# **Running TANGO**

## Running TANGO from the command line (for windows users: a dos box).

- 1) Open a command line window and go to the directory where you have put the executable.
- 2) Call tango as in the following example (use spaces, not tabs) tango P05100 nt="N" ct="N" ph="7.4" te="303" io="0.05" tf="0" stab="-10" seq="DNEWGYIAYHVSQDP"

formally this would translate as [executable\_name] [identifier] []...(parameter list)...[] [input sequence]

#### parameters:

nt: Protection at the C-terminus: can be N for no or Y for amidated

ct: Protection at the N-terminus: can be N for no, A for acetylated or S for succinilated.

ph: pH

te: Temperature in Kelvin

io: Ionic strength

tf: Percentage of the organic solvent TFE:i.e 20% is written 0.2

stab: Stability of your protein in Kcal/mol: for a standard protein it could be between -4 and -11 Kcal/mol

conc: Concentration in M of your protein or peptide.

### Running TANGO in batch mode under windows.

You can make a text file with many line of tango calls like the one shown above.

If you change the extention of this file to .bat, you can double click it to execute the commands inside.

# **TANGO** output.

The output of TANGO is in text format with the extension .out. You will get two classes of outputs. One with the name of the file you run that will contain the average aggregation per residue for every sequence you had in your file. The other will be a series of files with the names of the sequences you run that will contain the prediction at the residue level. Those files will have the following columns:

Sequence Number Amino acid in one-letter code Percentage of  $\beta$ -strand conformation Percentage of  $\beta$ -turn conformation Percentage of  $\alpha$ -helical conformation Percentage of Aggregation Percentage of Helical Aggregation.

