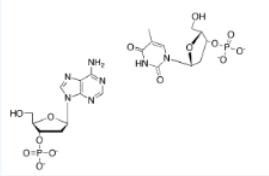
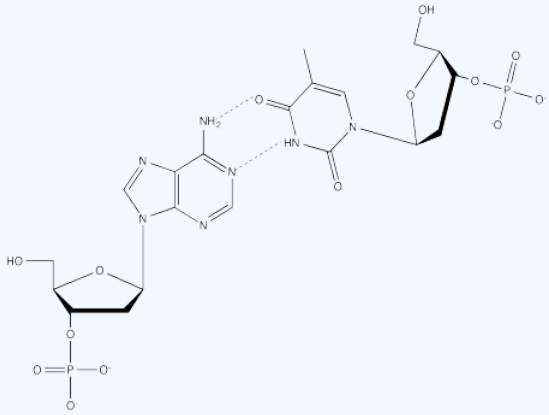
6.13: More Practice with Conformation

Exercise 6.13.1

Hydrogen bonding can have a strong influence on molecular shape. For example, it is a key factor in determining the shape of DNA. In DNA, "base pairs" in adjacent strands of DNA hydrogen bond to each other. Show how adenine and thymine, shown in the following drawing, hydrogen bond to each other.

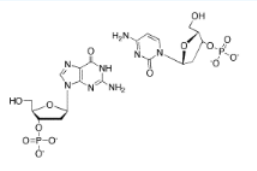


Answer

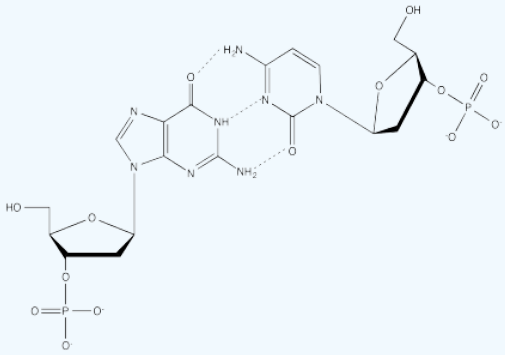


Exercise 6.13.2

Show how cytosine and guanine, shown in the following drawing, hydrogen bond to each other.

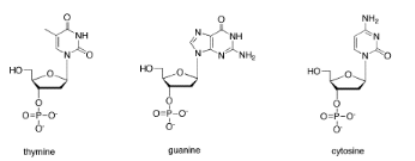


Answer

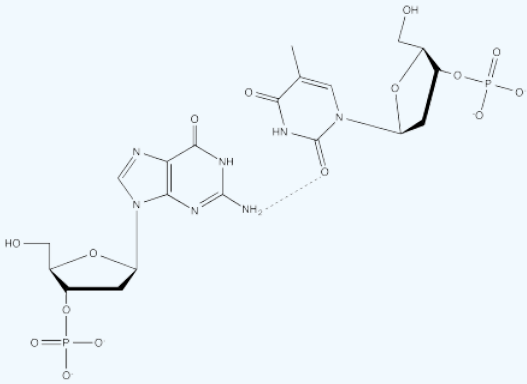


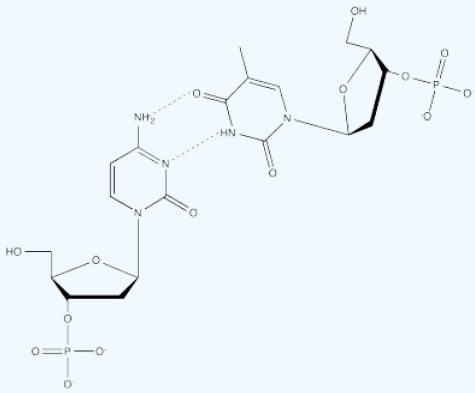
Exercise 6.13.3

Show why thymine is not well-suited to hydrogen bond to cytosine and guanine.



