



Louisiana Alliance for Simulation-Guided Materials Applications

# Simulation: The “CGI” of Science

Louisiana Tech University  
Engineering & Science Day  
4-10-13





Louisiana Alliance for Simulation-Guided Materials Applications



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## KEY INDUSTRIES

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# Key Industries

ADVANCED MANUFACTURING

AGRICULTURE

AVIATION AND AEROSPACE

CLEAN-TECH

DIGITAL MEDIA AND SOFTWARE

ENERGY

ENTERTAINMENT

SPECIALTY HEALTH CARE

WATER MANAGEMENT

**JOBs = MONEY!!**



**... but it's not just about the money.  
Scientists MAKE A  
DIFFERENCE!**

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## 27 SCIENCE FICTIONS THAT BECAME SCIENCE FACTS IN 2012

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We may never have our flying cars, but the future is here. From creating fully functioning artificial leaves to hacking the human brain, science made a lot of breakthroughs this year.

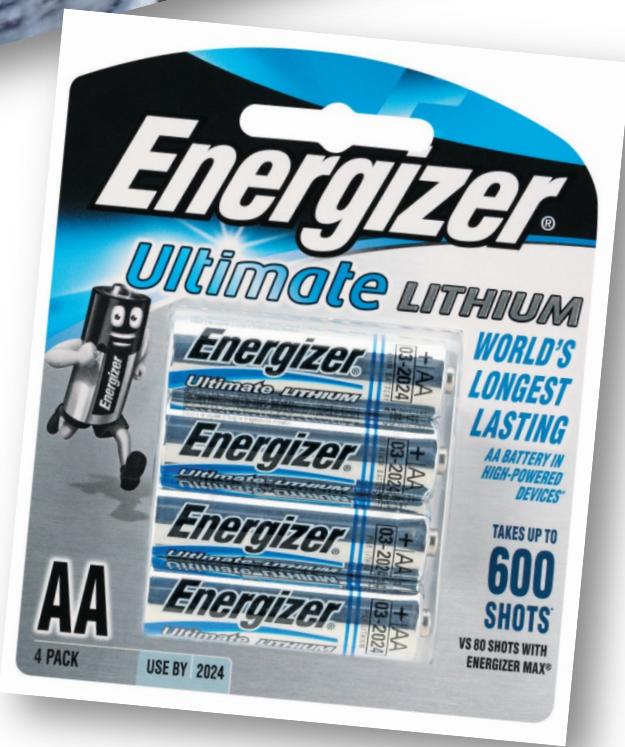
### 1. QUADRIPLEGIC USES HER MIND TO CONTROL HER ROBOTIC ARM





# LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications



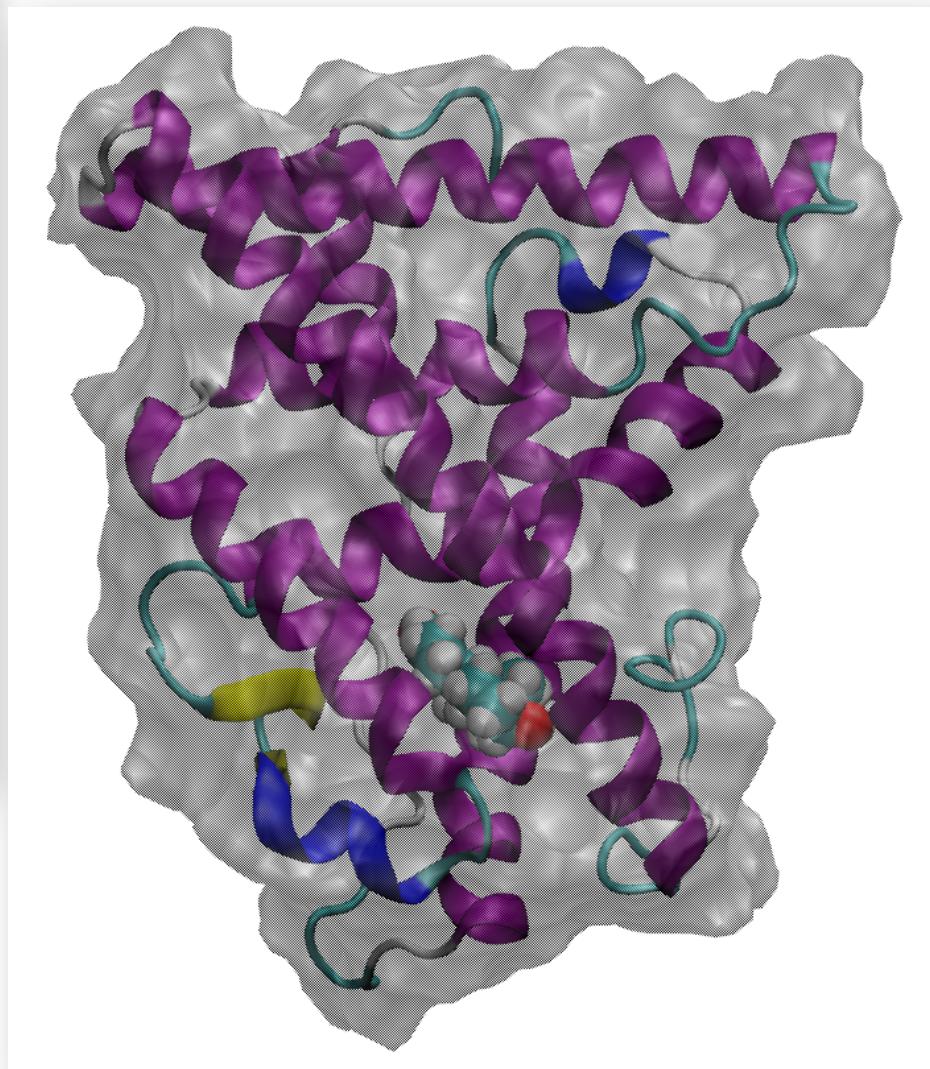
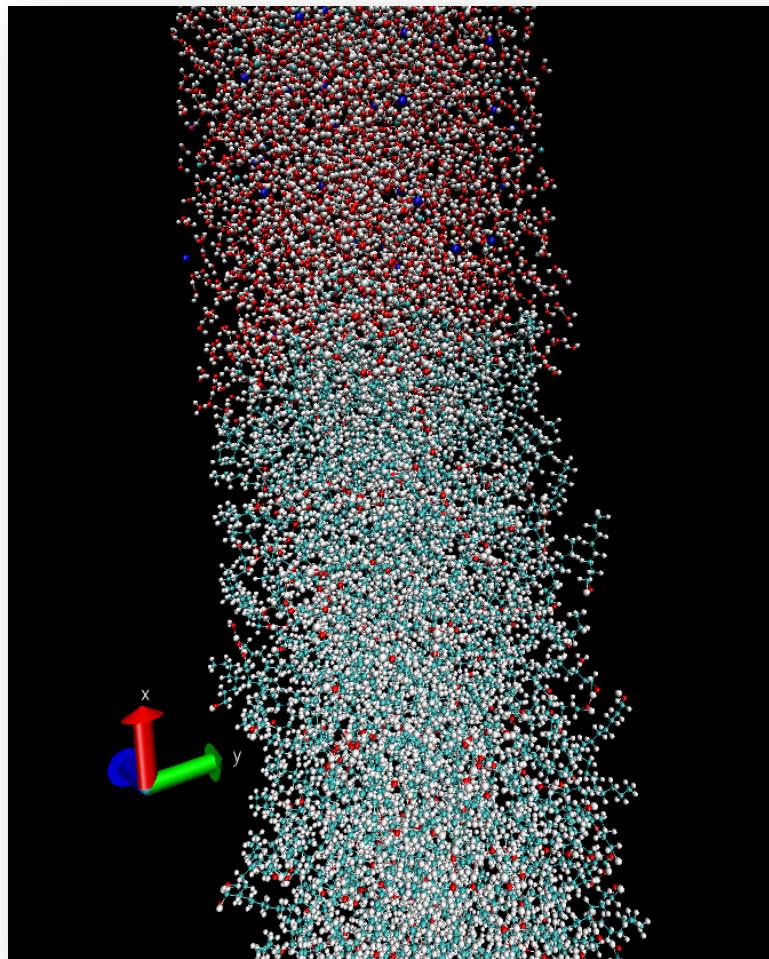


When you think of SCIENCE,  
which do you picture?



BOTH can be science!







# Victoria Bamburg

Freshman at LA Tech  
Chemical Engineering Major

Research on  
**Nucleosome Exclusion Sequences**



# A picture is worth a 1000 words



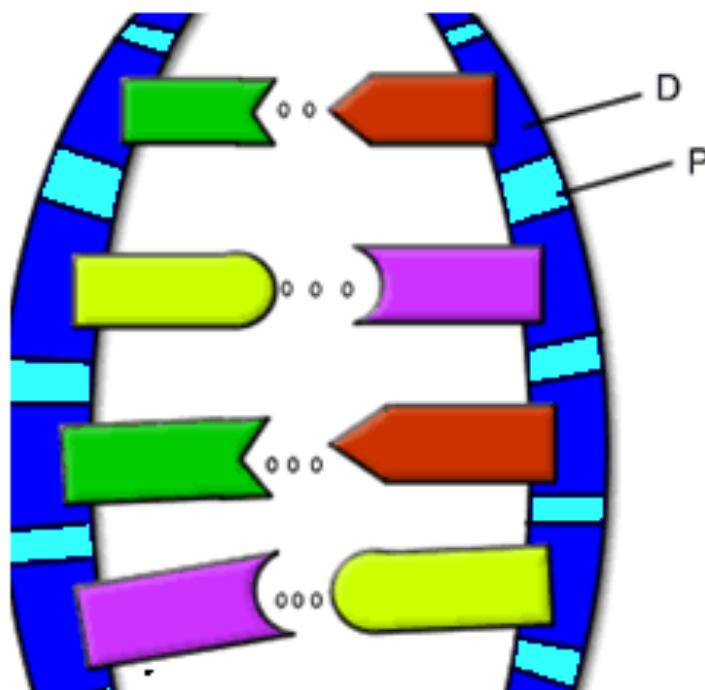
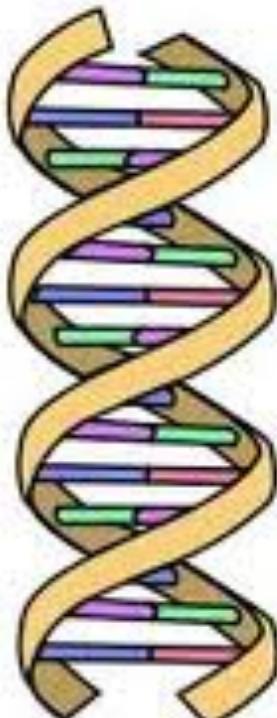
Do you see a musician or a girl's face?

