8.4	0.0	0.0	0.0	0.0
	2	66.0	3.3	8.2	0.2	67.8	0.0	0.0
	3	66.0	150.4	191.7	26.9	69.8	149.2	0.0
	4	66.0	0.0	583.8	247.0	86.9	194.5	0.0
	5	66.0	2.3	8.4	1,000,000,000.0	3,067.5	260.0	221.5
	6	66.0	0.0	0.0	0.0	0.0	2,408.6	853.3
$P_{r,i,j}$	1	1.0	1.0	0.8	1.0	1.0	1.0	1.0
	2	1.0	1.0	1.0	0.4	0.4	1.0	1.0
	3	1.0	0.9	0.7	0.3	0.5	0.8	1.0
	4	1.0	1.0	0.9	0.8	0.6	0.5	1.0
	5	1.0	1.0	1.0	0.9	0.9	0.6	0.5
	6	1.0	1.0	1.0	1.0	1.0	0.2	0.7
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	196.4	1.3	0.0	0.0	0.0	0.0
	2	0.0	324.9	1,036.2	0.1	935.5	0.0	0.0
	3	0.0	498.2	91.2	189.0	107.5	507.1	42.5
	4	0.0	0.0	88.4	93.2	286.1	321.4	0.0
	5	0.0	181.7	693.1	1,844.2	780.5	1,129.8	920.2
	6	0.0	0.0	6,226.3	39,377.8	506.4	3,677.7	2,828.4
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	25.3	0.2	0.0	0.0	0.0	0.0
	2	0.0	2.7	8.7	0.0	7.8	0.0	0.0
	3	0.0	142,679.0	10,954.7	12,479.4	18,129.1	17,681.0	42.5
	4	0.0	0.0	6,585.1	12,203.1	13,536.3	16,470.3	0.0
	5	0.0	181.7	132,742.0	19,392.0	13,687.8	18,459.4	23,556.6
	6	0.0	0.0	6,226.3	39,377.8	506.4	39,605.0	28,111.1
$P_{f,i,j}$	1	1.0	1.0	0.8	1.0	1.0	1.0	1.0
	2	1.0	1.0	1.0	0.4	0.4	1.0	1.0
	3	1.0	0.8	0.2	0.1	0.1	0.1	1.0
	4	1.0	1.0	0.2	0.1	0.1	0.1	1.0
	5	1.0	1.0	0.8	0.4	0.1	0.2	0.1
	6	1.0	1.0	1.0	1.0	1.0	0.3	0.3

Case 6: γ = 0.29 nm

Parameter	BP	Bond Number State								
		0	1	2	3	4	5	6	7	8
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	17.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	17.7	39.6	4.5	131.4	89.6	0.0	0.0	0.0
	3	66.0	17.7	14.3	100.6	75.8	50.9	259.0	0.0	0.0
	4	66.0	12.7	34.9	78.8	100.7	152.3	209.2	0.0	0.0
	5	66.0	0.0	55.1	51.1	116.8	183.7	311.0	188.4	0.0
	6	66.0	79.9	73.6	51.1	134.8	233.6	324.7	350.6	0.0
	7	66.0	0.0	0.0	0.0	250.3	237.9	296.0	287.1	0.0
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	0.3	0.6	0.1	2.1	1.4	0.0	0.0	0.0
	3	66.0	0.0	0.0	0.2	0.2	0.1	0.5	0.0	0.0
	4	66.0	106.9	887.8	2,306.2	298.0	474.4	383.3	0.0	0.0
	5	66.0	0.0	1,170.1	1,758.2	2,794.2	1,223.6	1,495.8	574.8	0.0
	6	66.0	79.9	3,456.1	1,189.4	3,132.8	1,470.6	2,000.3	2,657.8	0.0
	7	66.0	0.0	0.0	0.0	3,959.8	4,409.6	1,508.4	2,736.4	0.0
$P_{r,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.9	0.5	0.9	0.2	1.0	1.0	1.0
	3	1.0	1.0	0.8	0.6	0.5	0.4	0.8	1.0	1.0
	4	1.0	0.4	0.6	0.9	0.6	0.6	0.9	1.0	1.0
	5	1.0	1.0	0.8	0.9	0.8	0.7	0.6	0.2	1.0
	6	1.0	1.0	0.8	0.8	0.8	0.7	0.6	0.6	1.0
	7	1.0	1.0	1.0	1.0	0.4	0.6	0.6	0.6	1.0
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	10.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	218.7	449.1	1.4	0.1	1,037.4	0.0	0.0	0.0
	3	0.0	721.7	11,472.5	1,421.2	82.6	5.0	396.7	0.0	0.0
	4	0.0	351.9	238.3	429.7	543.1	659.6	771.4	0.0	0.0
	5	0.0	0.0	704.3	215.0	529.3	1,162.4	2,017.2	601.7	0.0
	6	0.0	9,364.1	262.1	178.6	617.4	1,693.9	2,330.9	3,765.0	0.0
	7	0.0	0.0	4,832.3	707.7	1,285.9	1,047.8	2,322.0	3,244.1	633.6
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	1.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	17.4	35.7	0.1	0.0	82.4	0.0	0.0	0.0
	3	0.0	1.0	16.1	2.0	0.1	0.0	0.6	0.0	0.0
	4	0.0	49,334.6	6,516.2	9,063.1	9,114.6	9,869.6	13,800.0	0.0	0.0
	5	0.0	0.0	7,764.5	7,361.5	9,335.9	12,449.1	18,350.1	34,439.1	0.0
	6	0.0	9,364.1	14,980.5	7,169.1	9,279.0	14,652.4	20,669.2	32,670.2	0.0
	7	0.0	0.0	4,832.3	707.7	9,642.1	12,840.1	19,803.0	33,471.0	633.6
$P_{f,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.9	0.5	0.9	0.2	1.0	1.0	1.0
	3	1.0	1.0	0.8	0.6	0.5	0.4	0.8	1.0	1.0
	4	1.0	0.7	0.2	0.1	0.1	0.1	0.2	1.0	1.0
	5	1.0	1.0	0.3	0.2	0.1	0.2	0.3	0.1	1.0
	6	1.0	1.0	0.5	0.2	0.1	0.2	0.3	0.2	1.0
	7	1.0	1.0	1.0	1.0	0.2	0.2	0.3	0.1	1.0

