

Biophysics Assignment - 2  
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18MS075

1) The data for the different molecules are arranged in different rows and the data for the position of one molecule on its random walk is given in the same row.

2)

	No of Time frames	No of Molecules	Size of each time frame(ps)	Total time of run(ps)
Pure Water	8000	30	0.1	800
Glucose	8000	45	0.1	800

3)i)

For Pure Water

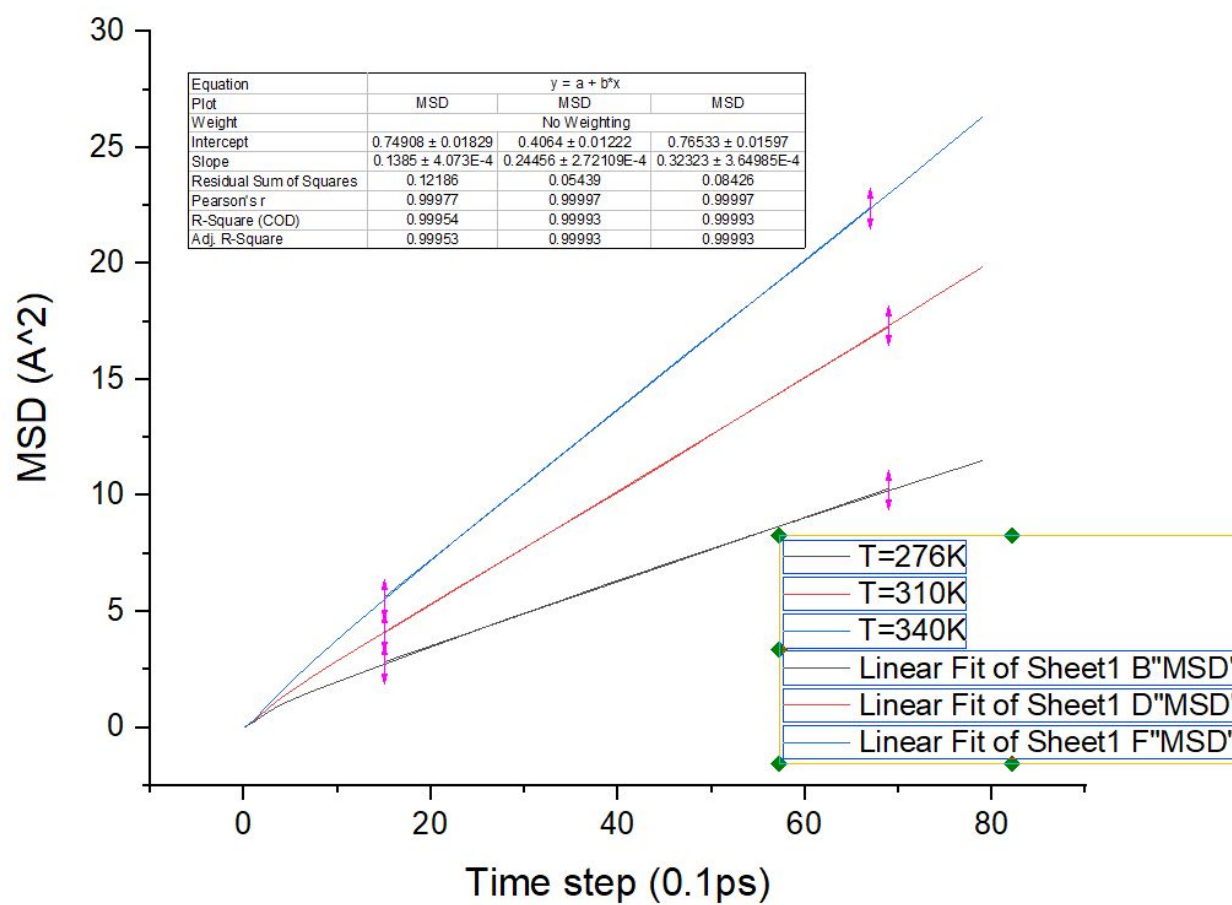
Tcor	Number of Molecules
80	5
400	15
800	20
800	30
2000	30

