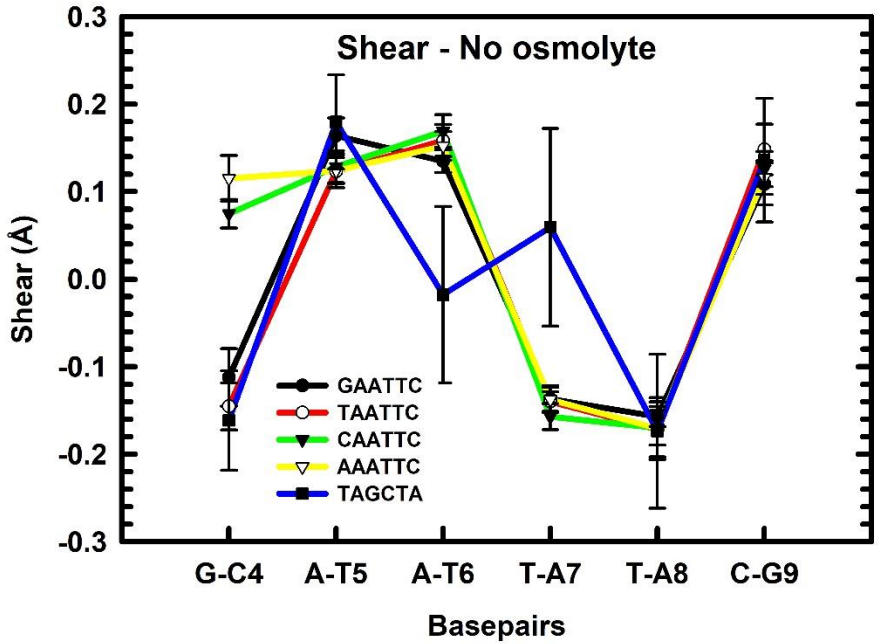
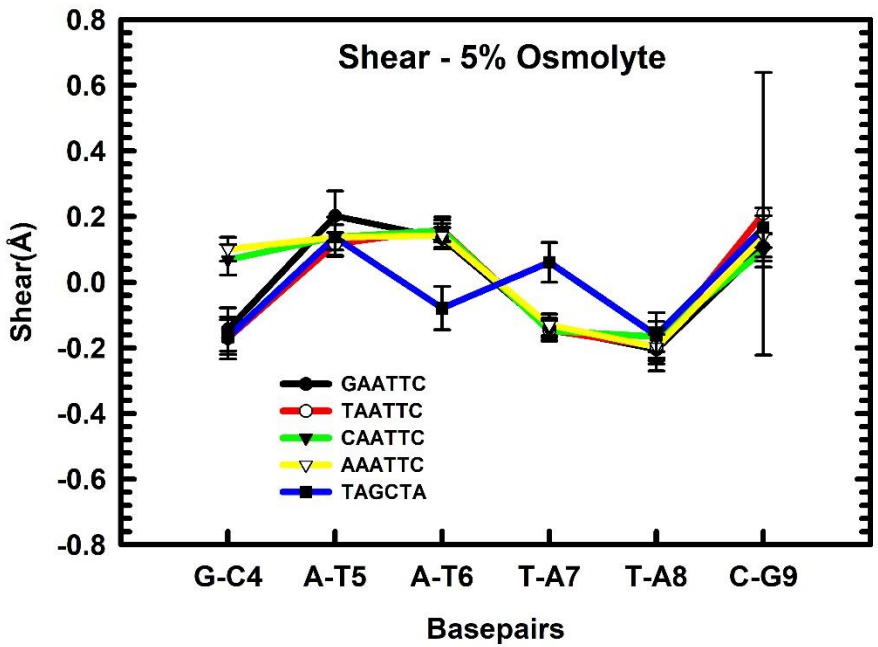
Average plot for 12 DNA conformational parameters and Groove widths

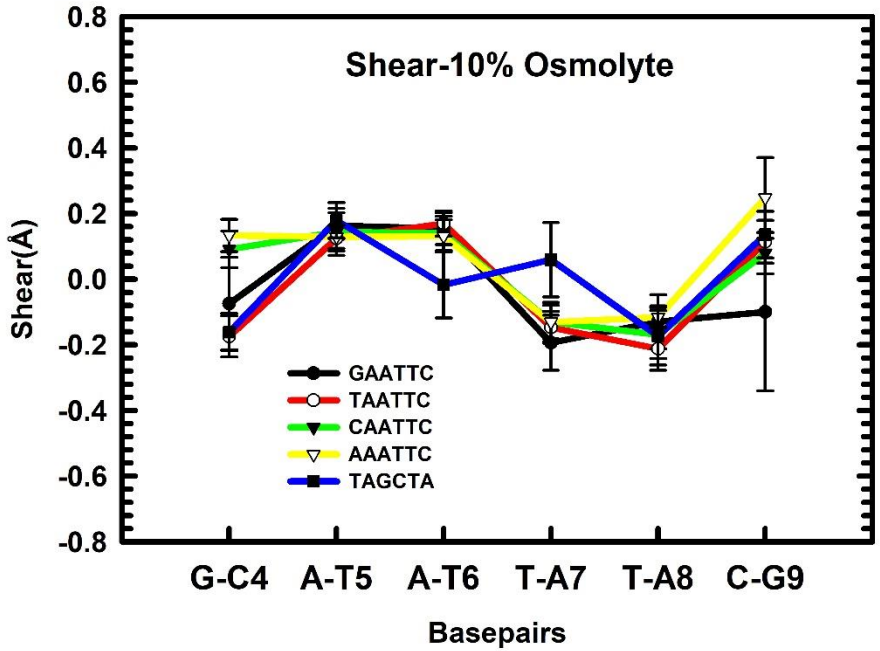
Basepair parameters (Shear, Stretch, Stagger, Buckle, Propeller and Opening)

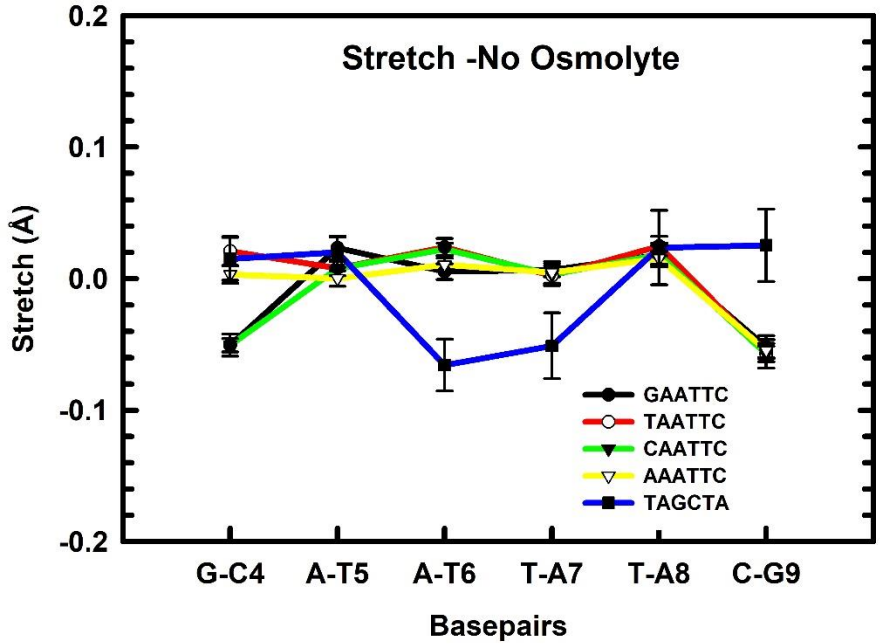
Basepair step parameters (Shift, Slide, Rise, Roll, Tilt and Twist)

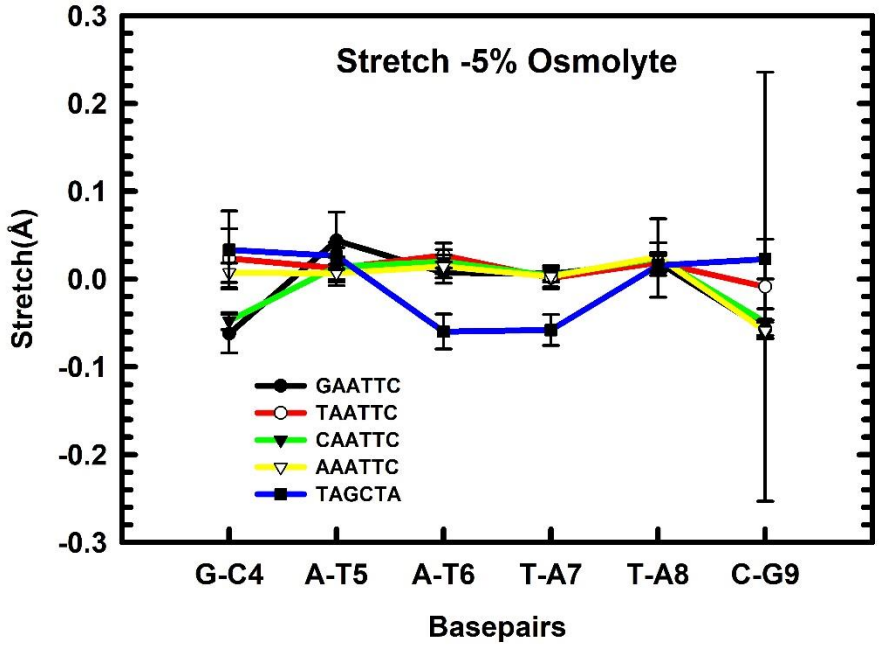
Groove widths (Major groove and Minor groove widths)