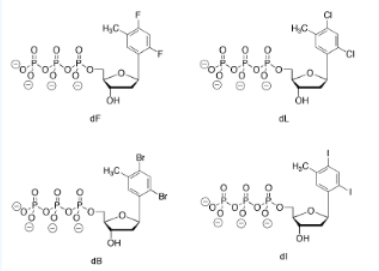
Answer





Exercise 6.13.4

Eric Kool at Stanford University has used "designer nucleotides" to study DNA polymerase and DNA repair mechanisms. He has been particularly interested in how sterics and hydrogen bonding affect these functions. The following set of nuleotides were designed to mimic a natural nucleotide. Perhaps surprisingly, these nucleotides are acceptable substrates as far as DNA polymerase is concerned, and they can be incorporated into the "correct" position in DNA.



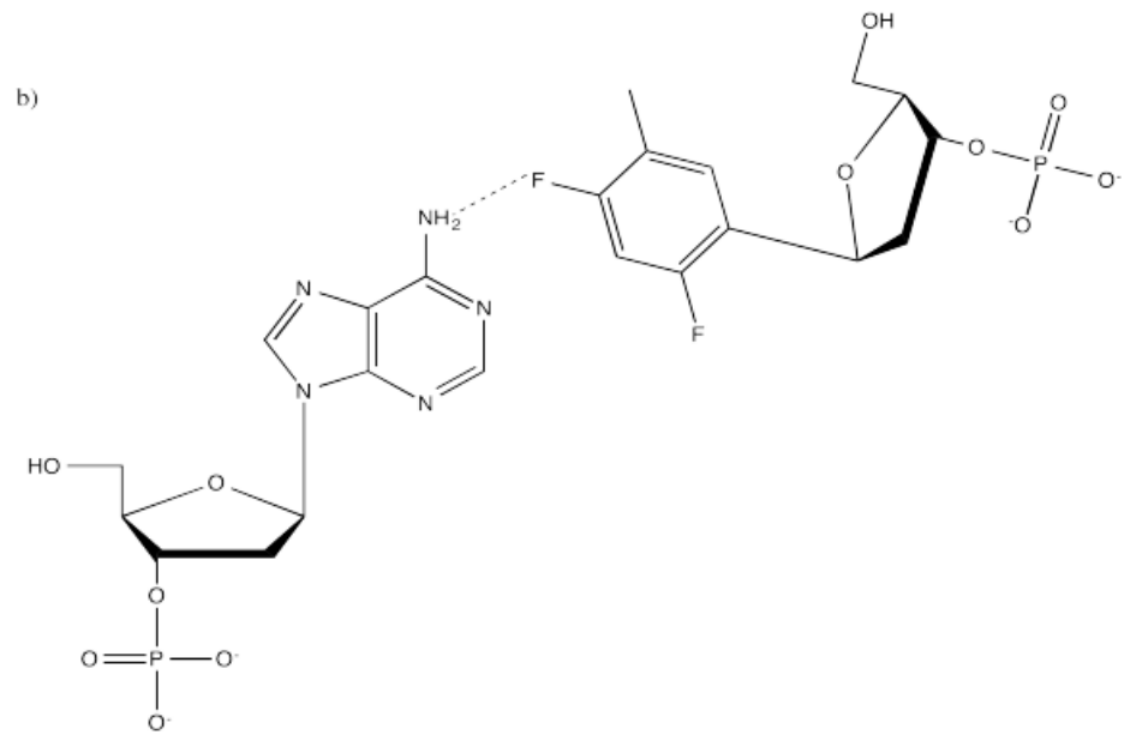
a. Which natural nucleotide do these designer molecules resemble most closely in shape?
b. Show how the designer nucleotide, dF, would fit together with the correct base pair partner for that natural nucleotide.

c. Compare and contrast these nucleotides with the natural one, in terms of their ability to hydrogen bond with the correct "base pair partner".
d. Compare and contrast these nucleotides with the natural one, in terms of their ability to fit together with the correct "base pair partner" in a DNA molecule.

