Homework 1

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Contents

1 Problem 1

- Name: SPERM WHALE MYOGLOBIN F46V N-BUTYL ISOCYANIDE AT PH 9.0
- ID: 101M

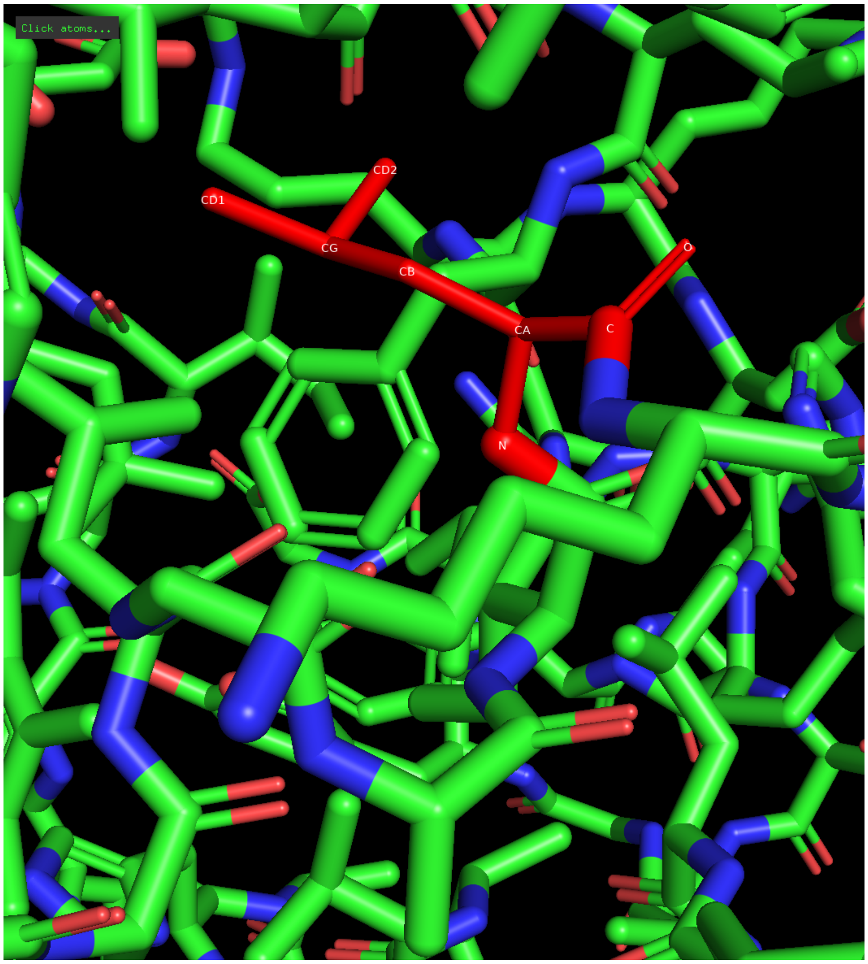


Figure 1: Illustration of molecule with sticks, atoms names of one amino acid labeled.

