

Structural and dynamical instability of DNA caused by high occurrence of d5SICS and dNaM Q2 unnatural nucleotides

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Supporting Information.

Curves library for the unnatural base-pairs.

Modified_b.lib

X R 11 'd5SICS'

-0.41200 1.66080 0.26050 'C1*'

0.83090 0.79030 0.23850 'N'

1.94260 1.27090 1.00210 'C14'

0.92910 -0.41280 -0.42360 'C19'

2.15950 -1.18030 -0.36130 'C18'

3.24130 -0.67570 0.38670 'C17'

3.09140 0.56370 1.07040 'C16'

4.45900 -1.40310 0.45990 'C12'

4.62450 -2.60490 -0.18640 'C10'

3.53520 -3.10650 -0.93450 'C9'

2.34460 -2.42400 -1.02110 'C7'

Y R 11 'dNaM'

-0.20240 1.84000 -0.40040 'C1*'

1.08260 1.03790 -0.27800 'C'

2.33570 1.69720 -0.11410 'C21'

1.08010 -0.32590 -0.30280 'C12'

3.50220 1.00390 -0.02470 'C16'

2.27590 -1.07980 -0.20300 'C13'

3.50700 -0.41190 -0.07300 'C14'

4.69790 -1.18270 0.01270 'C4'

2.24710 -2.50050 -0.24300 'C10'

4.64420 -2.54020 -0.02800 'C6'

3.40230 -3.21180 -0.15730 'C8'