... or maybe a lot of arguments.



# DeoxyriboNucleicAcid

## DNA : The Genetic Stuff



- Thymine
  - Adenine
  - Guanine
  - Cytosine
- D = Deoxyribose (sugar)
- P = Phosphate
- Hydrogen Bond

# How much DNA in a human cell?

Answer:

3,000,000,000 base pair in EVERY cell !

# How long is the DNA?

Hint: Each base pair is

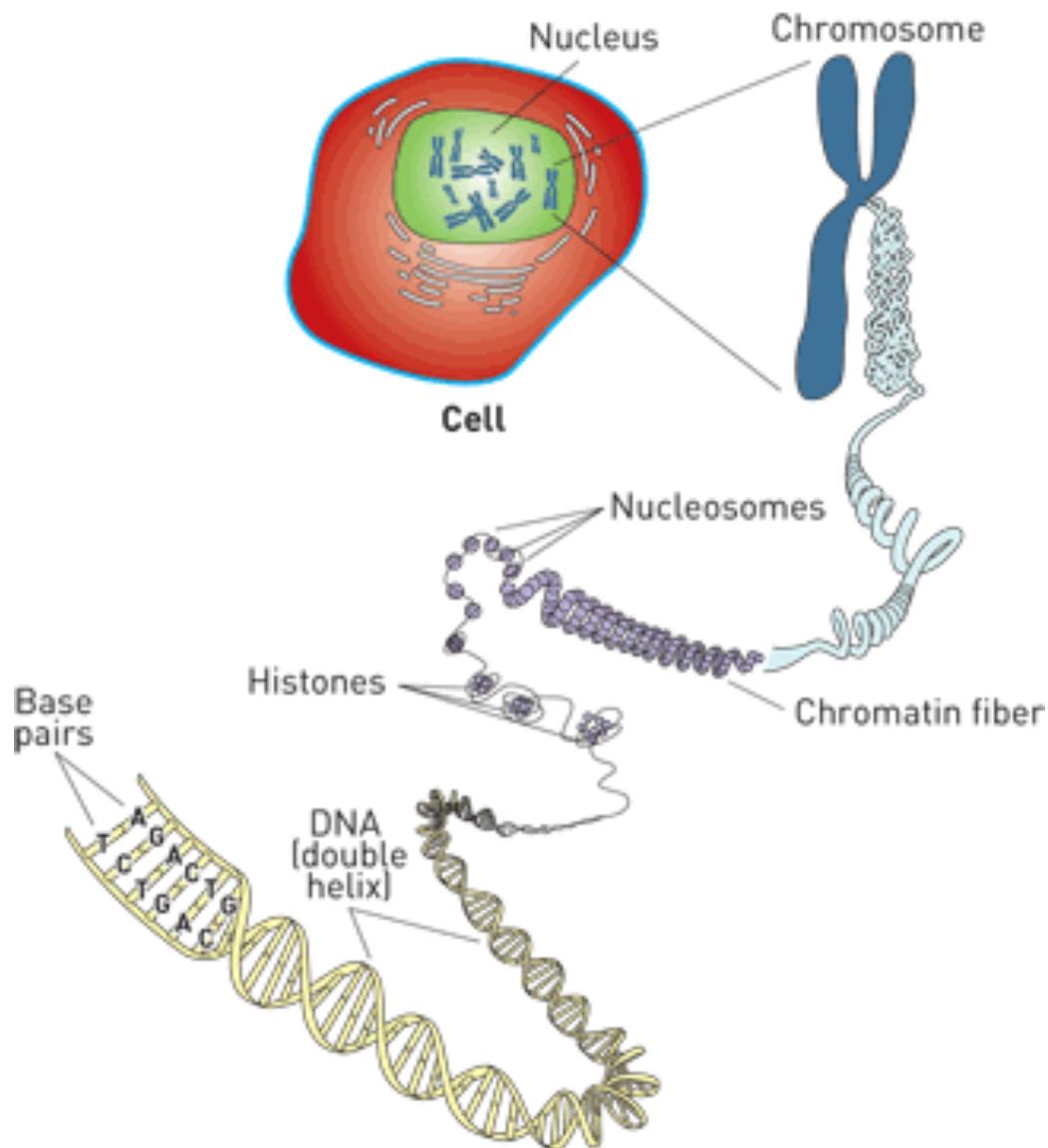
$\frac{1}{3,000,000,000}$  meters long

$$\frac{1m}{3,000,000,000} = \frac{1}{3} nm$$

# How long is the DNA?

Answer:

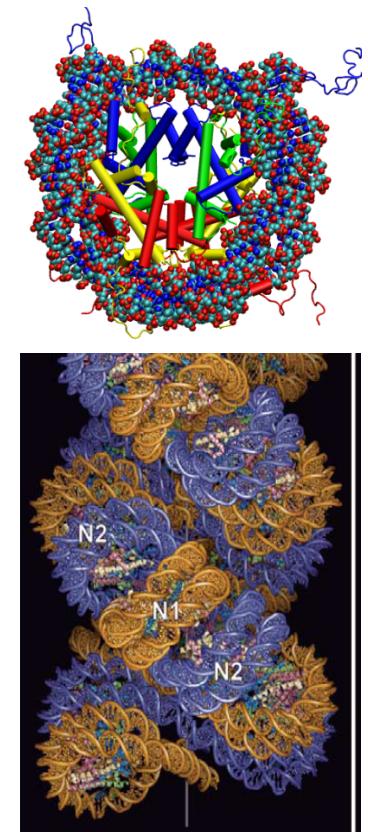
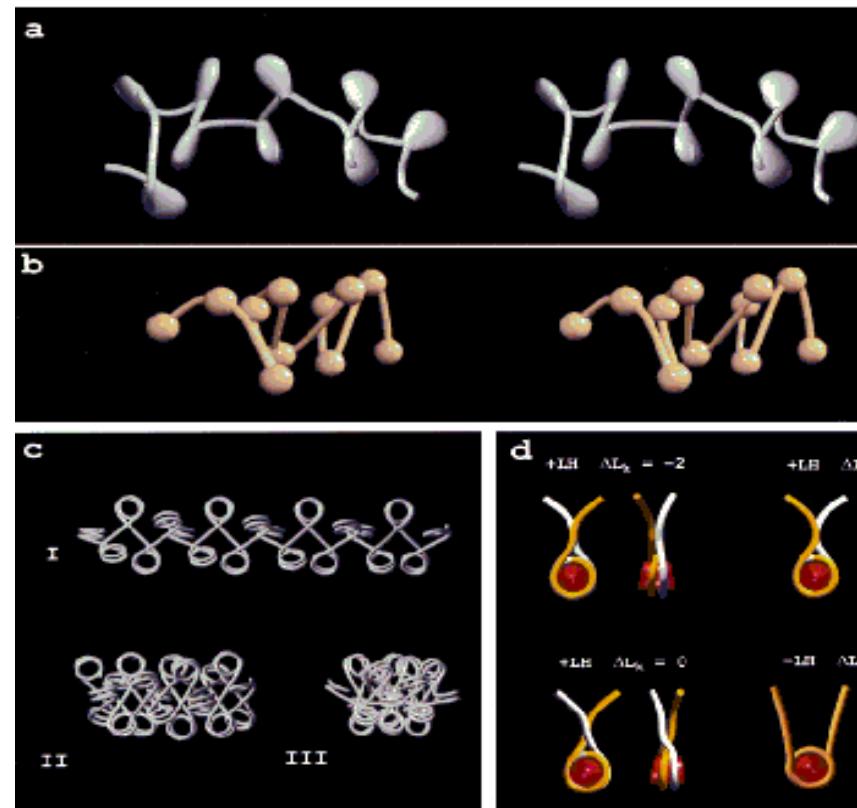
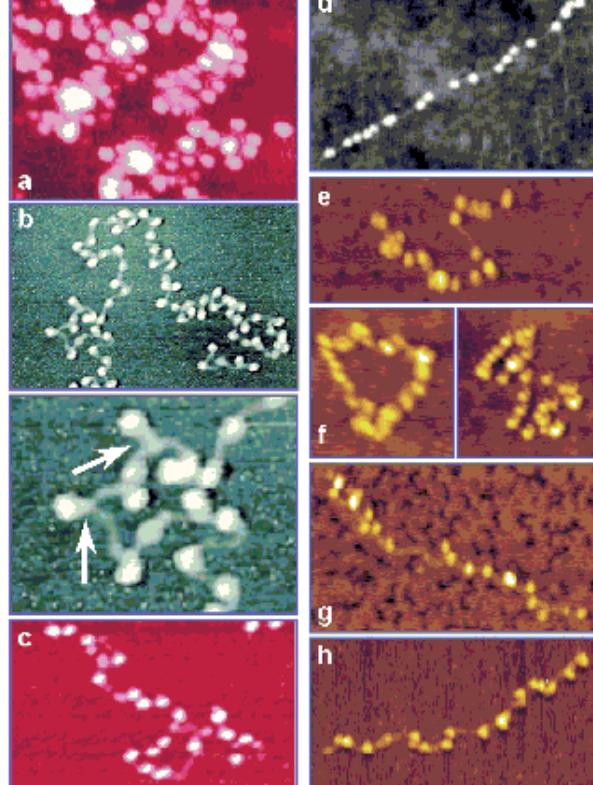
$$3,000,000,000\text{bp} \quad \times \quad \frac{1}{3,000,000,000\text{bp}} \frac{\text{m}}{\text{m}} \quad = \quad 1\text{m}$$



