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## **The mechanical genome : inquiries into the mechanical function of genetic information**

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## APPENDICES



# A

## A NOTE ON MODEL PARAMETERIZATION

As discussed in Section 1.1, the Rigid Base Pair (RBP) model can be parameterized in various ways. It has long had a standard parameterization in what we call the hybrid or mixed parameterization: intrinsic values from crystallography data [11] and stiffnesses from molecular dynamics simulations [13]. This is primarily due to the conclusions of Becker *et al.* [14], who benchmarked the predictions of various parameterizations for the nucleosome affinity of a set of sequences against experimental measurements, and found that this hybrid parameterization gave the best results.

This conclusion has led to the use of the hybrid parameterization in much subsequent research including most of that presented in this thesis. However, we have found that this parameterization does not work in all cases, as we will explain below.

Furthermore, in Chapters 4 and 6 we employed oligonucleotide distributions for the Markov-chain model for nucleosome affinity that were derived using MMC simulations at artificially low temperature. This helped the simulations converge more quickly. However, as we saw in Chapter 5 (the work for which was done after that for Chapters 4 and 6), temperature can be a subtle parameter to manipulate. We therefore also wish to briefly expand upon the effects of this artificially chosen temperature.

In light of what we learned during the research for Chapter 5, we later spent the computational time to generate sequence ensembles at room temperature, rather than at artificially low simulation temperatures. The analyses presented in this Appendix are all based on those room temperature simulations, to remove the complications in interpreting the results associated with temperature effects.

### A.1 PARAMETERIZATIONS: CRYSTALLOGRAPHY, MOLECULAR DYNAMICS, AND THEIR HYBRIDS

In Chapter 6 we switched from parameterizing our model using the hybrid parameterization to using the pure parameters obtained solely from crystallography data [11]. The reason for this switch is that the hybrid parameterization turned out not to be able to correctly capture long-range

effects. This is evident in Fig. A.1, which shows the same predictions as Figs. 6.2A-B, with various parameterizations.

We saw in Chapter 6 that the pure crystallography prediction corresponds well to the experimentally measured signals. However, the predictions made using the pure MD and hybrid parameterizations do not capture the nucleosome depletion signal at all. Even though the hybrid parameterization was deemed to be the most accurate in the benchmarks of Becker *et al.* [14], we find here a situation where it fails completely.

We also considered the reverse hybrid parameterization, which uses stiffness parameters derived from crystallography data and shape parameters from MD simulations. This reverse hybrid parameterization still captures the signal, albeit that the amplitude is too small. Apparently, switching out the crystallography shape parameters for the MD ones reduces the ability of the model to map the signals we are looking for. However, the stiffness parameters are more important: using MD stiffness parameters destroys the signal, regardless of which shape parameters are used.

The reason for this failure is suggested by the black dotted curves depicted in Fig. A.1, which shows the average GC content (averaged using a 147-bp window) in the regions of interest. As we saw in Chapter 6, the nucleosome occupancy signals in the promoter regions of organisms across the tree of life correlate well with GC content. The problem with the parameterizations that fail at predicting these signals seems to be a lack of correlation of their predictions with the average GC content.

We can understand this observation when we look at the dinucleotide distributions derived from MMC simulations using each set of parameters. Fig. A.2 shows the distributions of A/T-rich and G/C-rich dinucleotides for the pure crystallography parameterization and the reverse hybrid parameterization. We see that, apart from the oscillatory behavior, there is an overall preference for G/C-rich dinucleotides over the A/T-rich ones. On the other hand, the distributions of the pure MD parameterization and the hybrid parameterization, plotted in Fig. A.3, do not show a strong preference for G/C or A/T.

The sequences for which Becker *et al.* [14] analyzed the predictions of the different parameterizations were all relatively short. On short scales, the precise local positioning is important, and the most important feature that a parameterization needs to capture is the periodicity in the probability distributions of the dinucleotides. It may well be that the hybrid parameterization in this regard delivers superior performance. However, for the application we consider in Chapter 6 and in this section, our interest lies in mapping long-range effects. It seems that to capture these

