Programming project : Secondary Structure Assignment

Hélène Kabbech
Bioinformatics master student, Paris Diderot University

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1 Introduction

The purpose of this project is to generate a pattern-recognition program that assigns secondary structure elements (SSE) to a protein by using the dictionary of protein secondary structures (dssp)[1] fixed by Kabsch and Sander in the mid-80's. SSE are based on hydrogen-bonded and geometrical features extracted from atomic coordinates.

2 Material & Method

2.1 Programming tools

All scripts are written in Python 3.6. PDB files are easily manage thanks to the BioPython[2] library. GitHub has been used for the development of this program. It is a web-based hosting service for version control using Git. Therefore, this project (its documentation and source code) is available online at the following address : `https://www.github.com/kabhel/DSSP_implt`

2.2 Code structure

In addition to the main function (*dssp.py* file), three modules are implemented : *management* (Creation of the help, argument managment and display of results), *classes* (Residue class and its methods to calculate supplement parameters) and *structures* (Secondary structures assignment) (**see Figure 1**).

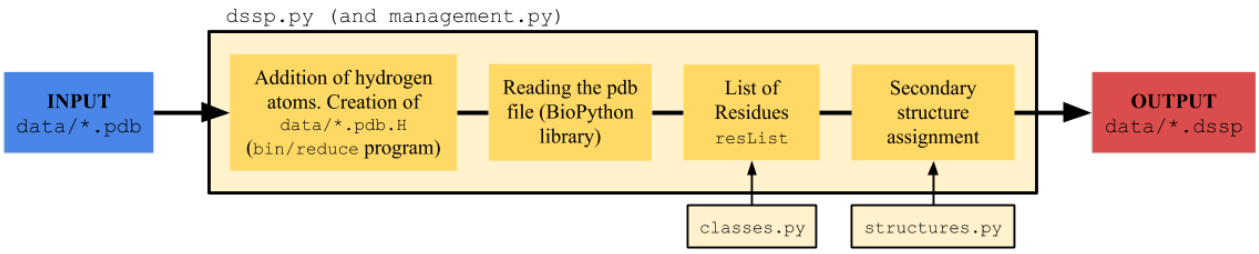


Figure 1. Schema of the implemented dssp program that assigns secondary structures from a pdb file.

2.3 Secondary Structure Assignment

As Kabsch and Sander described in their paper[1], the implemented dssp program assigns the SSE according to a specific priority order. First α-helices (**H**) are assign, follow by isolated β-bridges (**B**), extended strands (**E**), 3_{10}-helices (**G**), π-helices (**I**), H-bonded turns **T** and then bend (**S**). The assignment of a SSE depends mainly on H-bonded features.

2.4 Output parameters

Each line of a dssp output describes a residue and its assigned secondary structure (see dssp output **Annexe section**).

- **RESIDUE :** Residue sequence number and chain identifier.
- **AA :** One letter amino acid code.
- **STRUCTURE** :
  - Secondary structure element : '**H**', '**B**', '**E**', '**G**', '**I**', '**T**', '**S**' or ' '
  - 3-turn/helix pattern : '>' (start), '<' (end), '**X**' (start/end), '**3**' (middle), or ' '
  - 4-turn/helix pattern : '>', '**X**', '<', '**4**', or ' '
  - 5-turn/helix pattern : '>', '**X**', '<', '**5**' or ' '
  - Geometrical bend : '**S**' or ' '
  - Chirality : '+' or '-'
  - Bridge label : '**a,b,c.**' for parallel $\boldsymbol{\beta}$-bridge, '**A,B,C**.' for antiparallel $\boldsymbol{\beta}$-bridge
- **BP1 BP2 :** Residue number of first and second bridge partner.
- **TCO :** Cosine of angle between C=O of residue i and C=O of residue i-1. TCO is near +1 for α-helices, TCO is near -1 for β-sheets.
- **KAPPA :** Virtual bond angle (bend angle) defined by the three C_α atoms of residues i-2, i, i+2. Used to define bend.
- **ALPHA :** Virtual torsion angle (dihedral angle) defined by the C_α atoms of residues i-1, i, i+1 and i+2. Used to define chirality.
- **PHI PSI :** Peptide backbone torsion angles (dihedral angles).
- **X-CA Y-CA Z-CA :** C_α atom coordinates.