Chem. & Eng. News; July  
17, 2006

# Biology 101

## Nucleosomes and Chromatin

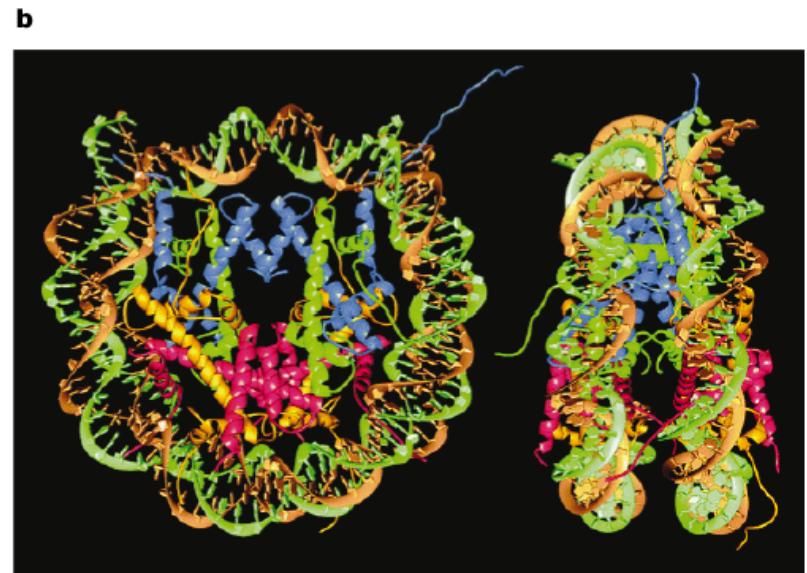
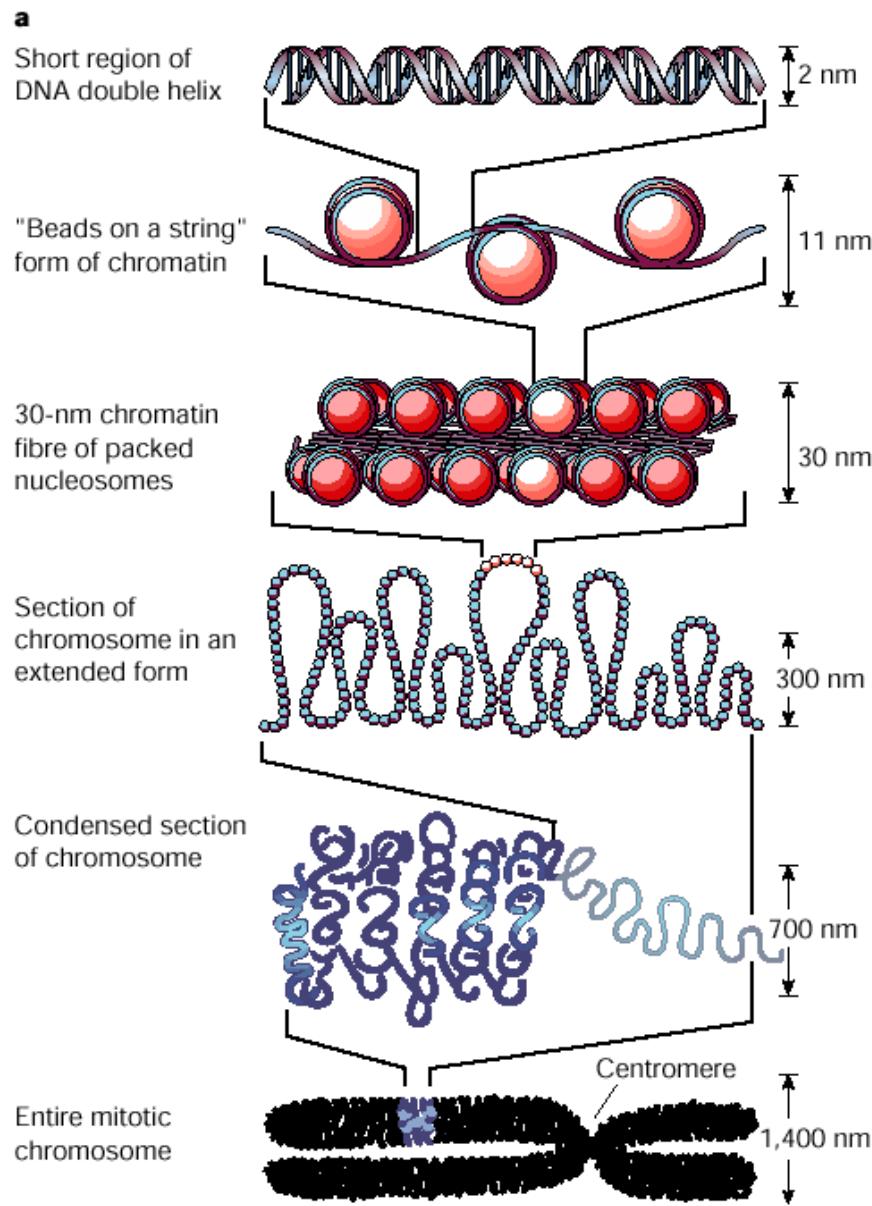


