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The range of fluctuations of number of zinc ions depends on the ligand binding reaction rate constant and the initial concentration

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We present the dependency of the range of fluctuations on the parameters of a reversible chemical association reaction in an equilibrium state. We derived the infinite system of equations describing the central moments from a set of equations called Chemical Master Equation. Next, we performed a series of numerical simulations in order to find appropriate assumptions in our model. Finally, by placing these assumptions into the equations, we derived the explicit formulas on the first two central moments. The second central moment determines the range of fluctuations of one partner of the reaction, thus, we are able to investigate the impact of the probability factor on the behavior of the system. We compared the obtained results with numerical simulations. The essential result is the mathematical formula describing the dependency of the range of fluctuations of the number of interacting molecules on the reaction rate constants and the initial concentrations. The mathematical model, as well as the method of the approximation, could be expanded to much more complicated systems. The method was tested on several experimental data available in literature for interactions of Zn(II) ions with biomolecules, including the reaction of formation of a zinc finger complex, for which K_d = k_off/k_on = 50 pM. For this particular example, the volume, in which the virtual experiment was performed, was V = 0.5 pL, initial concentrations of reagents were: [Zn] _Free =50 pM, [ZnP] = 50 M, [P] = 50 M and, as a result, the range of fluctuations of zinc ions was estimated to be ca. 26%, translating into the fluctuation of the Kd value in the range of 59% 190%.