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

```
PS C:\Users\M\Project\TDA507\Assignment3> python .\task1.py .\test_q1.txt
8.0
10.0
9.0
7.0
6.0
5.0
3.0
1.0
4.0
2.0
The total number of alpha-carbon atoms in the chain 10
```

```
PS C:\Users\M\Project\TDA507\Assignment3> python .\task1.py .\data_q1.txt
8.0
9.0
3.0
4.0
6.0
7.0
5.0
10.0
1.0
2.0
The total number of alpha-carbon atoms in the chain 10
```

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

```
PS C:\Users\M\Project\TDA507\Assignment3> python task2_method1.py
12
36
44
62
48
73
45
19
39
63
62
63
69
83
117
160
177
203
237
256
266
301
294
243
236
227
205
223
273
262
215
181
106
184
207
129
158
169
142
86
70
72
54
27
16
3
4
19
The total number of alpha-carbon atoms in the chain 48
```

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

```
PS C:\Users\M\Project\TDA507\Assignment3> python task2_method2.py
264.0
285.0
308.0
280.0
241.0
177.0
160.0
117.0
83.0
69.0
63.0
39.0
19.0
4.0
3.0
16.0
27.0
54.0
72.0
70.0
86.0
142.0
169.0
158.0
207.0
242.0
215.0
202.0
143.0
163.0
110.0
152.0
165.0
104.0
119.0
174.0
231.0
229.0
168.0
94.0
The total number of alpha-carbon atoms in the chain 40
```