Zlatanova and Leuba  
JMB 2003

Bednar, PNAS 1998

Luger, 1997  
Schalch Nature 2005

# DNA Folding



Felsenfeld, Nat.  
2003  
Luger Nat. 1997

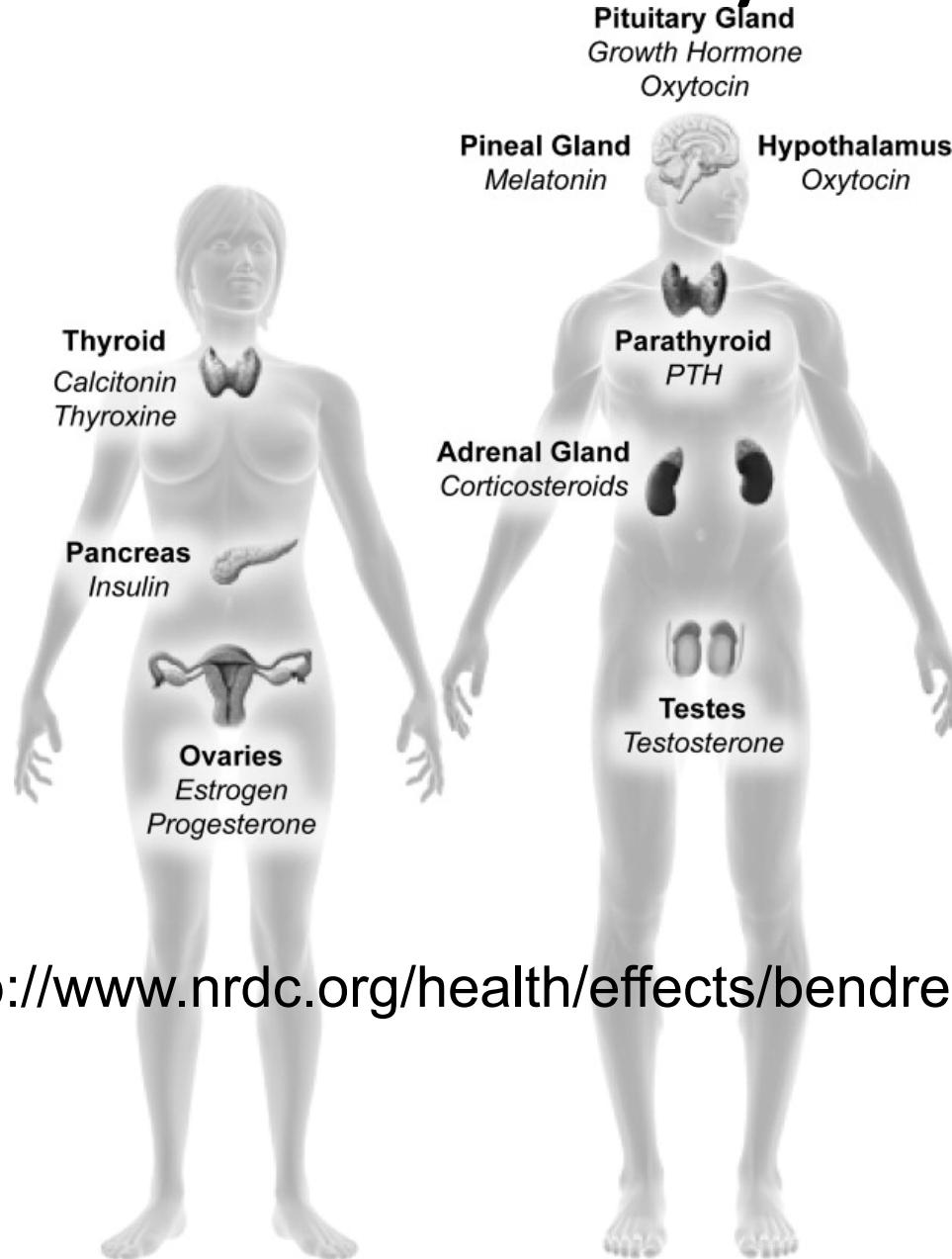
# Today's Assignment

Make a model of the

Mouse Mammary Tumor Virus  
Promoter Complex



# The Endocrine System

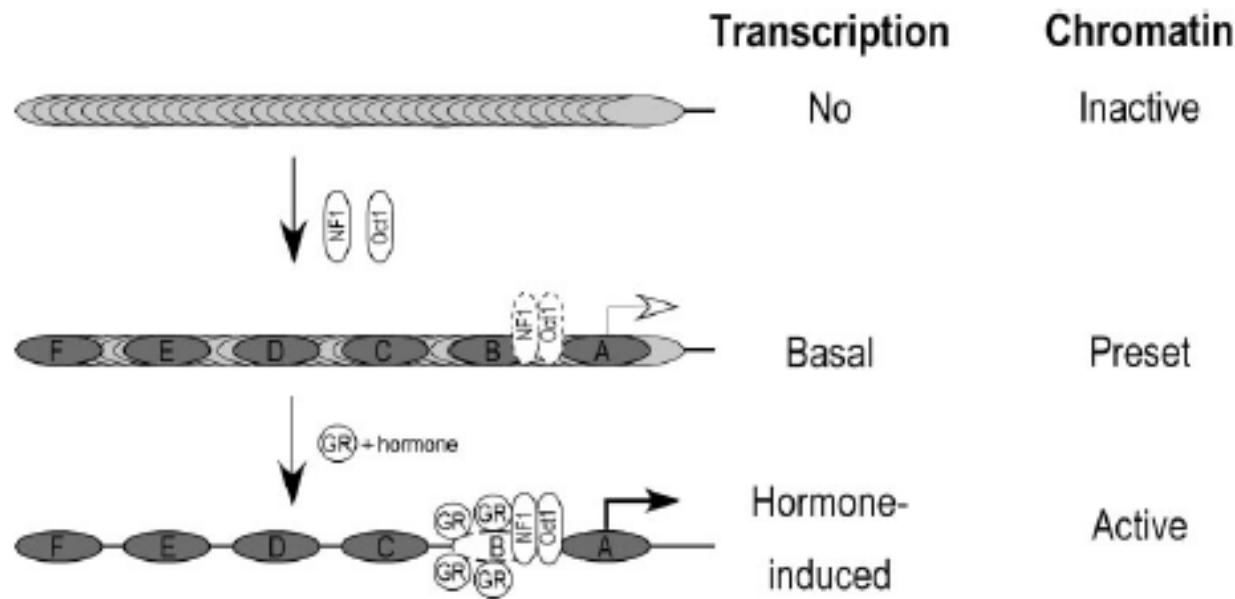


<http://www.nrdc.org/health/effects/bendrep.asp>

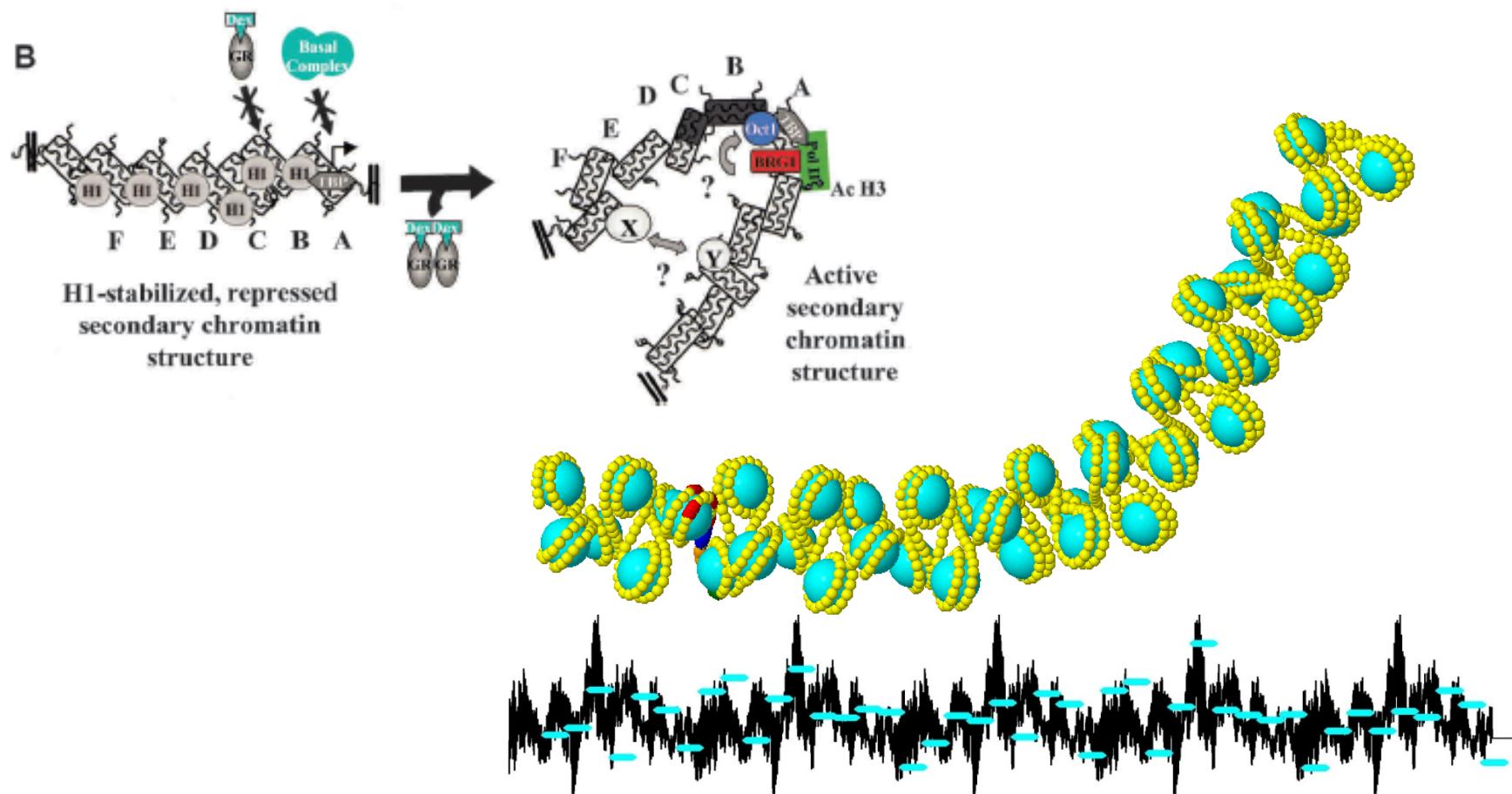
# Hormone Receptor Mechanism: MMTV

*NF1 and Oct1 Preset Chromatin in MMTV LTR*

4986



# Tandem Repeats of MMTV Yields Bent Chromatin



# MMTV Sequence Bioinformatics

**GRE**  
**NF1**  
**OCT**  
**TATA**

TGCTTCTTTAAAAA**AGAAAAAAAGGGGAAATGCCGCGCCTGCAGCAGAAATGGTTGAAC**  
TCCCAGAGTGTCCCTACACTTAGGGGAGAACGAGCCAAGGGGTGTTCCCACCAAGGAC  
GACCCGTCTGCGCACAAACGGATGAGCCCACAGACAAAGACATACTCATTCTGCTGC  
