



Fig 1. Potential of mean force along the correlated conformational coordinate λ . Fill lines: result of the harmonic umbrella sampling of [8]. Filled circles show points used for matching; open circles, the result of the adaptive procedure using the non-linear n -step optimized matching; - - - , the result of the new harmonic umbrella sampling calculation replacing run 2; -.-.-, the result of run 1 shifted to match the new run 2.