

Evidence for shared H-bond

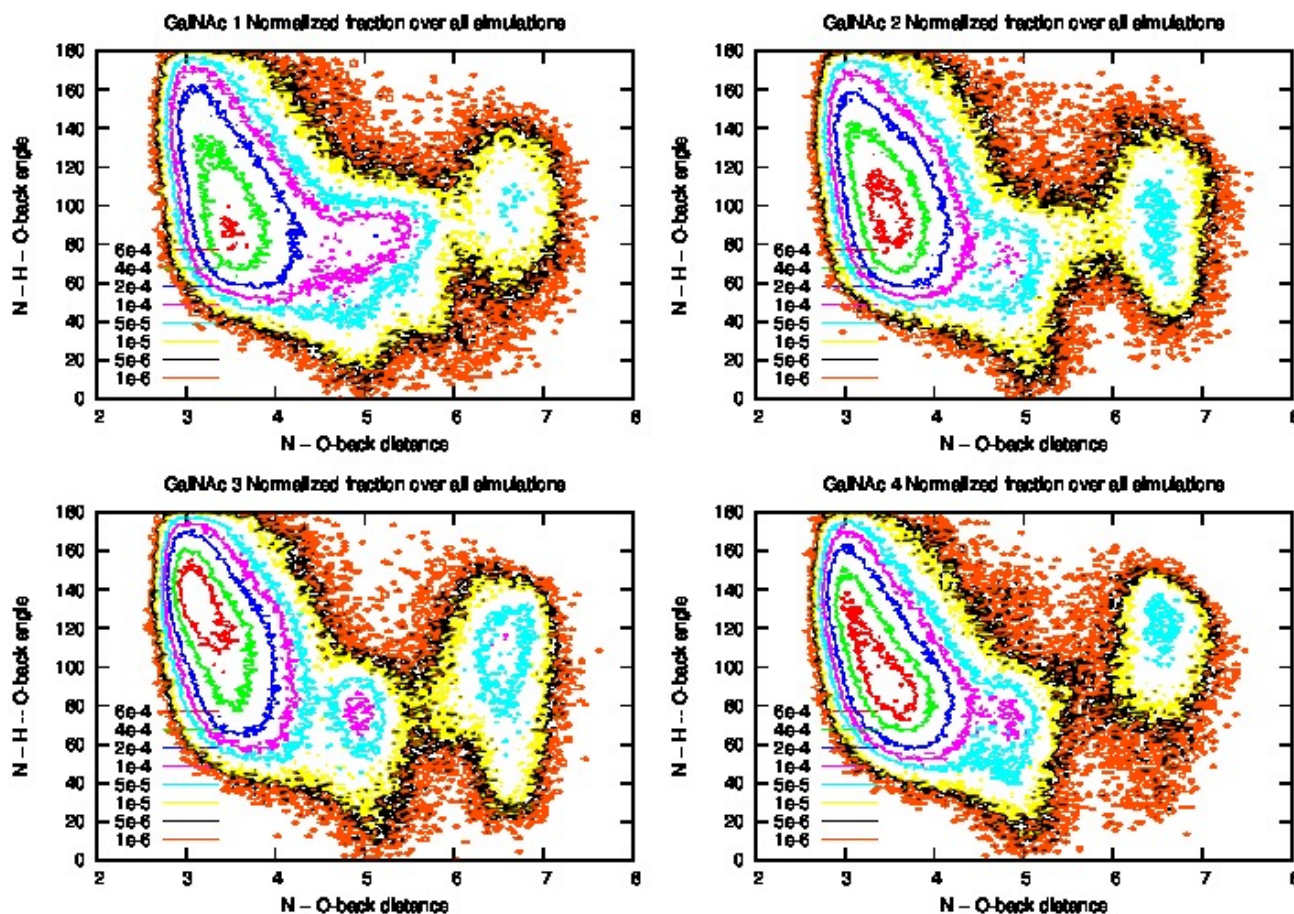
128.192.9.183/elnlachele/2013/08/22/evidence-for-shared-h-bond

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I finally got the program worked out and functioning. It's here: [do_GalNAc_analysis.c](#)
See the comments at the top of the file to see what all it does. I might make variations that save different sets of coordinates and such.