For Glucose

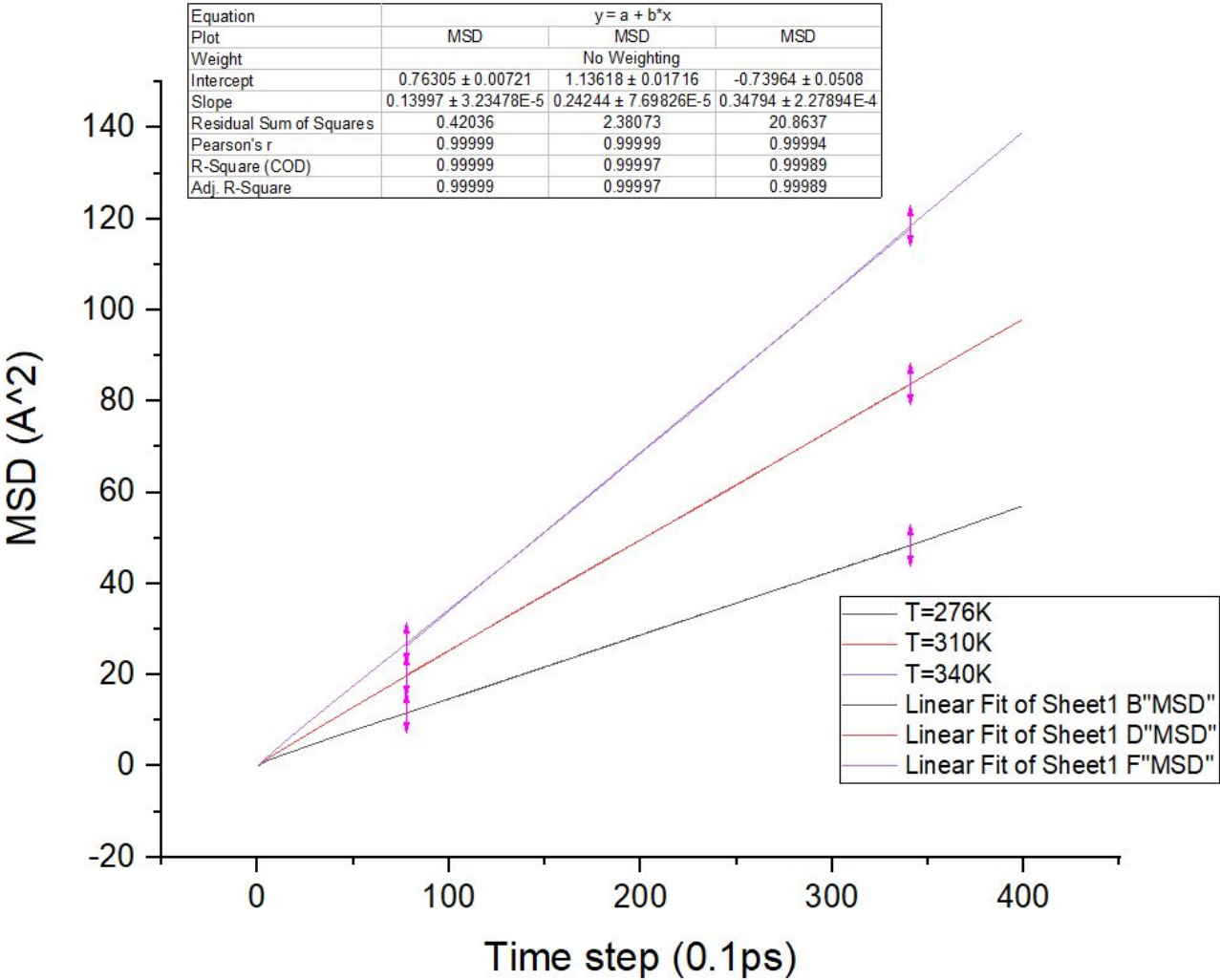
Tcor	Number of Molecules
800	5
4000	5
800	15
4000	15
800	30

ii)