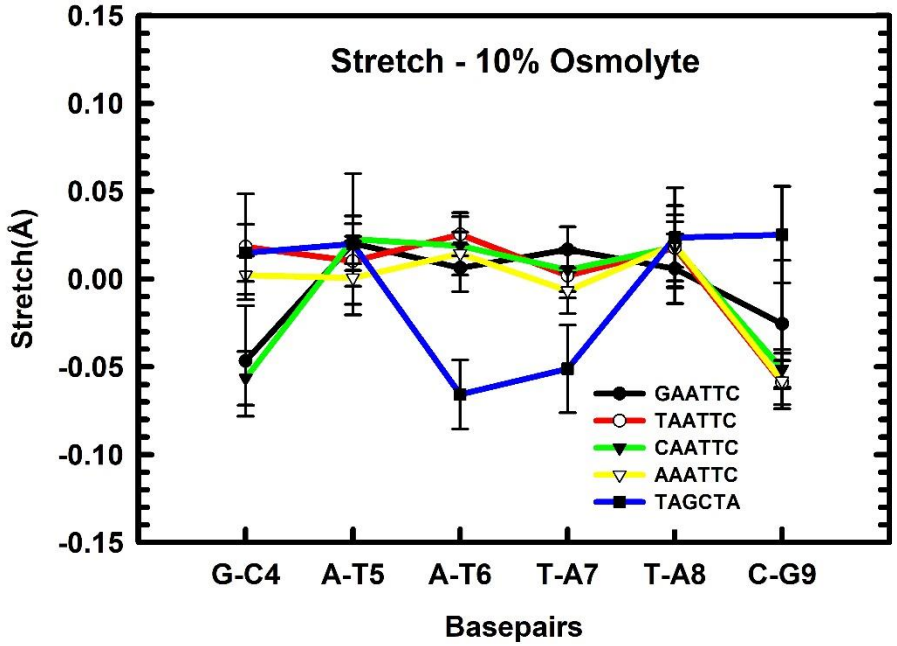

Shear - No osmolyte
Shear (Å)
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

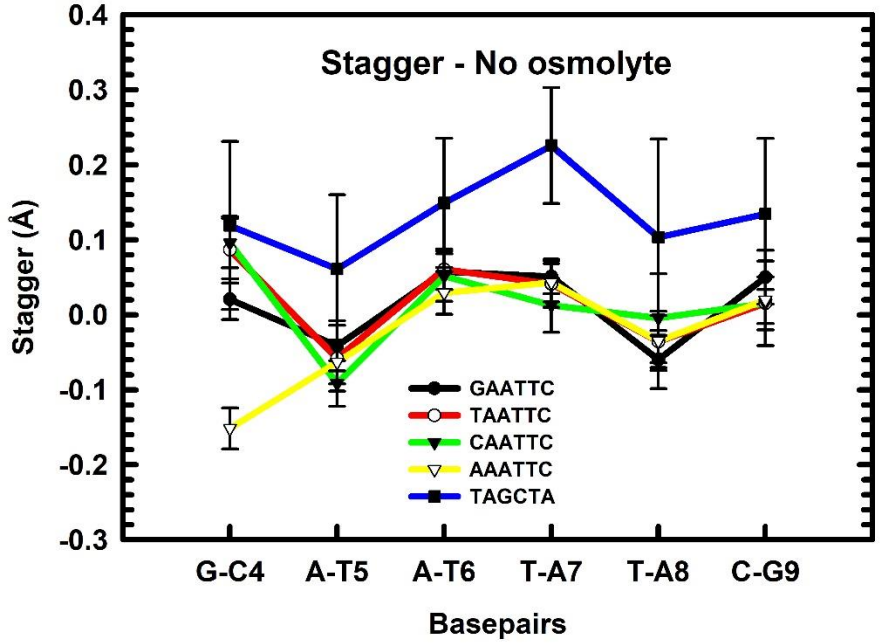

Shear - 5% Osmolyte
Shear(Å)
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

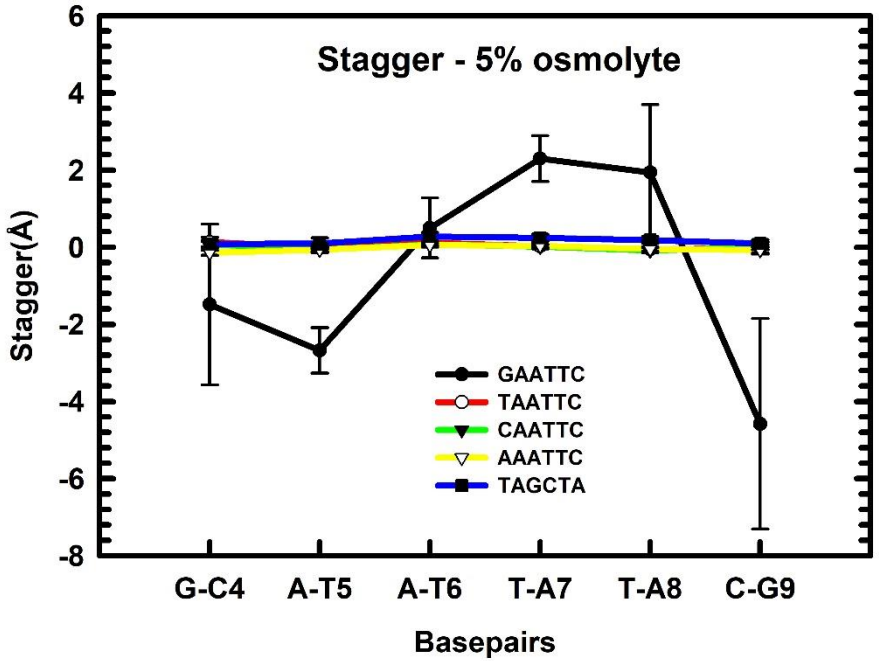

Shear-10% Osmolyte
Shear(Å)
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

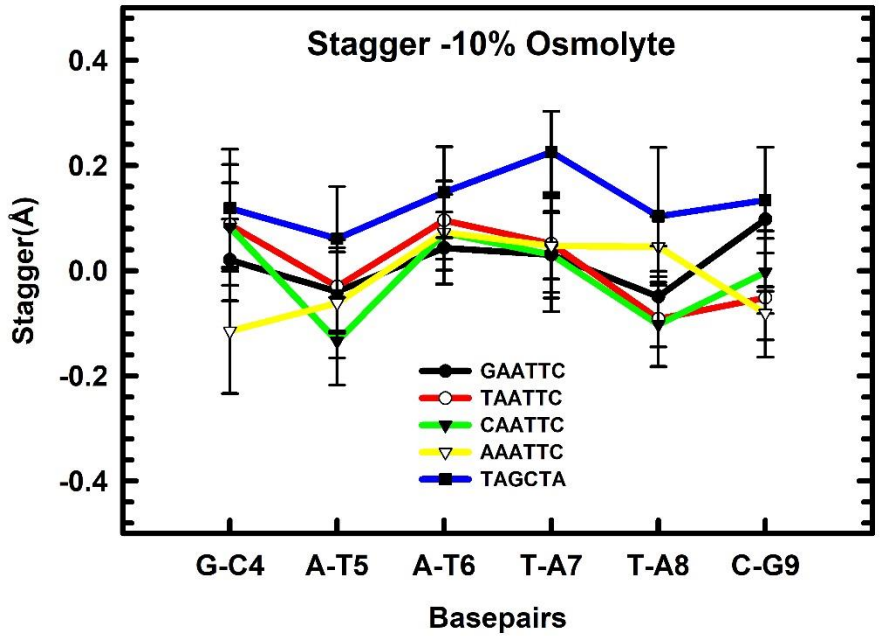

Stretch -No Osmolyte
Stretch (Å)
0.2
0.1
0.0
-0.1
-0.2
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA

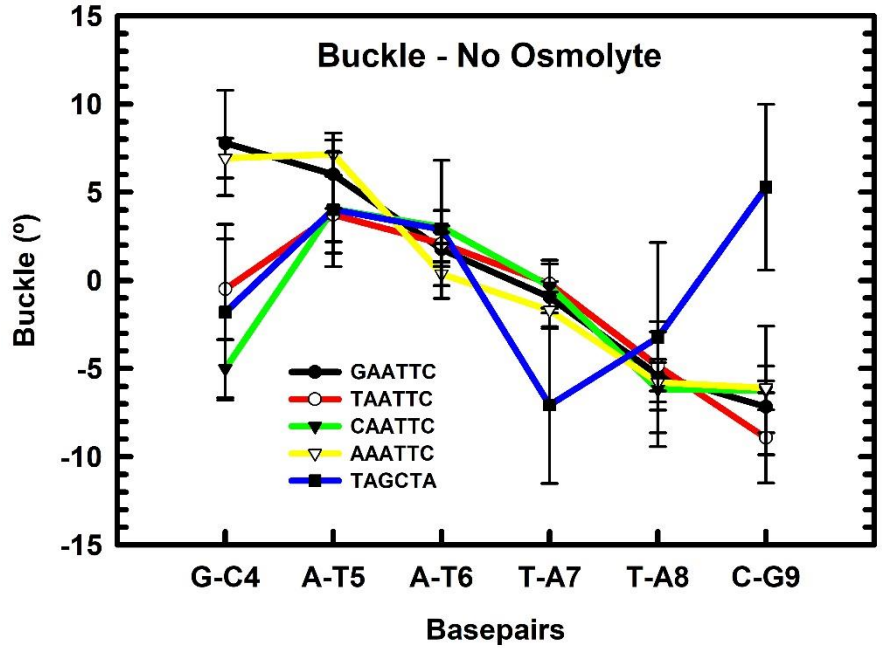

Stretch -5% Osmolyte
Stretch(Å)
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA

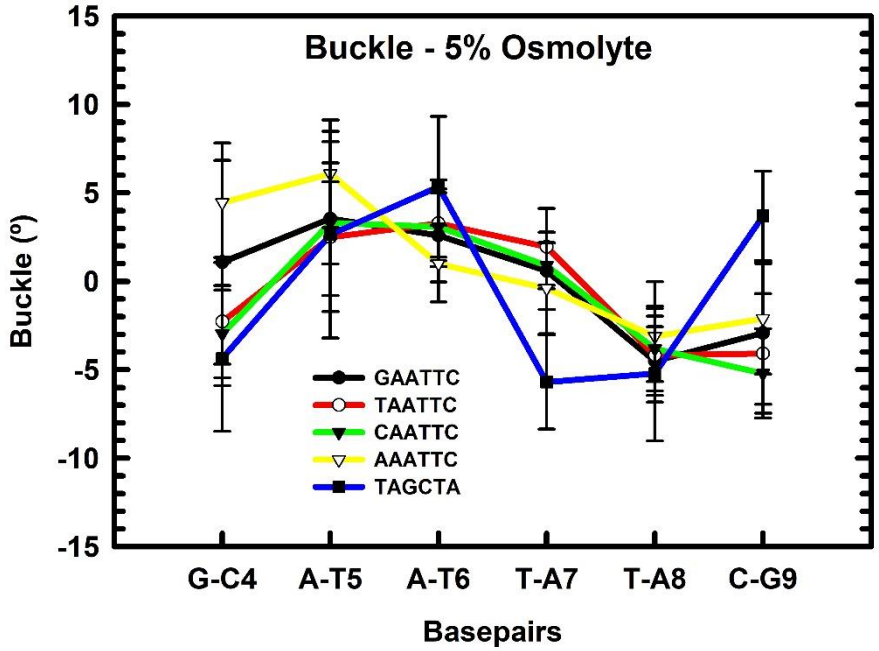

Stretch - 10% Osmolyte
Stretch(Å)
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA

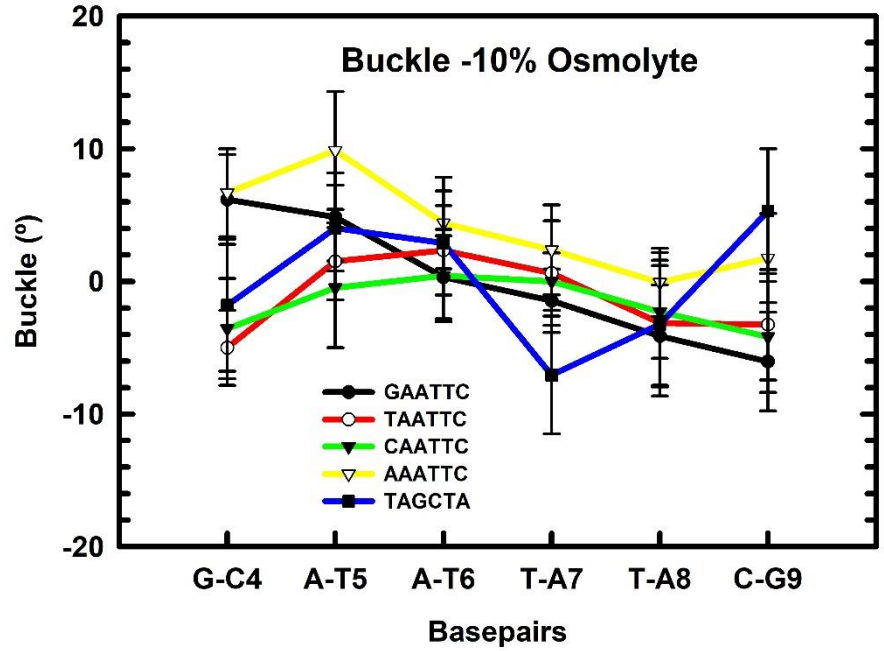

Stagger - No osmolyte
Stagger (Å)
0.4
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

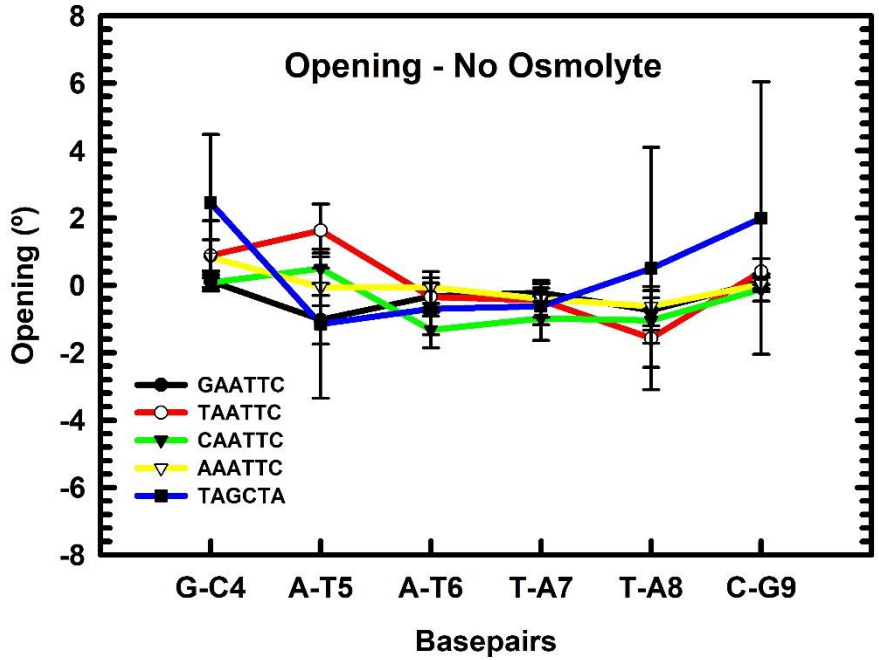

Stagger - 5% osmolyte
Stagger(Å)
6
4
2
0
-2
-4
-6
-8
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

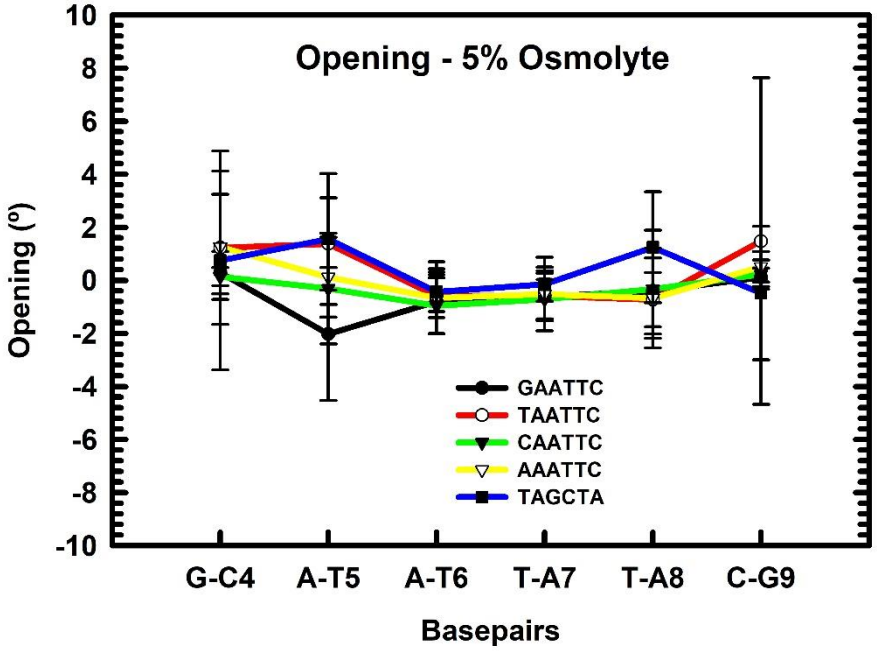

Stagger -10% Osmolyte
Stagger(Å)
0.4
0.2
0.0
-0.2
-0.4
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

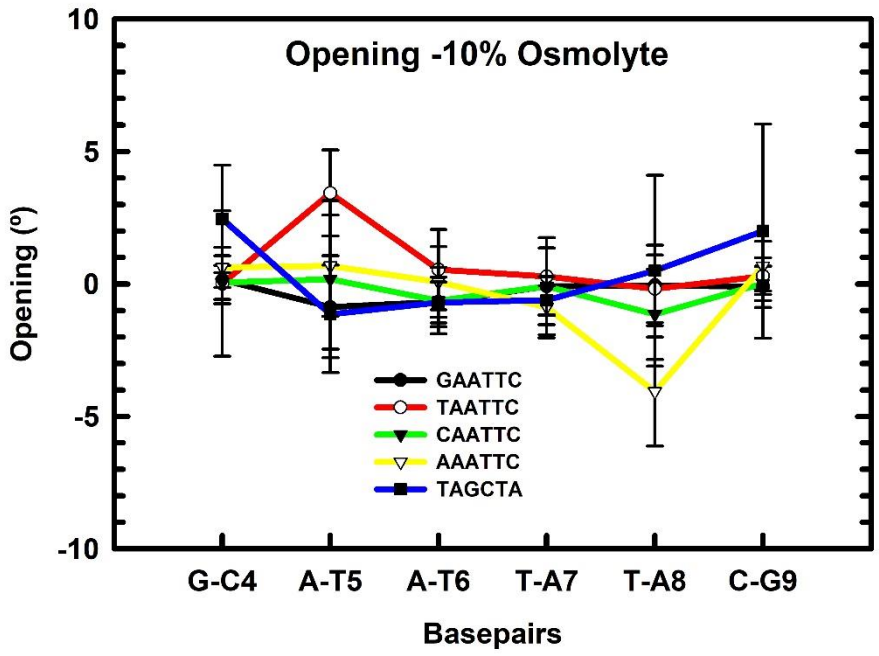

Buckle - No Osmolyte
Buckle (°)
15
10
5
0
-5
-10
-15
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

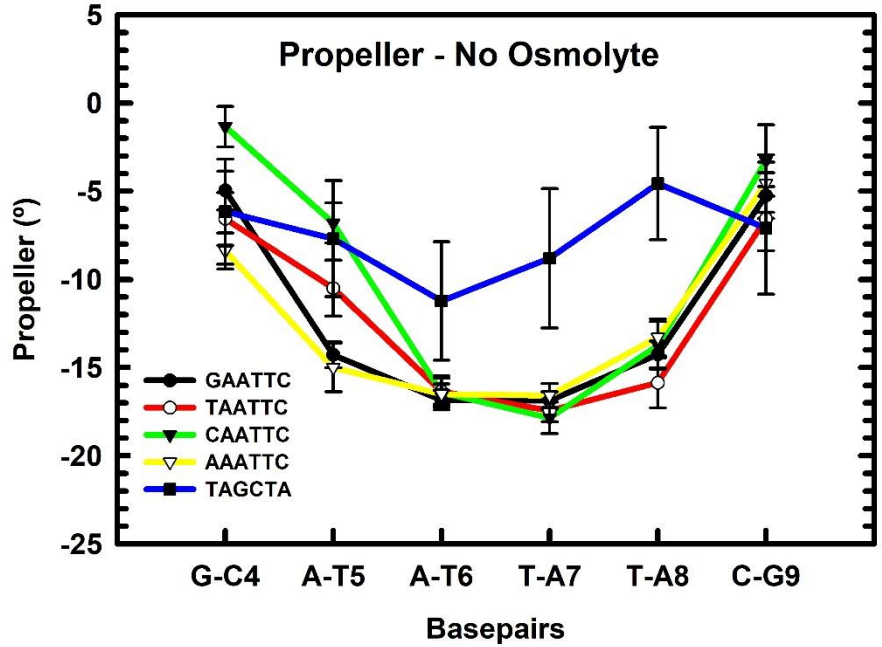

Buckle - 5% Osmolyte
Buckle (°)
15
10
5
0
-5
-10
-15
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