Case 7: γ = 0.3 nm

Parameter	BP	Bond Number State								
		0	1	2	3	4	5	6	7	8
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	8.9	2.7	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	8.9	140.3	1.2	213.5	0.0	0.0	0.0	0.0
	3	66.0	8.9	171.6	210.3	31.3	344.8	447.3	0.0	0.0
	4	66.0	8.9	111.1	111.0	243.9	351.4	467.5	499.8	0.0
	5	66.0	8.9	8.4	70.4	91.6	366.0	393.9	499.7	0.0
	6	66.0	0.0	4,633.8	152.1	392.1	472.5	645.9	955.4	0.0
	7	66.0	0.0	0.0	126.1	309.3	476.4	600.6	744.4	0.0
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	151.7	45.8	0.0	0.0	0.0	0.0	0.0	0.0
	2	66.0	0.1	2.2	0.0	3.3	0.0	0.0	0.0	0.0
	3	66.0	0.4	7.4	9.1	1.4	14.9	19.3	0.0	0.0
	4	66.0	0.1	0.7	0.7	1.6	2.3	3.0	3.2	0.0
	5	66.0	0.0	0.0	0.1	0.2	0.7	0.8	1.0	0.0
	6	66.0	0.0	4,633.8	8,009.1	4,398.1	2,229.4	4,249.5	7,355.8	0.0
	7	66.0	0.0	0.0	590.3	9,143.1	5,607.2	3,828.0	5,847.9	0.0
$P_{r,i,j}$	1	1.0	1.0	0.5	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	1.0	0.3	0.5	1.0	1.0	1.0	1.0
	3	1.0	1.0	0.5	0.5	0.6	0.7	0.9	1.0	1.0
	4	1.0	1.0	0.8	0.8	0.6	0.0	0.6	1.0	1.0
	5	1.0	1.0	0.8	0.8	0.7	0.6	0.4	1.0	1.0
	6	1.0	1.0	1.0	0.6	0.4	0.7	0.7	0.6	1.0
	7	1.0	1.0	1.0	0.1	0.9	0.4	0.7	0.6	1.0
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	21.5	4.9	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	301.3	627.6	0.5	4.9	0.0	0.0	0.0	0.0
	3	0.0	0.1	889.5	5,228.4	51.7	4.6	2,170.9	0.0	0.0
	4	0.0	16.7	717.3	274.6	80.2	103.3	70.1	295.4	0.0
	5	0.0	1,699.7	5,675.6	186.2	339.1	291.5	398.8	172.5	0.0
	6	0.0	0.0	307.2	1,707.9	2,127.3	2,187.9	2,536.5	5,348.2	0.0
	7	0.0	0.0	5,526.6	796.5	1,860.5	2,389.7	3,331.9	4,454.0	170,823.0
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	37.1	77.4	0.1	0.6	0.0	0.0	0.0	0.0
	3	0.0	0.0	18.3	107.3	1.1	0.1	44.6	0.0	0.0
	4	0.0	0.8	32.5	12.5	3.6	4.7	3.2	13.4	0.0
	5	0.0	5.5	18.3	0.6	1.1	0.9	1.3	0.6	0.0
	6	0.0	0.0	6,133.0	23,138.7	15,906.6	16,063.6	20,100.7	35,698.6	0.0
	7	0.0	0.0	5,526.6	8,464.8	18,210.3	18,931.6	23,042.0	33,404.5	170,823.0
$P_{f,i,j}$	1	1.0	1.0	0.5	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	1.0	0.3	0.5	1.0	1.0	1.0	1.0
	3	1.0	1.0	0.5	0.5	0.6	0.7	0.9	1.0	1.0
	4	1.0	1.0	0.8	0.8	0.6	0.0	0.6	1.0	1.0
	5	1.0	1.0	0.8	0.8	0.7	0.6	0.4	1.0	1.0
	6	1.0	1.0	0.1	0.3	0.2	0.3	0.2	0.2	1.0
	7	1.0	1.0	1.0	0.3	0.4	0.2	0.3	0.2	1.0

Case 8: $k_r^0 = 5x10^{-4}\ s^{-1}$

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}\ (s^{-1})$	1	66.0	21.8	12.4	0.0	0.0	0.0	0.0
	2	66.0	19.4	5.7	2.8	53.4	169.2	0.0
	3	66.0	20.7	270.0	43.8	37.2	231.3	277.4
	4	66.0	19.4	37.0	80.4	41.9	206.5	315.7
	5	66.0	0.0	137.5	142.4	158.7	222.8	370.9
	6	66.0	69.5	31.2	75.8	165.5	292.9	440.9
$k^{(2)}_{r,i,j}\ (s^{-1})$	1	66.0	15.2	8.7	0.0	0.0	0.0	0.0
	2	66.0	1.6	0.5	0.2	4.3	13.6	0.0
	3	66.0	0.3	3.4	0.5	0.5	2.9	3.5
	4	66.0	0.2	0.4	0.9	0.5	2.4	3.6
	5	66.0	0.0	2,050.9	3,134.7	3,889.8	1,128.0	1,700.3
	6	66.0	69.5	92.2	388.0	3,317.3	3,158.2	3,264.0
$P_{r,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.5	0.5	0.2	0.5	1.0
	3	1.0	1.0	1.0	0.6	0.5	0.3	0.5
	4	1.0	1.0	0.7	0.9	0.7	0.6	0.5
	5	1.0	1.0	0.2	0.7	0.9	0.7	0.7
	6	1.0	1.0	0.1	0.9	0.8	0.8	0.7
$k^{(1)}_{f,i,j}\ (s^{-1})$	1	0.0	53.8	33.0	0.0	0.0	0.0	0.0
	2	0.0	4.0	604.0	7.1	20.7	27.1	0.0
	3	0.0	20.9	5,060.1	83.7	38.4	19.4	248.5
	4	0.0	5.0	1,191.4	357.9	47.3	47.9	7.6
	5	0.0	0.0	484.0	771.1	535.4	871.0	2,281.6
	6	0.0	5,415.3	1,091.7	317.1	558.0	1,713.6	2,144.2
$k^{(2)}_{f,i,j}\ (s^{-1})$	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2	0.0	0.1	8.0	0.1	0.3	0.4	0.0
	3	0.0	0.2	44.7	0.7	0.3	0.2	2.2
	4	0.0	0.2	45.1	13.5	1.8	1.8	0.3
	5	0.0	0.0	6,529.1	9,583.1	9,965.3	12,025.0	19,913.9
	6	0.0	5,415.3	8,931.5	9,286.3	11,281.1	14,144.4	18,959.9
$P_{f,i,j}$	1	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	2	1.0	1.0	0.5	0.5	0.2	0.5	1.0
	3	1.0	1.0	1.0	0.6	0.5	0.3	0.5
	4	1.0	1.0	0.7	0.9	0.7	0.6	0.5
	5	1.0	1.0	0.2	0.1	0.1	0.1	0.3
	6	1.0	1.0	0.2	0.2	0.1	0.2	0.2

