Assignment 3

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**Task 1**

First, find the atoms pair which distance is between 3. 7 and 3. 9. Then, randomly choose the atom which has only one matching atom as the head, and then start to find the entire chain.

Command: python .\task1.py .\test\_q1.txt

Command: python .\task1.py .\data\_q1.txt

文本

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**Task 2 Method 1**

First, find the atoms pair which distance is between 3. 7 and 3. 9. This method looks for other main chain atoms in the peptide plane between two candidate alpha-carbons, the threshold is set to 1.2 according to the paper.

Command: python task2\_method1.py

The total number of alpha-carbon atoms in the chain 48

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**Task 2 Method 2**

First, find the atoms pair which distance is between 3. 7 and 3. 9. This method look for chain by consider the "pseudo-valence angles" defined by three consecutive alpha-carbon atoms. The angle is between 75-160 according to the paper.

Command: python task2\_method2.py

The total number of alpha-carbon atoms in the chain 40

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