

Supplementary Materials

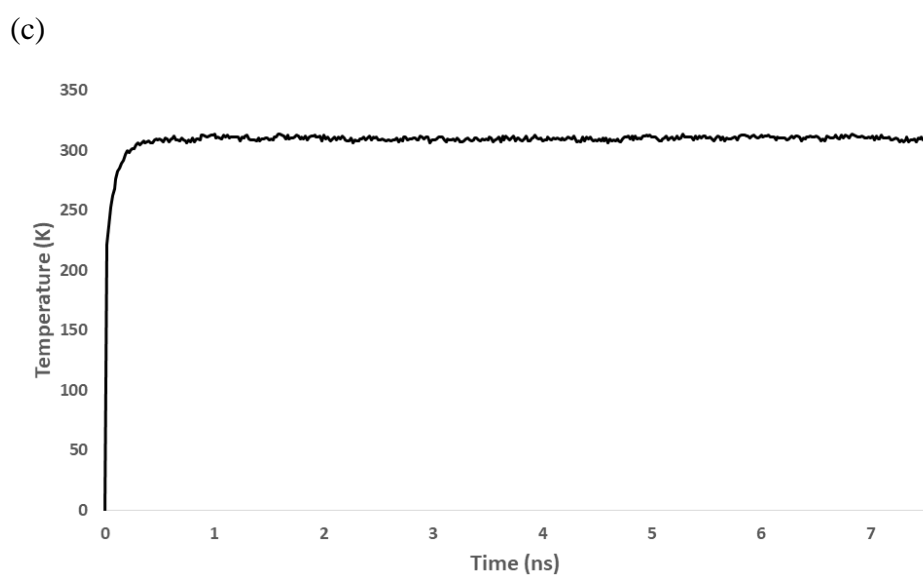
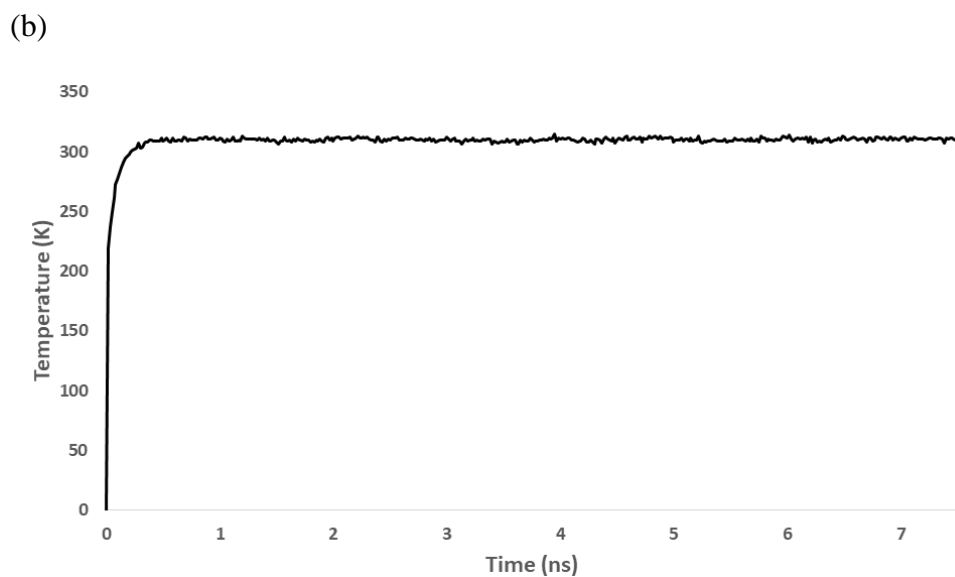
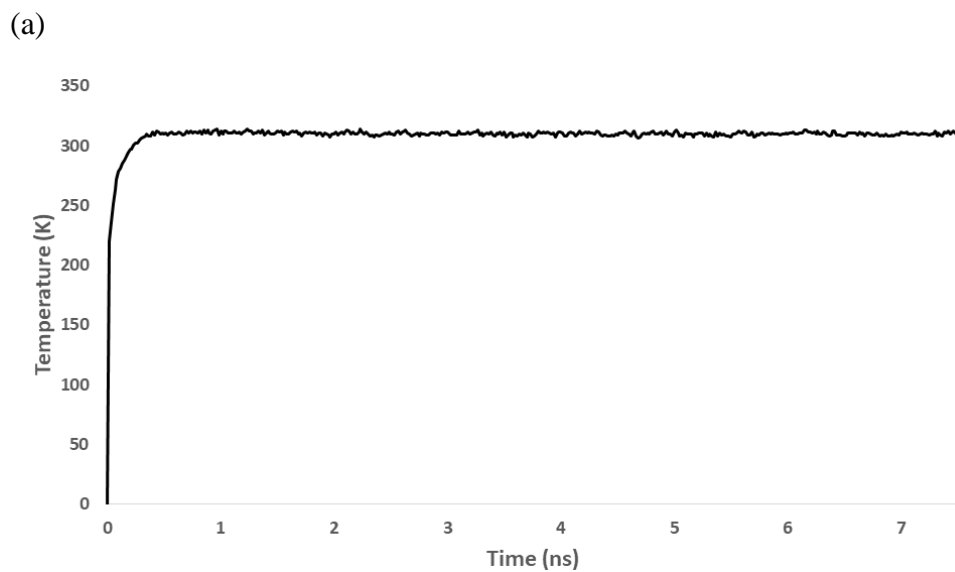