Case 9: $k_r^0 = 10^{-3}$ s^{-1}

Parameter	BP	Bond Number State						
		0	1	2	3	4	5	6
$k^{(1)}_{r,i,j}$ (s^{-1})	1	66.0	16.3	385.7	0.0	0.0	0.0	0.0
	2	66.0	14.2	407.8	3.7	118.1	0.0	0.0
	3	66.0	14.5	131.7	185.6	232.6	362.4	0.0
	4	66.0	15.8	162.3	181.9	295.7	258.7	500.0
	5	66.0	14.8	203.5	155.9	304.8	485.5	500.0
	6	66.0	14.7	68.9	164.4	399.8	488.8	465.3
$k^{(2)}_{r,i,j}$ (s^{-1})	1	66.0	79.2	1,877.8	0.0	0.0	0.0	0.0
	2	66.0	0.2	6.4	0.1	1.8	0.0	0.0
	3	66.0	0.8	7.1	10.0	12.6	19.6	0.0
	4	66.0	0.5	5.2	5.9	9.5	8.3	16.1
	5	66.0	0.3	4.0	3.0	5.9	9.5	9.7
	6	66.0	1.2	5.7	13.5	32.8	40.1	38.2
$P_{r,i,j}$	1	1.0	1.0	0.1	1.0	1.0	1.0	1.0
	2	1.0	1.0	1.0	0.4	0.6	1.0	1.0
	3	1.0	1.0	0.7	0.8	0.5	0.5	1.0
	4	1.0	1.0	0.5	0.6	0.6	0.6	0.5
	5	1.0	1.0	0.5	0.6	0.8	0.6	0.6
	6	1.0	1.0	0.8	0.8	0.4	0.8	0.6
$k^{(1)}_{f,i,j}$ (s^{-1})	1	0.0	68.6	108.6	0.0	0.0	0.0	0.0
	2	0.0	258.6	2,200.6	1.3	6.6	0.0	0.0
	3	0.0	21.0	947.0	827.9	255.9	17.7	0.0
	4	0.0	0.9	3,179.0	4,125.3	3,021.2	1,099.1	55.5
	5	0.0	29.3	3,090.1	1,864.3	1,233.9	249.7	405.3
	6	0.0	12,604.9	166.8	46.7	11,098.8	8,022.9	326.7
$k^{(2)}_{f,i,j}$ (s^{-1})	1	0.0	3.6	5.7	0.0	0.0	0.0	0.0
	2	0.0	5.9	49.9	0.0	0.1	0.0	0.0
	3	0.0	2.1	92.6	80.9	25.0	1.7	0.0
	4	0.0	0.0	15.5	20.1	14.7	5.3	0.3
	5	0.0	0.6	68.4	41.2	27.3	5.5	9.0
	6	0.0	155.3	2.1	0.6	136.8	98.9	4.0
$P_{f,i,j}$	1	1.0	1.0	0.1	1.0	1.0	1.0	1.0
	2	1.0	1.0	1.0	0.4	0.6	1.0	1.0
	3	1.0	1.0	0.7	0.8	0.5	0.5	1.0
	4	1.0	1.0	0.5	0.6	0.6	0.6	0.5
	5	1.0	1.0	0.5	0.6	0.8	0.6	0.6
	6	1.0	1.0	0.8	0.8	0.4	0.8	0.6

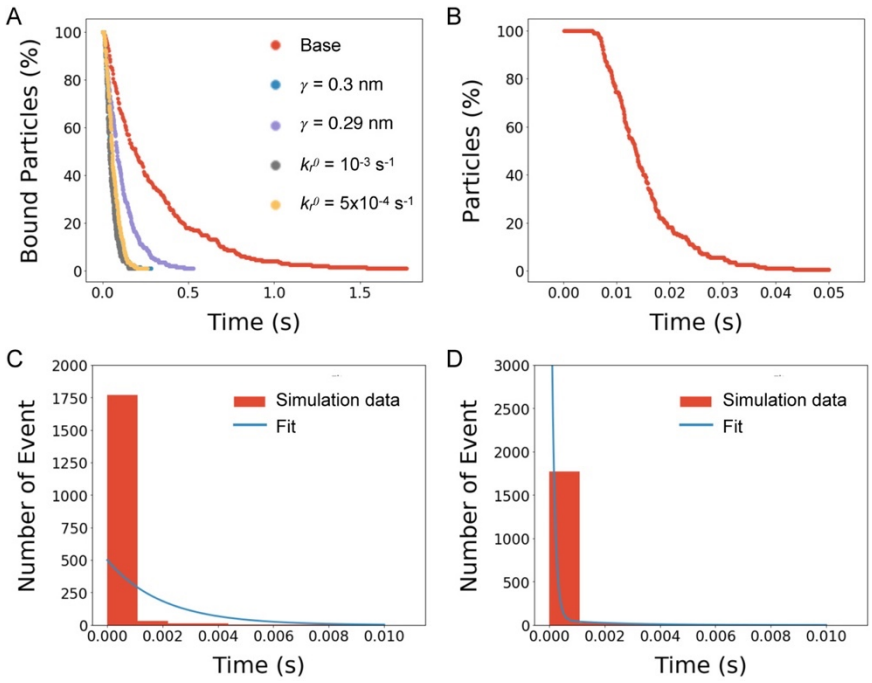


Figure S1. Bond transition rate model fitting parameters. (A,B) Single bond tether simulations to determine values for (A) $k_{r1,1}$ and (B) k_{diff}. (C,D) Representative example of simulation pause time fitting to determine initial transition rate values for ODE model fits using (C) one and (D) two sub-components.

