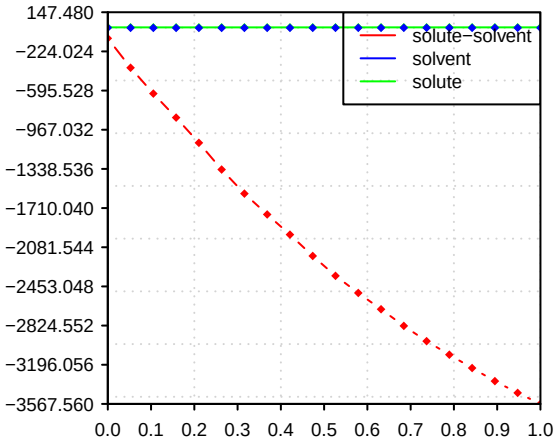
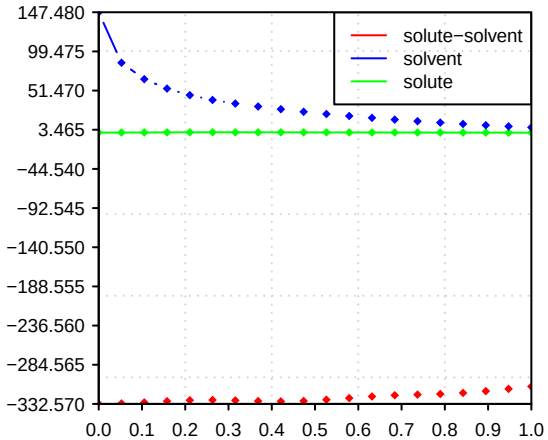
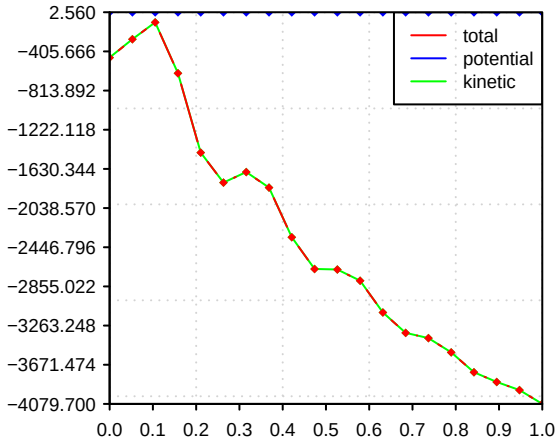
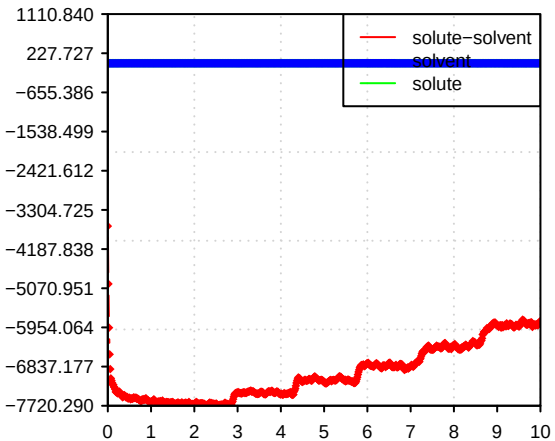
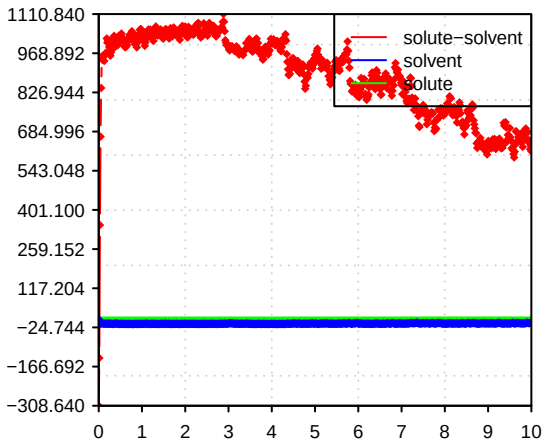
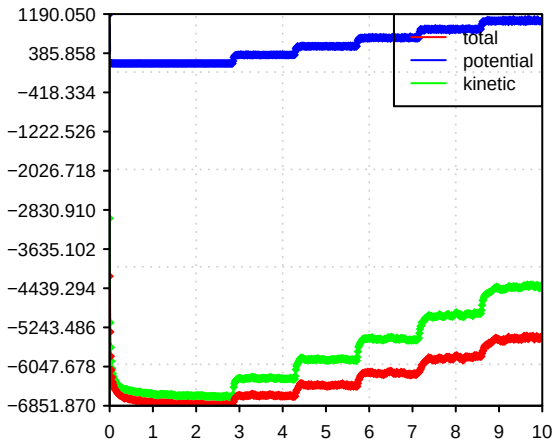

