APPENDIX A
(Supplementary material)
The following is a specimen topology file for the units of PNA. CYP represents the
PNA topology for the CYT base associated with the PNA backbone. We have used
the automatic assignment of the angles and the dihedrals in CHARMM package. The
initial coordinates of the non-hydrogen atoms were obtained by mapping the
respective atoms of the corresponding DNA molecules.

RESI  CYP     0.00
GROUP
ATOM  C1'  C     0.33
ATOM  O1'  O    -0.25
GROUP
ATOM  C2'  CT2    -0.35
ATOM  H2'  HB     0.18
ATOM  H2'' HB    0.18
GROUP
ATOM  N2'  NH3    -0.09
GROUP
ATOM  C5'  CT2    -0.33
ATOM  H5'  HB     0.17
ATOM  H5'' HB    0.17
GROUP
ATOM  C6'  CT2    -0.06
ATOM  H6'  HB     0.10
ATOM  H6'' HB    0.10
GROUP
ATOM  N1'  NH1    -0.37
ATOM  H1'  H      0.24
GROUP
ATOM  C3'  C      0.25
ATOM  O3'  O    -0.27
GROUP
ATOM  C4'  CT2    -0.34
ATOM  H4'  HB     0.17
ATOM  H4'' HB    0.17
!BASE ATOMS START HERE
GROUP
ATOM  N1  NN2    -0.16
ATOM  C6  CN3     0.11
ATOM  H6  HN3     0.05
GROUP
ATOM  C2  CN1     0.53
ATOM  O2  ON1C   -0.48
ATOM  N3  NN3    -0.67
ATOM  C4  CN2     0.62
GROUP
ATOM N4 NN1 -0.58
ATOM H41 HN1  0.31
ATOM H42 HN1  0.27
GROUP
ATOM C5 CN3 -0.10
ATOM H5 HN3  0.10

BOND +N1' C1' C1' O1' C1' C2' C2' H2' C2' H2'' C2' N2'
BOND N2' C5' C5' H5' C5' H5'' C6' C5' C6' H6' C6' H6''
BOND C6' N1' N1' H1' !N1' -C1'
BOND N2' C3' C3' O3' C3' C4' C4' H4' C4' H4''
BOND C4' N1 N1 C2 N1 C6 C2 O2
BOND C2 N3 N3 C4 C4 N4 N4 H41 N4 H42
BOND C4 C5 C5 C6 C5 H5 C6 H6

IMPH O2 N1 N3 C2 N4 N3 C5 C4
IMPH H5 C4 C6 C5 H6 C5 N1 C6
IMPH H42 C4 H41 N4
!impropers for PNA backbone.
IMPH C6' H1' -C1' N1'
IMPH N1' -O1' -C2' -C1'
IMPH N2' O3' C4' C3'
IMPH C2' O1' +N1' C1'
IMPH C1' +H1' +C6' +N1'
IMPH C4' C2 C6 N1 !PNA-BASE linkage

DONO H42 N4
DONO H41 N4
DONO H1' N1'
ACCE O2 C2
ACCE N3
ACCE O1' C1'
ACCE O3' C3'