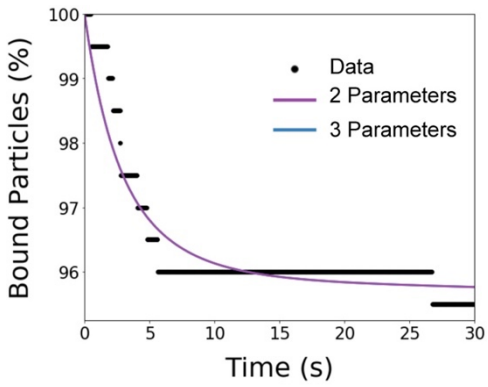


Figure S2. Population heterogeneity detachment model fits for two sub-components using 2 and 3 degrees of freedom. Two degrees of freedom (2 DOF) assumes that one component does not detach while three degrees of freedom (3 DOF) assumes that both can detach, and the fits were identical. Results shown are for the base case (medium antibody and ICAM-1 density, γ = 0.274 nm, k_r^0 = 1.1x10^{-4} s^{-1}).

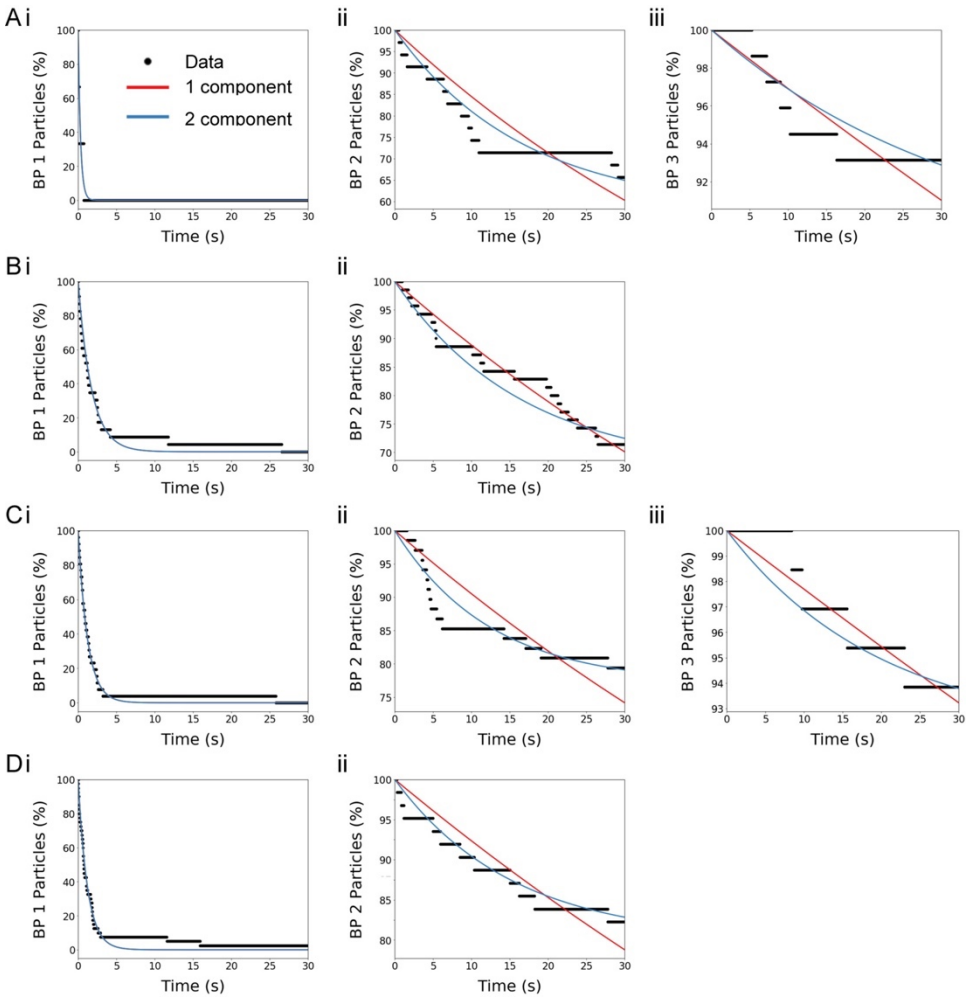


Figure S3. Population heterogeneity detachment model fits for individual BPs of cases 2-5. Base case parameters were modified to (A) low antibody density, (B) low ICAM-1 density, (C) ICAM-1 dimers, and (D) clustered ICAM-1 dimers. Detachment data and fits performed using one and two sub-components for (i) BP 1, (ii) BP 2, and (iii) BP 3.

