

Mucin data collection time/frame stats

 128.192.9.183/elin/lachele/2013/08/29/mucin-time-stats

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Just to have this conveniently in a location...

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Overall data:

Trajectory data was saved every 5000 steps. Each of these saved trajectory steps is a “frame.” Each simulation step represents 0.002 ps. So, frames were saved every 10 ps. Quick calculation to determine time in microseconds: move decimal in number of frames to the left five spaces. That is, 7654321 frames is 76.54321 microseconds.

There was a hardware malfunction during the runs. This caused data corruption on a few frames throughout the simulations. The corrupt frames were identified and removed. Specific numbers of frames reported here represent only the uncorrupted frames.

Also, some runs that failed (for reasons unrelated to the simulation) were restarted from the failure point, but for times longer than necessary to merely complete the simulation. For this reason, and the issue mentioned in the last paragraph, there is some variability in number of frames collected from each simulation.

The GalNAc Runs

- 32 simulations (runs) total.
- Runs 1-16 were begun from starting structures 1-16. Runs 17-32 were also begun from starting structures 1-16.

- Total frames saved in all simulations: 317739 (3.17739 microseconds)
 - 1: 9951
 - 2: 9960
 - 3: 9909
 - 4: 9942
 - 5: 9267
 - 6: 9908
 - 7: 9951
 - 8: 9251
 - 9: 9936
 - 10: 9946
 - 11: 9377
 - 12: 9928
 - 13: 12820
 - 14: 9913
 - 15: 9929
 - 16: 9935
 - 17: 9950
 - 18: 9940
 - 19: 9403
 - 20: 9925
 - 21: 9954
 - 22: 9392
 - 23: 9933
 - 24: 9950
 - 25: 9948
 - 26: 9922
 - 27: 9902
 - 28: 9945
 - 29: 9914
 - 30: 9908
 - 31: 9899
 - 32: 9931

The Mannose Runs

- 36 simulations (runs) total.
- Runs 1-36 were begun from starting structures 1-36.

- Total frames saved in all simulations: 355642 (3.55642 microseconds)
 - 1: 9943
 - 2: 9953
 - 3: 9929
 - 4: 9949
 - 5: 9938
 - 6: 9950
 - 7: 9920
 - 8: 9963
 - 9: 9950
 - 10: 9941
 - 11: 9961
 - 12: 9927
 - 13: 9924
 - 14: 9954
 - 15: 9947
 - 16: 9298
 - 17: 9915
 - 18: 9935
 - 19: 9913
 - 20: 9936
 - 21: 9952
 - 22: 9915
 - 23: 9951
 - 24: 9923
 - 25: 9953
 - 26: 9931
 - 27: 9911
 - 28: 9930
 - 29: 9910
 - 30: 9906
 - 31: 9931
 - 32: 9946
 - 33: 9692
 - 34: 10935
 - 35: 10206
 - 36: 7504

The Peptide Runs

- 48 simulations (runs) total.
- Runs 1-48 were begun from starting structures 1-48.

- Total frames saved in all simulations: 520407 (5.20407 microseconds)
 - 1: 9999
 - 2: 10865
 - 3: 10835
 - 4: 10945
 - 5: 10939
 - 6: 11241
 - 7: 10490
 - 8: 11007
 - 9: 11219
 - 10: 11151
 - 11: 10600
 - 12: 10900
 - 13: 10528
 - 14: 11266
 - 15: 10547
 - 16: 10801
 - 17: 10638
 - 18: 10365
 - 19: 10775
 - 20: 11300
 - 21: 11168
 - 22: 10626
 - 23: 11088
 - 24: 10493
 - 25: 10848
 - 26: 10164
 - 27: 10792
 - 28: 11429
 - 29: 10788
 - 30: 10729
 - 31: 10484
 - 32: 10264
 - 33: 10862
 - 34: 10925
 - 35: 11463
 - 36: 10776
 - 37: 10458
 - 38: 10659
 - 39: 11096
 - 40: 10680

- 41: 11882
- 42: 11148
- 43: 11317
- 44: 10946
- 45: 11335
- 46: 10883
- 47: 10685
- 48: 10008