Suplementary Material of 'P-NIPAM in water-acetone mixtures: Experiments and simulations"

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I. SIMULATION BUILDING FILES

In this section we provide the necessary files to build the systems we are studying through the Gromacs simulation package. The coordinate files for a 30-mer of pNIPAM and acetone are given in *Protein Data Bank*(.pdb) format. Note that **pdb** is just a file format and not necessarily a protein molecule obtained from databases. The *.pdb* files are passed through the Gromac's tool *gmx pdb2gmx* from where the corresponding structure file (.gro) and topology (.top) are generated. The *gmx pdb2gmx* tool searches into the selected forcefield rtp-files for the residues named at the *.pdb* files. Thus, it is necessary to add these residues to the rtp-formated file, i. e. names given in the rtp-file must match names given at the pdb-file, which contain the definitions of atom types, bounds, and a few missing dihedral angles (proper and improper) from the forcefield. The residue definitions for the OPLS-AA forcefield are also given further below in this document.

oligomer.pdb

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TITLE Initial configuration
REMARK THIS IS A SIMULATION BOX
CRYST1 50.000 50.000 180.000 90.00 90.00 90.00 P 1 1
MODEL 1 ATOM 1 CAL ipaB 1 -5.799 -1.324 93.057 1.00 0.00
ATOM 2 CAK ipaB 1 -7.017 -1.150 93.947 1.00 0.00
ATOM 3 CAM ipaB 1 -7.791 0.102 93.531 1.00 0.00
ATOM 4 NAJ ipaB 1 -7.899 -2.330 93.837 1.00 0.00
ATOM 5 HAW ipaB 1 -8.819 -2.256 94.218 1.00 0.00
ATOM 6 CAH ipaB 1 -7.503 -3.468 93.242 1.00 0.00
ATOM 7 OAI ipaB 1 -6.359 -3.645 92.806 1.00 0.00
ATOM 8 CAD ipaB 1 -8.575 -4.571 93.234 1.00 0.00
ATOM 9 CAE ipaB 1 -8.653 -5.413 94.524 1.00 0.00
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ATOM 12 CAM ipaM 2 -7.791 0.102 96.115 1.00 0.00
ATOM 13 NAJ ipaM 2 -7.899 -2.330 96.421 1.00 0.00
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ATOM 14 HAW ipaM 2 -8.819 -2.256 96.802 1.00 0.00
ATOM 15 CAH ipaM 2 -7.503 -3.468 95.826 1.00 0.00
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ATOM 69 CAH ipaM 8 -7.503 -3.468 111.331 1.00 0.00
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ATOM 223 OAI ipaM 25 -6.359 -3.645 154.828 1.00 0.00
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ATOM 268 OAI ipaT 30 -6.359 -3.645 167.749 1.00 0.00
ATOM 269 CAD ipaT 30 -8.575 -4.571 168.178 1.00 0.00
ATOM 270 CAE ipaT 30 -8.653 -5.413 169.468 1.00 0.00
TER
ENDMDL
```

acetone.pdb

```
TITLE Acetone molecule
ATOM 1 HC11 Acet 1 1.275 -1.463 -0.789 1.00 0.00
ATOM 2 CT1 Acet 1 1.289 -0.699 -0.001 1.00 0.00
ATOM 3 HC12 Acet 1 2.146 -0.036 -0.141 1.00 0.00
ATOM 4 HC13 Acet 1 1.394 -1.231 0.953 1.00 0.00
ATOM 5 C Acet 1 -0.000 0.097 -0.000 1.00 0.00
ATOM 6 O Acet 1 0.000 1.320 0.000 1.00 0.00
ATOM 7 CT2 Acet 1 -1.290 -0.699 0.001 1.00 0.00
ATOM 8 HC21 Acet 1 -1.276 -1.461 0.790 1.00 0.00
ATOM 9 HC22 Acet 1 -2.146 -0.035 0.139 1.00 0.00
ATOM 10 HC23 Acet 1 -1.394 -1.232 -0.953 1.00 0.00
END
```

After the insertion of water and acetone one must procede with an energy minimization. These following

lines must be append in the aminoacids.rtp file of the OPLS-AA forcefield.

