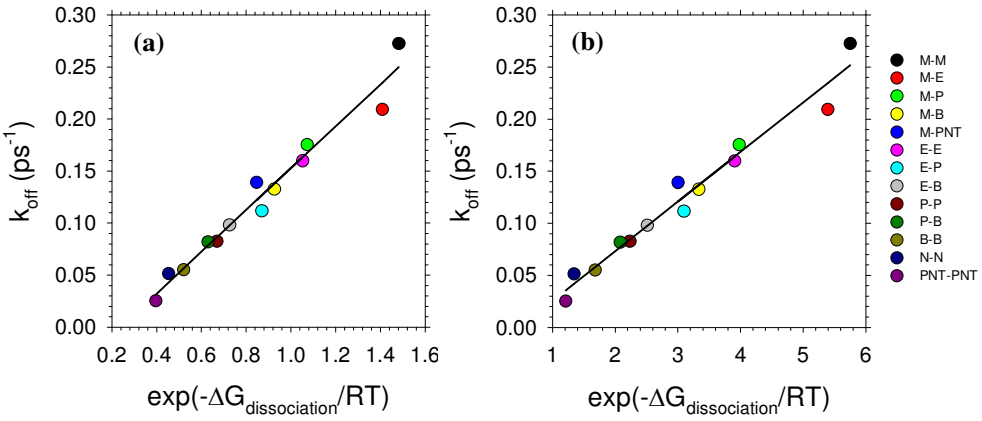

Figure S1. The dissociation kinetics of the 13 alkane-pairs. Correlations between the computed dissociation rate constant (k_{off}) and the free energy change for dissociation ($\Delta G_{dissociation}$) computed using the center-of-mass reaction coordinate. In panel (a), the free energy changes are calculated from association constants, 'K_{eq}', which have been defined and calculated according to the procedure outlined in Reference 15 of the main text. In panel (b), the free energy changes are calculated from association constants, 'K_2', which have been defined and calculated according to the procedures outlined in References 26 and 27 of the main text. r^2 values for the linear fits are both 0.966.