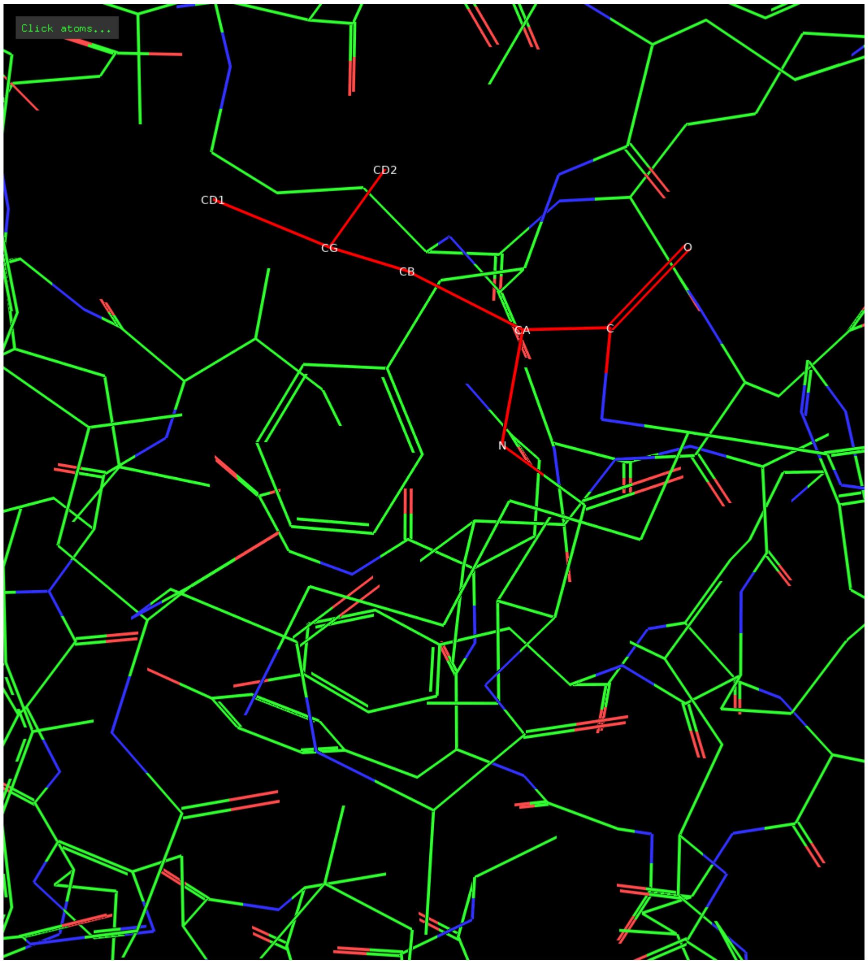


Figure 2: Illustration of molecule with lines, atoms of one amino acid labelled

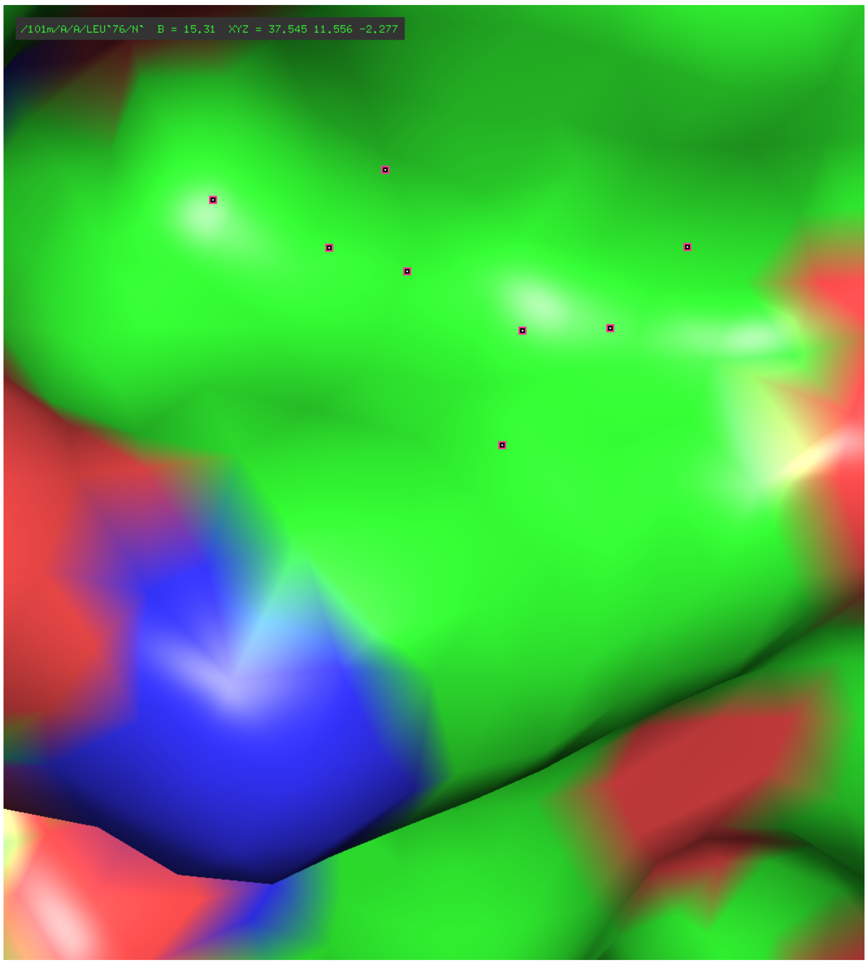


Figure 3: Illustration of molecule with surfaces, atoms and names hidden under surface

