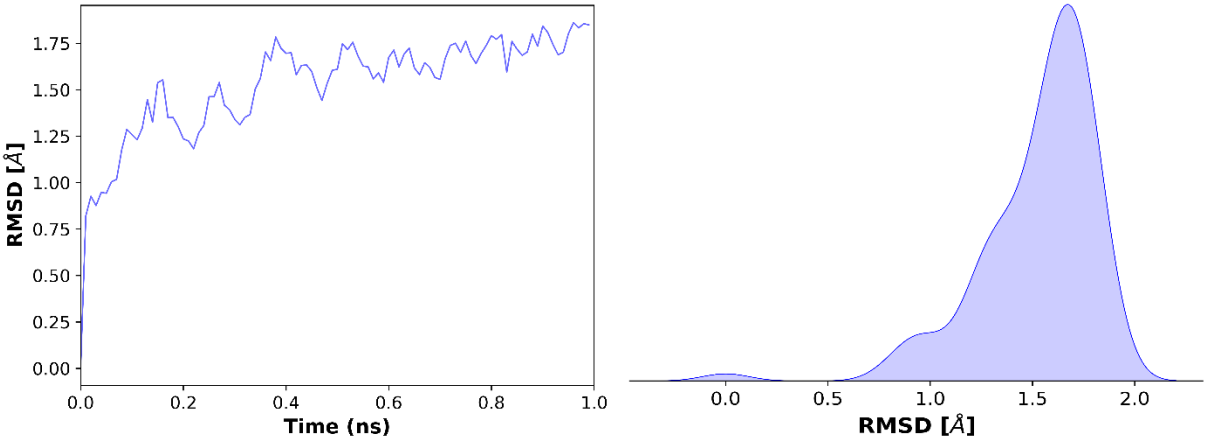
Molecular Dynamics Simulation

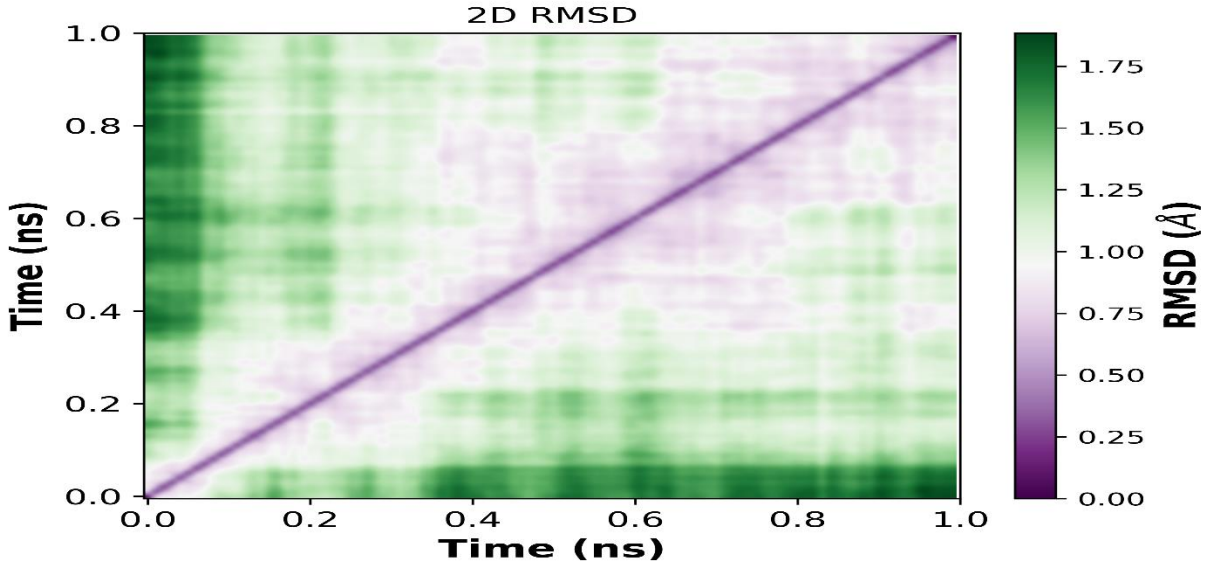
This MD (Molecular Dynamics) simulation run has a Delta total of -4.0777 kcal/mol, which suggest that tremulone binds favorably to caspase 3 indicating a stable interaction.
This was calculated using MM-GBSA (Molecular Mechanics- Generalized Born Surface Area)

This was ran at 1ns, with minimization of 5000 using Pablo Arantes github Jupyter notebook on googlecolab T4 GPU.