Figure S1: MD simulation: Temperature profile during 7 ns for the (a) **TAK-285**, (b) **1a**, (c) **1d**.

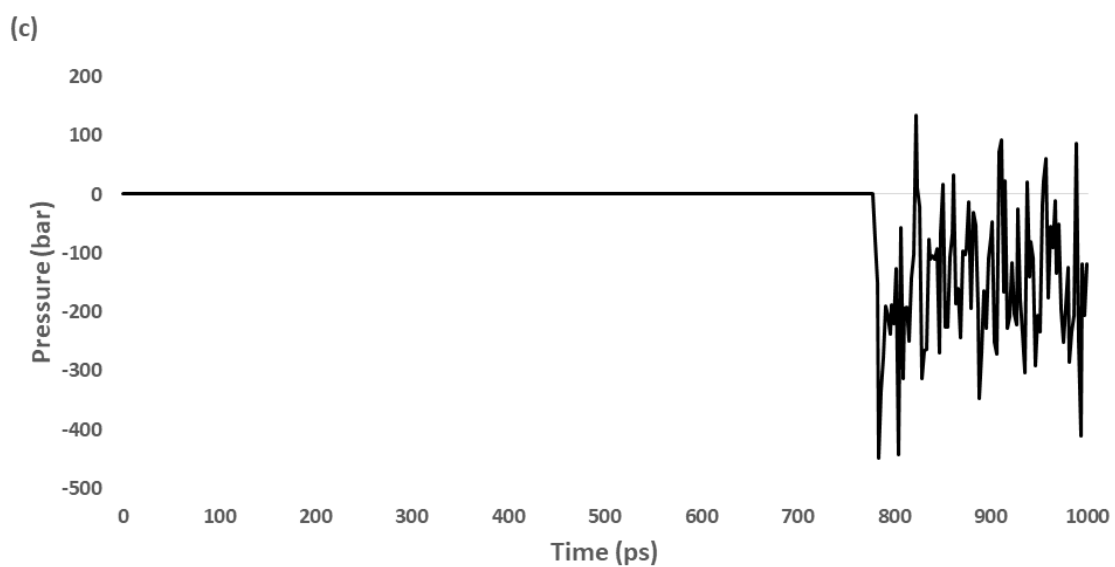
