• Dnase
  → For the DNase project, I worked on reanalyzing some data. In order to find correlation between cleavage rate of hexamers and minor groove width. By looking at minor groove width of 108 hexamers, previously we had found the strongest correlation for position -2, which we now attributed to the flank sites used for our simulations since MC (Fig 1) or HT (Fig 2) holds similar results for those 108 hexamers, but HT alone of all hexamers does not show the same correlation. However, the result for position +1 still holds. This is because for position +1 we still see correlation when looking at simulations of all possible hexamers, what does not happen for position -2. In another test we wanted to relate both methods, which is shown in the scatter plot MC vs HT (Fig 3).

  We also found correlation between torsion angles and cleavage rate, but such correlation might not be real - it could also be due to the flank sites used since the same effect was seen for minor groove width (Fig 4). I also look at results for methylated sequences, and one of the goals for this week is to look at results from 256 sequences from Yan.

• bax and p21RE
  → Helped with figure of model but still need to finish it;
  → Got program for constraint simulation, now I need to run simulations for p21 RE;

• polymerase
  → After meeting with Cathy, next step is to check position, run new curves and review figure;
MC simulation for hexamers

**Fig 1.** Correlation between minor groove width and DNase I cleavage rate. MC simulations for hexamers.
HT prediction for hexamers

Fig 2. Correlation between minor groove width and DNase I cleavage rate. HT prediction for hexamers.
Fig 3. Scatter plot – relation between MC and HT for 108 hexamers.
Fig 4. Torsion angles and correlation between them and cleavage rate of DNase I