```
; Additions
;PNIPAm - this is an internal residue
[ ipaM ]
[ atoms ]
CAL opls_135 -0.180 1
HAL1 opls_140 0.060 1
HAL2 opls_140 0.060 1
HAL3 opls_140 0.060 1
CAM opls_135 -0.180 2
HAM1 opls_140 0.060 2
HAM2 opls_140 0.060 2
HAM3 opls_140 0.060 2
CAK opls_224B 0.140 3
HAK1 opls_140 0.060 3
NAJ opls_238 -0.500 3
HAW opls_241 0.300 3
CAH opls_235 0.500 4
OAI opls_236 -0.500 4
CAD opls_137 -0.060 5
HAD1 opls_140 0.060 5
CAE opls_136 -0.120 6
HAE1 opls_140 0.060 6
HAE2 opls_140 0.060 6

[ bonds ]
CAL HAL1
CAL HAL2
CAL HAL3
CAL CAK
CAK HAK1
CAK NAJ
CAK CAM
CAM HAM1
CAM HAM2
CAM HAM3
NAJ HAW
NAJ CAH
CAH OAI
CAH CAD
CAD HAD1
CAD -CAE
CAD CAE
CAE HAE1
CAE HAE2
CAE +CAD

[ dihedrals ]
HAL1 CAL CAK CAM 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAL2 CAL CAK CAM 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAL3 CAL CAK CAM 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAM1 CAM CAK CAL 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAM2 CAM CAK CAL 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAM3 CAM CAK CAL 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
```

```
[ impropers ]
OAI CAH CAD NAJ improper_Z_N_X_Y
HAW NAJ CAK CAH improper_O_C_X_Y

; Terminal PNIPAm residue ("beginning" of chain)
[ ipaB ]
[ atoms ]
CAL opls_135 -0.180 1
HAL1 opls_140 0.060 1
HAL2 opls_140 0.060 1
HAL3 opls_140 0.060 1
CAM opls_135 -0.180 2
HAM1 opls_140 0.060 2
HAM2 opls_140 0.060 2
HAM3 opls_140 0.060 2
CAK opls_224B 0.140 3
HAK1 opls_140 0.060 3
NAJ opls_238 -0.500 3
HAW opls_241 0.300 3
CAH opls_235 0.500 4
OAI opls_236 -0.500 4
CAD opls_136 -0.120 5
HAD1 opls_140 0.060 5
HAD2 opls_140 0.060 5
CAE opls_136 -0.120 6
HAE1 opls_140 0.060 6
HAE2 opls_140 0.060 6

[ bonds ]
CAL HAL1
CAL HAL2
CAL HAL3
CAL CAK
CAK HAK1
CAK NAJ
CAK CAM
CAM HAM1
CAM HAM2
CAM HAM3
NAJ HAW
NAJ CAH
CAH OAI
CAH CAD
CAD HAD1
CAD HAD2
CAD CAE
CAE HAE1
CAE HAE2
CAE +CAD

[ dihedrals ]
HAL1 CAL CAK CAM 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAL2 CAL CAK CAM 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAL3 CAL CAK CAM 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAM1 CAM CAK CAL 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAM2 CAM CAK CAL 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
```

