1 The effects of methylation on the shape of DNA

Figure 1 shows (a) Minor groove width of the 256 methylated CG hexmer (red) and the 256 unmethylated CG hexmer (blue), which is NNNCGGN with CGCG flank on the two ends. The solid line is the average over the 256 trajectories. (b) RMSD is the root mean square deviation, while MD is mean deviation which is the minor groove width of methylated sequence minus the minor groove width of the corresponding unmethylated sequence. We can see that most of the MDs are less than 0 which means, on average, methylated sequence has a narrower minor groove width. But the RMSD is not just the square of MD, which means some methylated sequences have wider minor groove width than unmethylated ones. So we divided the 256 sequences into two sets based on the minor groove width at M point, then we get the seq-logo (frequency plot). (c) is the seq-logo that methylated sequences have a narrower minor groove width and (d) is that the methylated sequences have a wider minor groove width at position M. (e) is the logo of sequences, in which all the positions have a narrowed minor groove width in methylated sequences than the corresponding unmethylated ones (totally 18 sequences, while 0 for wider minor groove width). (f) is the logo of sequences, in which the middle 6 positions have a narrower minor groove width in methylated sequences than the corresponding unmethylated ones (totally 23 sequences, while 1 for wider minor groove width, which is GTG—CGG).(g) and (h) are the sequences in which, the minor groove width difference is less than 0.12 Å between the methylated sequence and the corresponding unmethylated one. (g) consider all the position, while (h) consider only the middle hexmer. The total number of sequences in (g) is 7 and in (h) is 13.
Figure 1: Statistical results of the effects of methylation on the 256 hexmers.
Figure 2: Seq-logo of sequences which have a narrow/wide minor groove width at each position.
Figure 3: Minor/major groove width and also the fluctuation of minor/major groove width for the three sequences from Lieber’s cell paper 2008.
Figure 4: Roll/twist and also the fluctuation of roll/twist for the three sequences from Lieber’s cell paper 2008. From this figure we can see that the methylated CpG step (MpG) always have a higher roll compared to unmethylated CpG step.