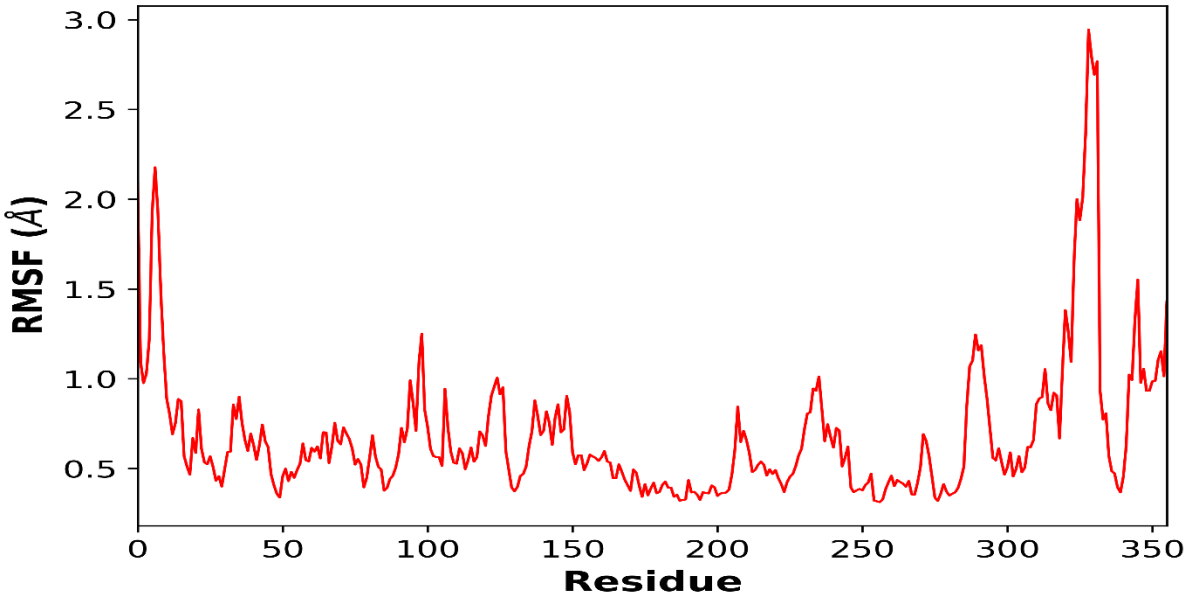
Values generated are shown in the next slides: showing the RMSD, RMSF and Cross Correlation.
I conducted this study on my HP Personal Computer.