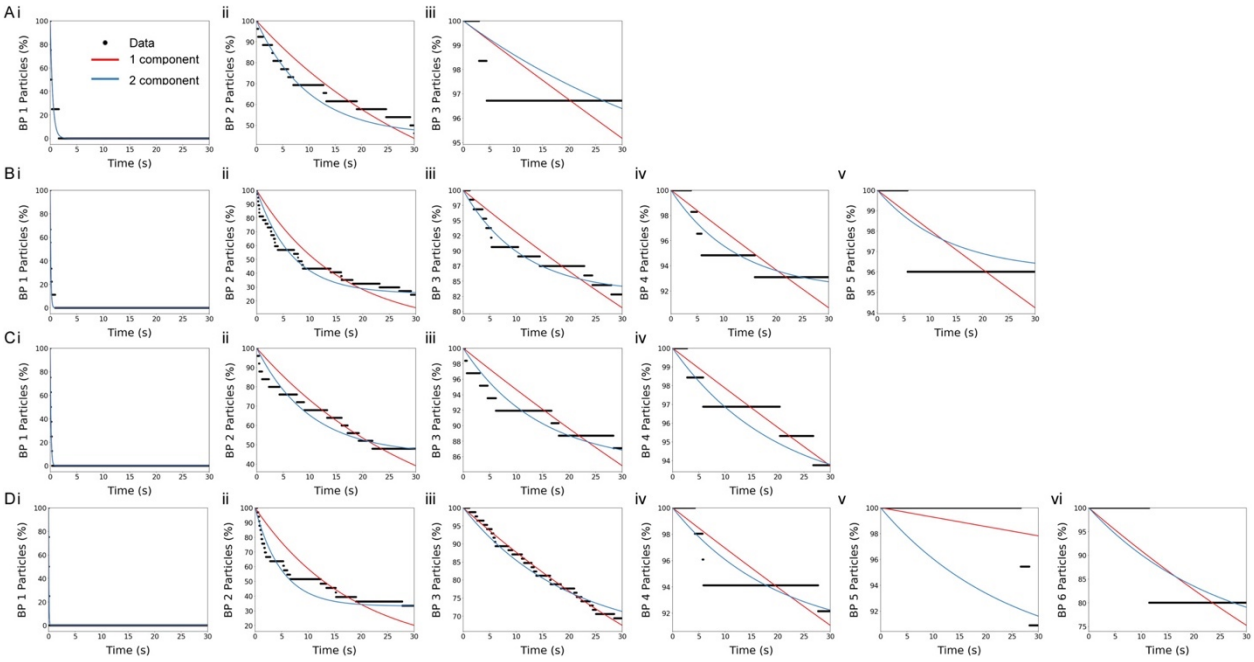


Figure S4. Population heterogeneity detachment model fits for individual BPs of cases 6-9. Base case parameters were modified to (A) γ = 0.29 nm, (B) γ = 0.3 nm, (C) k_r^0 = 5x10^{-4} s^{-1}, and (D) k_r^0 = 10^{-3} s^{-1}. Detachment data and fits performed using one and two sub-components for (i) BP 1, (ii) BP 2, (iii) BP 3, (iv) BP 4, (v) BP 5, and (vi) BP 6.

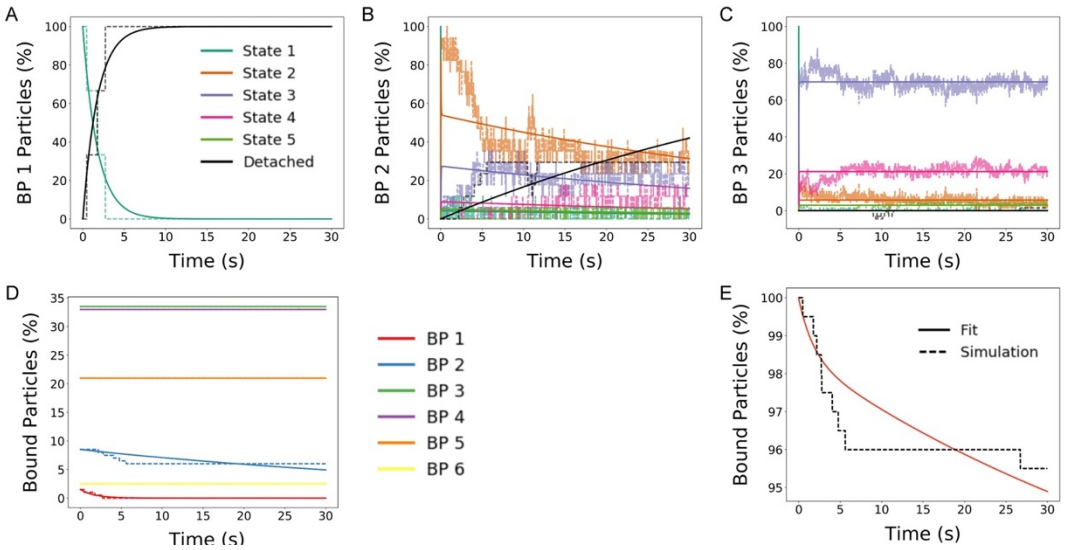


Figure S5. Bond transition rate modeling for the base case using one sub-component. (A-C) Simulation data and fits for NPs within each bond number state for (A) BP 1, (B) BP 2, and (C) BP 3. The detachment profile is also overlaid in black for each BP category. (D,E) Detachment data from the simulation and fits for (D) each BP category and (E) the full population.