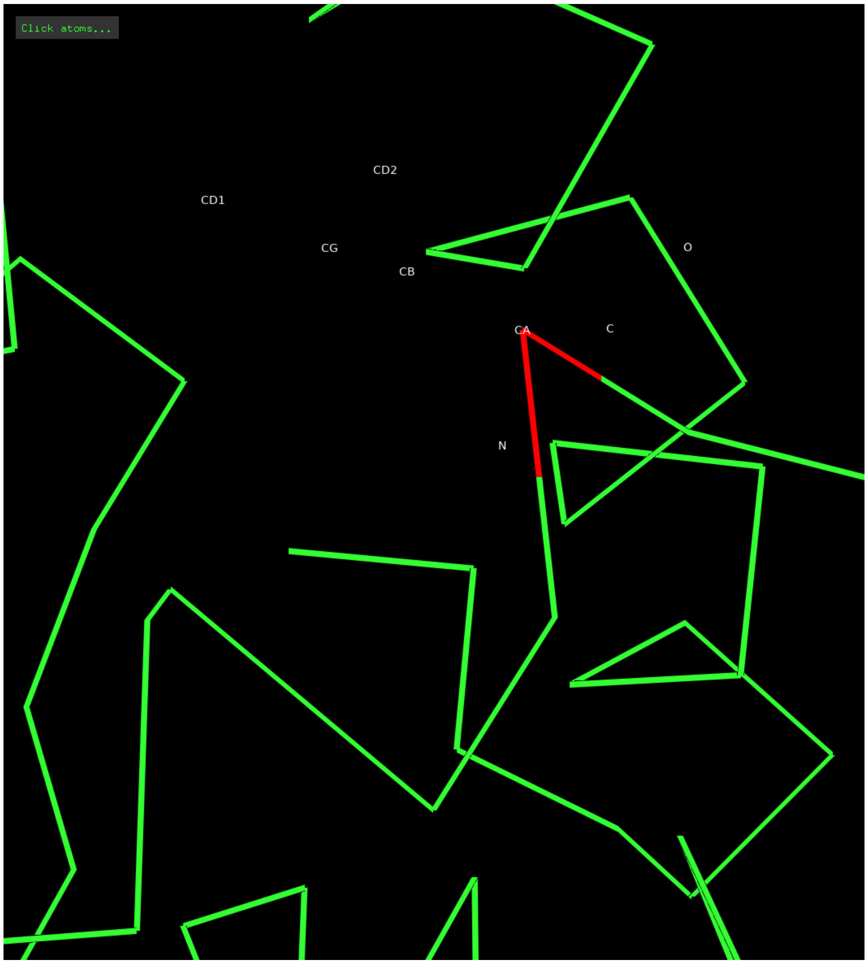


Figure 4: Illustration of molecule with ribbons, atoms hidden but labels are in view.

2 Problem 2

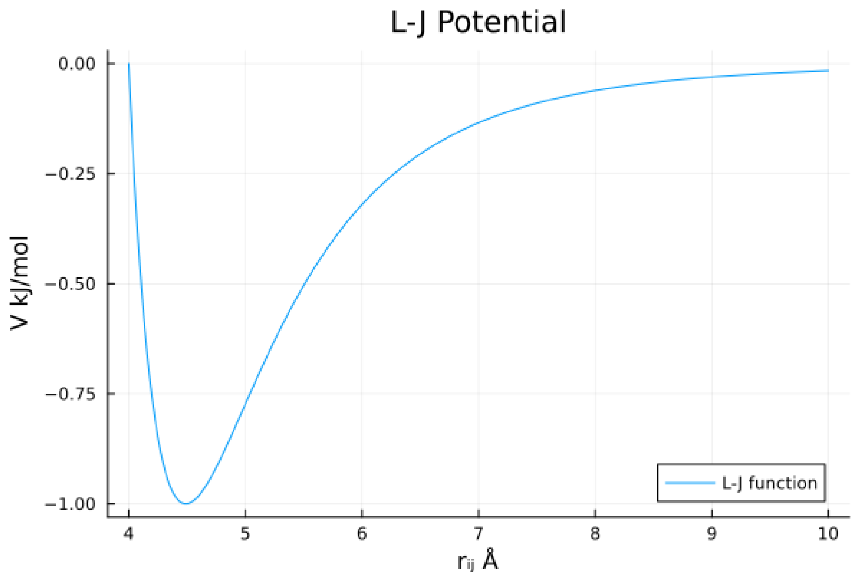
Since $\beta \equiv 1/(k_B T)$, $\partial\beta = -\frac{1}{k_B T^2}\partial T$.

$$\begin{aligned}
c_v &\equiv \frac{\partial < U >}{\partial T} && (1)\\
&= -\frac{1}{k_B T^2}\frac{\partial < U >}{\partial\beta} && (2)\\
&= \frac{1}{k_B T^2}\frac{\partial}{\partial\beta}(\frac{\partial ln(Z)}{\partial\beta}) && (3)\\
&= \frac{1}{k_B T^2}\frac{\partial}{\partial\beta}(\frac{\partial Z/\partial\beta}{Z}) && (4)\\
&= \frac{1}{k_B T^2}\frac{\frac{\partial^2 Z}{\partial\beta^2}Z - (\frac{\partial Z}{\partial\beta})^2}{Z^2} && (5)\\
&= \frac{1}{k_B T^2}(\frac{\frac{\partial^2 Z}{\partial\beta^2}}{Z} - (\frac{\partial Z}{\partial\beta}/Z)^2) && (6)\\
&= \frac{1}{k_B T^2}(< U^2 > - < U >^2) && (7)
\end{aligned}$$

For the last step, we used the fact that $Z = \sum e^{-U\beta}$, taking derivative with respect to β twice will bring down U^2.