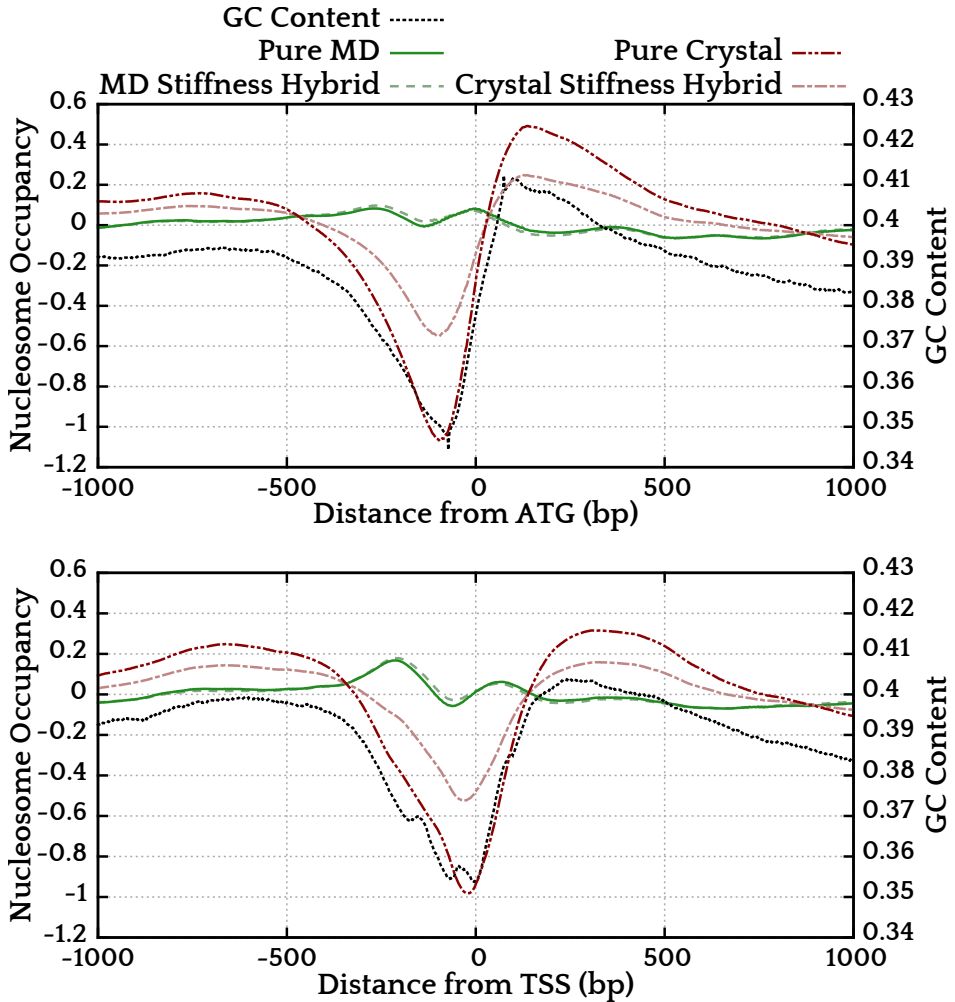


Figure A.1: Nucleosome occupancy signals in the promoter regions of *S. cerevisiae* (analogous to Figs. 6.2A-B) as predicted using the model of Chapter 4 using various parameterizations: pure MD parameters [13] (solid green curve), pure crystallography parameters [11] (dash-dot-dotted dark red curve), and the two possible hybrids: the MP parameterization in [14], using MD stiffness parameters with crystallography shape parameters (dashed pale green curve); and the reverse of this hybrid, using crystallography stiffness parameters with MD shape parameters (dash-dotted pale red curve). Also shown for reference is the average GC content in the promoter regions, smoothed over a 147-base-pair window (black dotted curve).

