The Psi-Blast alignment scoring matrix

Parts of the active site of the 1K7C, and 1WAB esterase proteins consist of the amino acids HTHT and YLHL, respectively.

1) Calculate the alignment score of the two amino acids segments using the BLOSUM50 scoring matrix

```
        HTHT
        YLHL
```

How many of the alignment scores are positive (>=0)?

```
    A  R  N  D  C  Q  E  G  H  I  L  K  M  F  P  S  T  W  Y  V
A   4 -1 -2 -2  0 -1 -1  0 -2 -1 -1 -1 -1 -2 -1  1  0 -3 -2  0
R  -1  5  0 -2 -3  1  0 -2  0 -3 -2  2 -1 -3 -2 -1 -1 -3 -2 -3
N  -2  0  6  1 -3  0  0  0  1 -3 -3  0 -2 -3 -2  1  0 -4 -2 -3
D  -2 -2  1  6 -3  0  2 -1 -1 -3 -4 -1 -3 -3 -1  0 -1 -4 -3 -3
C   0 -3 -3 -3  9 -3 -4 -3 -3 -1 -1 -3 -1 -2 -3 -1 -1 -2 -2 -1
Q  -1  1  0  0 -3  5  2 -2  0 -3 -2  1  0 -3 -1  0 -1 -2 -1 -2
E  -1  0  0  2 -4  2  5 -2  0 -3 -3  1 -2 -3 -1  0 -1 -3 -2 -2
G   0 -2  0 -1 -3 -2 -2  6 -2 -4 -4 -2 -3 -3 -2  0 -2 -2 -3 -3
H  -2  0  1 -1 -3  0  0 -2  8 -3 -3 -1 -2 -1 -2 -1 -2 -2  2 -3
I  -1 -3 -3 -3 -1 -3 -3 -4 -3  4  2 -3  1  0 -3 -2 -1 -3 -1  3
L  -1 -2 -3 -4 -1 -2 -3 -4 -3  2  4 -2  2  0 -3 -2 -1 -2 -1  1
K  -1  2  0 -1 -3  1  1 -2 -1 -3 -2  5 -1 -3 -1  0 -1 -3 -2 -2
M  -1 -1 -2 -3 -1  0 -2 -3 -2  1  2 -1  5  0 -2 -1 -1 -1 -1  1
F  -2 -3 -3 -3 -2 -3 -3 -3 -1  0  0 -3  0  6 -4 -2 -2  1  3 -1
P  -1 -2 -2 -1 -3 -1 -1 -2 -2 -3 -3 -1 -2 -4  7 -1 -1 -4 -3 -2
S   1 -1  1  0 -1  0  0  0 -1 -2 -2  0 -1 -2 -1  4  1 -3 -2 -2
T   0 -1  0 -1 -1 -1 -1 -2 -2 -1 -1 -1 -1 -2 -1  1  5 -2 -2  0
W  -3 -3 -4 -4 -2 -2 -3 -2 -2 -3 -2 -3 -1  1 -4 -3 -2 11  2 -3
Y  -2 -2 -2 -3 -2 -1 -2 -3  2 -1 -1 -2 -1  3 -3 -2 -2  2  7 -1
V   0 -3 -3 -3 -1 -2 -2 -3 -3  3  1 -2  1 -1 -2 -2  0 -3 -1  4
```

2) Next, use the sequence profile calculated for 1K7C shown below to calculate the alignment score

```
          A   R   N   D   C   Q   E   G   H   I   L   K   M   F   P   S   T   W   Y   V
1     T  -1  -2  -1  -2  -2  -2  -2  -2  -3  -2  -3  -2  -2  -3  -2   3   6  -4  -3  -2
2     T  -2   0  -2  -3  -3  -2  -3  -4  -4  -3  -3   1  -3  -4  -3  -1   7  -5  -4  -2
...
193 H  -3   3   4   0  -5  -2  -3   1   6  -4  -4  -2  -4  -2  -2  -2   0  -5   2  -5
194 T  -3  -4  -3  -4  -3  -3  -4  -4  -4  -2   0  -3   1  -1  -4  -1   7  -5  -4   1
195 H  -4  -3  -2  -4  -6  -2  -2  -5  10  -6  -5  -3  -4  -4  -5  -3  -4  -5  -1  -6
196 T  -3  -4  -4  -5  -4  -4  -4  -5  -1  -2   2  -4  -1   6   2  -2   4  -3  -1  -1
...
232 C  -1  -3  -2  -3   9  -3  -3  -2  -3  -2  -2  -3  -2  -3  -3   2  -1  -3  -3  -2
233 L  -2  -3  -4  -4  -2  -3  -4  -4  -4   3   5  -3   1   0  -4  -3  -2  -2  -2   1
```

Note, that the PSSM is calculated for 1K7C.

How many of the alignment scores are now positive (>=0)?

Can you understand why Psi-Blast is able to make a correct alignment of the two proteins?