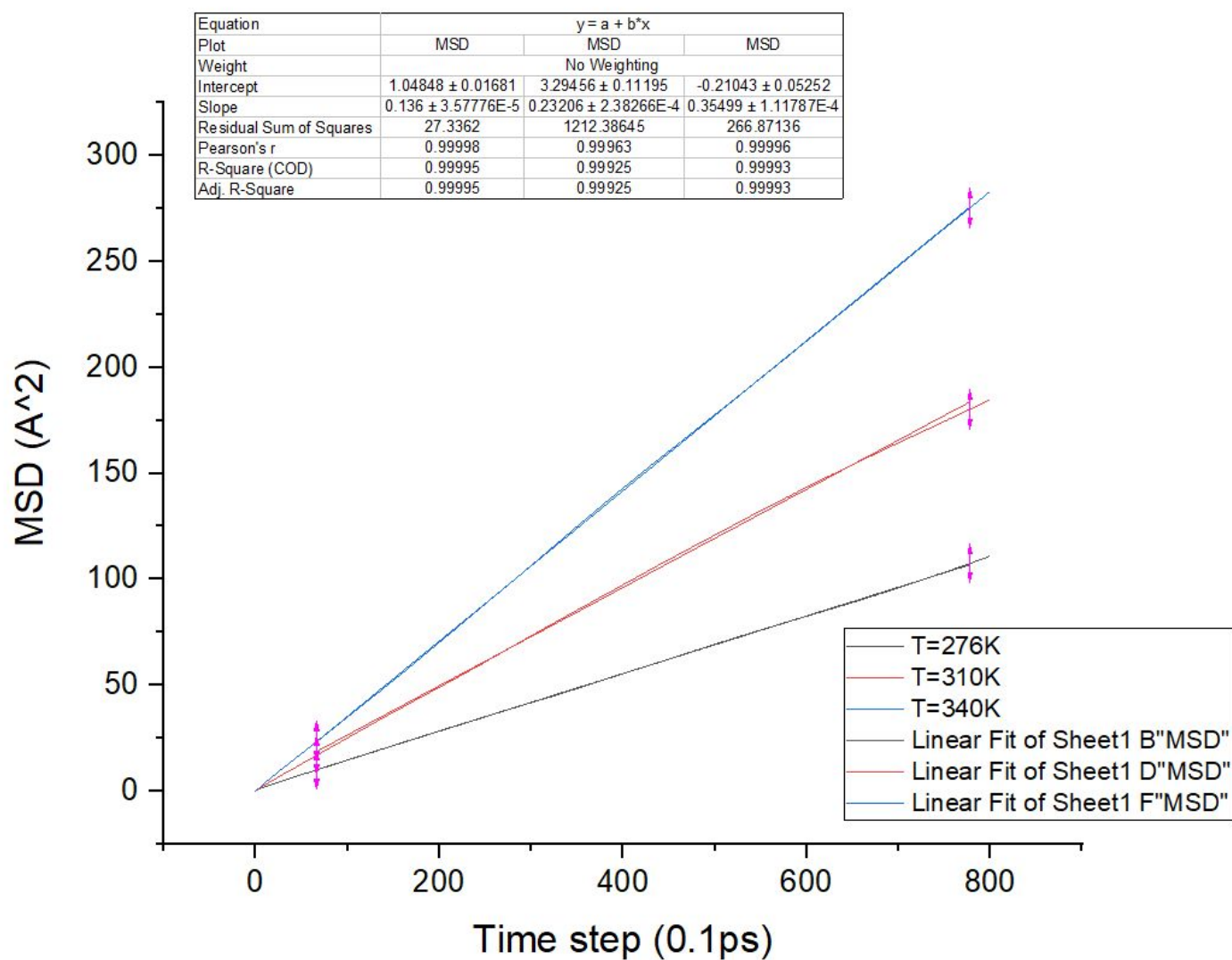
Pure water (molecules= 5, tcor= 80)



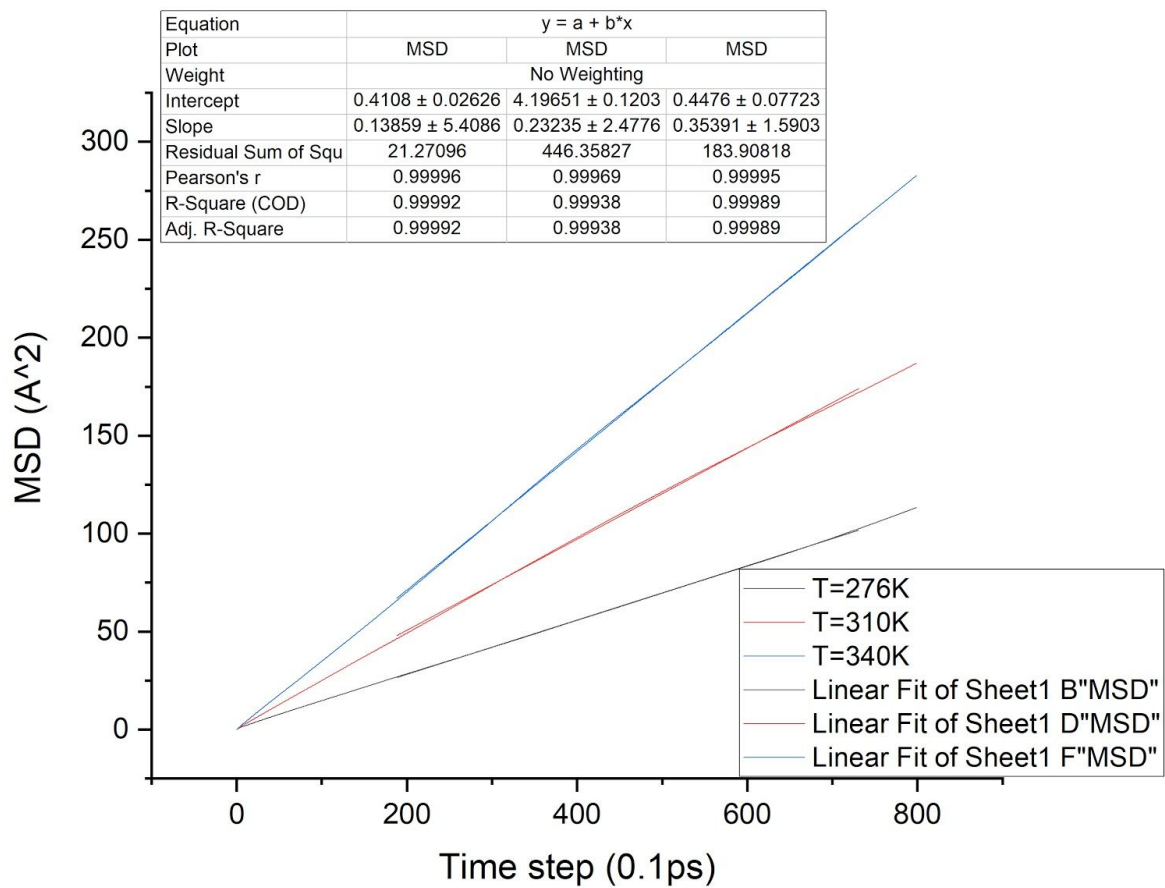
Pure water (molecules= 15, tcor= 400)



