

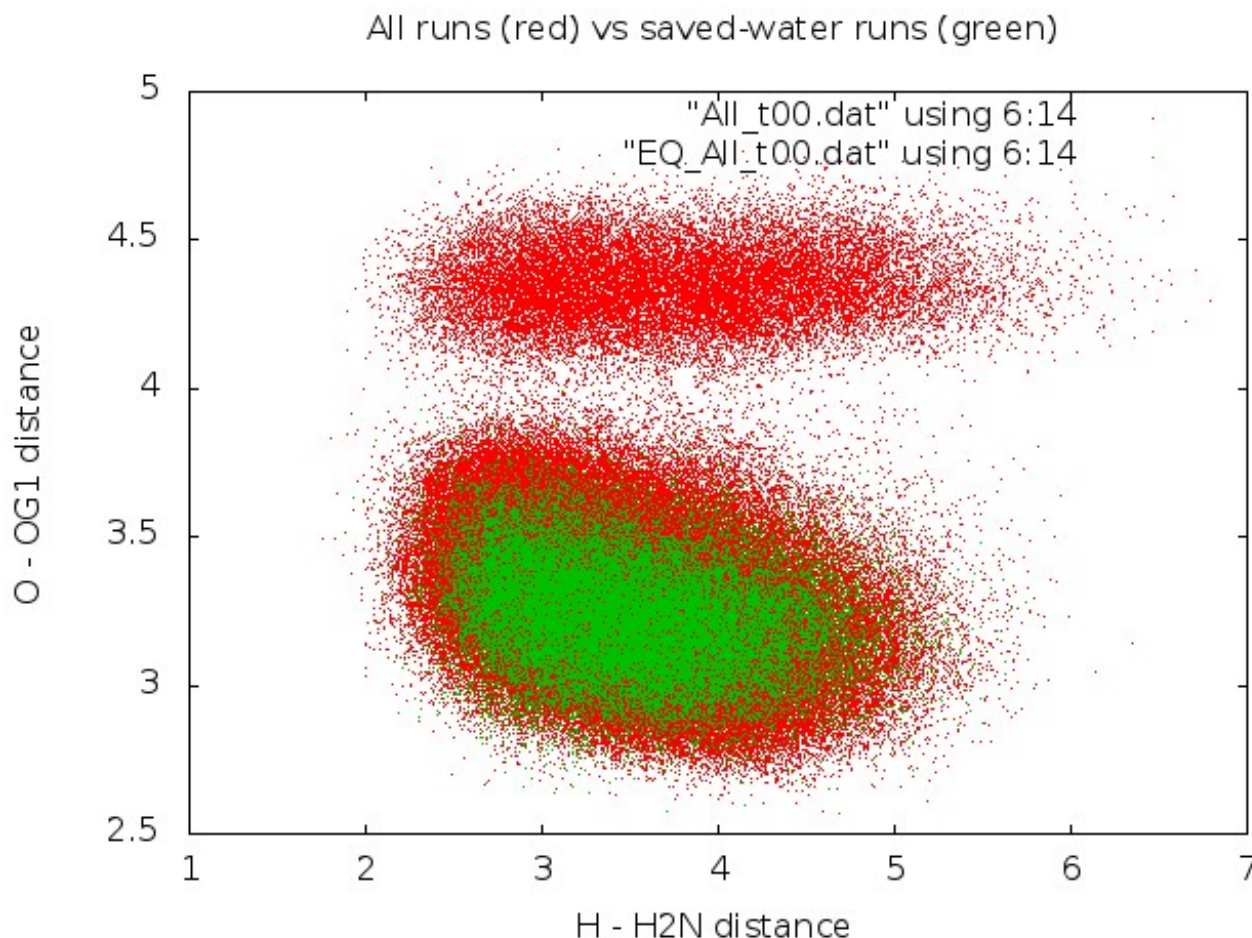
First look at water vs no-water runs

128.192.9.183/elin/lachele/2014/09/18/first-look-at-water-vs-no-water-runs

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Most runs were saved without waters. I want to know if the smaller number that were saved with waters are a reasonable approximation to the ones without. This first look says yes. So, I'll be publicly happy about it now in case the other plots aren't so supportive.

The first plot (below) shows, for the 3rd TRH/GalNAc site, that the combinations of O(backbone) – O(glycosidic) and H(backbone) – H(NAc) distances are very similar in both sets of runs. The second plot shows that the data points with O-O distances over about 4 Angstroms are a very small part of the overall set of points. There are only about 6 “green” runs for every 100 “red” ones. So, it isn't necessarily expected that there will be any green points in that region, and it's ok that there aren't. I hope the other plots turn out as nicely. BTW, the other three THR/GalNAc sites have similar plots, so I'm not showing them.



For all runs, concatenated (32 total)

