

A scientific investigation of the bases & their interactions

This worksheet is divided into 7 tasks and is accompanied by a rubric that totals 100 points. It is the first of a two-part assignment

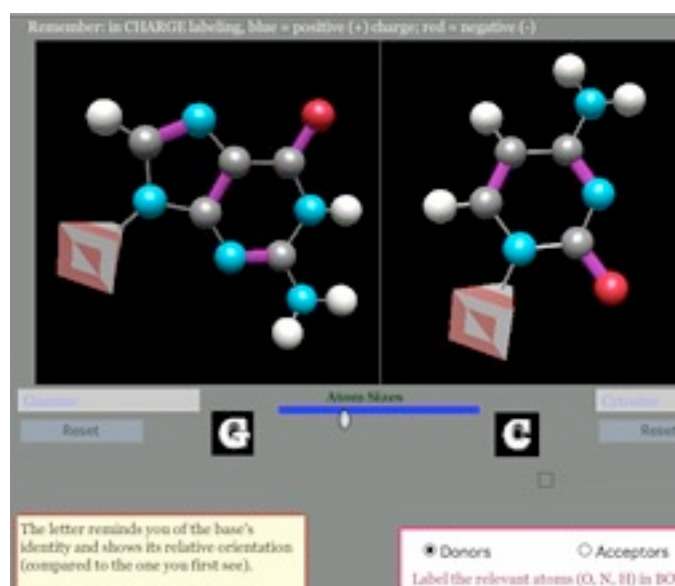
****Note** that in this guide, **questions in purple** need to be typed/written by you when doing this as homework; **things in orange** are steps you must record in the software if you wish to receive credit.

Launch **BasePairer**. When doing this for credit (logged in), the background should be light blue (not pink). As you save each pairing, you should receive an acknowledgment message and see the pairing and a code appear in the text box at the lower right of the screen. In lab, launch from the 'Not-for-credit' ContCent menu

Task 1: Selecting bases to pair

a) Choose Guanine from the left 'Bases' menu. Note the big pyramid with its 'butt' to you. This represents the ribose/phosphate structure that would be connected to the next base in line; it can also remind you of which way the base is oriented. FYI, this stuff would be as big as a base.

b) Choose Cytosine from the now-active 'Bases' menu on the right



Task 2: Identifying 'feel' (partial charges)

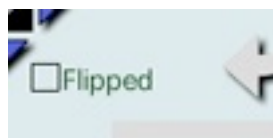
A second page, will be ask you to identify H-bond *donors* (partially positively charged hydrogens) and H-bond *acceptors* (oxygen and nitrogens bonded to C or H) that could participate in interactions. Click the appropriate atoms in the structures. In the image at left, the 'Donors' radio button is currently selected. Once you have correctly identified *all* donors and acceptors, you'll be returned to the manipulations page. Donors [partial (+)] will be marked as **blue cubes**; acceptors [partial (-)] as **red cubes**, indicating charge.

Rotation arrows

Movement



arrows



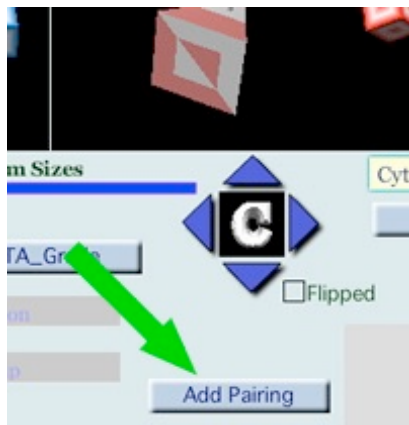
Flip checkbox (right structure only) **This will need to be done for every pairing for the rest of the assignment

Task 3: Creating interactions: pairing guanine & cytosine

Purpose: Science is understanding. You need to manipulate the bases and CREATE the pairings in order to make meaning for yourself. They're kind of little, so we'll work on the computer. Feel free to consult the physical models we provide if they help you 'connect' better with the on-screen images. The driving question here: **?How/Why do Gua & Cyt go together?** The easiest way to do this is to *characterize* the 'feel' of the right side of Gua and ask what the corresponding feel for a partner should be, then consider where these bits are on Cyt and how you need to manipulate Cyt to line things up.