Answer a:

Thymine 5'-triphosphate

Answer b:



Answer c:

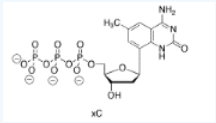
dF is only able to hydrogen bond with adinine in one position while thymine can hydrogen at two positions with thymine.

Answer d:

dF is similar in size and electronic nature to thymine. The fluorine groups on dF are somewhat smaller than oxygen on thymine, but present a comprable polar group that is able to act as a hydrogen bond acceptor. dF lacks the hydrogen bond donating ability as seen in thymine.

Exercise 6.13.5

Another one of Kool's "designer nucleotides" is shown below.

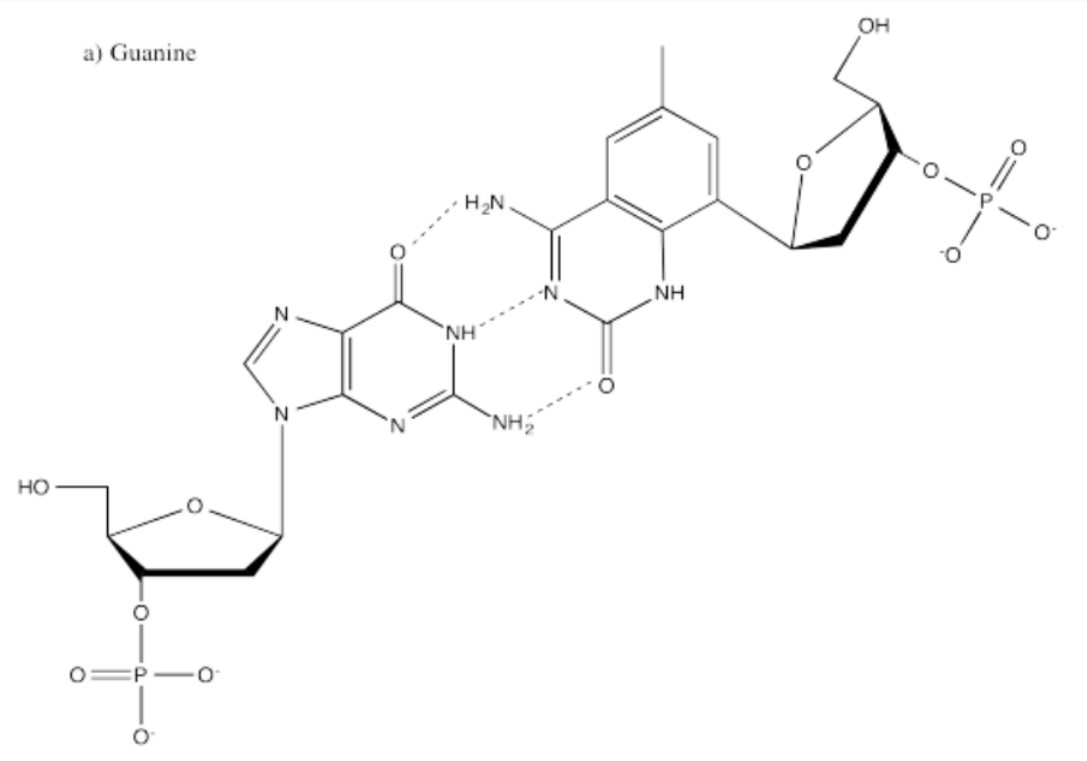


a) Which natural nucleotide would xC interact with most strongly? Show the interaction.

b) Compare and contrast xC with its natural analog, in terms of their ability to hydrogen bond with the correct "base pair partner".

c) Compare and contrast xC with its natural analog, in terms of their ability to fit together with the correct "base pair partner" in a DNA molecule.

Answer a:



Answer b:

xC is similar to cytosine. Both molecules present hydrogen bond donors and acceptors in the same positions.

Answer c:

While xC is similar to cytosine in terms of placement of hydrogen bond donors and acceptors, the additional ring creates steric problems in that the hydrogen bond donors and acceptors are placed too close to the correct "base pair partner".