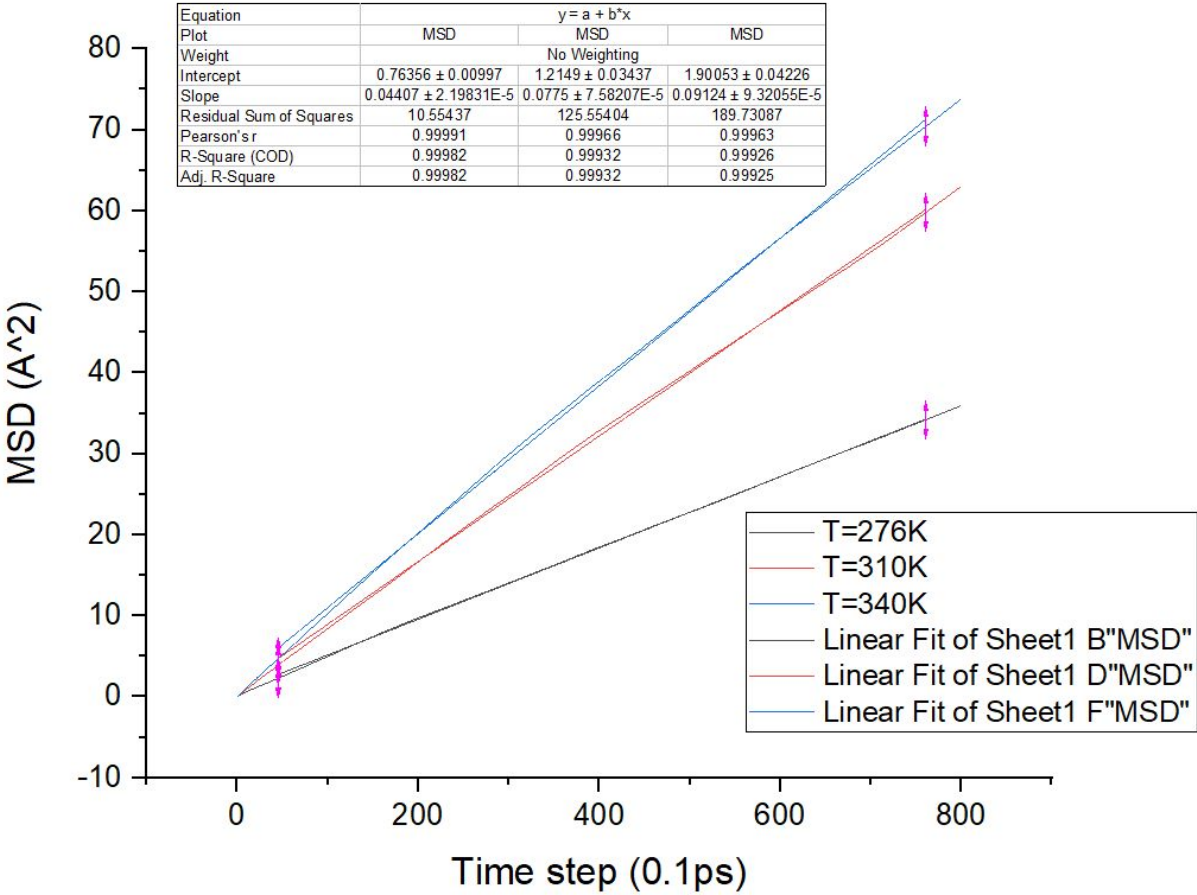
Pure water (molecules= 20, tcor= 800)