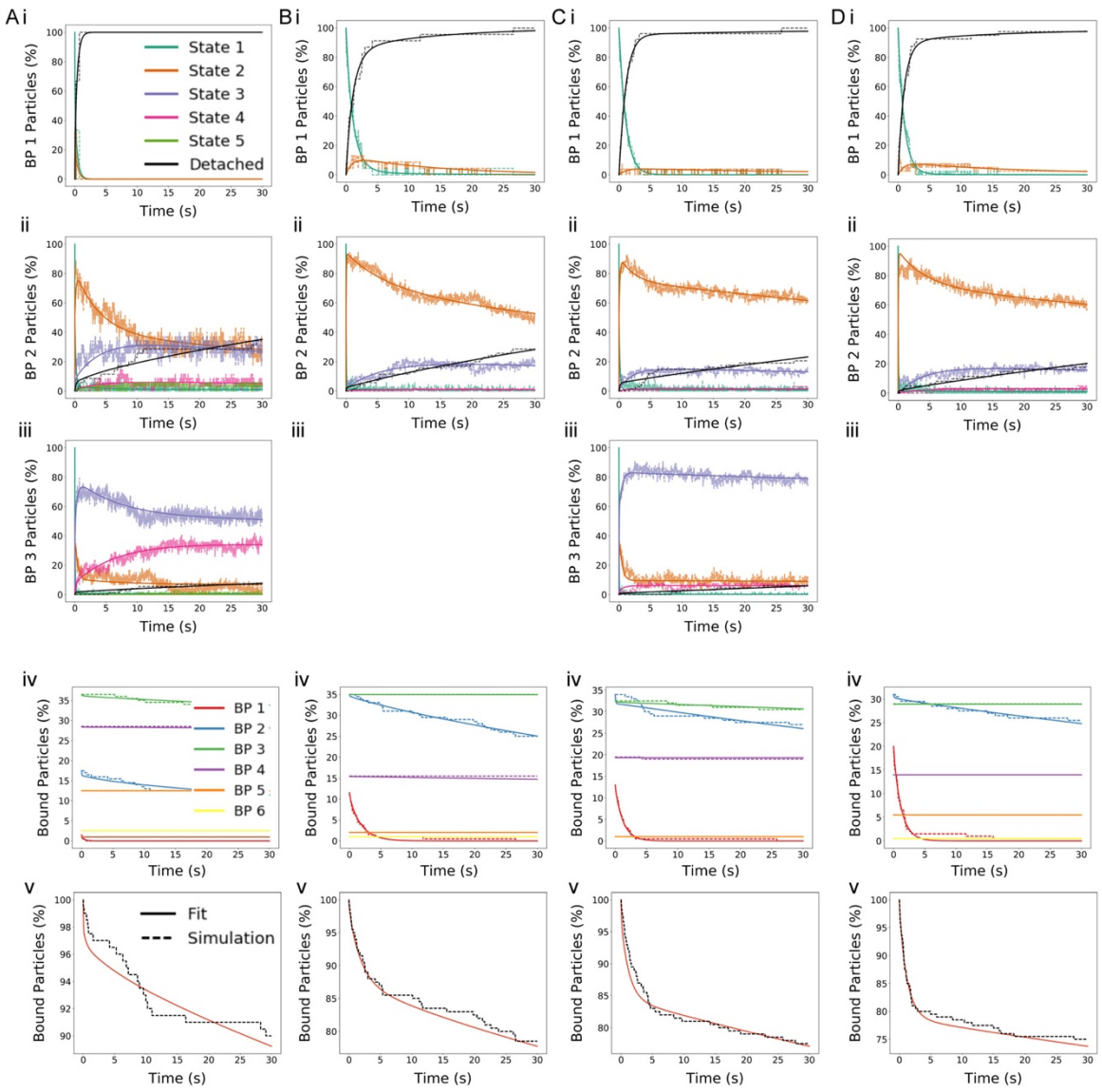
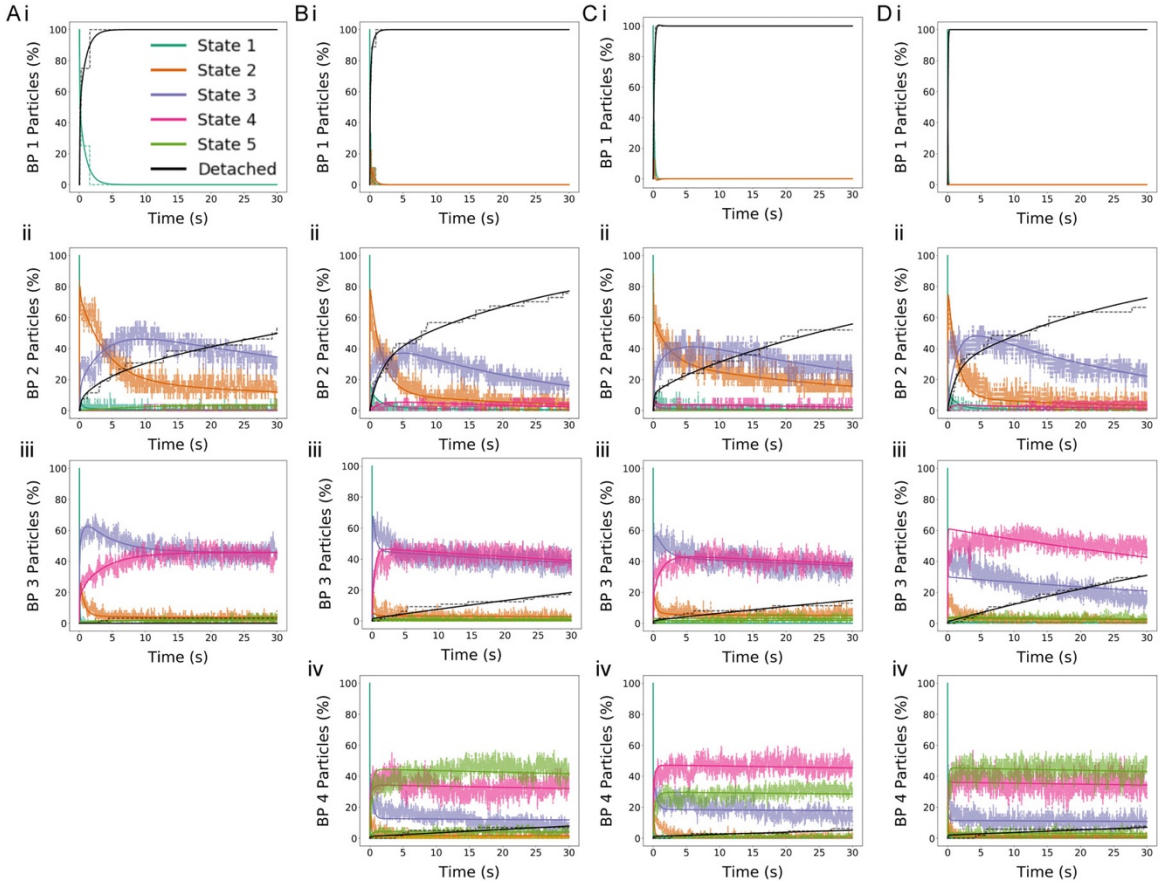


Figure S6. Bond transition rate modeling for cases 2-5. Base case parameters were modified to (A) low antibody density, (B) low ICAM-1 density, (C) ICAM-1 dimers, and (D) clustered ICAM-1 dimers. (i-iv) Simulation profiles and fits for NPs within each bond number state for (i) BP 1, (i) BP 2, and (i) BP 3. The detachment profile is also overlaid in black for each BP category. (iv-v) Detachment data from the simulation and fits for (iv) each BP category and (v) the full population.