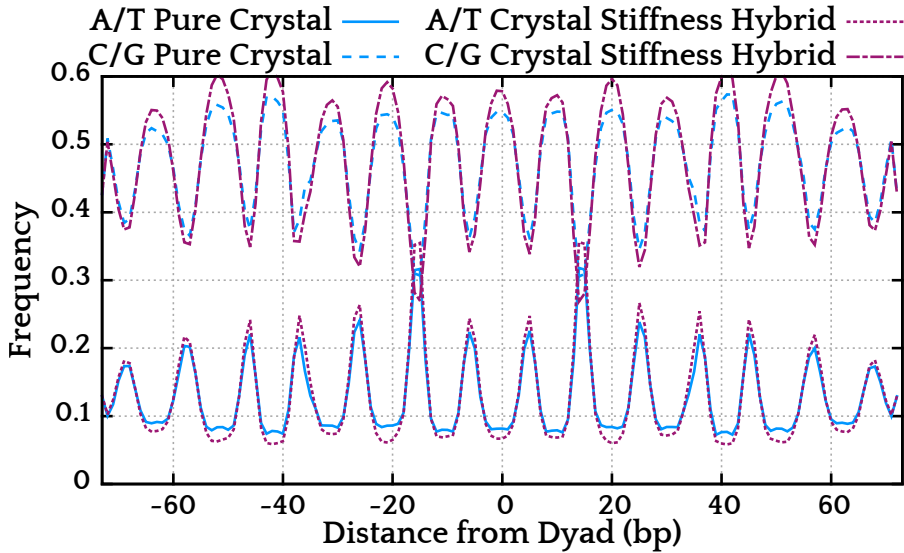


Figure A.2: Dinucleotide distributions along the nucleosome (modeled as in [1] and the rest of this thesis), with the nucleosome model parameterized by the pure crystallography parameters and the reverse hybrid parameterization (crystallography stiffness parameters, MD shape parameters). The label A/T indicates the combined probabilities of the dinucleotides AA, AT, TA and TT. The label G/C corresponds to CC, CG, GC and GG. Both parameterizations lead to a nucleosome with a significant preference for GC-rich dinucleotides.

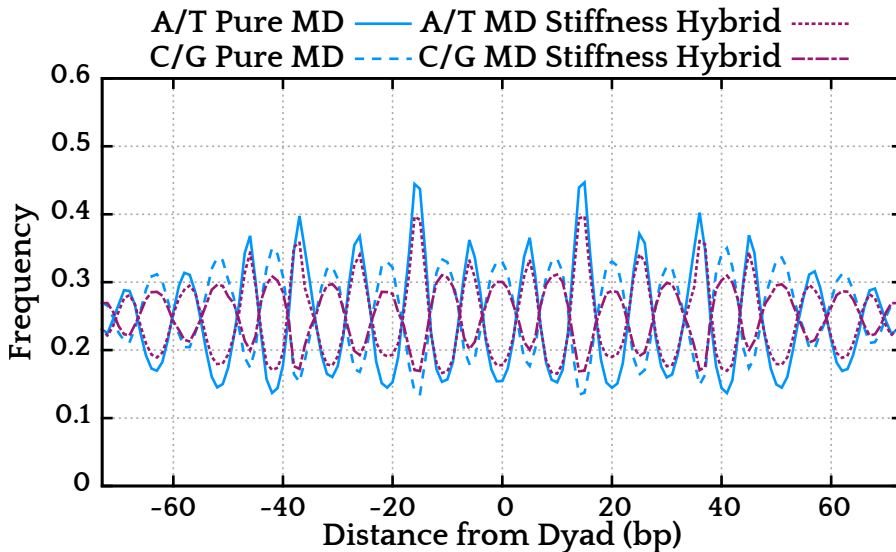


Figure A.3: As Fig. A.2 for the pure MD parameterization and the hybrid parameterization (MD stiffness parameters, crystallography shape parameters). These parameterizations show no significant preference for GC- or AT-rich dinucleotides.



long-range signals correctly, a proper correlation with GC content, and therefore a preference for high GC content, is required.

The pure crystallography parameterization does prefer high GC, but the hybrid parameterization lacks this preference. On the other hand, the pure crystallography parameterization, judging by the results of Becker *et al.* [14], does not capture the periodic signal in the distributions as well as does the hybrid parameterization. Therefore, these two parameterizations (pure crystallography and the original hybrid) may be taken to be complementary: neither performs optimally in all situations and for any given application, a careful choice should be made.

## A.2 THE EFFECT OF MMC TEMPERATURE ON THE MARKOV-CHAIN MODEL

The probability distributions that inform the Markov-chain model introduced in Chapter 4 depend not only on the chosen parameterization, but also on the temperature at which the MMC simulation is run. The effect of temperature, qualitatively, is predictable: a lower simulation temperature leads to stronger preferences of the nucleosome for accommodating sequences.

Running the MMC at temperatures lower than room temperature (which is the temperature we are generally interested in) is desirable because the simulations converge more quickly. In Chapters 4 and 6 we utilized probability distributions gained from MMC simulations run at artificially low temperatures, and in which we scaled the results back up to room temperature (Eq. 4.7). The discerning reader may have noticed that this trick is in fact the same technique used in Chapter 5 to change the mutation temperature separately from the physical temperature.