```
HAM3 CAM CAK CAL 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom

[ impropers ]
OAI CAH CAD NAJ improper_Z_N_X_Y
HAW NAJ CAK CAH improper_O_C_X_Y

; Terminal PNIPAm residue (“end” of chain)
[ ipaT ]
[ atoms ]
CAL opls_135 -0.180 1
HAL1 opls_140 0.060 1
HAL2 opls_140 0.060 1
HAL3 opls_140 0.060 1
CAM opls_135 -0.180 2
HAM1 opls_140 0.060 2
HAM2 opls_140 0.060 2
HAM3 opls_140 0.060 2
CAK opls_224B 0.140 3
HAK1 opls_140 0.060 3
NAJ opls_238 -0.500 3
HAW opls_241 0.300 3
CAH opls_235 0.500 4
OAI opls_236 -0.500 4
CAD opls_137 -0.060 5
HAD1 opls_140 0.060 5
CAE opls_135 -0.180 6
HAE1 opls_140 0.060 6
HAE2 opls_140 0.060 6
HAE3 opls_140 0.060 6

[ bonds ]
CAL HAL1
CAL HAL2
CAL HAL3
CAL CAK
CAK HAK1
CAK NAJ
CAK CAM
CAM HAM1
CAM HAM2
CAM HAM3
NAJ HAW
NAJ CAH
CAH OAI
CAH CAD
CAD HAD1
CAD -CAE
CAD CAE
CAE HAE1
CAE HAE2
CAE HAE3

[ dihedrals ]
HAL1 CAL CAK CAM 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAL2 CAL CAK CAM 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAL3 CAL CAK CAM 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
```

```
HAM1 CAM CAK CAL 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAM2 CAM CAK CAL 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom
HAM3 CAM CAK CAL 0.6276 1.8828 0 -2.51 0 0; hydrocarbon all-atom

[ impropers ]
OAI CAH CAD NAJ improper_Z_N_X_Y
HAW NAJ CAK CAH improper_O_C_X_Y

;Acetone addition
[ Acet ]
[ atoms ]
O opls_253 -0.42 1
C opls_252 0.42 1
CT1 opls_256 -0.18 2
HC11 opls_140 0.06 2
HC12 opls_140 0.06 2
HC13 opls_140 0.06 2
CT2 opls_256 -0.18 3
HC21 opls_140 0.06 3
HC22 opls_140 0.06 3
HC23 opls_140 0.06 3

[ bonds ]
O C
C CT1
C CT2
CT1 HC11
CT1 HC12
CT1 HC13
CT2 HC21
CT2 HC22
CT2 HC23
```

The lines to be appended in the aminoacids.hdb (hydrogen database) read:

```
ipaM 5
3 4 HAL CAL CAK CAM
3 4 HAM CAM CAK CAL
1 5 HAK1 CAK CAL CAM NAJ
1 5 HAD1 CAD CAH CAE -CAE
2 6 HAE CAE CAD +CAD
ipaB 5
3 4 HAL CAL CAK CAM
3 4 HAM CAM CAK CAL
1 5 HAK1 CAK CAL CAM NAJ
2 6 HAD CAD CAH CAE
2 6 HAE CAE CAD +CAD
ipaT 5
3 4 HAL CAL CAK CAM
3 4 HAM CAM CAK CAL
1 5 HAK1 CAK CAL CAM NAJ
1 5 HAD1 CAD CAH CAE -CAE
3 4 HAE CAE CAD -CAE
```

Note that making use of the hydrogen database is unnecessary for the acetone molecule since the appended lines for

residue type [*Acet*] already contain all hydrogen atoms.

II. RADIUS OF GYRATION

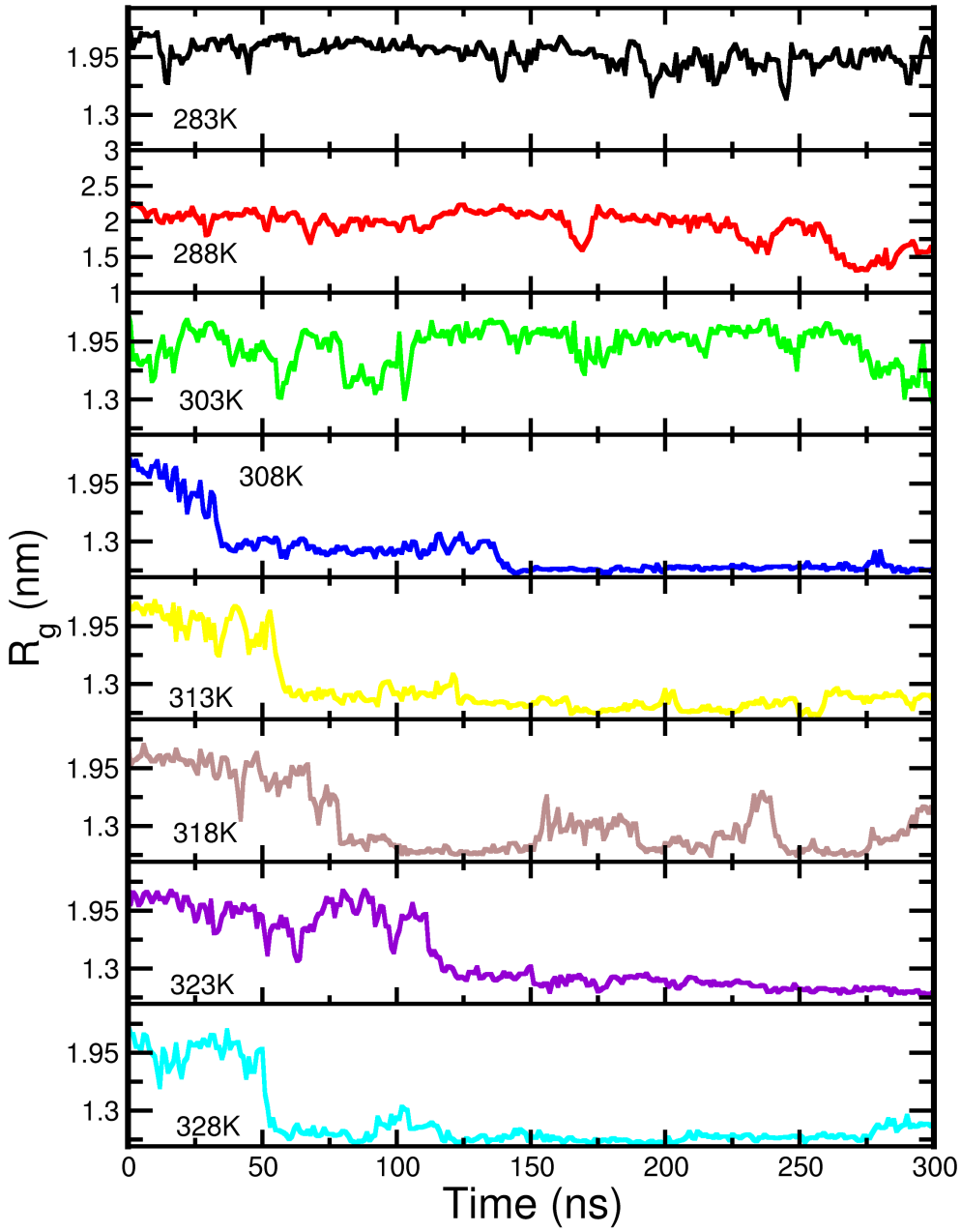

