Supporting Information

(10 pages)

Title: Network of Receptors Characterize B Cell Receptor Macro- and Micro- Clustering in a Monte Carlo Model

Authors: A. Srinivas Reddy¹, Sandeep Chilukuri^{1,5}, Subhadip Raychaudhuri^{1,2,3,4}[†]

¹Department of Biomedical Engineering, ²Biophysics Graduate Group, ³Graduate Group in Immunology, ⁴Garduate Group in Applied Mathematics, University of California-Davis, Davis,

⁵Department of Biotechnology, Indian Institute of Technology Madras, Chennai, India USA.

† Address correspondence to: raychaudhuri@ucdavis.edu

Figure S1: Snapshots of the receptor molecules at the regular time intervals (1 X 10^7 time steps) of the clustering simulations for N=100; L=30; T= 10^8 considering four neighboring nodes.

Figure S2a: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 400 for L=30; K=1; T= 10^8 considering four neighboring nodes.

Figure S2b: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 500 for L=30; K=2; T= 10^8 considering four neighboring nodes.

Figure S2c: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 500 for L=30; K=3; T= 10^8 considering four neighboring nodes.

Figure S3: Snapshots of the macro clusters formed due to biased diffusion toward the largest cluster receptors for various sets of receptor concentrations from 100 to 500 for L=30; K=4; $T=10^8$ considering four neighboring nodes.

Figure S4a: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 400 for L=30; K=1; T= 10^8 considering eight neighboring nodes.

Figure S4b: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 400 for L=30; K=2; T= 10^8 considering eight neighboring nodes.

Figure S4c: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 400 for L=30; K=3; T= 10^8 considering eight neighboring nodes.



1 X 10⁷







 $4 \ge 10^{7}$

 5×10^{7}





8 X 10⁷

 $9 \ge 10^{7}$

6 X 10⁷

10⁸

Figure S1: Snapshots of the receptor molecules at the regular time intervals (1 X 10⁷ time steps) of the clustering simulations for N=100; L=30; K=1; T= 10^8 considering four neighboring nodes.



N=400

Figure S2a: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 400 for L=30; K=1; T= 10^8 considering four neighboring nodes.



Figure S2b: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 500 for L=30; K=2; T= 10^8 considering four neighboring nodes.



Figure S2c: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 500 for L=30; K=3; T= 10^8 considering four neighboring nodes.



Figure S3: Snapshots of the macro clusters formed due to biased diffusion toward the largest cluster receptors for various sets of receptor concentrations from 100 to 500 for L=30; K=4; $T=10^8$ considering four neighboring nodes.



Figure S4a: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 400 for L=30; K=1; T= 10^8 considering eight neighboring nodes.



Figure S4b: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 400 for L=30; K=2; T= 10^8 considering eight neighboring nodes.



Figure S4c: Snapshots of micro-clustering for various sets of receptor concentrations from 100 to 400 for L=30; K=3; T= 10^8 considering eight neighboring nodes.