Differential utilization of binding loop flexibility in T cell receptor ligand selection and cross-reactivity

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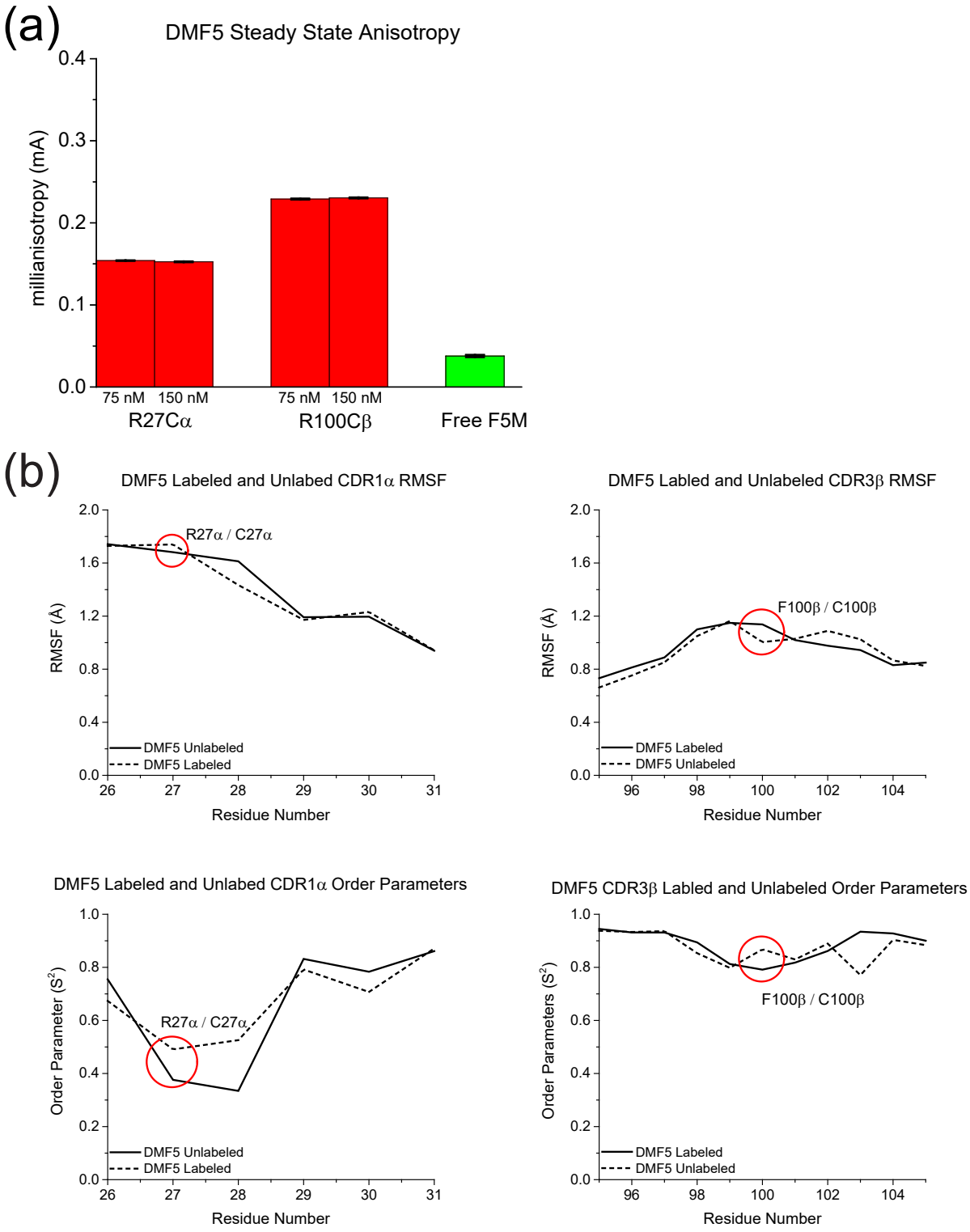

Fig. S1. Fluorescence anisotropy measurements validate the simulation methodology for DMF5. **A)** Steady state anisotropy measurments for DMF5 fluorescently labeled at position 27 in CDR1α or position 100 in CDR3β. Consistent with the simulation results, position 27α is more mobile on the nanosecond timescale (lower anisotropy) than position 100β. Measurements for two protein concentrations are shown. Error bars reflect the standard deviation of 50 measurments. Green shows the anisotropy of free fluorescein. **B)** Incorporation of a cysteine mutation and fluorescent label does not significantly perturb the simulation results for position 27α and neighboring residues or position 100β and neighboring residues. The two panels show α carbon RMSF values and the bottom two show Cα-Cβ order parameters, with solid lines the results from the simulations of unlabeled protein and the dashed lines the simulations of labeled protein. Values for positions 27α or 100β are circled.