A i
B i
C i
D i
ii
iii
iv
State 1
State 2
State 3
State 4
State 5
Detached
BP 1 Particles (%)
BP 2 Particles (%)
BP 3 Particles (%)
BP 4 Particles (%)
Time (s)

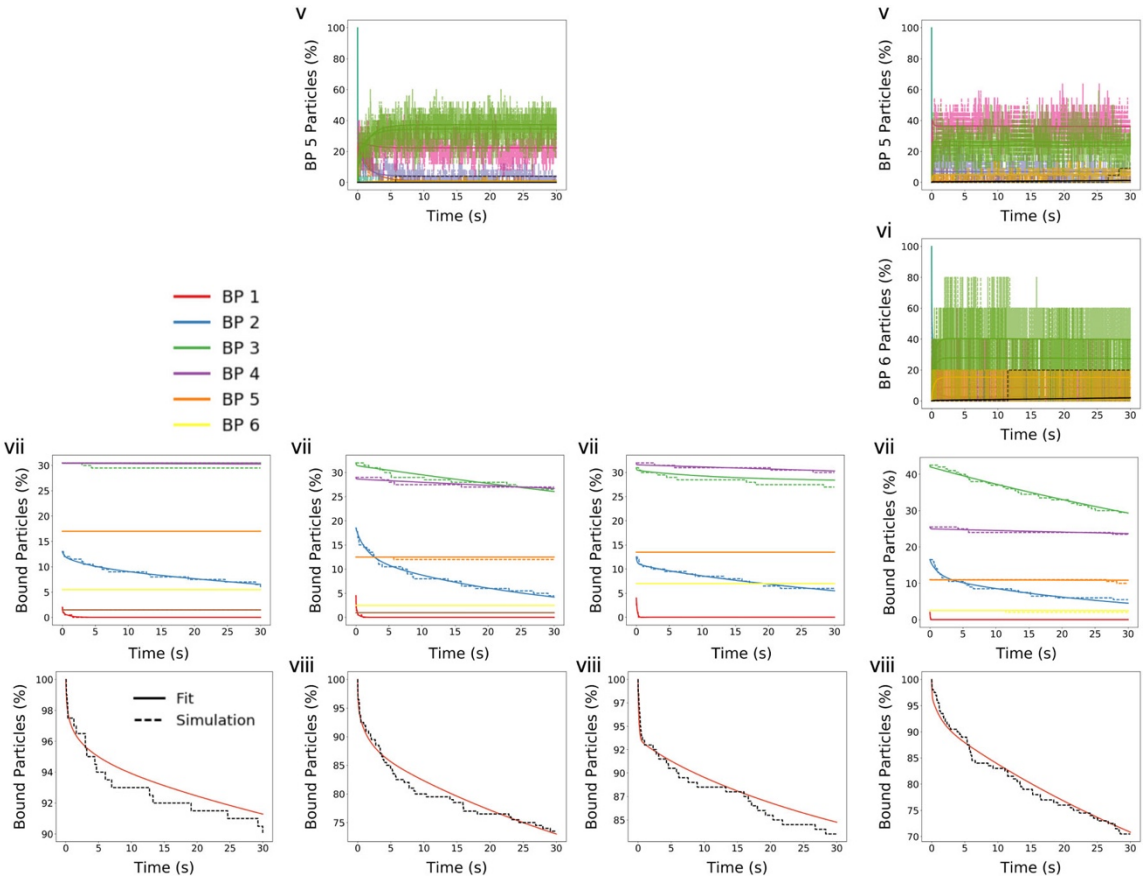


Figure S7. Bond transition rate modeling for cases 2-5. Base case parameters were modified to (A) γ = 0.29 nm, (B) γ = 0.3 nm, (C) k_r^0 = 5x10^{-4} s^{-1}, and (D) k_r^0 = 10^{-3} s^{-1}. (i-iv) Simulation profiles and fits for NPs within each bond number state for (i) BP 1, (i) BP 2, (i) BP 3, (iv) BP 4, (v) BP 5, and (vi) BP 6. The detachment profile is also overlaid in black for each BP category. (vii-viii) Detachment data from the simulation and fits for (vii) each BP category and (viii) the full population.

