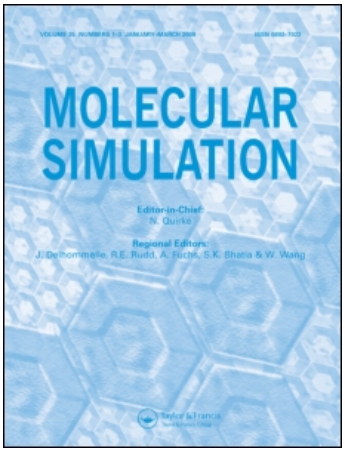

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Consequences of Sequential Ca^2 Occupancy for the Structure and Dynamics of $Calbindin_{D9K}$: Computational Simulations and Comparison to Experimental Determinations in Solution (*10*, 309, (1993))

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Clarification

CONSEQUENCES OF SEQUENTIAL CA^{2+} OCCUPANCY FOR THE STRUCTURE AND DYNAMICS OF $CALBINDIN_{D9K}$: COMPUTATIONAL SIMULATIONS AND COMPARISON TO EXPERIMENTAL DETERMINATIONS IN SOLUTION (*10*, 309, (1993))

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Due to the slow convergence of the atomic rms fluctuations with the length of time for which they are calculated, the entropic contribution to the cooperativity of Ca^{2+} binding to $calbindin_{D9k}$, discussed on pp. 329–330, has to be evaluated for a longer interval than used for the rms values given in Table 5. The value of $\triangle\triangle G$ obtained from the rms fluctuations given in Table 5 is about 0.5 Kcal/mole. For the longer interval of 179 ps the average rms values calculated for CAB_0, CAB_1 and CAB_2 (see original article for definitions) are 4.5 Å, 0.9 Å and 0.8 Å, respectively. The value of $\triangle\triangle G$ calculated from these rms fluctuations according to the equations in the the original article is about 1.0 Kcal/mole. It is noted that these trends do not affect the interpretation or conclusions regarding the significance of the configurational entropy for the cooperativity of binding in $calbindin_{D9k}$.