3 Problem 3

```
begin
using Plots
epsilon_ij = 1.0
delta_ij = 4.0
V(r) = 4 * epsilon_ij * ((delta_ij/r)^12 - (delta_ij/r)^6)
r = 4:0.01:10
vs = V.(r)
plot(r,vs,title="L-J Potential",label="L-J function")
xlabel!("r\_ij Å")
ylabel!("V kJ/mol")
savefig("./potential.png")
end
```




```
F(r) = -98304.0 *(r^6 - 8192)/r^13
println(F(4*(2)^(1/6) + 0.5))
println(F(4*(2)^(1/6) - 0.5))
```

```
F (generic function with 1 method)
-0.5989510746437929
6.2953600398067096
```

3.1 a

- The global minimum is at $\frac{\partial V(r_{ij})}{\partial r_{ij}} = 0$. Solving this equation we get $r_{ij} = 4 * 2^{1/6} \approx 4.4898$
- By definition of the force $F = -\frac{\partial V}{\partial r}$, there should be no force at r_m
- When $r_{ij} = r_m + 0.5$, $F = -\frac{\partial V}{\partial r} = -0.5989510746437929$, it's attractive force, they should pull towards each other.
- When $r_{ij} = r_m - 0.5$, $F = -\frac{\partial V}{\partial r} = 6.2953600398067096$, it's repulsive force, they should push them away from each other.

3.2 b

The mixing rule says: $\sigma_{AB} = 1/2(\sigma_A + \sigma_B) = 4$ angstrom. And, $\epsilon_{AB} = \sqrt{\epsilon_A \epsilon_B} \approx 0.98 kJ/mol$

4 Problem 4

4.1 a

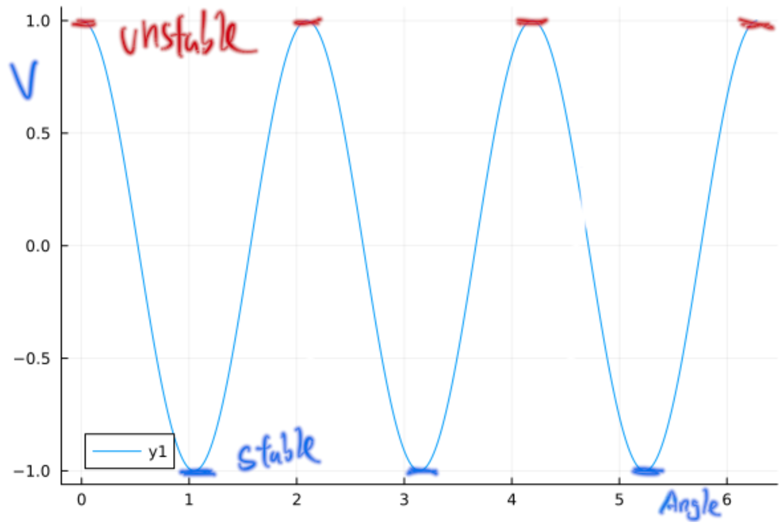
- Bond terms: $4 + 1 = 5$, 4 C-H and 1 C-C.
- Angles: $4 + 2$, 4 H-C-C, 2 H-C-H
- Dihedrals: 4, 4 H-C-C-H

4.2 b

- For a single molecule, there are 4 distinct pairs of hydrogen that has 1-4 interactions.
- For two molecules, there are $8 + 36$ non-bonded interactions terms. 8 from 1-4 interactions, and 36 from inter-molecular atomic interactions.

5 Problem 5

- There are three hydrogens, so the period of the potential is $2\pi/3$.
- The stable states occurs at $\pi/3, \pi, 5pi/3$ angles, they are **staggered conformation**
- The un-stable states occurs at $0, 2\pi/3, 4\pi/3, 2\pi$ angles, they are **eclipsed conformation**.
- I referenced this website to answer this question.

- 

V
unstable
stable
Angle
y1
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6