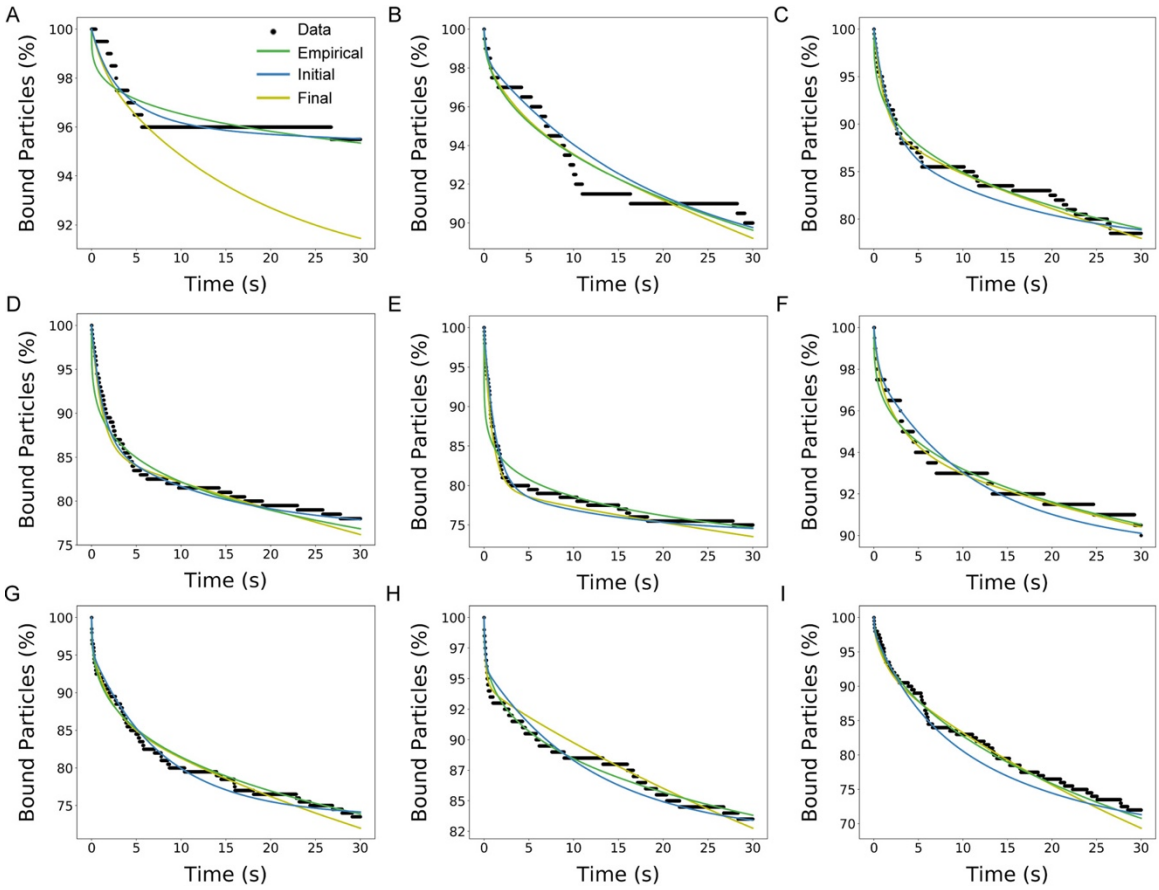


Figure S8. Final population heterogeneity model fitting results. Results are shown for all 9 cases including (A) base case, (B) low antibody density, (C) low ICAM-1 density, (D) ICAM-1 dimers, (E) clustered ICAM-1 dimers, (F) γ = 0.29 nm, (G) γ = 0.3 nm, (H) k_r^0 = 5x10^{-4} s^{-1}, and (I) k_r^0 = 10^{-3} s^{-1}. Utilizing the mean first passage time criterion improved long-term predictions of the BP model relative to the initial results obtained in which the second sub-component did not detach. Empirical fits are also included for comparison.

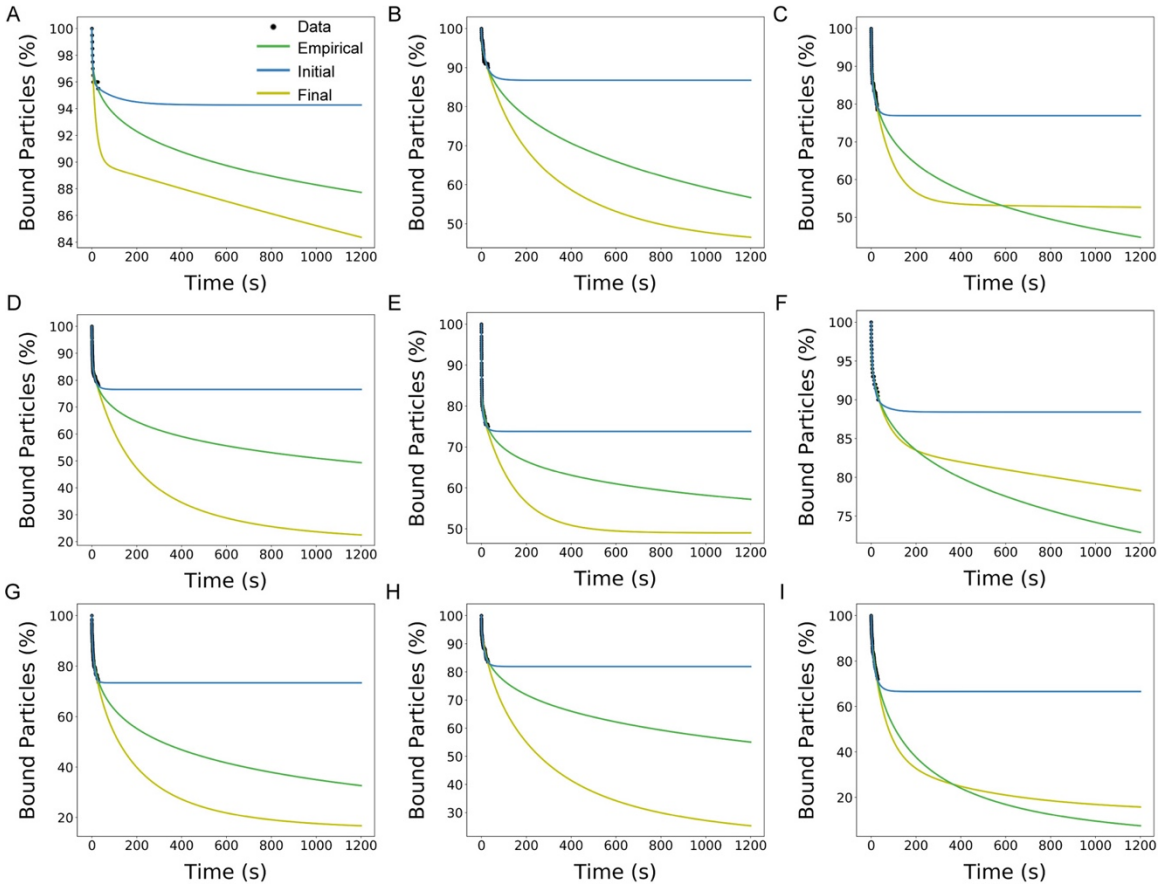


Figure S9. Final population heterogeneity model predictions. Extrapolations were made out to 20 min for all 9 cases including (A) base case, (B) low antibody density, (C) low ICAM-1 density, (D) ICAM-1 dimers, (E) clustered ICAM-1 dimers, (F) γ = 0.29 nm, (G) γ = 0.3 nm, (H) k_r^0 = 5x10^{-4} s^{-1}, and (I) k_r^0 = 10^{-3} s^{-1}. The initial population heterogeneity model predicted that no further detachment would occur beyond the 30 s simulation time. The final population heterogeneity model, using the mean first passage time criterion, enabled long-term predictions that were similar, but not exactly equal, to the empirical model.