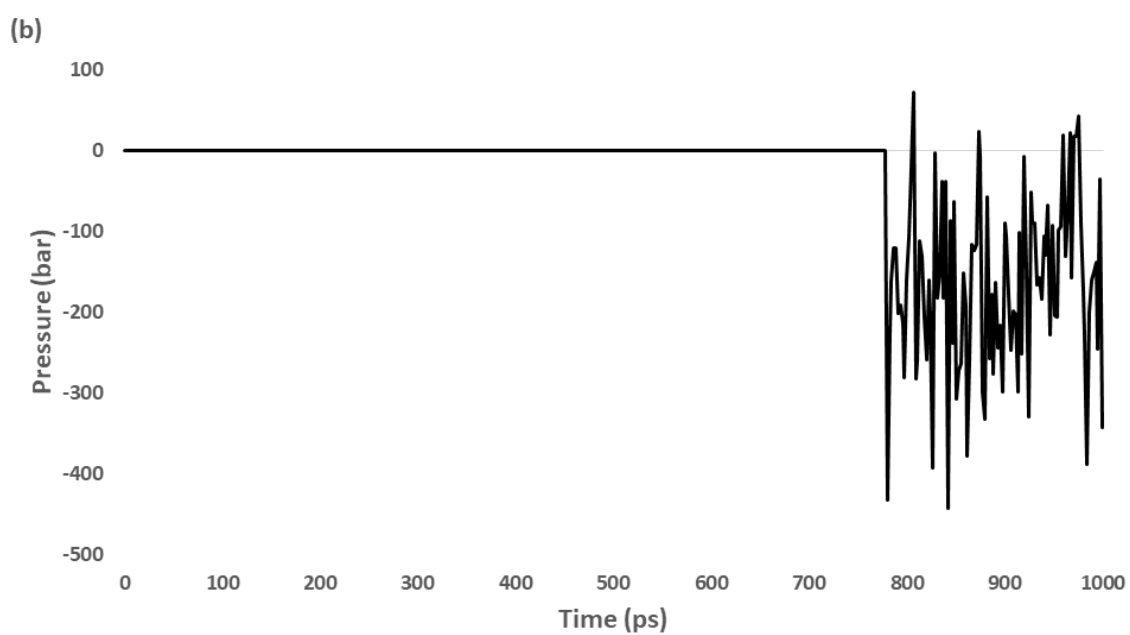
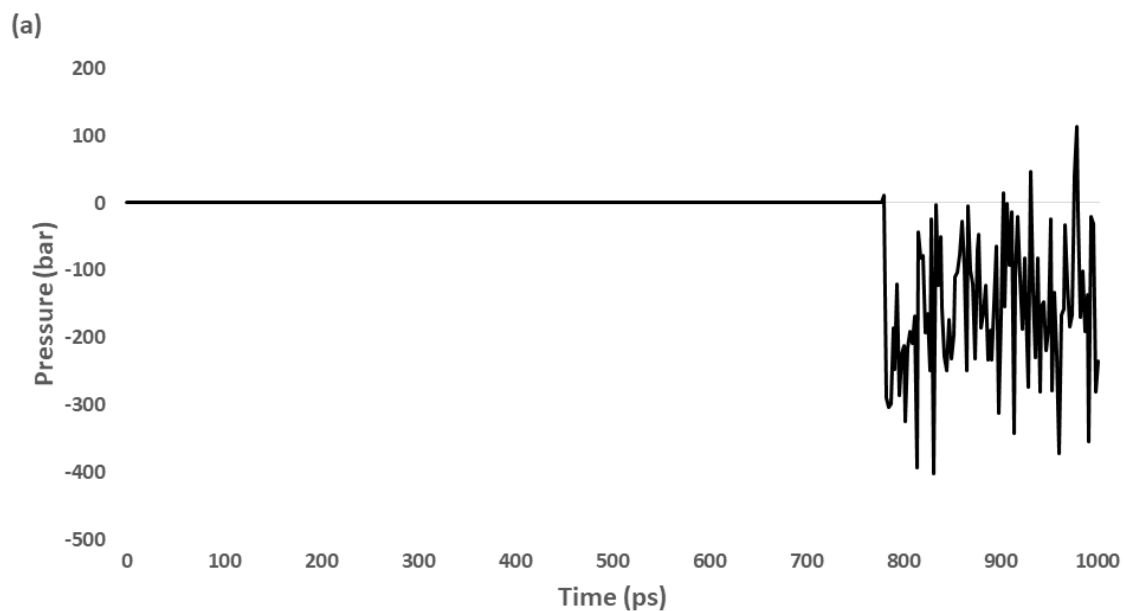


Figure S2: MD simulation: pressure profile during equilibration for the (a) TAK-285, (b) 1a, (c) 1d.