AAACTTGGCATAGCTCTGCTTGCTAGGGCTATTGGGGGAAGTTGCGGTTGTCGCTCGC  
**AGGGCTCTCACCCCTGATTCTTCATAATAACTCTCTGTGCAAGATTACAATCTAAAC**  
GATTGGAGAACTCGACCTCCTCTGGGGCAAGGACCACAGCCAACCTCCTCTTACAAG  
CCGCATCGAATTGTCCTT**AGAAATAGAAATAAGAATGCTGCTAAAAGTATATTTT**  
ACCAATAAGACCAATCCAATAGTCGATTATTAGTCACTATGTTAAGAAATGAATCATT  
TCTTTAGTACTATTTTACTCAAATT**CAGAAGTTAGAAATGGGAATAGAAATAGAAAG**  
AGACGCTAAAATCAATTGAAGAGCAGGTACAAGGACTATTGGCCTCAGGCCTAGAAGTA  
**AAAAAGGGAAAAAAGAGTGTGTTGCAAATAGGAGACAGGGTGGCAACCAAGGACT**  
TATAGGGGACCTTACATCTACAGACCAACAGATGCCCTTACCATATACAGGAAGATAT  
GA**CTTAAATTGGGATAGGTGGTCACAATCAACGGCTATAAAGTGTATACAGATCCCTC**  
**CCCTTCGTGAAAGACTCGCCAGAGCTAGACCTCCTGGTGTATGCTAACTGAGAAAGAG**  
**AAAGACGACATGAAACAACAGGTACATGATTATTTATCTAGGAA**CAGGAATGCACTT  
TGGGAAAGGTTTCCATACCAAGGAAGGGCAGTGGCTGGACTGATAGAACATTATTCT  
GCAAAAACCTATGGTATGAGTTATTGATTAGCCTTATTGCCAACCTGCGGTTCC  
