HIV-1 Reverse Transcriptase Structure with RNase H Inhibitor Dihydroxy Benzoyl Naphthyl Hydrazone Bound at a Novel Site

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http://pubs.acs.org/cgi-bin/article.cgi/acbcct/2006/1/i11/html/cb600303y.html

Figure 1 of the paper referenced and linked above is available in a web-enhanced version using the Jmol software. This interactive figure nicely shows that the inhibitor binds far away from the RNase active site. This is kind of weird, since the inhibitor inhibits the RNase activity but not the polymerase activity. Using the molecular visualization software of your choice, create 3 rendered images of the HIV-1 reverse transcriptase structure described in this paper as follows:

1. A Cα backbone trace similar to that shown on p.138 of the notes.
   - use a white background
   - no color (grayscale only) for protein portion
   - show the non-H atoms of DHBNH

2. A cartoon (i.e., ribbon type representation as shown on p.138) representation.
   - use a white background
   - show the non-H atoms of DHBNH
   - the finger domain, thumb domain and RNase domain should each be clearly identified through the use of color
   - indicate the location of the polymerase and ribonuclease active sites through the use of color and/or some other trick (e.g., rendering active site residues)

3. A zoomed in view of the DHBNH binding site that emphasizes the shape and electrostatic properties of the protein cavity where the DHBNH is bound. This could best be achieved with showing the protein as an electrostatic surface representation and the DHBNH in some sort of stick, ball-and-stick, or space filling representation. Alternatively, the protein could be shown in a space-filling representation with atoms colored by type and the DHBNH in a stick or ball-and-stick representation.

These instructions are purposely vague because you are encouraged to customize the images in the way that you find best represents the structure.

The rendered images should be inserted into powerpoint or some other figure preparation software. Please save and insert images as opposed to copy and paste if you are using powerpoint. One image per slide. You should then add labels (or short legends) inside of powerpoint to make it as clear as possible just what is being represented. The N and C termini should also be labeled where appropriate.