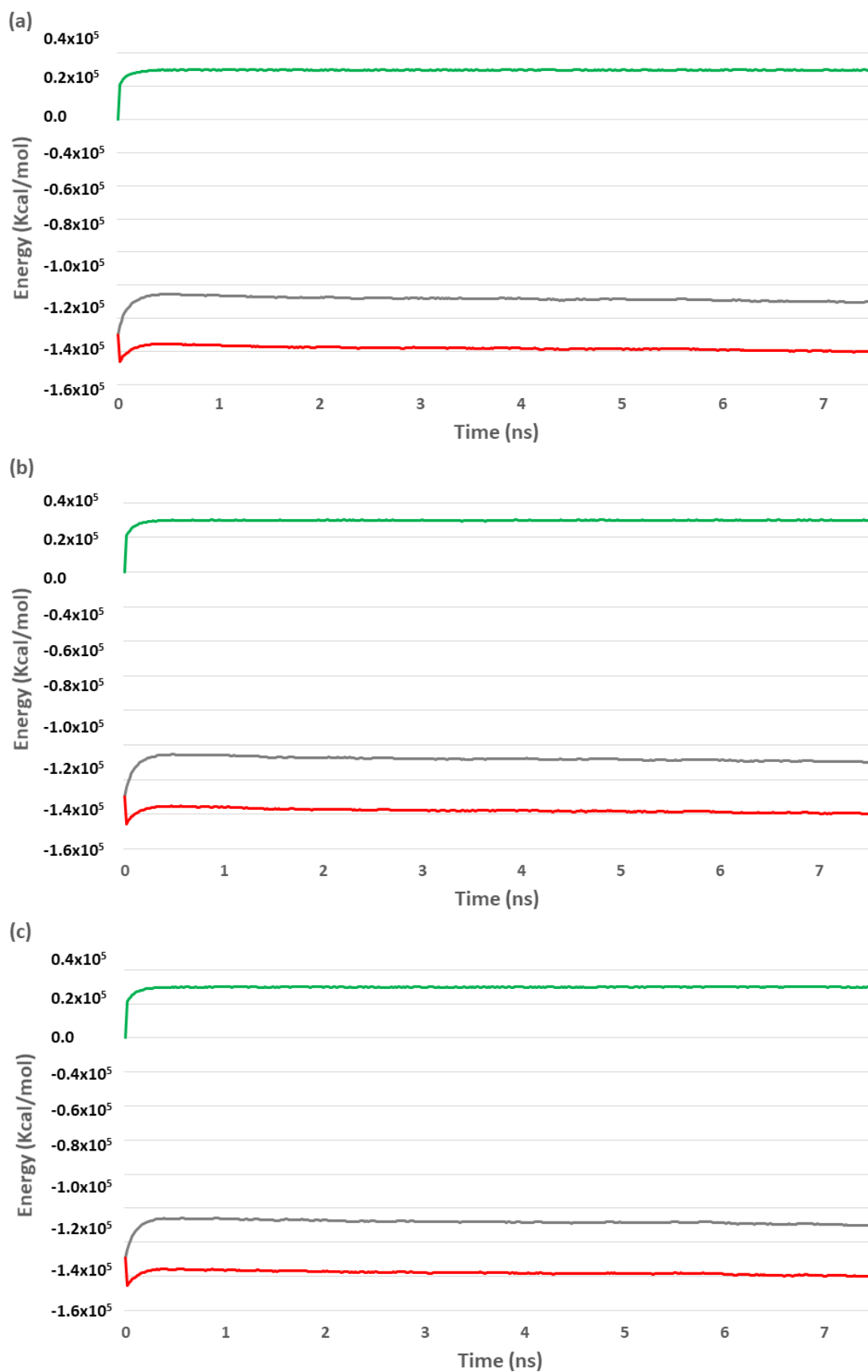


Figure S3. MD simulation: Energy profile for the (a) TAK-285, (b) 1a, (c) 1d. total energy (grey color), potential energy (red color), kinetic energy (green color)