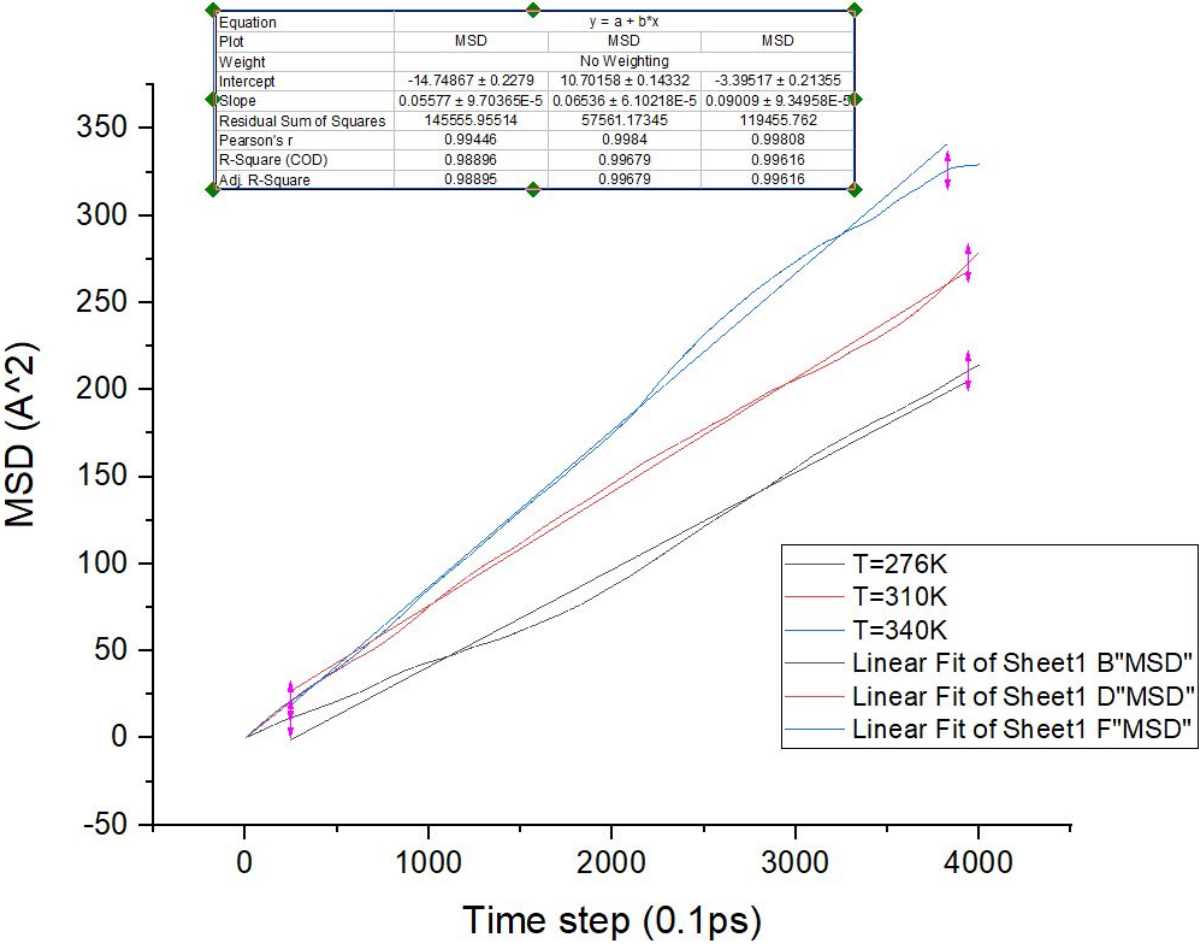
Pure water (molecules= 30, tcor= 800)



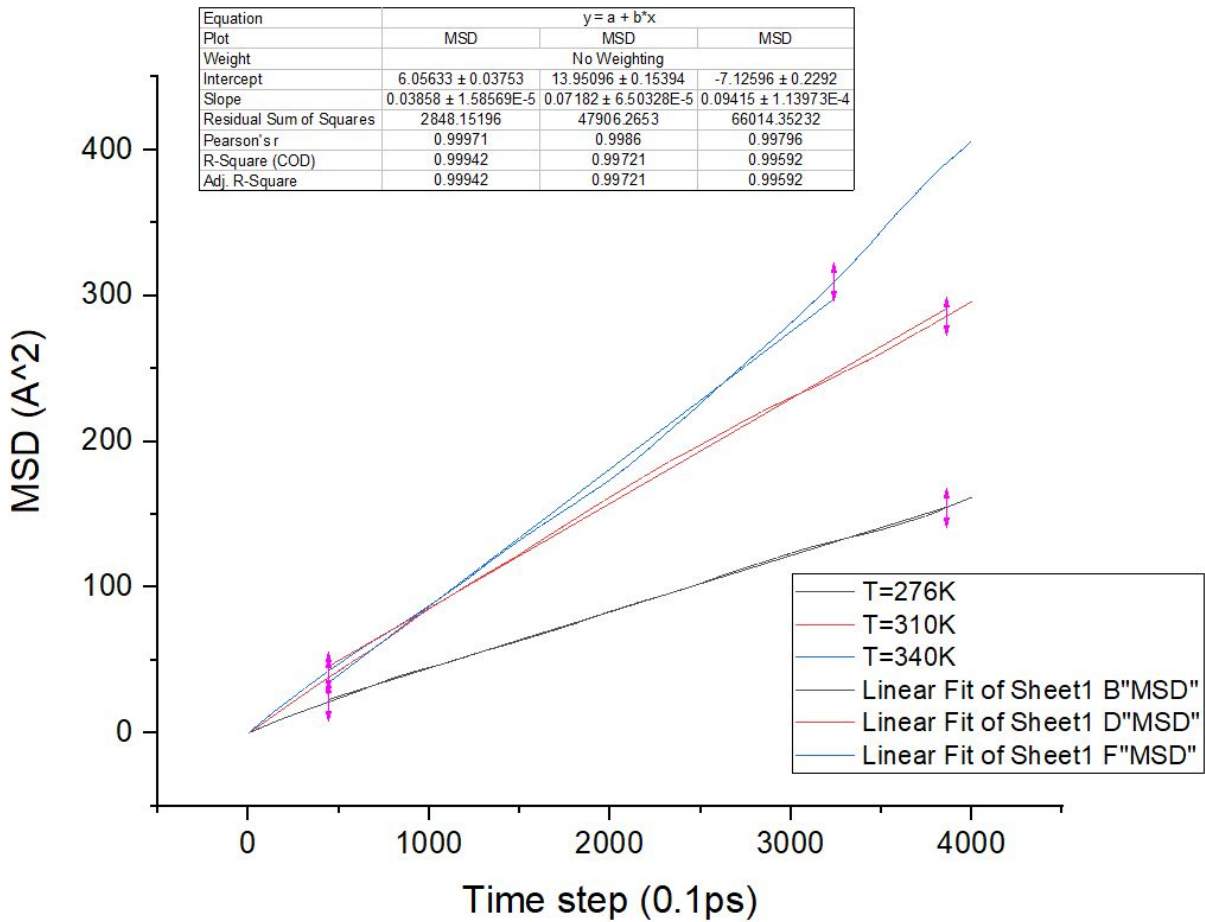
Glucose (molecules= 5, tcor= 800)