FIG. 1: Radius of gyration of a 30-mer in pure water as function of time for different temperatures

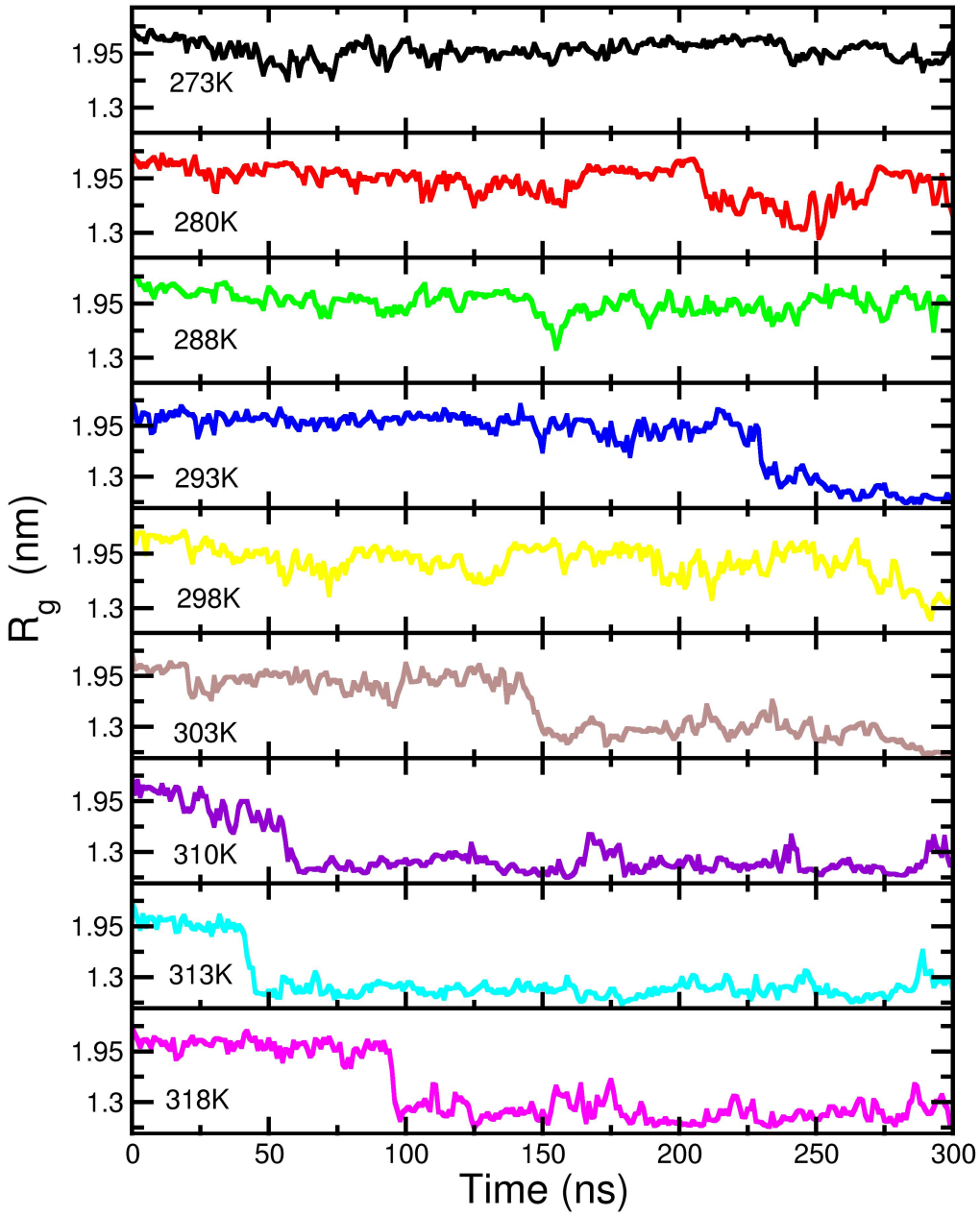

FIG. 2: Radius of gyration of a 30-mer in a water-acetone mixture with X_{Acet}=0.05 as function of time for different temperatures

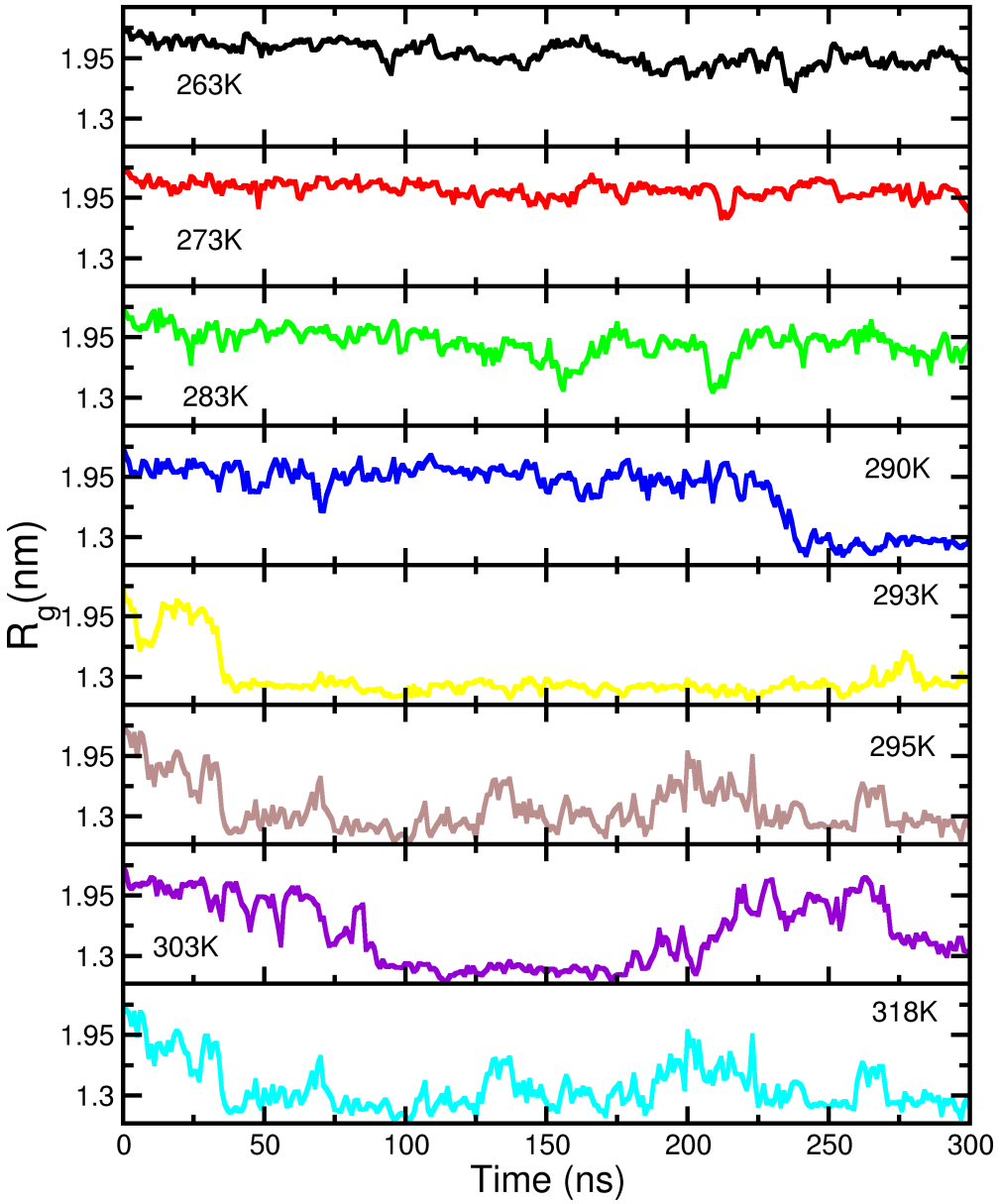