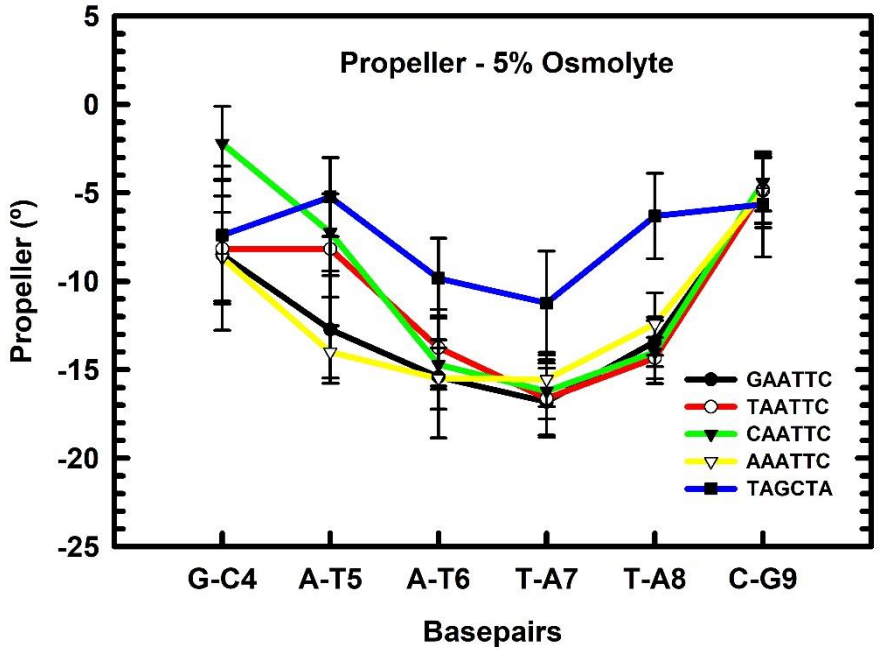

Buckle -10% Osmolyte
Buckle (°)
20
10
0
-10
-20
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

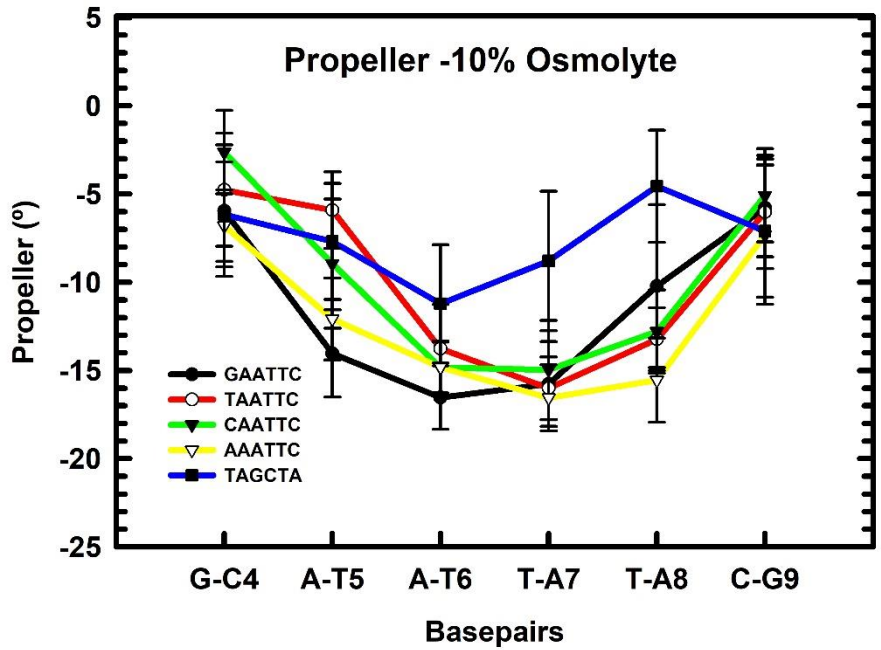

Opening - No Osmolyte
Opening (°)
8
6
4
2
0
-2
-4
-6
-8
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

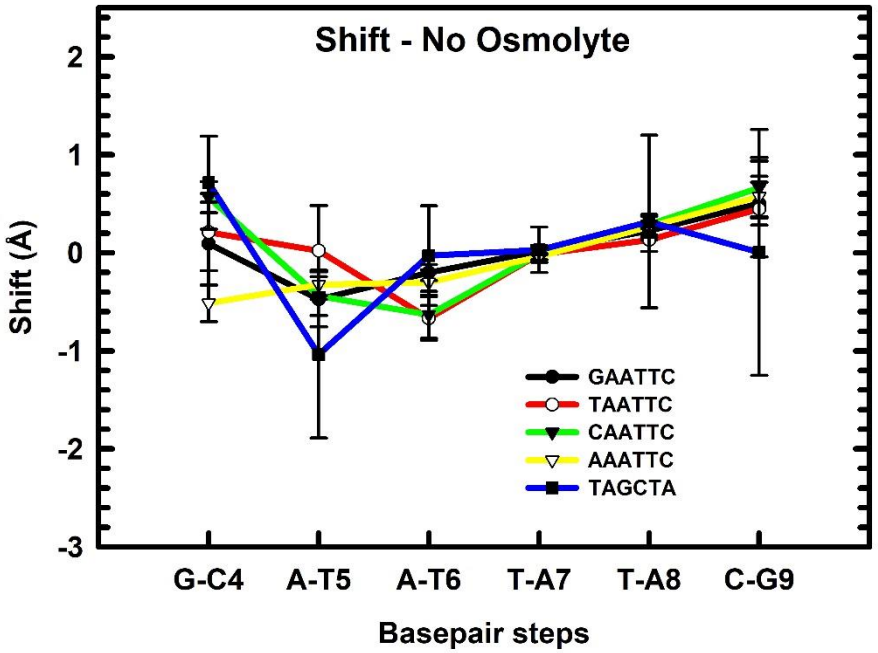

Opening - 5% Osmolyte
Opening (°)
10
8
6
4
2
0
-2
-4
-6
-8
-10
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

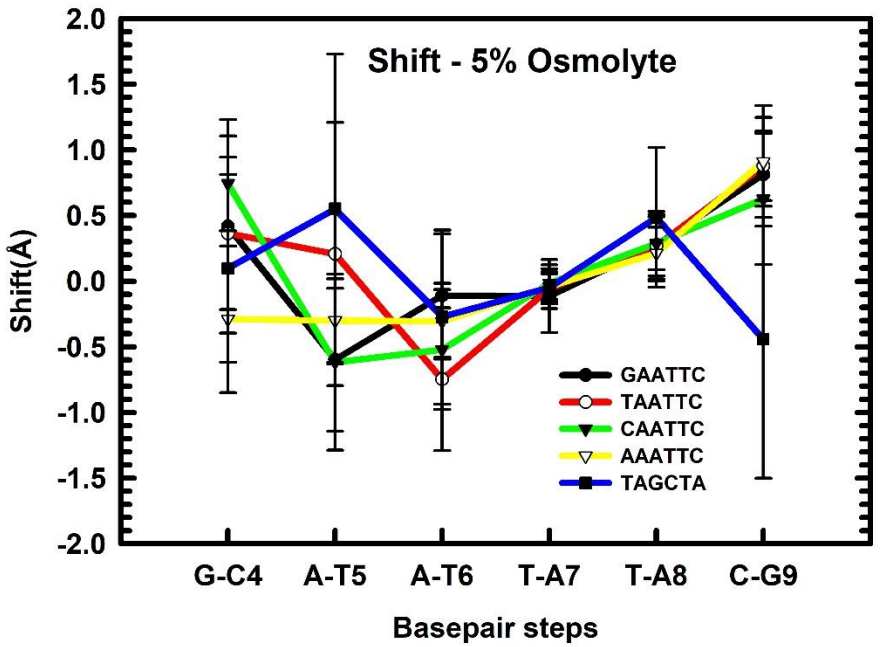

Opening -10% Osmolyte
Opening (°)
10
5
0
-5
-10
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

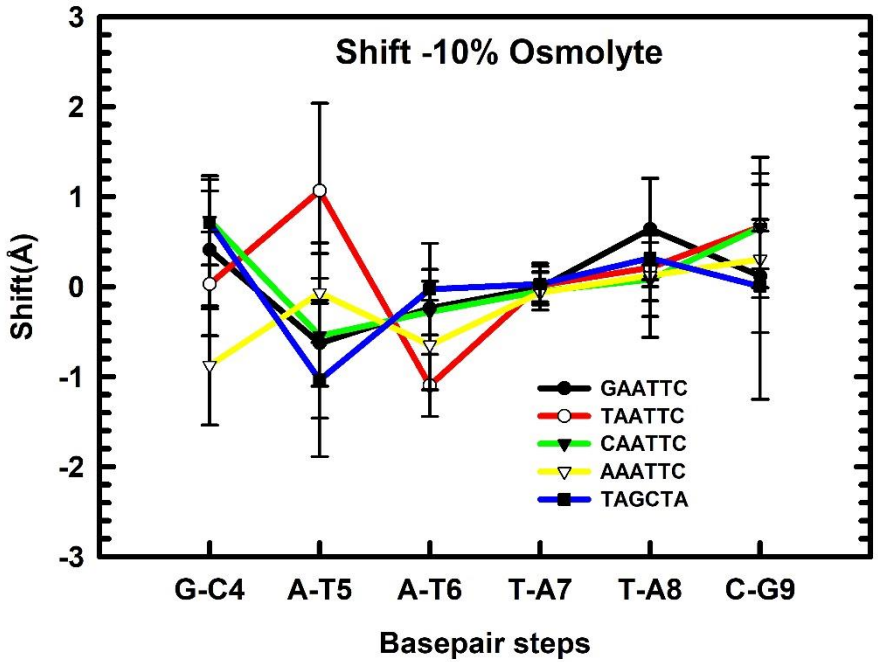

Propeller - No Osmolyte
Propeller (°)
5
0
-5
-10
-15
-20
-25
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

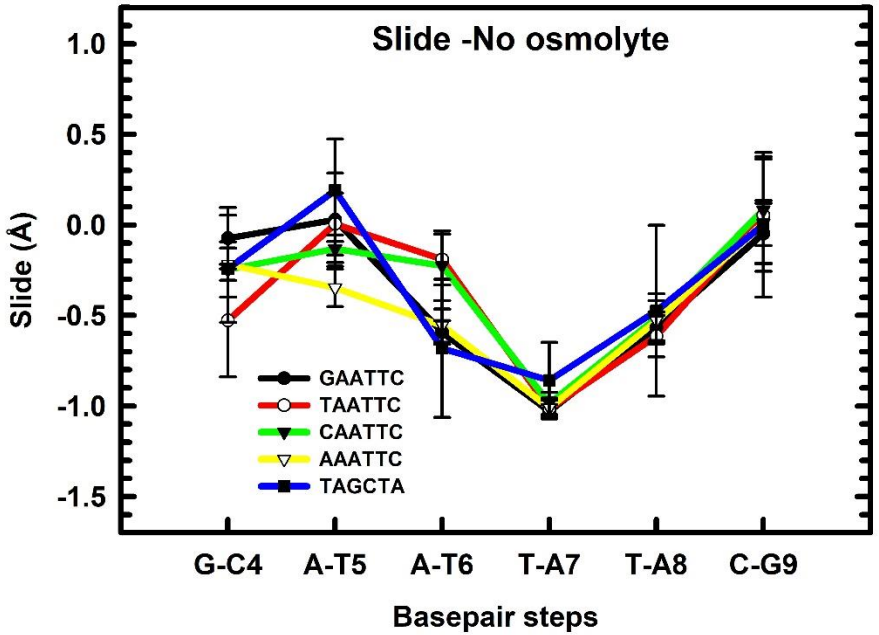

Propeller - 5% Osmolyte
Propeller (°)
5
0
-5
-10
-15
-20
-25
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

