Supplementary information, Table S4

Table S4 The windows and the corresponding simulation steps in FEP calculations

λ	[0,0.0001]	[0.0001,0.001]	[0.001,0.005]	[0.005,0.01]	[0.01,0.0125]	[0.0125,0.015]
Steps($\times 10^4$)	4	4	4	4	3	3
λ	[0.015,0.0175]	[0.0175,0.02]	[0.02,0.025]	[0.025,0.03]	[0.03,0.035]	[0.035,0.04]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.04,0.045]	[0.045,0.05]	[0.05,0.055]	[0.055,0.06]	[0.06,0.0625]	[0.0625,0.065]
Steps($\times 10^4$)	3	3	3	3	4	4
λ	[0.065,0.0675]	[0.0675,0.07]	[0.07,0.075]	[0.075,0.08]	[0.08,0.085]	[0.085,0.09]
Steps($\times 10^4$)	4	4	3	3	3	3
λ	[0.09,0.095]	[0.095,0.1]	[0.1,0.105]	[0.105,0.11]	[0.11,0.115]	[0.115,0.12]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.12,0.125]	[0.125,0.13]	[0.13,0.135]	[0.135,0.14]	[0.14,0.145]	[0.145,0.15]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.15,0.155]	[0.155,0.16]	[0.16,0.165]	[0.165,0.17]	[0.17,0.175]	[0.175,0.18]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.18,0.185]	[0.185,0.19]	[0.19,0.195]	[0.195,0.2]	[0.2,0.205]	[0.205,0.21]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.21,0.215]	[0.215,0.22]	[0.22,0.225]	[0.225,0.23]	[0.23,0.235]	[0.235,0.24]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.24,0.245]	[0.245,0.25]	[0.25,0.255]	[0.255,0.26]	[0.26,0.265]	[0.265,0.27]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.27,0.275]	[0.275,0.28]	[0.28,0.285]	[0.285,0.29]	[0.29,0.295]	[0.295,0.3]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.3,0.305]	[0.305,0.31]	[0.31,0.315]	[0.315,0.32]	[0.32,0.33]	[0.33,0.34]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.34,0.35]	[0.35,0.36]	[0.36,0.37]	[0.37,0.38]	[0.38,0.39]	[0.39,0.4]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.4,0.405]	[0.405,0.41]	[0.41,0.415]	[0.415,0.42]	[0.42,0.425]	[0.425,0.43]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.43,0.435]	[0.435,0.44]	[0.44,0.445]	[0.445,0.45]	[0.45,0.455]	[0.445,0.46]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.46,0.465]	[0.465,0.47]	[0.47,0.475]	[0.475,0.48]	[0.48,0.485]	[0.485,0.49]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.49,0.495]	[0.495,0.5]	[0.5,0.505]	[0.505,0.51]	[0.51,0.515]	[0.515,0.52]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.52,0.525]	[0.525,0.53]	[0.53,0.535]	[0.535,0.54]	[0.54,0.545]	[0.545,0.55]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.55,0.555]	[0.555,0.56]	[0.56,0.565]	[0.565,0.57]	[0.57,0.575]	[0.575,0.58]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.58,0.585]	[0.585,0.59]	[0.59,0.595]	[0.595,0.6]	[0.6,0.605]	[0.605,0.61]
Steps($\times 10^4$)	3	3	3	3	3	3

λ	[0.61,0.615]	[0.615,0.62]	[0.62,0.625]	[0.625,0.63]	[0.63,0.635]	[0.635,0.64]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.64,0.645]	[0.645,0.65]	[0.65,0.655]	[0.655,0.66]	[0.66,0.665]	[0.665,0.67]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.67,0.675]	[0.675,0.68]	[0.68,0.685]	[0.685,0.69]	[0.69,0.695]	[0.695,0.7]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.7,0.705]	[0.705,0.71]	[0.71,0.715]	[0.715,0.72]	[0.72,0.725]	[0.725,0.73]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.73,0.735]	[0.735,0.74]	[0.74,0.745]	[0.745,0.75]	[0.75,0.755]	[0.755,0.76]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.76,0.765]	[0.765,0.77]	[0.77,0.775]	[0.775,0.78]	[0.78,0.785]	[0.785,0.79]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.79,0.795]	[0.795,0.8]	[0.8,0.805]	[0.805,0.81]	[0.81,0.815]	[0.815,0.82]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.82,0.825]	[0.825,0.83]	[0.83,0.835]	[0.835,0.84]	[0.84,0.845]	[0.845,0.85]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.85,0.855]	[0.855,0.86]	[0.86,0.865]	[0.865,0.87]	[0.87,0.875]	[0.875,0.88]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.88,0.885]	[0.885,0.89]	[0.89,0.895]	[0.895,0.9]	[0.9,0.905]	[0.905,0.91]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.91,0.915]	[0.915,0.92]	[0.92,0.925]	[0.925,0.93]	[0.93,0.935]	[0.935,0.94]
Steps($\times 10^4$)	3	3	3	3	3	3
λ	[0.94,0.945]	[0.945,0.95]	[0.95,0.955]	[0.955,0.96]	[0.96,0.965]	[0.965,0.97]
Steps($\times 10^4$)	3	3	3	3	4	4
λ	[0.97,0.975]	[0.975,0.98]	[0.98,0.985]	[0.985,0.99]	[0.99,0.995]	[0.995,0.999]
Steps($\times 10^4$)	4	4	4	4	4	4
λ	[0.999,0.9999]	[0.9999,1]				
Steps($\times 10^4$)	4	4				

The 4000 steps in pre-equilibration are included here in each window. In free energy

estimation, the pre-equilibration steps are excluded from the calculation.