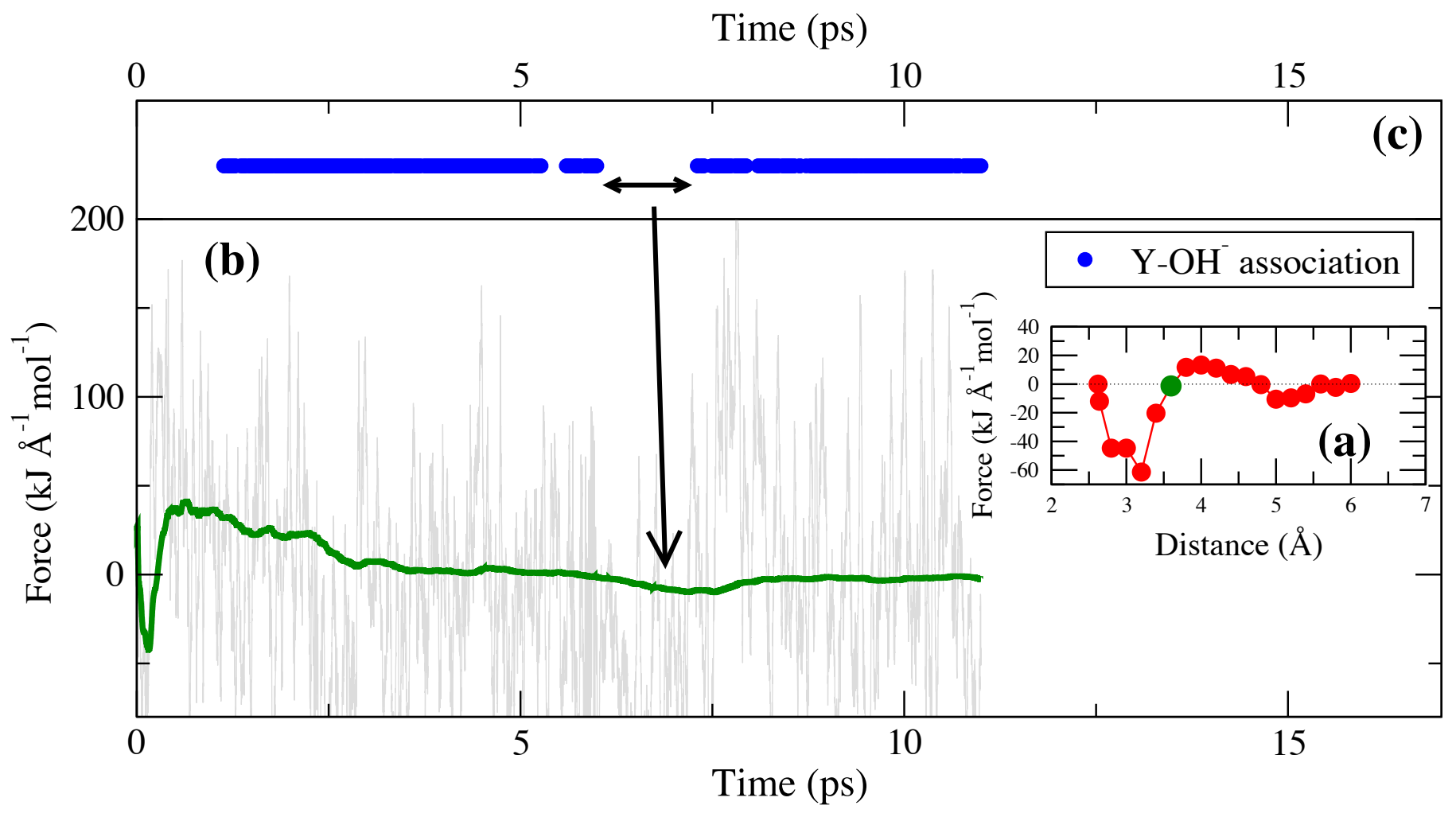
Time (ps)
0
5
10
15
(c)
200
(b)
Y-OH⁻ association
100
0
Force (kJ Å⁻¹mol⁻¹)
40
20
0
-20
-40
-60
(a)
2
3
4
5
6
7
Distance (Å)
Time (ps)