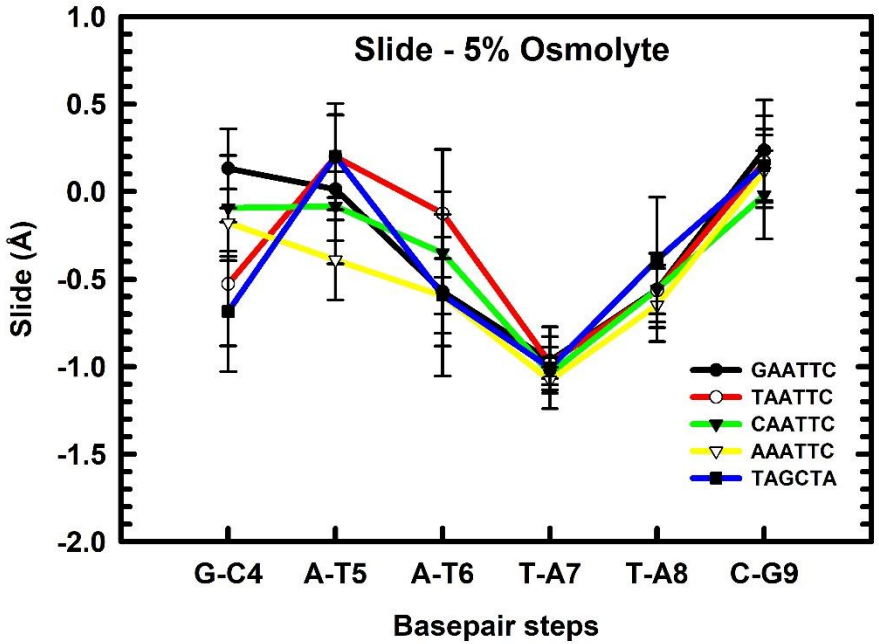

Propeller -10% Osmolyte
Propeller (°)
5
0
-5
-10
-15
-20
-25
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepairs

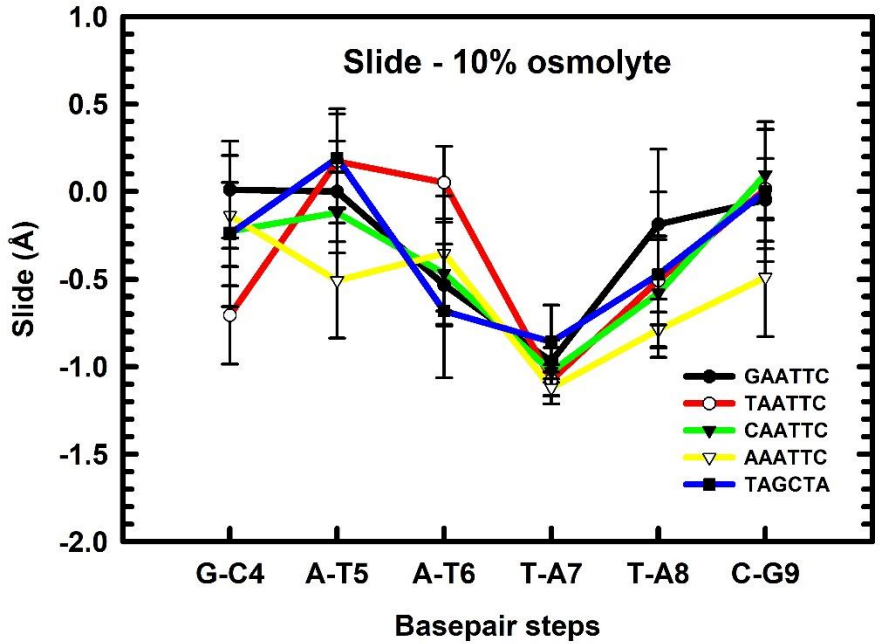

Shift - No Osmolyte
Shift (Å)
2
1
0
-1
-2
-3
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

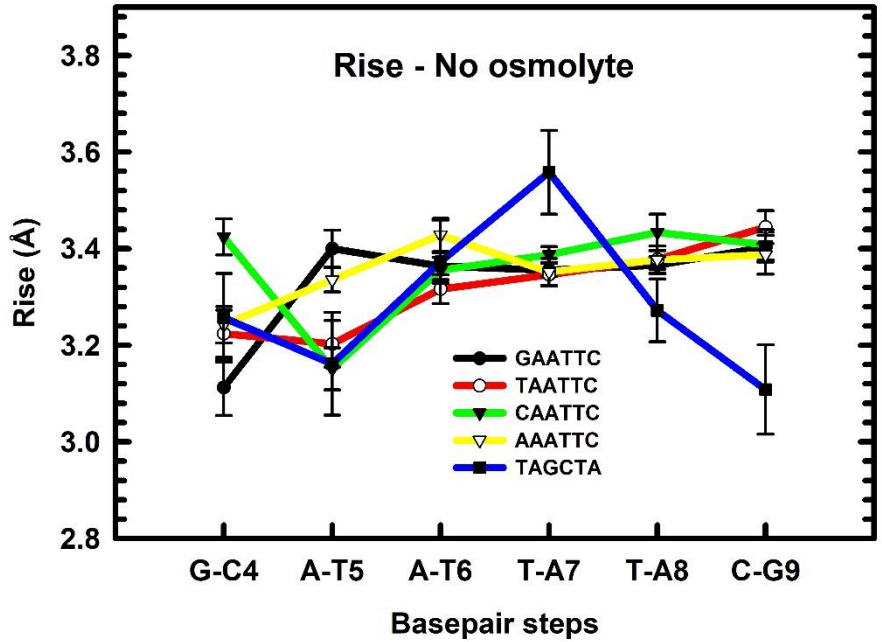

Shift - 5% Osmolyte
Shift(Å)
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

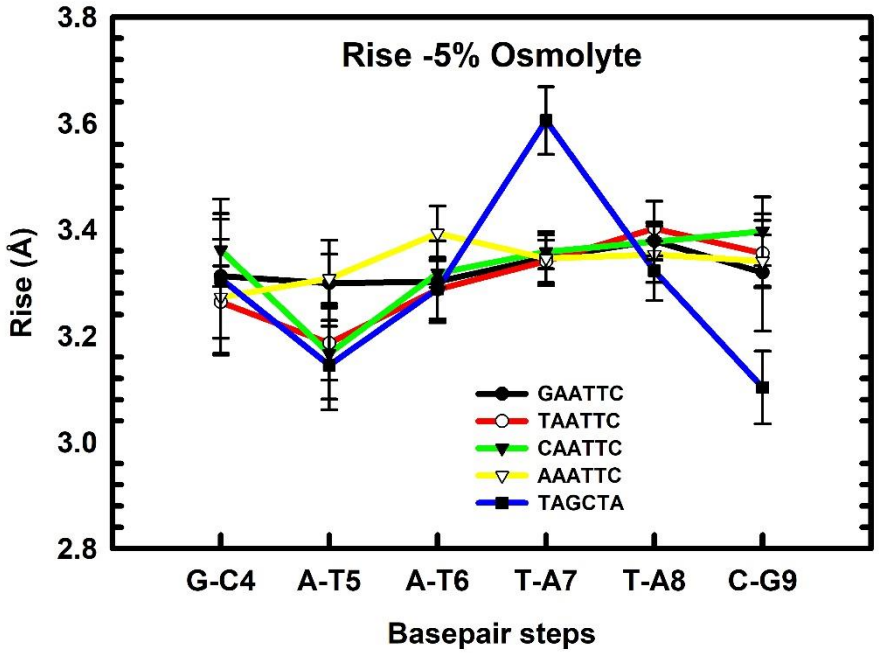

Shift -10% Osmolyte
Shift(Å)
3
2
1
0
-1
-2
-3
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

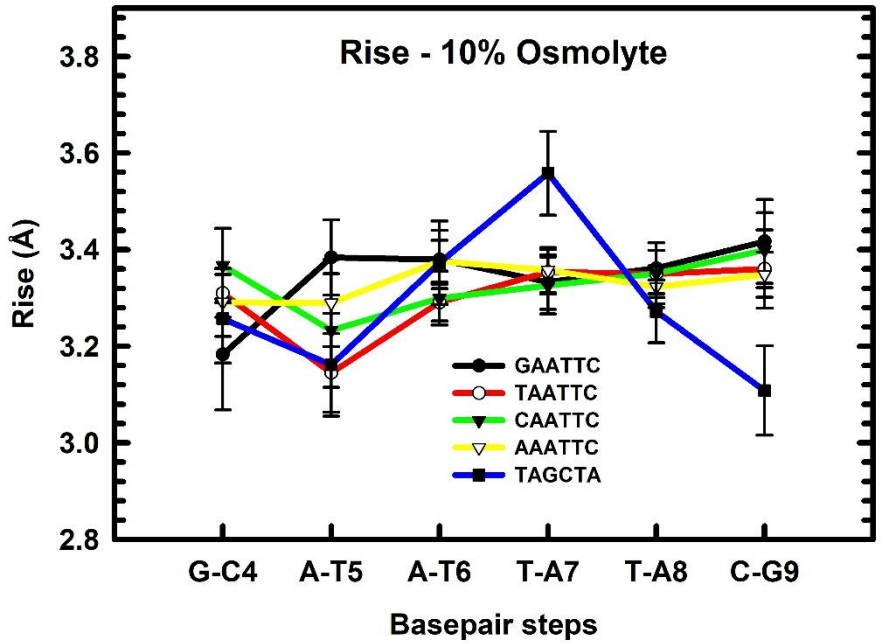

Slide -No osmolyte
Slide (Å)
1.0
0.5
0.0
-0.5
-1.0
-1.5
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

