Question 5

In this question, we first calculate the initial energy of the system,

$E_0 = -99337.24954027531 kcal/mol$

To calculate this we evaluate the sum of energies corresponding to each pair of molecules.

After that, we try to minimise the energy by changing the spatial configuration using simulated randomised translations.

After 50 simulations, we propose the minimal energy of the system to be

$E_{min} = -99557.230624$

We also add the corresponding configuration to the notebook.