

Electronic Supplementary information.

Evaluation of Water Displacement Energetics in Protein Binding Sites with Grid Cell Theory

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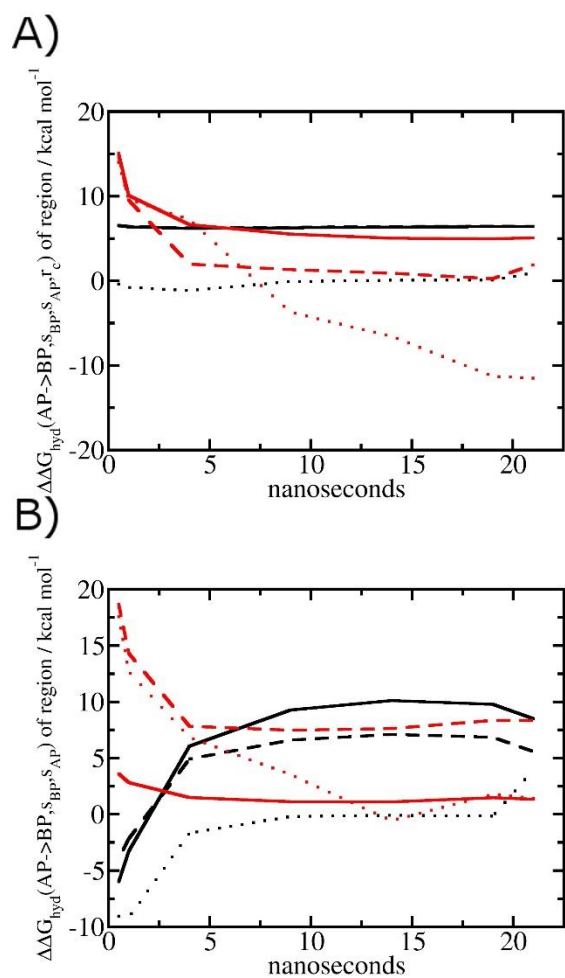


Fig S1. Convergence of the differences in holo hydration energies of congeneric pairs. (A) shows the convergence of three medoid volumes of p38 MAP kinase. In black is the convergence at fullr while red with bbr conditions. The solid line is when $X_{\text{medoid}} = 1 \text{ \AA}$, dashed line is at $X_{\text{medoid}} = 4 \text{ \AA}$, and the dotted line is at $X_{\text{medoid}} = 8 \text{ \AA}$. (B) shows the convergence of three medoid volumes of EGFR kinase with the same symbols used.