Pure water (molecules= 5, tcor= 4000)

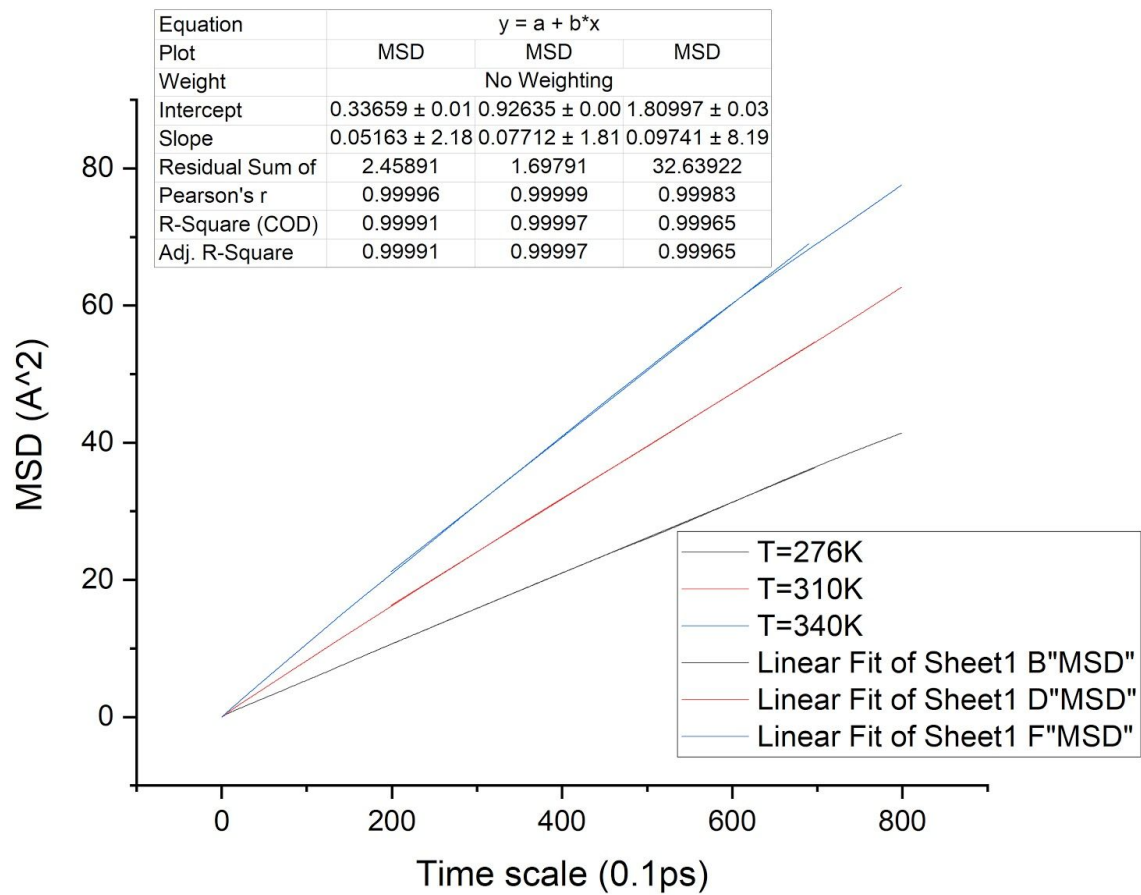


Glucose (molecules= 15, tcor= 4000)