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Keeping a record of your manipulations, figure out what is needed to maximize the amount of hydrogen bonding between guanine & cytosine. Note that since red = (-) and blue = (+), you're trying to match blue cubes on one molecule to reds on another.



Once you have done this, click the 'Add pairing' button at lower right (adds a code that starts with 'GC'). *Failing to do this means failing to receive credit for the assignment.* Make sure you show it to your Lab Instructor to ensure you're on the right track!

?What is the basis of the 'matching' of G and C?

?What manipulations did you perform to achieve G::C?

Note that you can revisit this pairing anytime by clicking its encoded form in the box next to 'Add Pairing' button (each basepair encoding starts with the bases used).

You'll find it useful at this point to click the 'show back path' button on the right side of the screen. It places yellow spheres where you've probably ended up placing the phosphate backbone (red & white pyramids).

Check out the 'assistance' checkbox as well.

-----!!!!**Critical note:** for the rest of the assignment, excepting only G:T, whenever you are asked to create a 'canonical pairing' or 'like Gua-Cyt' or anything of the sort, it will be in parallel to this situation--with one of the partners 'flipped', and with the ribose-phosphate groups (the pyramids) on the bottom corners, when possible with the pyramids in the yellow 'show backpath' indicators. This is the way 'proper' bases match up. Any pair that can comfortably achieve this is 'good enough' for the copying machinery, and good enough to escape notice of your repair machinery!!!!

Task 4: The other paired pair: Adenine & Thymine

To complete your set, create a correctly aligned (i.e., having the same relative orientation as Gua + Cyt) pairing of **Ade & Thy** and satisfy yourself that this 'works', remembering to flip Thy.

Again, click the 'add pairing' button to record your work (adds **AT**).

?Why do Ade & Thy form only two hydrogen bonds? Whose 'fault' is it, and what chemical change (alteration/addition/removal) could give rise to 3 bonds between these partners?

Task 5: Doing it wrong

When you think of a happy relationship, you often focus on how well you'll get along with your Significant Other. But there's the dark side, too. Most folks generally aren't all that keen on their partner spending a lot of time bumping basepairs with anybody else. The principle also applies to nucleic acids: it's all well and good that Ade & Thy pair, and that Gua and Cyt pair, but if the 'wrong' partnerships were comfortable, you'd already be dead. Take a gander at the 'wrong' pairing of Ade & Cyt.

See what Ade + Cyt does in the 'classical' orientation (following the steps you executed for G+C originally--flip the Cyt.). You'll see that there's little or no attraction there. Click the 'Add Pairing' button (adds **AC**).

?Working from top to bottom, report on the charge-charge match-ups at each potential basepairing position. Why do/don't they 'go together'?

Task 6: Guanine & Thymine doing it wrong

Everybody has memorized "A goes with T, G goes with C". This is a science course; talk counts for nothing. First, take a look at G pairing with T when aligned 'as usual'. How does that work out?

?Working from top to bottom, report on the charge-charge match-ups at each potential basepairing position. Why do GC 'go together', but GT don't?

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Task 7: can G & T pair like a pair? Can you move thymine, still properly 'flipped' so that it can form 2 H-bonds with guanine? *note: this time, you're allowed to move thymine up and down as much as you need to in order to discover good pairing!* (Hint: good = just as many H interactions as A with T!). **Once you get it, go with the 'Add pairing' button again to record your work! (Adds GT)**

Look closely & discover the *difference* between GC vs. GT pairs. You can click your saved GT structure (the code at lower right) to go back and forth between the two.

?How does a Gua-Thy pairing differ from Gua-Cyt?