Please be aware that the latest is calculated independently of the first four and therefore you could get a number higher than 1 if you sum the 5 columns. Below you have an example of the sequence output.

```
01,
     M, 0.14,
                0.08, 0.00, 0.00,
                                    0.00
                       0.00,
02,
         0.24,
                0.11,
                             0.00,
                                    0.00
                0.11,
                       0.00,
                             0.00,
03,
         0.44,
                                    0.00
04,
         0.45,
                0.27,
                       0.00,
                             0.87,
                                    0.00
05,
         0.36,
                0.19,
                       0.00,
                             0.87,
                                    0.00
06,
     T, 1.14,
                0.16,
                       0.00,
                             1.40,
                                    0.00
07,
     F, 1.08,
                0.16,
                       0.00, 1.61,
                                    0.00
08,
     V, 1.08,
                0.62,
                       0.00,
                             1.61,
                                    0.00
09,
     G, 1.03,
                0.66,
                       0.00,
                             0.74,
                                    0.00
     D, 0.18,
                0.67,
                       0.00,
                             0.74,
                                    0.00
10,
         0.14,
                0.67,
                       0.00,
                             0.74,
                                    0.00
11,
12,
         0.39,
                0.05,
                       0.00,
                             3.80,
                                    0.00
13,
         0.64,
                0.00,
                       0.00,
                             3.80,
                                    0.00
                0.00,
14,
     E, 0.73,
                       0.00,
                             3.31,
                                    0.00
     I, 0.75,
                0.00, 0.00,
                             3.31,
15,
                                    0.00
     V, 0.48,
                0.00, 0.00,
                             3.31,
                                    0.00
16,
17,
     P, 0.23,
                0.22,
                       0.00,
                             3.04,
                                    0.00
18,
     S, 0.12, 0.24, 0.00,
                             0.62,
                                    0.00
19,
     N, 0.00,
                0.35, 0.00, 0.00,
                                    0.00
```

```
20,
      Ε,
          0.00,
                  0.38, 0.00, 0.00,
                                         0.00
21,
      Ε,
          0.00,
                  0.17,
                         0.00,
                                 0.00,
                                         0.00
22,
      Q,
          0.33,
                  0.15,
                         0.00,
                                 0.00,
                                         0.00
23,
      I,
          0.39,
                  0.14,
                         0.00,
                                 0.00,
                                         0.00
24,
                  0.12,
      Κ,
          0.40,
                         0.00,
                                 0.00,
                                         0.00
25,
      N.
          0.40,
                  0.12,
                         0.00,
                                 0.00,
                                         0.00
26,
      L,
          0.11,
                  0.12,
                         0.00,
                                 0.00,
                                         0.00
27,
      L,
          0.34,
                  0.03,
                         0.00,
                                 0.00,
                                         0.00
28,
                  0.02,
      Ο,
          0.59,
                         0.00,
                                 0.00,
                                         0.00
29,
          0.63,
                  0.04,
                         0.00,
                                 0.00,
                                         0.00
      L,
                         0.00,
                                 0.00,
30,
          0.62,
                  0.04,
                                         0.00
31,
      Α,
          0.33,
                  0.06,
                         0.00,
                                 0.00,
                                         0.00
32,
      0,
          0.09,
                  0.12,
                         0.00,
                                 0.00,
                                         0.00
33,
                  0.10,
                         0.00,
      Ε,
          0.06,
                                 0.00,
                                         0.00
34,
      Η,
          0.16,
                  0.10, 0.00,
                                 0.00,
                                         0.00
                  0.09,
35,
          0.44,
                         0.00,
                                 0.00,
                                         0.00
36,
      Ο,
          0.56,
                  0.04,
                         0.00,
                                 0.00,
                                         0.00
                                 0.00,
37,
      L,
          0.78,
                  0.03,
                         0.00,
                                         0.00
38,
      D,
          0.82,
                  0.03,
                         0.00,
                                 0.00,
                                         0.00
39,
                  0.00, 0.00,
      F,
          0.70,
                                 0.00,
                                         0.00
40,
      W,
          0.76,
                  0.00,
                         0.00,
                                 0.00,
                                         0.00
41,
      Κ,
          0.54,
                  0.00,
                         0.00,
                                 0.00,
                                         0.00
42,
      S,
          0.38,
                  0.25,
                         0.00,
                                 0.00,
                                         0.00
43,
      Ρ,
          0.20,
                  0.25,
                         0.00,
                                 0.00,
                                         0.00
44,
      Τ,
          0.05,
                  0.25,
                         0.00,
                                 0.00,
                                         0.00
45,
      Τ,
          0.04,
                  1.47,
                         0.00,
                                 0.00,
                                         0.00
46,
                  1.36,
      Ρ,
          0.04,
                         0.00,
                                 0.00,
                                         0.00
                                 0.00,
47,
      G,
          0.04,
                  1.48,
                         0.00,
                                         0.00
48,
      Ε,
          0.01,
                  1.48,
                         0.00,
                                 0.00,
                                         0.00
49,
          0.14,
                  0.27,
                         0.00,
                                 0.00,
                                         0.00
          0.20,
                  0.12,
                         0.00,
50,
      Α,
                                 0.00,
                                         0.00
51,
      Η,
          0.49,
                  0.00,
                         0.00,
                                 0.00,
                                         0.00
52,
      V,
          2.69,
                  0.00,
                         0.00,
                                 0.00,
                                         0.00
53,
      R,
          2.57,
                  0.00,
                         0.00,
                                 0.00,
                                         0.00
      V,
          2.50,
                  0.00,
                         0.00, 6.27,
54,
                                         0.00
55,
      Ρ,
          2.21,
                  0.00,
                         0.00, 6.27,
                                         0.00
                  0.00,
56,
          0.00,
                         0.00, 11.61,
                                         0.00
57,
          0.00,
                  0.00, 0.00, 11.93,
      V,
                                         0.00
58,
          0.00,
                  0.00, 0.00, 11.93,
                                         0.00
59,
      V,
          0.00,
                  0.01,
                         0.33, 11.69,
                                         0.00
60,
      Q,
          0.00,
                  0.01, 0.33, 8.01,
                                         0.00
61,
      Α,
          0.00,
                  0.01,
                         0.33,
                                 7.08,
                                         0.00
62,
      V,
          0.00,
                  0.01,
                        0.33,
                                 6.80,
                                         0.00
      Κ,
          0.00,
                  0.00,
                         0.00,
63,
                                 0.00,
                                         0.00
64,
      V,
          0.00,
                  0.00,
                         0.00,
                                 4.17,
                                         0.00
65,
      F,
          0.00,
                  0.00,
                         0.00, 4.39,
                                         0.00
```

```
66,
     L,
         0.00, 0.09, 0.00, 4.39, 0.00
67,
         0.00,
                0.19, 0.00, 4.39,
                                     0.00
68,
     S,
         0.00,
                0.38, 0.00, 4.53,
                                     0.00
69,
                0.40, 0.00, 5.02,
         0.00,
                                     0.00
70,
                0.31, 0.00, 12.27,
     G,
         0.00,
                                     0.00
71,
                0.21, 0.00, 64.25,
         0.00,
                                     0.00
72,
     Α,
         0.00,
                0.02, 0.00, 68.13,
                                     0.00
     Υ,
73,
         0.00,
                0.01, 0.00, 70.91,
                                     0.00
74,
                0.01, 0.00, 70.91,
      S,
         0.00,
                                     0.00
75,
                0.01, 0.00, 70.91,
     I,
         0.00,
                                     0.00
76,
         0.00,
                0.01, 0.00, 67.35,
                                     0.00
77,
     I,
         0.00,
                0.12, 0.00, 62.97,
                                     0.00
78,
         0.00,
                0.12, 0.00, 4.98,
                                     0.00
      Ε,
79,
         0.00,
                0.12, 0.00, 1.93,
     D,
                                     0.00
80,
     V,
                0.12, 0.00, 1.85,
         0.00,
                                     0.00
81,
         0.00,
                0.00, 0.00, 0.00, 0.00
```