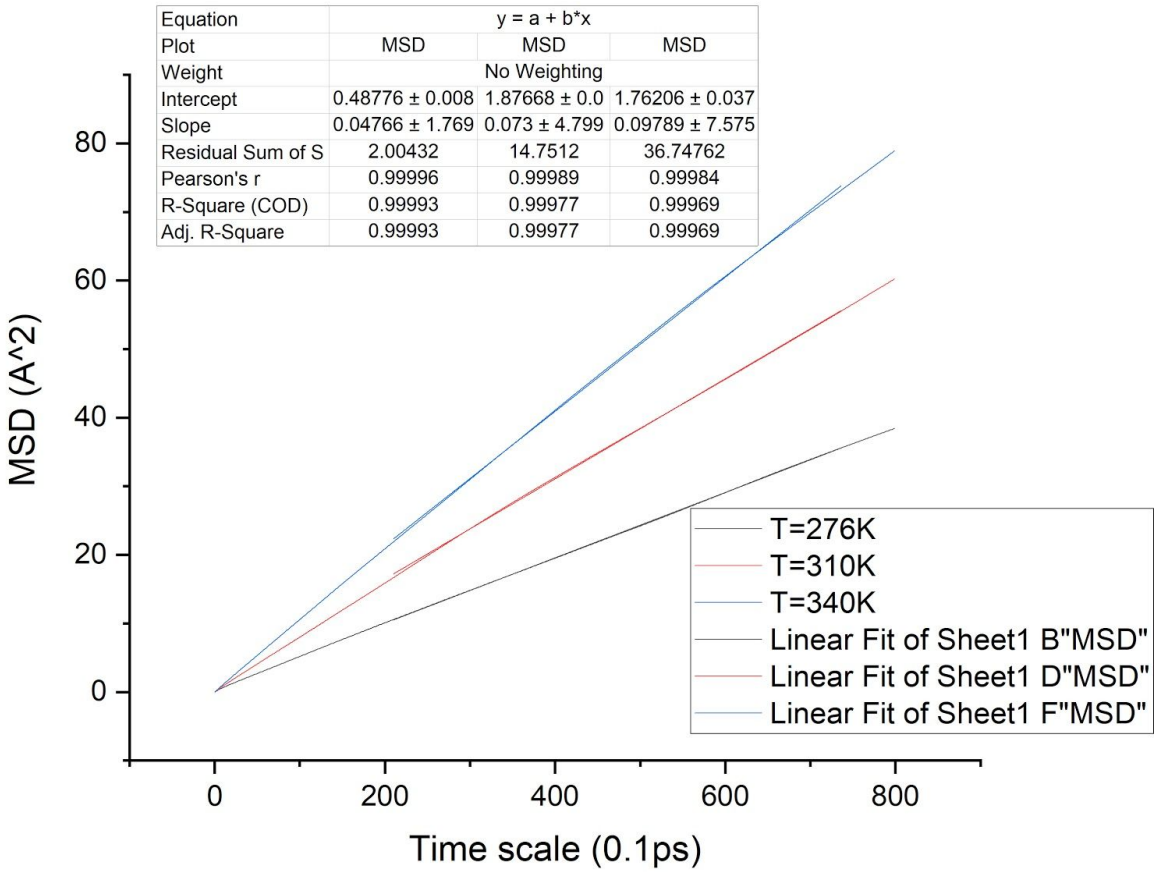




Glucose (molecules= 15, tcor= 800)



Glucose (molecules= 30, tcor= 800)



iii) Pure Water

	No. of Molecules	<u>Tcor</u>	Slope of the fit ( $A^2/0.1$ <u>ps</u> )	Diffusion constant ( $A^2/0.1$ <u>ps</u> )	Diffusion constant ( $cm^2/sec$ )
Temperature = 276 K	5	80	0.1385	0.02	0.02e-3
	15	400	0.13997	0.02333	0.02333e-3
	20	800	0.136	0.02266	0.02266e-3
	30	800	0.13859	0.02309	0.02309e-3
	30	2000	0.15549	0.025915	0.025915e-3
Temperature = 310K	5	80	0.24456	0.04076	0.04076e-3
	15	400	0.24244	0.040406	0.040406e-3
	20	800	0.23206	0.03867	0.03867e-3
	30	800	0.23235	0.038725	0.038725e-3
	30	2000	0.23212	0.03868	0.03868e-3
Temperature = 340 K	5	80	0.32323	0.05387	0.05387e-3
	15	400	0.34794	0.05799	0.05799e-3
	20	800	0.35499	0.059165	0.059165e-3
	30	800	0.35391	0.05898	0.05898e-3
	30	2000	0.36885	0.06147	0.06147e-3

