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Crowding and hydrodynamic interactions likely dominate in vivo macromolecular motion

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To begin to elucidate the principles of intermolecular dynamics in the crowded environment of cells, employing brownian dynamics (BD) simulations, we examined possible mechanism(s) responsible for the great reduction in diffusion constants of macromolecules in vivo from that at infinite dilution. In an Escherichia coli cytoplasm model comprised of 15 different macromolecule types at physiological concentrations, BD simulations of molecular-shaped and equivalent sphere representations were performed with a soft repulsive potential. At cellular concentrations, the calculated diffusion constant of GFP is much larger than experiment, with no significant shape dependence. Next, using the equivalent sphere system, hydrodynamic interactions (HI) were considered. Without adjustable parameters, the in vivo experimental GFP diffusion constant was reproduced. Finally, the effects of nonspecific attractive interactions were examined. The reduction in diffusivity is very sensitive to macromolecular radius with the motion of the largest macromolecules dramatically slowed down; this is not seen if HI dominate. In addition, long-lived clusters involving the largest macromolecules form if attractions dominate, whereas HI give rise to significant, size independent intermolecular dynamic correlations. These qualitative differences provide a testable means of differentiating the importance of HI vs. nonspecific attractive interactions on macromolecular motion in cells.