RMSD

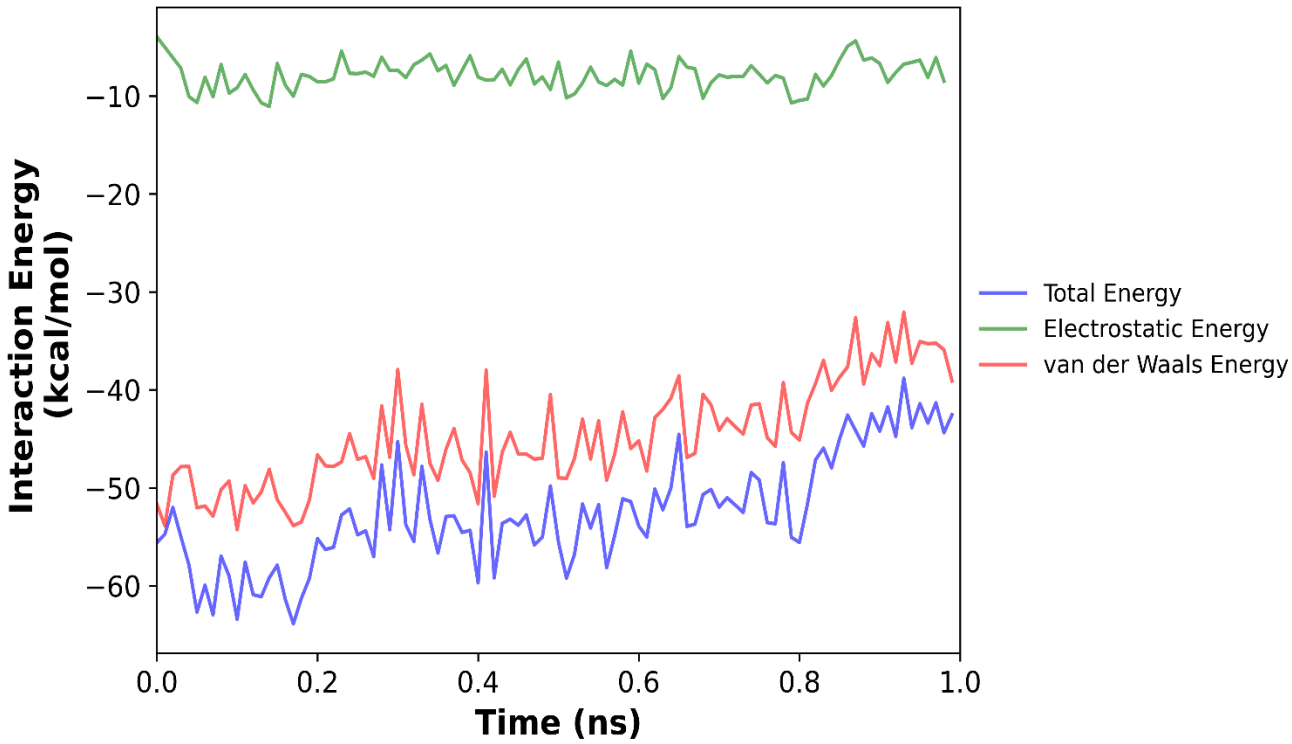


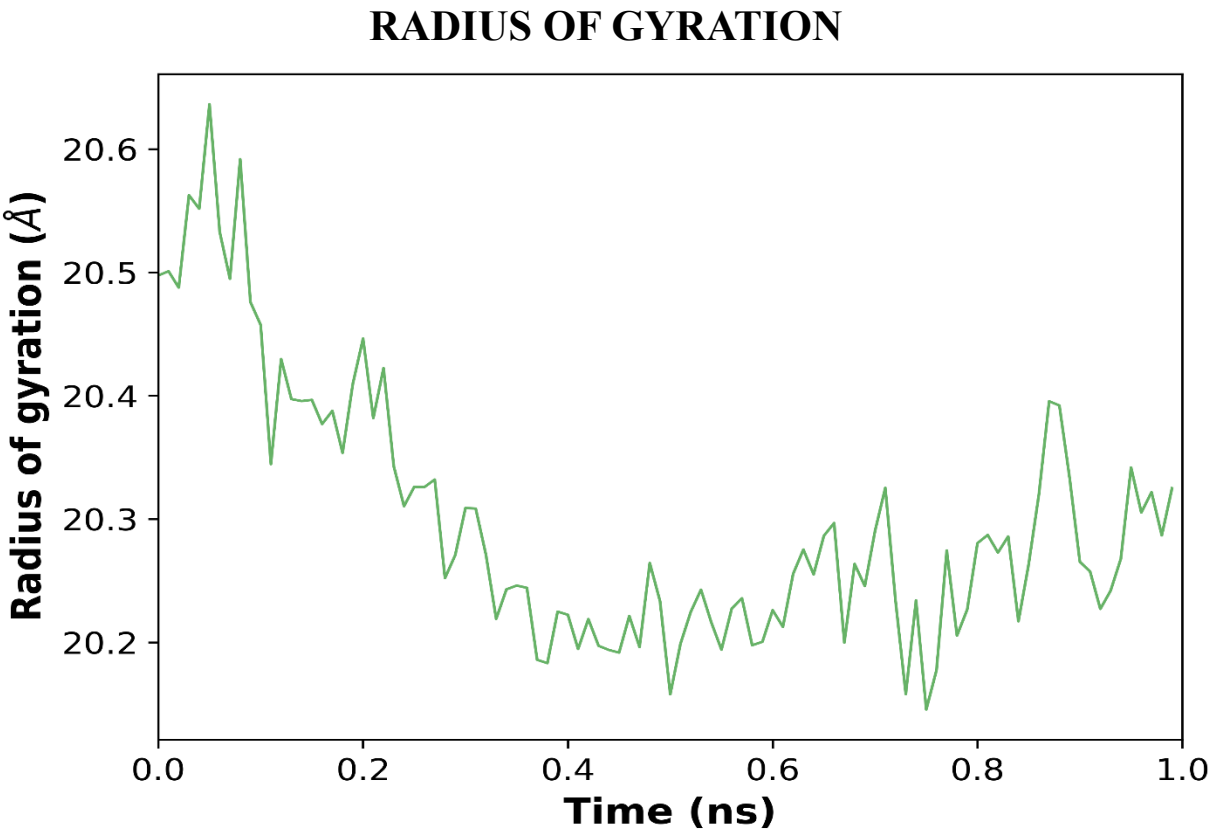


RMSF



INTERACTION ENERGY




RADIUS OF GYRATION
Radius of gyration (Å)
20.6
20.5
20.4
20.3
20.2
0.0
0.2
0.4
0.6
0.8
1.0
Time (ns)