Chapter 5 presents a far deeper understanding of the role of temperature in MMC simulations than was available at the time when the work for Chapters 4 and 6 was performed. Knowing now that our rescaled probabilities in fact represent the probabilities found using a low temperature for the configurational moves, and room temperature for the mutations, we should check what the effects are. We already showed in Section 5.4 that for nucleosomes, the spatial temperature has only a moderate effect on the sequence preferences (see Fig. 5.1A-C). Still, we would do well to check what effect this has on the results of Chapter 6.

To do so, we have now invested the computational time to run our MMC simulations at room temperature (all the results shown in this appendix

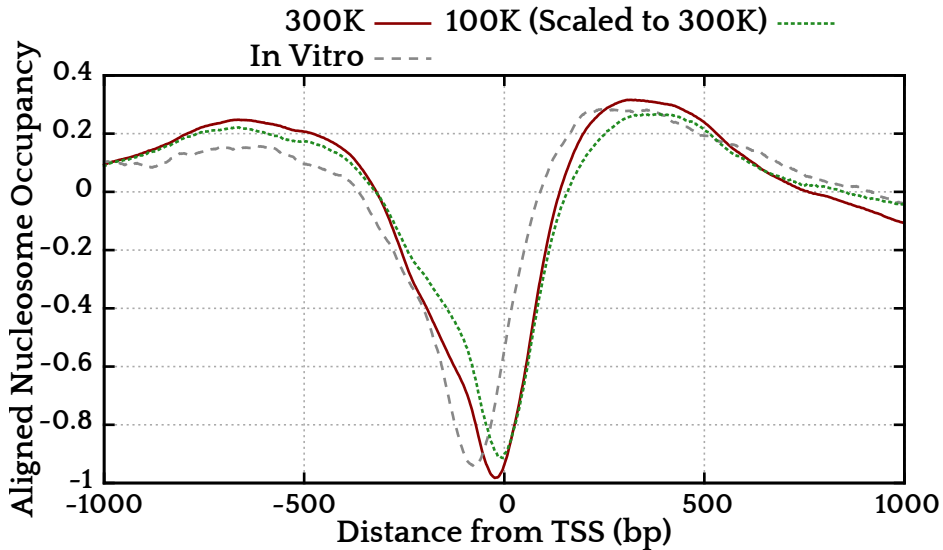


Figure A.4: As Fig. 6.2A, with the prediction using distributions derived at room temperature added. Correlation with GC content is very similar for the pure room temperature model and the low temperature model, and the predicted nucleosome occupancy signals differ little.

were derived at room temperature.) In Fig. A.4 we see that using the pure room temperature distributions leads to a slightly stronger nucleosome depletion signal. However, the differences between the two predictions are minimal, and both provide agreement with the *in vitro* data of similar quality. While this does not constitute a full do-over of the analyses performed in Chapter 6, this agreement indicates that the results of Chapter 6 are unlikely to be strongly affected by the temperature of the configurational moves in the MMC simulation, at least down to 1/3 of room temperature.

# B | A LIST OF SEQUENCES OF INTEREST

For reference, this appendix lists in full detail the nucleotide sequences of particular interest mentioned in the chapters of this thesis.

- [1] The Widom 601 sequence [85]:

```
CTGGAGAATC CCGGTGCCGA GGCCGCTCAA TTGGTCGTAG ACAGCTCTAG
CACCGCTTAA ACGCACGTAC GCGCTGTCCC CCGCGTTTTA ACCGCCAAGG
GGATTACTCC CTAGTCTCCA GGCACGTGTC AGATATATAC ATCCTGT
```

- [2] The kinetoplast DNA sequence [96, 107]:

```
GAATTCCCAA AAATGTCAAA AAATAGGCAA AAAATGCCAA AAATCCCAAA
```

- [3] The artificial, strongly curved, sequence found through MMC in Chapter 2 and Ref. [86]:

```
AACCCCTTT AAAGAGCTTT TTAGAGCTTT TAAAGCCTCT TTAACCTCT
TTAAACCTC TAAAAGCTC TTTAAGCCC TTTT
```