147.480
−224.024
−595.528
−967.032
−1338.536
−1710.040
−2081.544
−2453.048
−2824.552
−3196.056
−3567.560
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
solute−solvent
solvent
solute

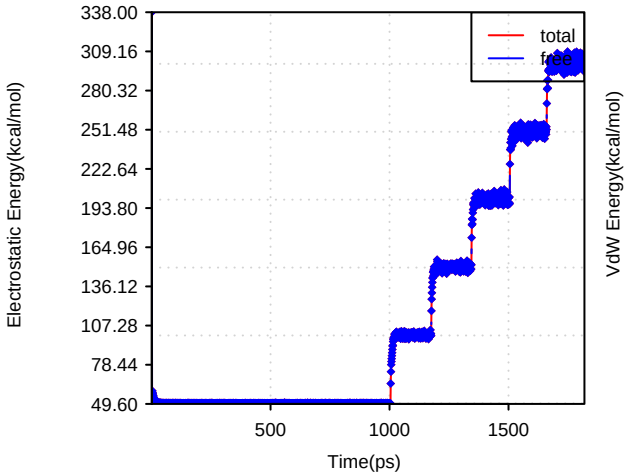

147.480
99.475
51.470
3.465
−44.540
−92.545
−140.550
−188.555
−236.560
−284.565
−332.570
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
solute−solvent
solvent
solute

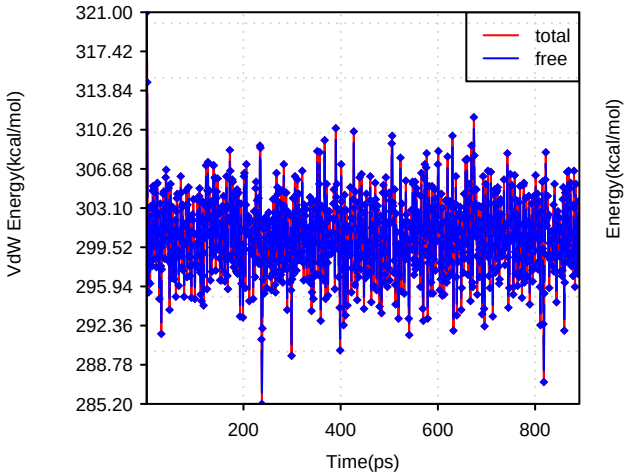

2.560
−405.666
−813.892
−1222.118
−1630.344
−2038.570
−2446.796
−2855.022
−3263.248
−3671.474
−4079.700
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
total
potential
kinetic

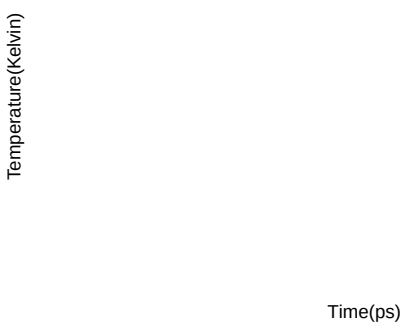

1110.840
227.727
−655.386
−1538.499
−2421.612
−3304.725
−4187.838
−5070.951
−5954.064
−6837.177
−7720.290
0 1 2 3 4 5 6 7 8 9 10
solute−solvent
solvent
solute


1110.840
968.892
826.944
684.996
543.048
401.100
259.152
117.204
−24.744
−166.692
−308.640
0 1 2 3 4 5 6 7 8 9 10
solute−solvent
solvent
solute


1190.050
385.858
−418.334
−1222.526
−2026.718
−2830.910
−3635.102
−4439.294
−5243.486
−6047.678
−6851.870
0 1 2 3 4 5 6 7 8 9 10
total
potential
kinetic


Electrostatic Energy(kcal/mol)
338.00
309.16
280.32
251.48
222.64
193.80
164.96
136.12
107.28
78.44
49.60
500
1000
1500
Time(ps)
total
free


VdW Energy(kcal/mol)
321.00
317.42
313.84
310.26
306.68
303.10
299.52
295.94
292.36
288.78
285.20
200
400
600
800
Time(ps)
total
free


Temperature(Kelvin)
Time(ps)

Energy(kcal/mol)
Time(ps)