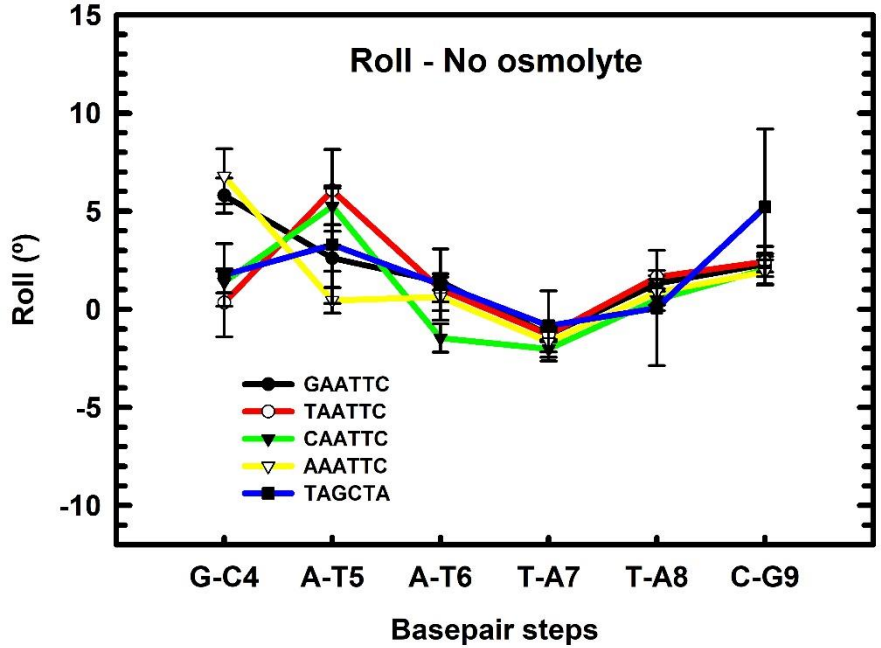

Slide - 5% Osmolyte
Slide (Å)
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

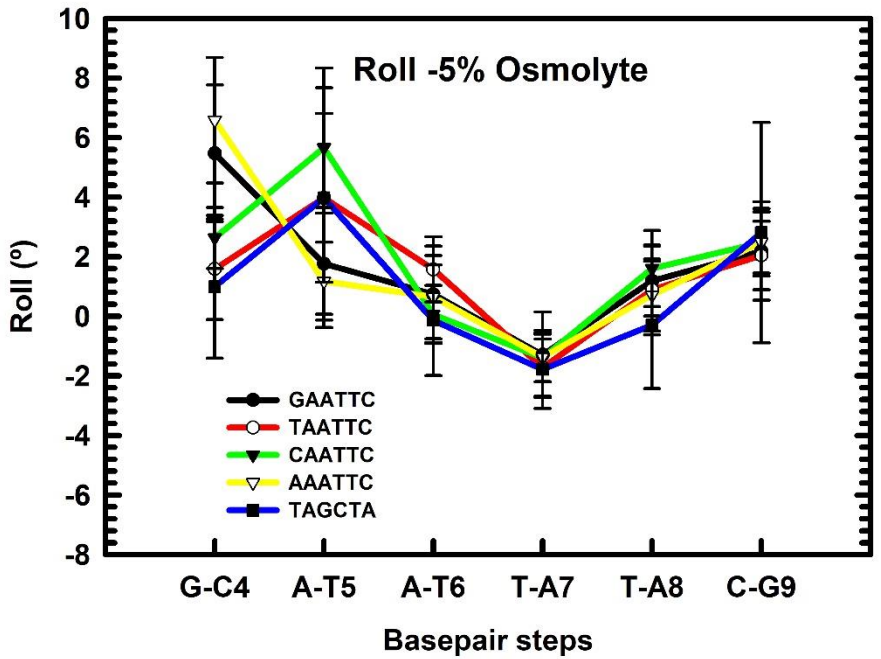

Slide - 10% osmolyte
Slide (Å)
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

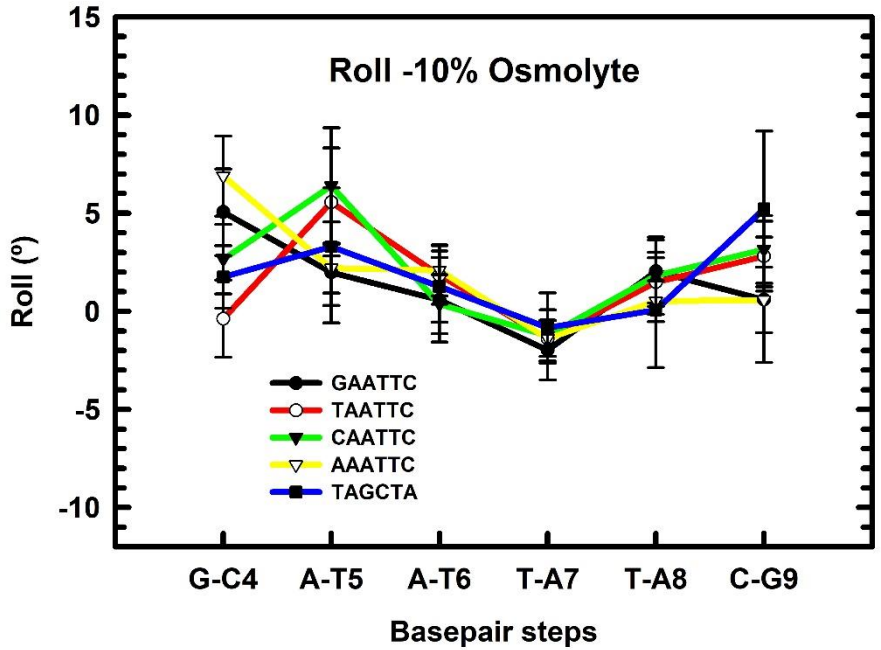

Rise - No osmolyte
Rise (Å)
3.8
3.6
3.4
3.2
3.0
2.8
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

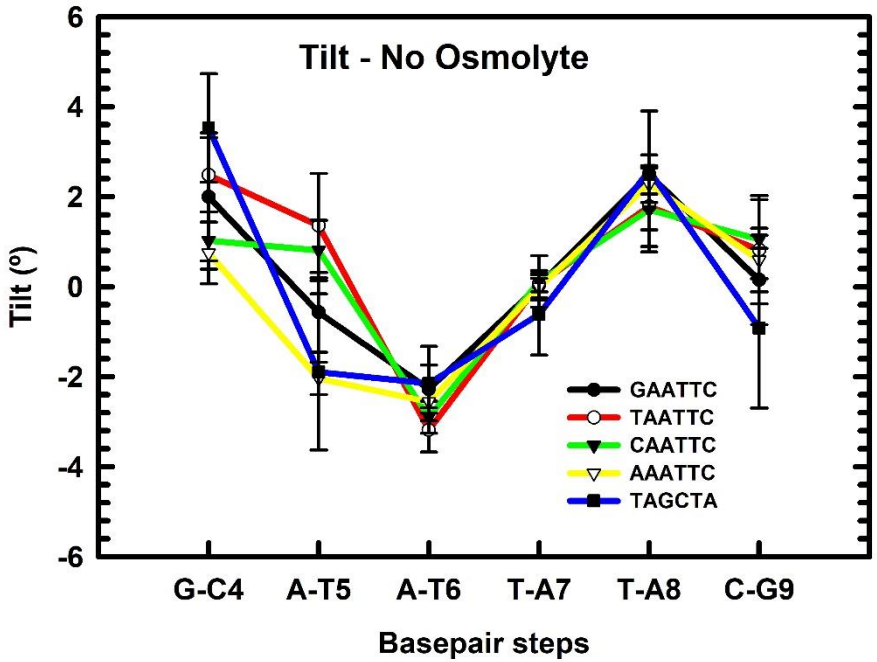

Rise -5% Osmolyte
Rise (Å)
3.8
3.6
3.4
3.2
3.0
2.8
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

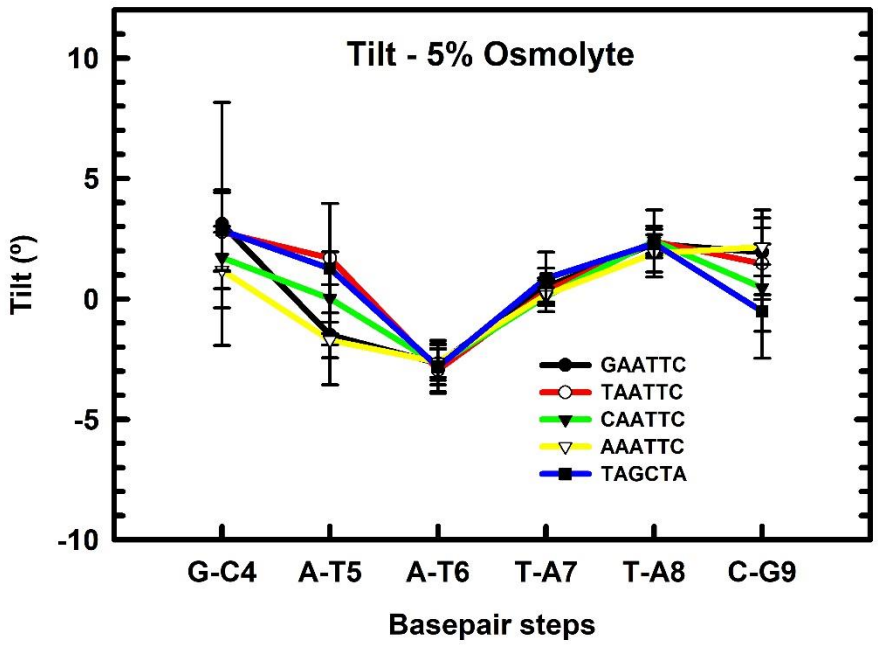

Rise - 10% Osmolyte
Rise (Å)
3.8
3.6
3.4
3.2
3.0
2.8
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