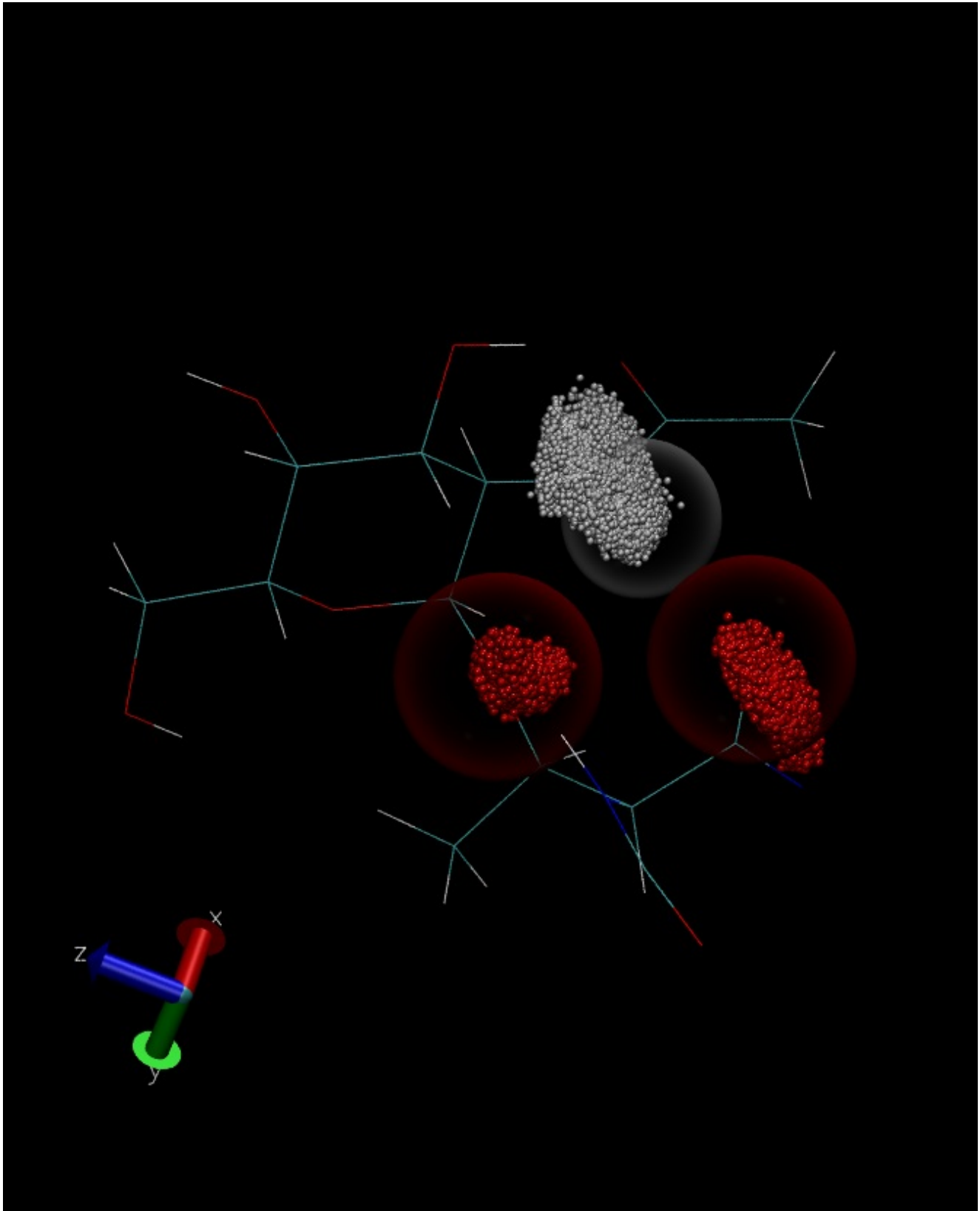
The most interesting thing I found is some pretty good evidence for a shared H-bond. The H is from the NAc on the GalNAc and the two O's are the nearest backbone O and the glycosidic O.

Consider the plot below. It shows, for all four GalNAc's, the N – O-back distance versus N – H – O-back angle. Note that all three GalNAc's seem to exist primarily in three conformations, at least with respect to those two observables. The three states are best separated for GalNAc 3.



