

Supplementary Information

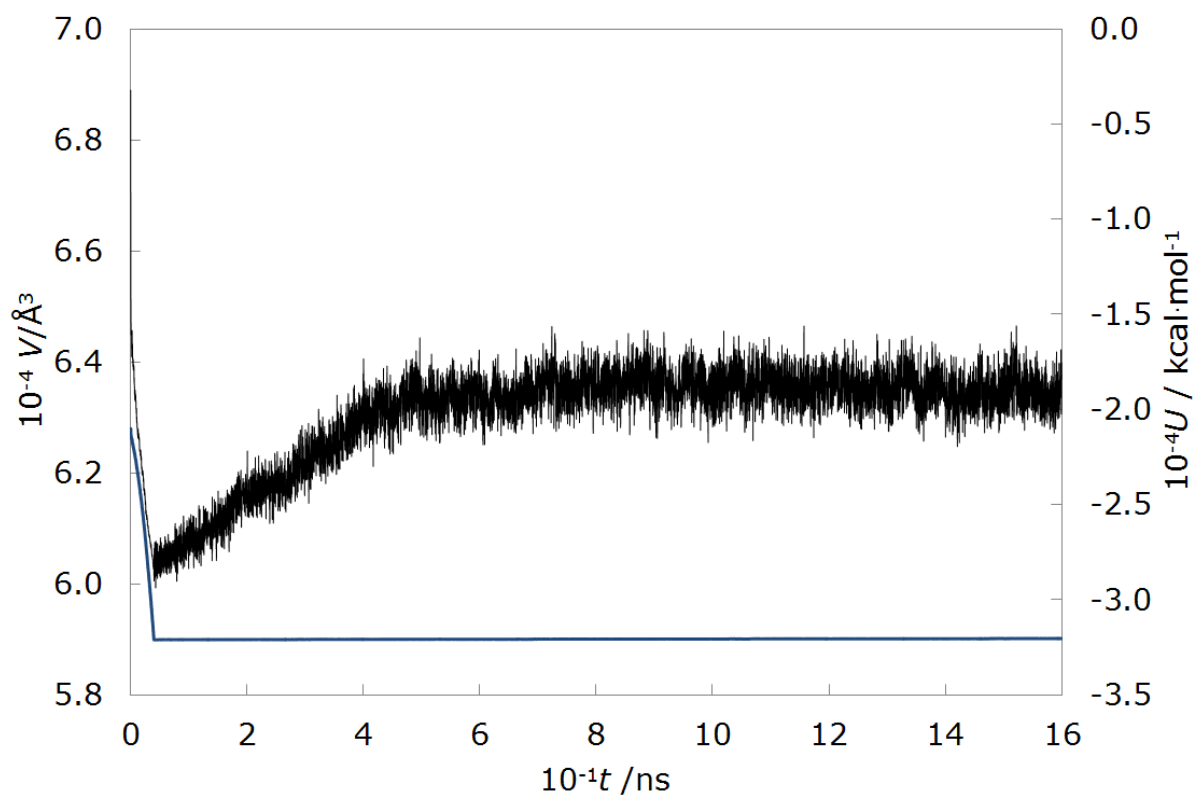


Figure. S1. Total energy (U) (blue line) and total volume (V) (black line) as a function of time (t) in NPT simulation at 298.15 K.