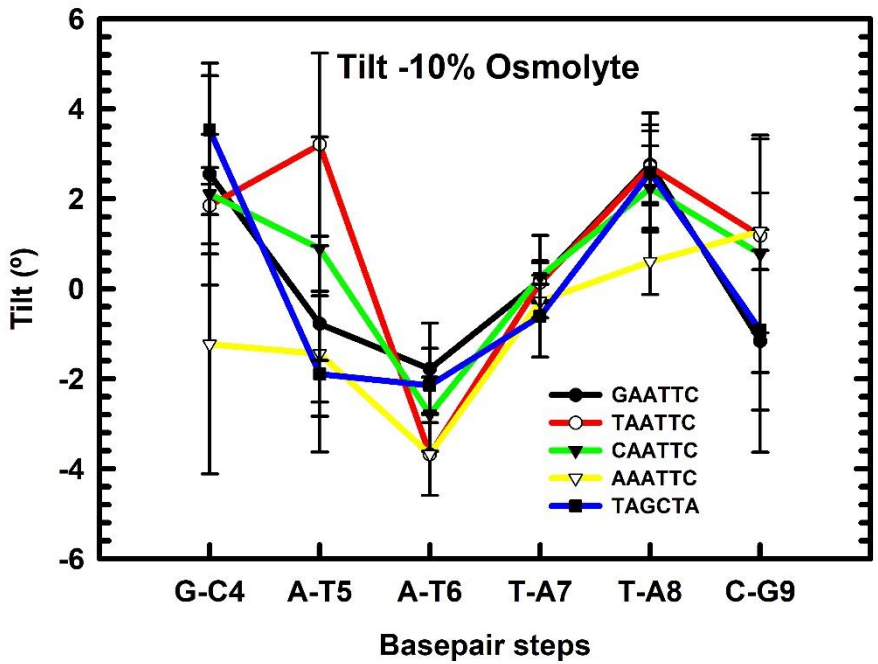

Roll - No osmolyte
Roll (°)
15
10
5
0
-5
-10
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

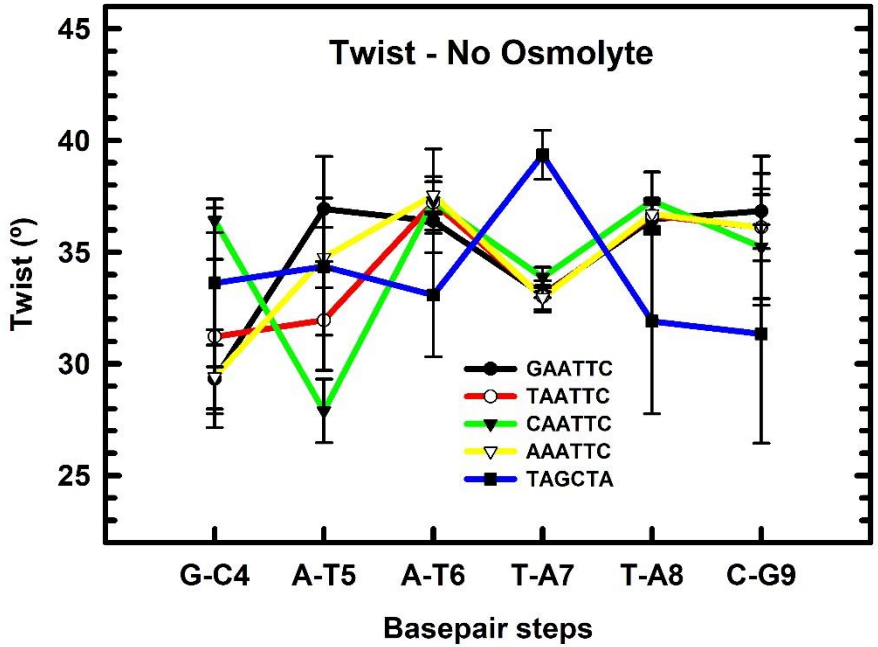

Roll -5% Osmolyte
Roll (°)
10
8
6
4
2
0
-2
-4
-6
-8
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

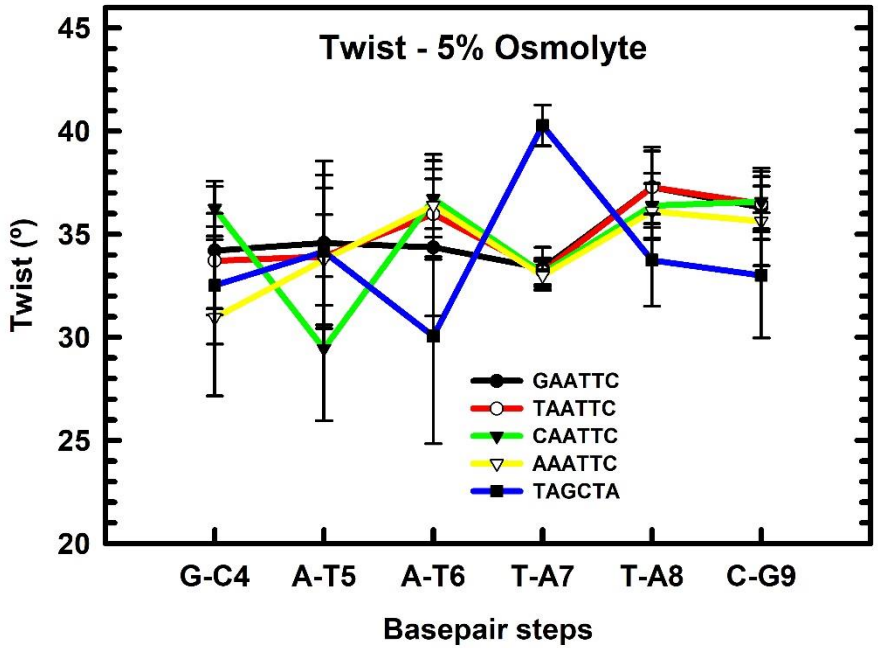

Roll -10% Osmolyte
Roll (°)
15
10
5
0
-5
-10
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

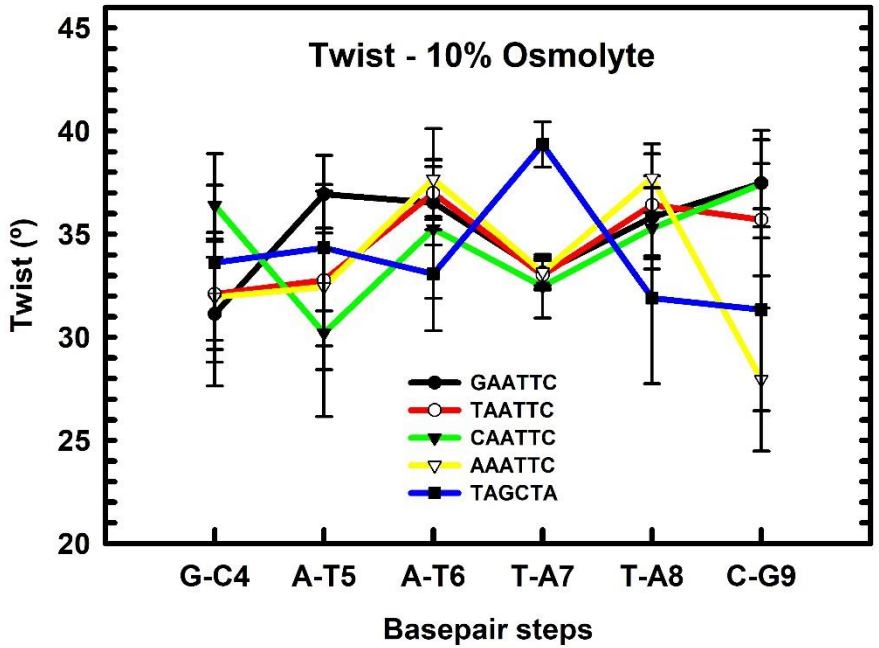

Tilt - No Osmolyte
Tilt (°)
6
4
2
0
-2
-4
-6
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA


Tilt - 5% Osmolyte
Tilt (°)
10
5
0
-5
-10
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA


Tilt -10% Osmolyte
Tilt (°)
6
4
2
0
-2
-4
-6
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA


Twist - No Osmolyte
Twist (°)
45
40
35
30
25
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

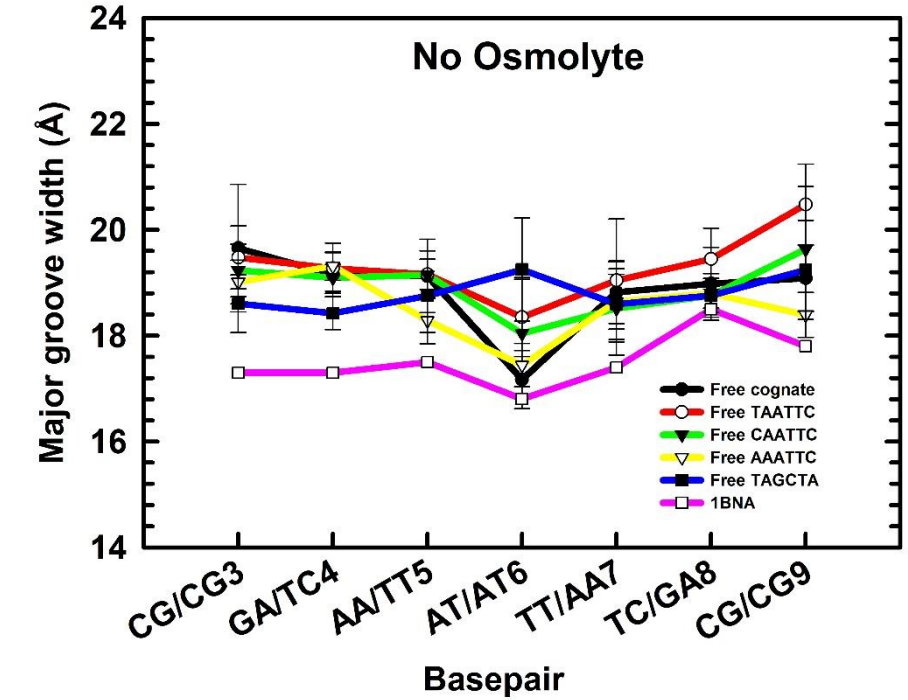

Twist - 5% Osmolyte
Twist (°)
45
40
35
30
25
20
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