FIG. 3: Radius of gyration of a 30-mer in a water-acetone mixture with X_{Acet}=0.08 as function of time for different temperatures

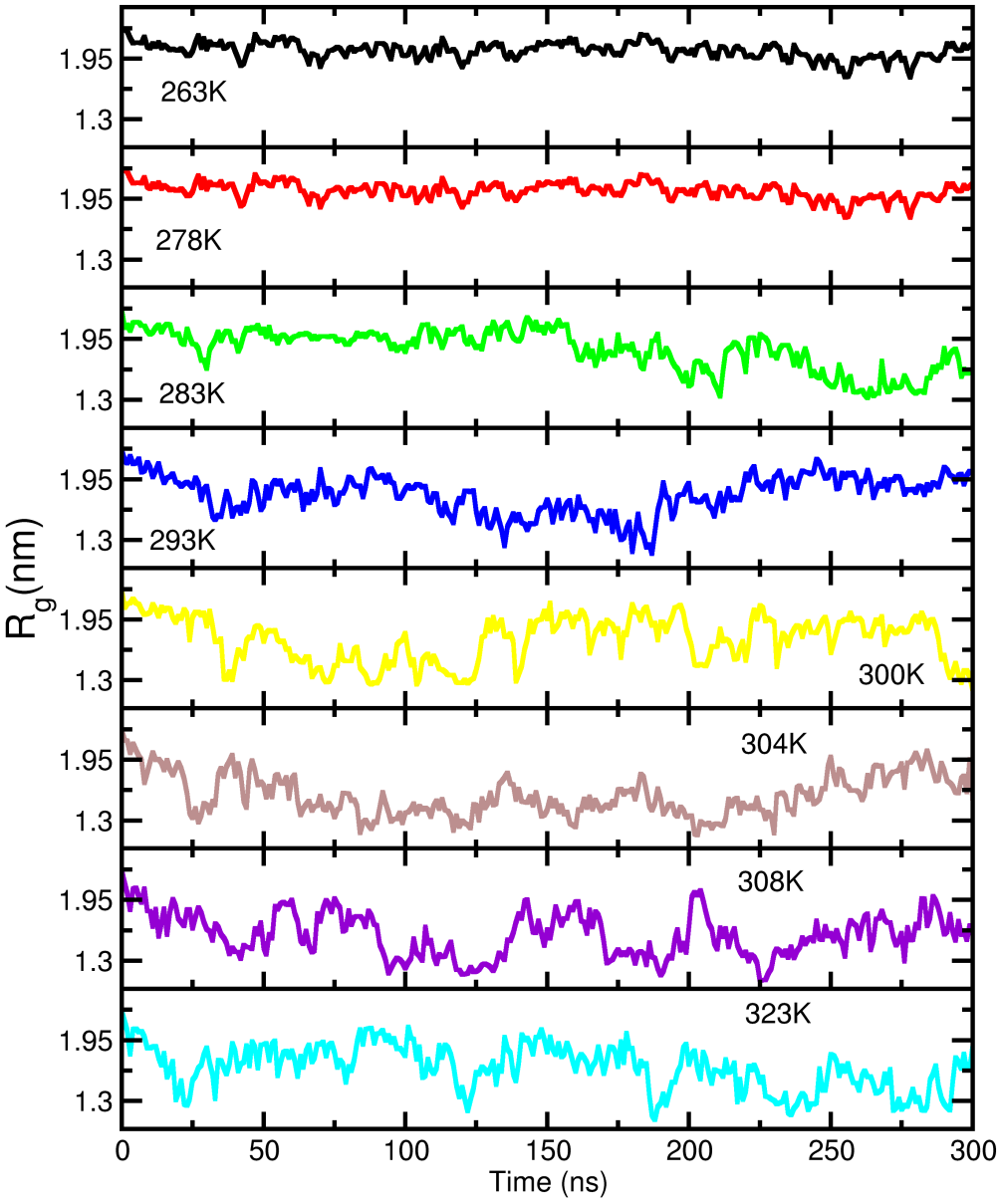

FIG. 4: Radius of gyration of a 30-mer in a water-acetone mixture with X_{Acet}=0.15 as function of time for different temperatures