- [4] The straight sequence with the same dinucleotide content as (a tandem repeat of) Seq. [3], also from Chapter 2 and Ref. [86]. The entire sequence consists of 4700 nucleotides; only a fragment is given here:

```
AACCCCTTT AAAGAGCTTT TAACCCCTT TAAAGAGCTT TTAGAGCTT
TTAAAGCCTC CCTTAAAGCT CTTTACCCT CTTTAAACCC TCTAAGCTTT
TTAGAGCTTT TAAAGCCTTA AAGAGCTTTT TAGAAGCCTC TTTAAGCTCT
TTTAAAGCTC TTTAAGCCC CCCTTAAAA AGAGCTTTTT AAAAAGCTCT
TTTAAAGCTTT AAACCTCTT TAAAAGAAG CCTCTTTTT AAGCTTTTTT
AACCTCTTA AAAGCTCTTT TAAGCTTTAA ACCCCTTAAC CCTCTTT...
```

- [5] The sequence YALoo2W-826, which starts at base pair position 826 of the YALoo2W gene of *S. cerevisiae*. The sequences [6]-[23] are all modifications to this sequence, through either free MMC (in which case the starting sequence is actually irrelevant, but we mention it for the sake of coherence) or synonymous MMC, in various nucleosomal unwrapping states (see Chapter 3). The names follow the pattern Y826-LR{syn}, where L is the number of binding sites opened from the left, and R the number of sites opened from the right, and

syn is either present or not, indicating whether the sequence results from synonymous mutations or not. Nucleotides that have remained unchanged from the original sequence are printed in gray, while nucleotides that have been altered are printed in black.

CATTTTGCCC TTATTTTATT ATCGCCACAC GTTCTTTTGA TGTTTCAAGA  
AACTGTTGAA CCCTCAGTAC AAAATTCTCT AGTCGTGAAT AGCTCTATTT  
CATGGACTCA AAAGTGTTC AGGGTTGCTT ATTCCGTAAA TAATAAA

[6] Y826-o8

AAGATAAAAAG CTCTTTATAA GCCTCTTAAC CCCTATTTAA AGAGTTTTAA  
GAGCCTTTAA CGGTTTAAAA GGGGTTTTGA GGGTATATTA CCCC GCGGCC  
CGGCGCGCGC GCGCGCGCGC GCCGACGCGC GCGCGACCGG CGCGGTA

[7] Y826-o8syn

CACTTTGCCC TCATTTTATT GAGTCCTCAC GTCTCTTTGA TGTTCCAAGA  
GACCGTCGAA CCGTCTGTAC AGAACTCGTT AGTCGTTAAT TCCTCGATAT  
CGTGGACGCA GAACTGTAGT CGCGTAGCGT ACAGCGTGAA TAACAAA

[8] Y826-17

ACCCCTTTT AAGAGGAAAA GCCTCTTTAC CCCGGGTAA AGCTCTTTAA  
AGCCCTTTAA CGAGCGTTAC CTCTTTAAAG AGGGTTAAAC CGGCTACCCC  
GCCCGTCCG CGCGTCCGTC GCGCTCCGCG ACGCTCGGCG GCGCGCG

[9] Y826-17syn

CAC TTCGCTT TAATATTATT GAGTCCACAC GTCTCTTTGA TGTTCCAAGA  
GACCGTCGAA CCGAGCGTAC AGAATTCGCT AGTCGTAAAC AGCAGTATCA  
GCTGGACGCA GAACTGCAGC CGCGTCGCGT ACTCCGTCAA TAACAAA

[10] Y826-26

GAGCGGCAAA ACCCCCTTTT AACCGGTAA CCGGGGTAA AGAGTTTTAA  
GAGCCTTTAA TGCTCGTTA GAGCTCTTAA CCGTTTAAAG AGGGTTAATG  
CGGTCTTGA CCGCTCGGGC TATACTCCGC GGGCGTCCGC GCGGAG

[11] Y826-26syn

CAC TTCGCTT TAATCCTTTT AAGCCCTCAC GTCTCTTTGA TGTTCCAAGA  
GACCGTCGAA CCGTCGGTAC AGAACTCTT AGTCGTAAAC AGCTCTATAA  
GCTGGACGCA GAACTGTTTCG CGCGTAGCGT ACAGCGTTAA TAATAAA

**[12]** Y826-35

GCGCGCTCGT CGCCGCTCAA AAACCCCTTT TAAAGGTTAA AGCTCTTTAA  
 GACCTCTTAA AAGCTCATAA AGAGCTTATA ACGAGTTTAA ACTCTTAAAG  
 AGGGCTTTGA GGCTACGACG CGCGCGCCGC CGGCCGGCCG CCCGCGG