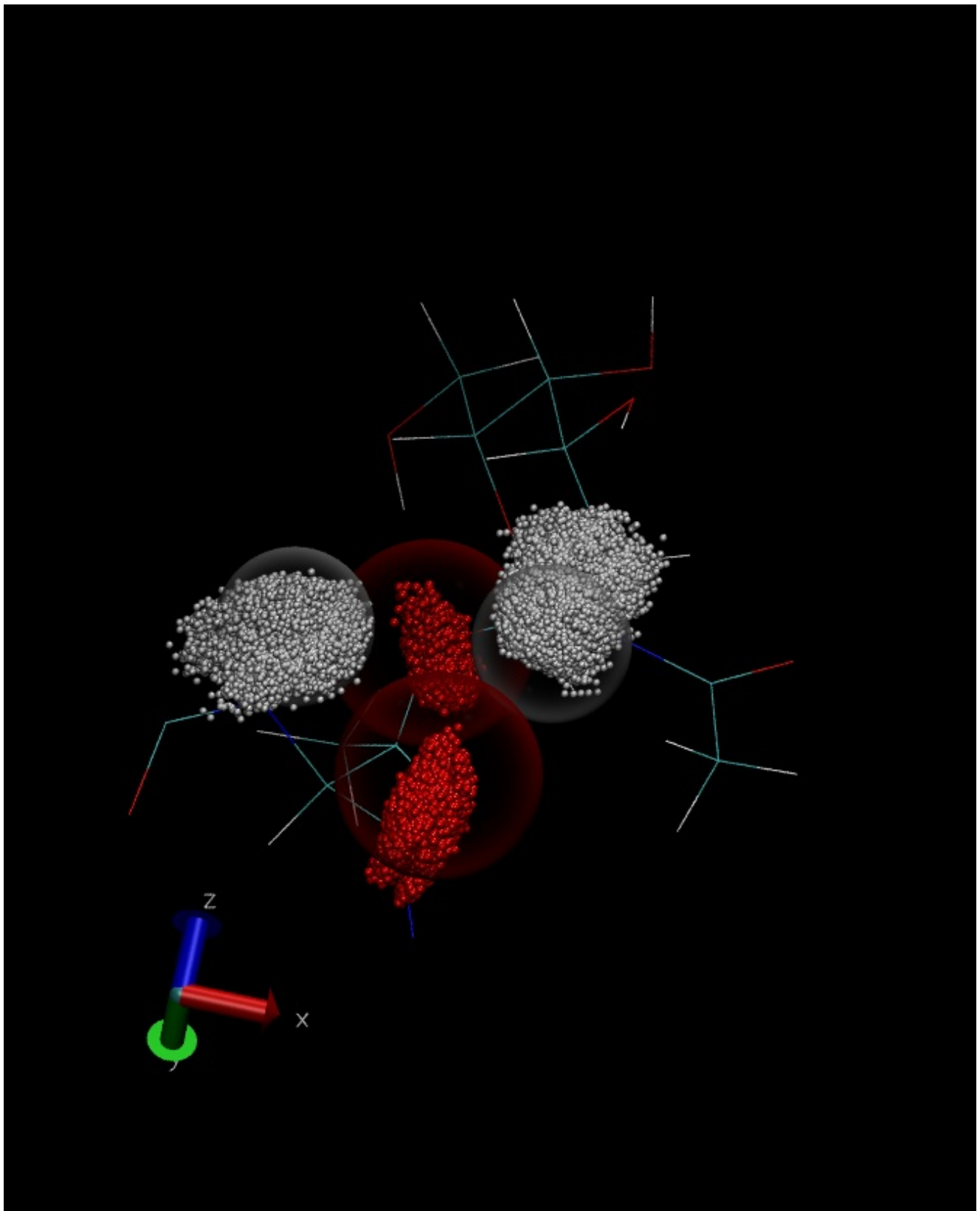
So, out of curiosity, I saved all frames, over all simulations, where the N – O-back distance was less than 4.5 (seemed a decent division between that state and the others). I aligned all trajectory frames on the NO & OG1 in the THR and the NH and H2N in the GalNAc.

Then, I had VMD represent simultaneously all the positions of the O-bak (O), O-gly (OG1) and H-NAc (H2N) over all of the frames. I represented them as small spheres in red for the O's and light gray for the H's. This is what I got:



The large, transparent spheres represent approximate van der Waals radii for the O's and the H. The center represents the last frame in the set, with that frame chosen only for convenience. This is a pretty fair representation, too. If you turn to other perspectives, the spread of the spheres doesn't change significantly (it will increase or decrease a little, of course).

Also of interest to me, though David didn't seem as impressed, is the plot below. In it, I have also represented the H from the backbone. Notice that it seems shared between the O-bak and O-glyc, but from the other side. Since the GalNAc seems to stabilize the peptide in an extended conformation, this shows one way in which it might have such influence.



I believe that the GalNAc-GalNAc interactions also play a role in stabilizing the extended structure, but haven't investigated that in as much detail or with nearly as much success.

Now, I need to get back to other analyses. I also need to remake the images above in a nicer way. I'll put a current to-do list in the next post.