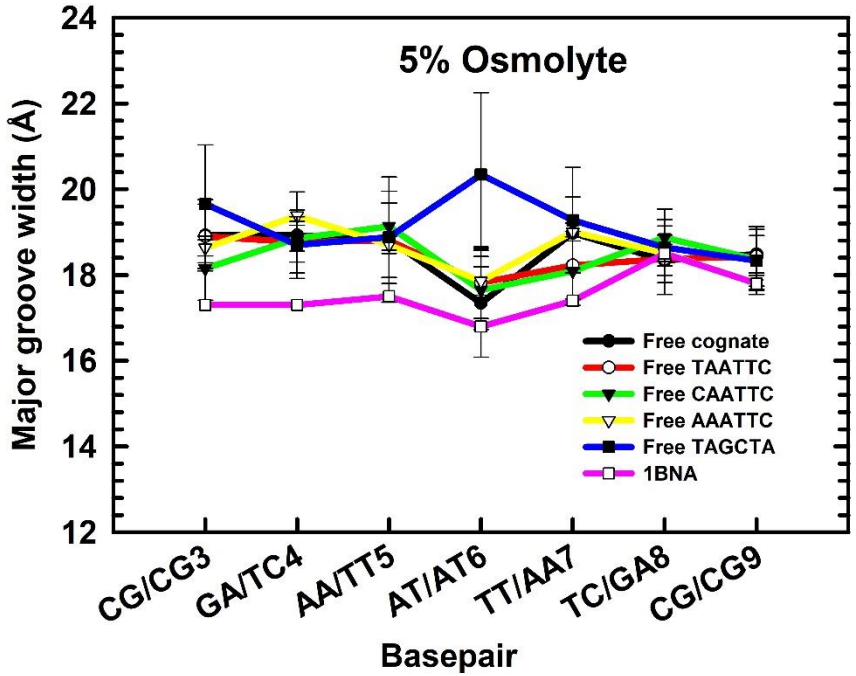

Twist - 10% Osmolyte
Twist (°)
45
40
35
30
25
20
GAATTC
TAATTC
CAATTC
AAATTC
TAGCTA
G-C4
A-T5
A-T6
T-A7
T-A8
C-G9
Basepair steps

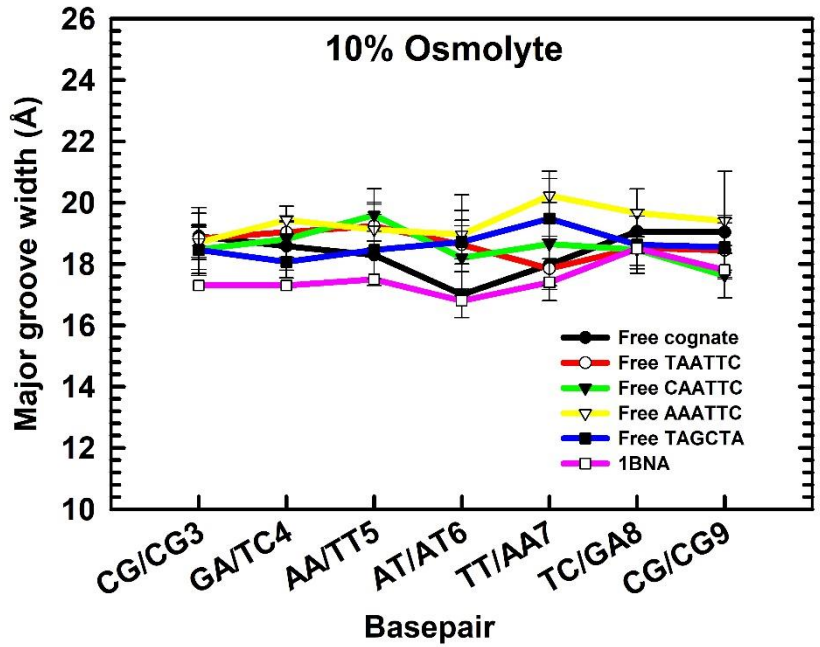
Average plot for groove width

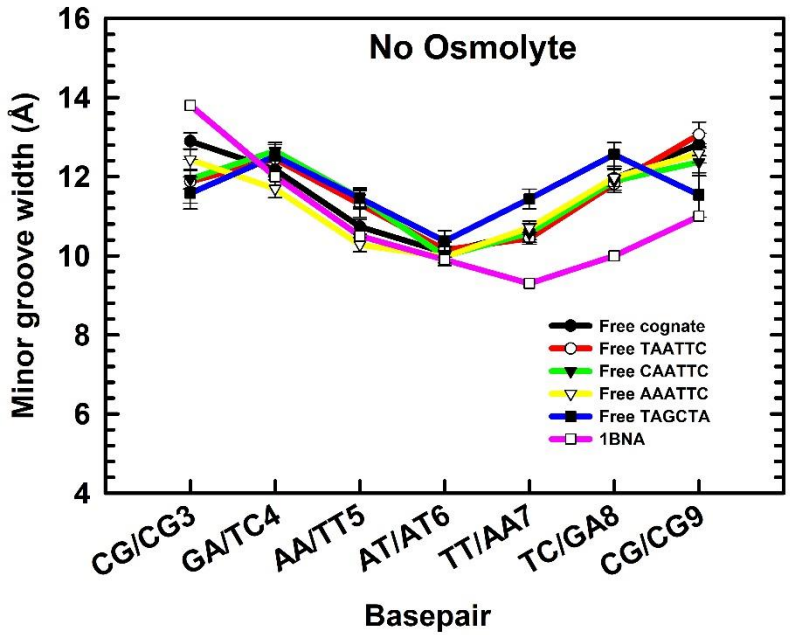
Major groove width

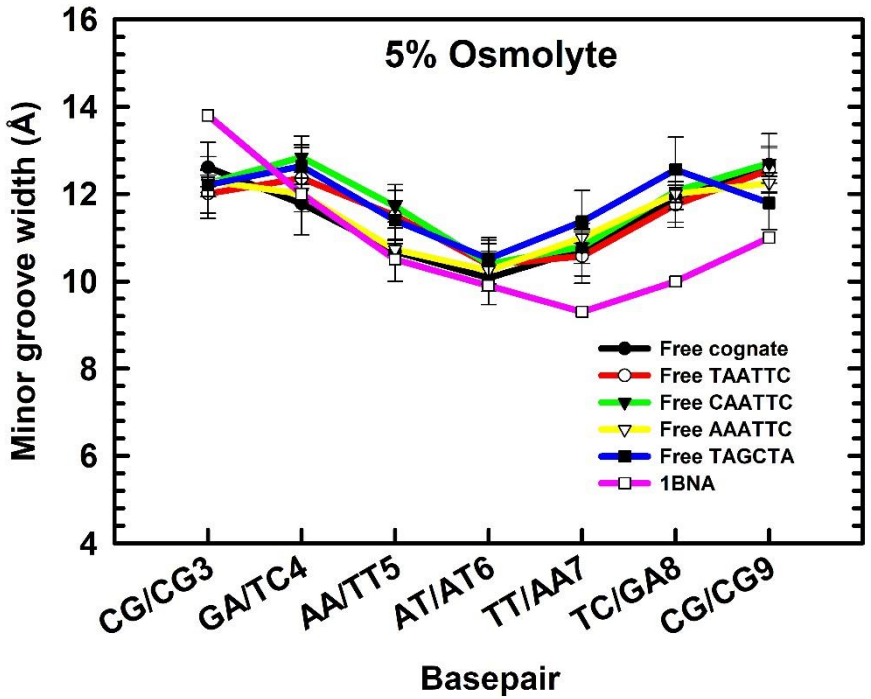
Minor groove width

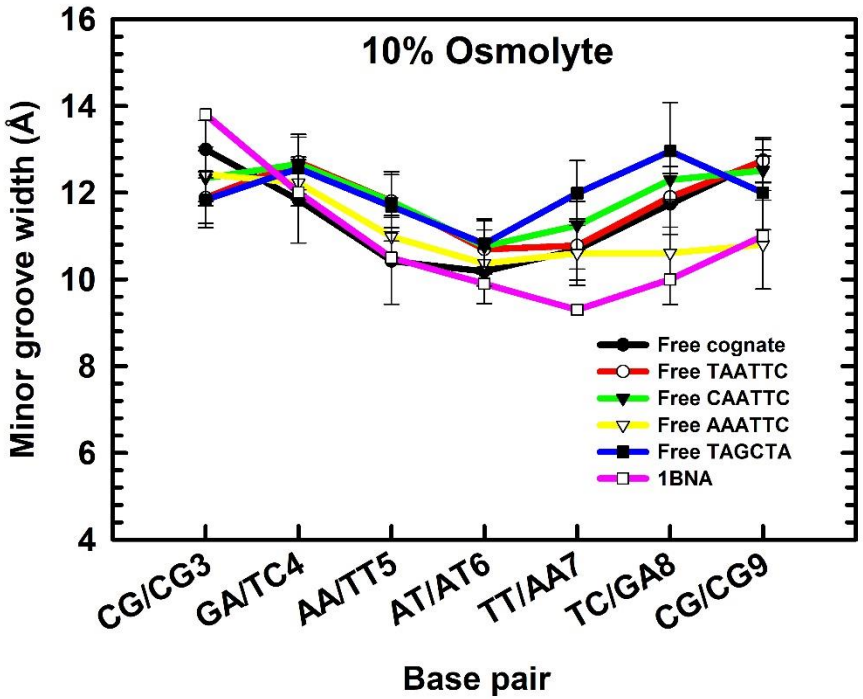

No Osmolyte
Major groove width (Å)
24
22
20
18
16
14
CG/CG3
GA/TC4
AA/TT5
AT/AT6
TT/AA7
TC/GA8
CG/CG9
Basepair
Free cognate
Free TAATTC
Free CAATTC
Free AAATTC
Free TAGCTA
1BNA


5% Osmolyte
Major groove width (Å)
24
22
20
18
16
14
12
CG/CG3
GA/TC4
AA/TT5
AT/AT6
TT/AA7
TC/GA8
CG/CG9
Basepair
Free cognate
Free TAATTC
Free CAATTC
Free AAATTC
Free TAGCTA
1BNA


10% Osmolyte
Major groove width (Å)
26
24
22
20
18
16
14
12
10
CG/CG3
GA/TC4
AA/TT5
AT/AT6
TT/AA7
TC/GA8
CG/CG9
Basepair
Free cognate
Free TAATTC
Free CAATTC
Free AAATTC
Free TAGCTA
1BNA


No Osmolyte
Minor groove width (Å)
16
14
12
10
8
6
4
CG/CG3
GA/TC4
AA/TT5
AT/AT6
TT/AA7
TC/GA8
CG/CG9
Basepair
Free cognate
Free TAATTC
Free CAATTC
Free AAATTC
Free TAGCTA
1BNA


5% Osmolyte
Minor groove width (Å)
16
14
12
10
8
6
4
CG/CG3
GA/TC4
AA/TT5
AT/AT6
TT/AA7
TC/GA8
CG/CG9
Basepair
Free cognate
Free TAATTC
Free CAATTC
Free AAATTC
Free TAGCTA
1BNA


10% Osmolyte
Minor groove width (Å)
16
14
12
10
8
6
4
CG/CG3
GA/TC4
AA/TT5
AT/AT6
TT/AA7
TC/GA8
CG/CG9
Base pair
Free cognate
Free TAATTC
Free CAATTC
Free AAATTC
Free TAGCTA
1BNA