**[13]** Y826-35syn

CACTTCGCGT TGATCCTTTT AAGCCCTCAC GTAAGTTTAA TGTTCCAAGA  
 GACCGTCGAA CCGAGCGTAC AGAACTCTTT AGTGGTTAAT AGCTCTATAA  
 GCTGGACGCA GAACTGTTCG CGGGTCGCGT ACTCCGTGAA CAATAAG

**[14]** Y826-44

CCGGCTCGGG CGCGGTCGTA TACGCCCTTA AACCCCTTT AAAGAGGTAA  
 AGCCCTTTAT AAGCTCGTTT AAGCTCTTTA CCGCTCGTTA AAGGGCTTTT  
 CCGGTTTAAAG AGGGGTTTAA GCCTCTATCG CCGGTCGGGT CGCGCGC

**[15]** Y826-44syn

CACTTCGCCC TGATCCTATT AAGCCCGCAC GTATCTCTTA TGTTCCAAGA  
 GACCGTCGAA CCGTCGGTAC AGAACTCTTT AGTGGTTAAT AGTAGTATTT  
 CCTGGACGCA GAACTGTTCG AGGGTCGCGT ACAGCGTAAA CAATAAA

**[16]** Y826-53

CCGCGCCCCG CCGCGTCGTC GCGCGCCGCGA CGAGACTCTT TAACCCCTTT  
 TAAGAGTTAA CCGCGGGTAA AAGCTCTATA ACGAGCATTAA AAGGCTCTTT  
 TAAGCGTTTA ACCTTTTAAA GGGGCTTAAA CGCGTCGGCG CGTCGCG

**[17]** Y826-53syn

CACTTCGCCC TGATCCTGCT AAGTCCTCAC GTATCTCTTA TGTTCCAGGA  
 AACCGTCGAA CCCAGCGTAC AGAACTCTTT AGTGGTTAAT AGTAGTATTT  
 CGTGGACTCA AAACGTTCG AGGGTCGCGT ACTCCGTAA TAACAAA

**[18]** Y826-62

CCCCGTCGGG TAACGCGTCC CGTACGCGGT ACGCCCGCGC GTCCCCCTCA  
 AAAACCTCTT TAAAAGGTAA AGAGCTCTAA ACGCGCGTTA AAGGGCTTTT  
 ATGAGCTTTA ACCCGGGTTT ACCGGTAAA AGGGGTTTAA CAGCTCT

**[19]** Y826-62syn

CACTTCGCGT TGATCCTGCT GAGCCCTCAC GTGAGCCTTA TGTTCCAGGA  
 AACAGTCGAA CCAAGTGTAC AGAACTCTTT AGTGGTTAAT AGTAGTATTT  
 CGTGGACACA AAACGTTCG CGCGTCGCGT ACAGCGTTAA TAACAAA

**[20]** Y826-71

GCGGCTAGCG GGCCGAGAGG CGAGTCGCGG CGCCGATCGT TCGCCGACCG  
 ACCCCGCCTT TTACCCTCTT TAAACCGGTA ACGCGCATAA AAGGCTCTTA  
 AAACGCTTTA ACCCGGGGTA AAAGAGGTTA TTCGGTTTAA AGGGGGT

**[21]** Y826-71syn

CATTTGCGGC TGATCTTGCT AAGCCCGCAC GTCTCGCTCA TGTTCCAGGA  
 AACGGTCGAA CCGAGCGTTC AAAATAGTTT AGTGGTTAAT AGTAGTATTT  
 CGTGGACTCA AAAGTCTCG AGAGTCGCTT ACTCGGTTAA CAACAAA

**[22]** Y826-80

GTCCGAGGTC CGTCCGTCTA GGCCGCGCGG CGCCGCGATC GGGACGCGCG  
 ATACGGTCGC GCCCCGCTT AAACCCCTTT TAAACCGGTA AGAGGCTTTT  
 AAAGTCTTTA ACCCGGGGTA AAGAGGGTTA TTAAAGGCTT TAATCTT

**[23]** Y826-80syn

CACTTCGCGC TCATACTACT ATCGCCGCAC GTGAGCCTGA TGTTCCAGGA  
 AACGGTGGAA CCGTCCGTTC AAAACTCTCT CGTAGTAAAT AGTAGTATTT  
 CGTGGACACA AAAGTCTCG CGAGTCGCTT ATAGCGTCAA TAACAAA

**[24]** The 36-base-pair locking sequence from Rosanio *et al.* [93], providing a directional bias to their DNA rings:

TATCTGGTGG GAAACAAGCT TCAGCGATGA GATGAG







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