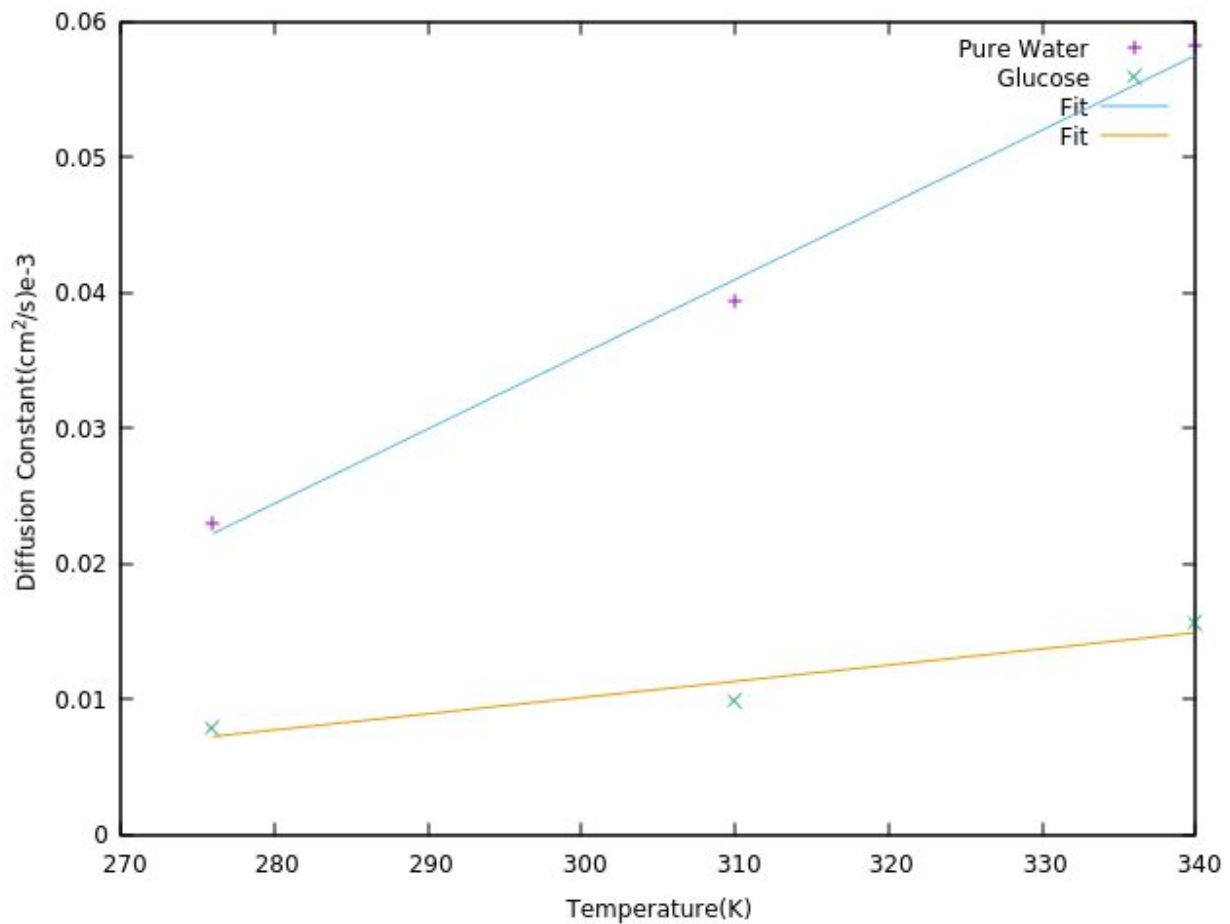
Glucose

	No. of Molecules	<u>Tcor</u>	Slope of the fit ( $A^2/0.1$ <u>ps</u> )	Diffusion constant ( $A^2/0.1$ <u>ps</u> )	Diffusion constant ( $cm^2/sec$ )
Temperature = 276 K	5	800	0.04407	0.007345	0.007345e-3
	5	4000	0.0557	0.00928	0.00928e-3
	15	800	0.05163	0.008605	0.008605e-3
	15	4000	0.03858	0.00643	0.00643e-3
	30	800	0.04766	0.007943	0.007943e-3
Temperature = 310K	5	800	0.0775	0.01291	0.01291e-3
	5	4000	0.06536	0.01089	0.01089e-3
	15	800	0.00712	0.00118	0.00118e-3
	15	4000	0.07182	0.01197	0.01197e-3
	30	800	0.073	0.01216	0.01216e-3
Temperature = 340 K	5	800	0.09124	0.0152	0.0152e-3
	5	4000	0.09009	0.01501	0.01501e-3
	15	800	0.09741	0.01623	0.01623e-3
	15	4000	0.09415	0.01569	0.01569e-3
	30	800	0.09789	0.01631	0.01631e-3

iv)

	Temperature = 276K	Temperature = 310K	Temperature = 340K
Pure Water	0.0229e-3	0.03944e-3	0.05829e-3
Glucose	0.00792e-3	0.0098e-3	0.01568e-3

4.



From the graph, it can be seen that the diffusion coefficient increases with temperature because the temperature increases the thermal fluctuations which are the reason for diffusion.

The slope of the graph gives the value of  $k/z$  where  $z$  is the friction coefficient and  $k$  is Boltzmann coefficient, which will give us the value of  $z$  using the equation:

$$D.z = k.T$$

Where

T: Temperature

D: Diffusion Coefficient