CAGGGTTT**AAATAAGTTATGGTACAAACTGTTCT****TAAAACGAGGATGTGAGACAAGTG**  
**GTTTCTGACTGGTTGGTATCAAATGTTCT****GATCTGAGCTCTAGTGTCTAATTTCC**  
**TATGTTCTTTGGAATCTATCCAAGTCTTATGTAATGCTTATGTAACACATA**TTT  
AGAGTGCTGATTTTGAGTAAAC**TTGCAACAGTCCTAACATTCTCTCGTGTGTTTG**  
**TGTCGTTGCCATCCCGTCTCGCTCGTCACTTATCCTTCAC**TTTCAGAGGGTCCCC  
CGCAGATCCGGTCACCTCAGGCGGCCACTGCGCAGCTGGCGCCCGA**ACAGGGACC**  
CTCGGATAAGTGACCTGTCTTATTCTACTATTTGTGTTGCTTGTCTCT  
ATCTGTCTGGCTATCATCACAAGAGCGGAACGGACTCACCTCAGGGAA

# Interactive Chromatin Modeling

ICM ~ I see 'em

<http://localhost/icm/>

<http://www.latech.edu/~bishop>

# Thank You!



*This material is based upon work supported by the National Science Foundation under the NSF EPSCoR Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents.”*

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