

Supplemental information for

Evaluating the FEP+ protocol for predicting binding affinity of congeneric ligands towards various soluble proteins

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Figure S1: Representative image of overlap of work distributions for transformation with “good overlap”

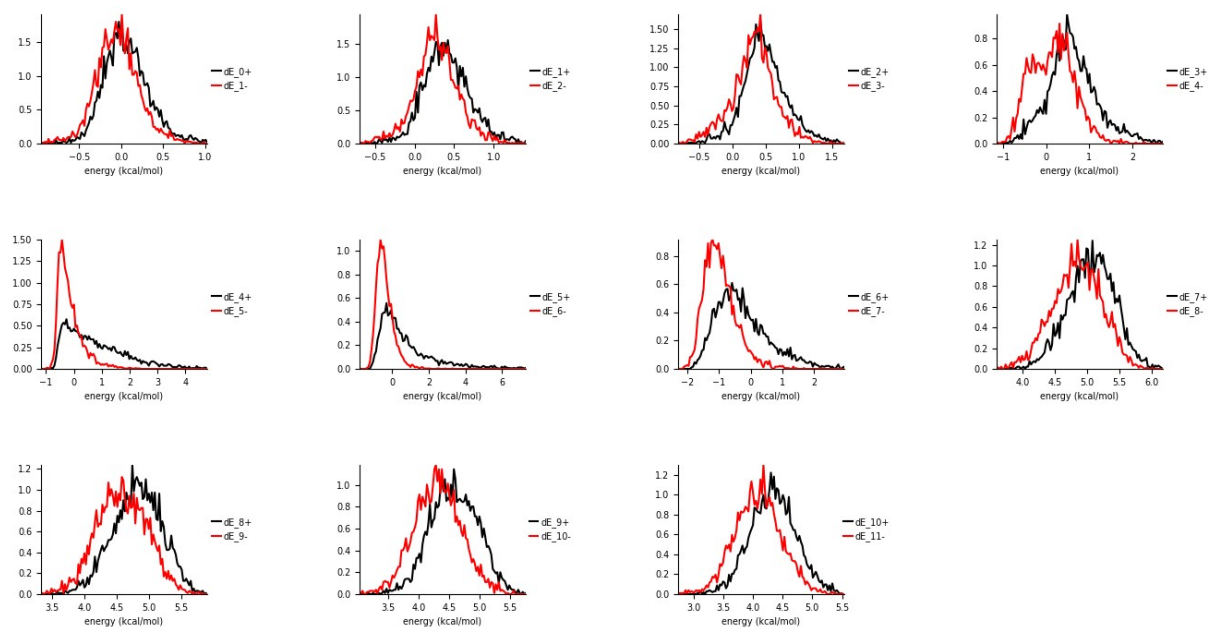


Figure S2: Representative image of overlap of work distributions for transformation with “poor overlap”

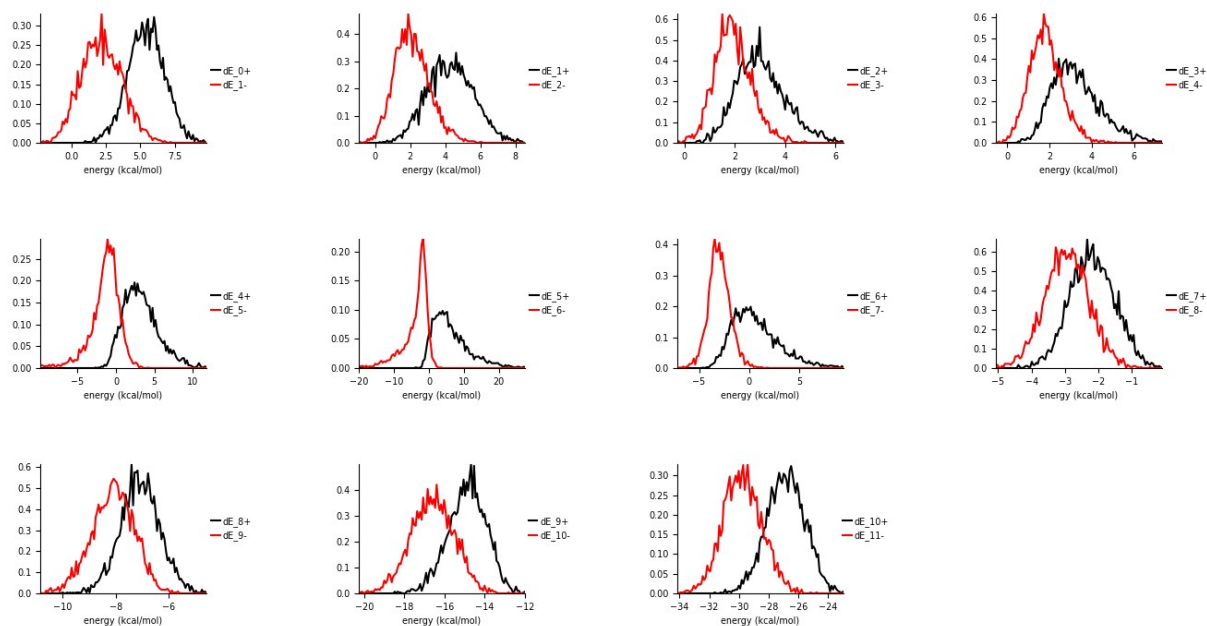


Figure S3: Overall free energy difference (dG) as a function of time of a transformation showing convergence