2.5 Input data

The input file must be in PDB (Protein Data Bank) format. Our program is illustrate by two examples : 1BTA[3] the three-dimensional structure of barstar Secondly and 1ITV[4] the dimeric form of the haemopexin domain of MMP9 (see **Results section**).

3 Results

3.1 1BTA : A simple case

1BTA is a simple structure with four α-helices and one β-sheet containing three parallel β-strands (see **Figure 2**). By comparing the dssp output (see **Annexe section**) with the original output (**dssp program 3.0.0**), we notice the same assignment of the secondary structures for each residues, except an isolated beta-bridge (at index 7 and 9) that is not determined by the original program.

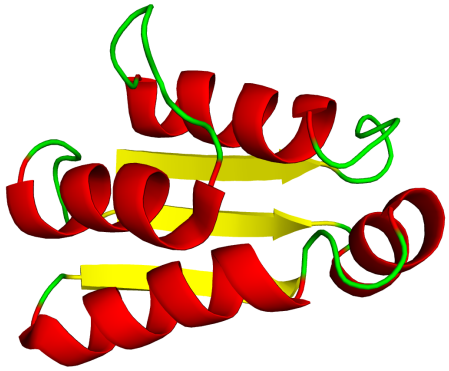


Figure 2. Structure of 1BTA colored by secondary structure in PyMol[5].

3.2 1ITV : A more complex case

1ITV is a more complex example because it contains two chains. Each chain has four β-sheets of three/four antiparallel β-strands and five small helices of α and 3_{10} types (see **Figure 3**). As well as previously, the main secondary structures (helices and strands) are well assigned. However, there are some differences/mistakes at some points.

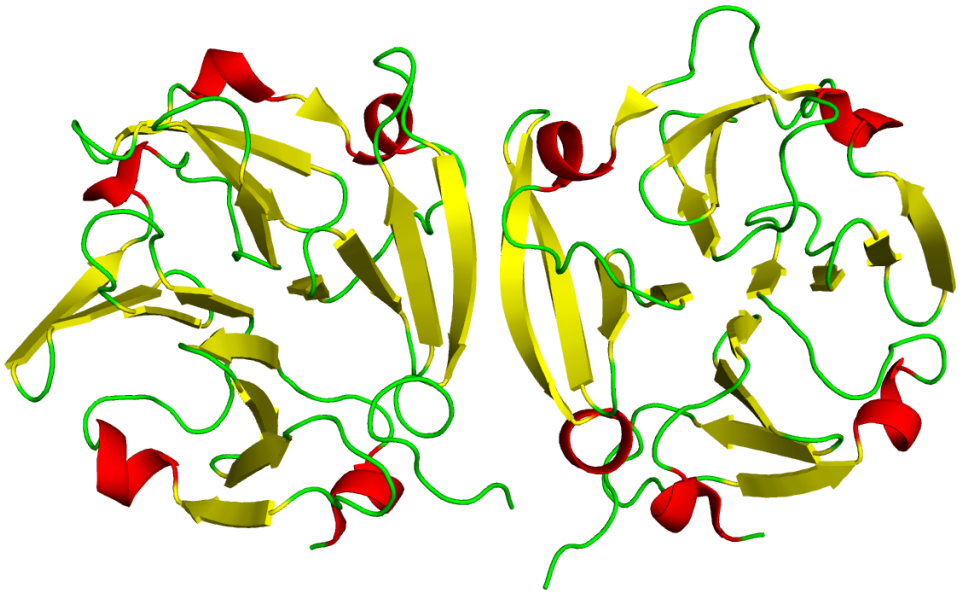


Figure 3. Structure of 1ITV colored by secondary structure in PyMol[5].

4 Conclusion

The dssp program implemented in python 3.6 performs almost similarly the original dssp program. It assigns secondary structure elements for each residues.

5 References

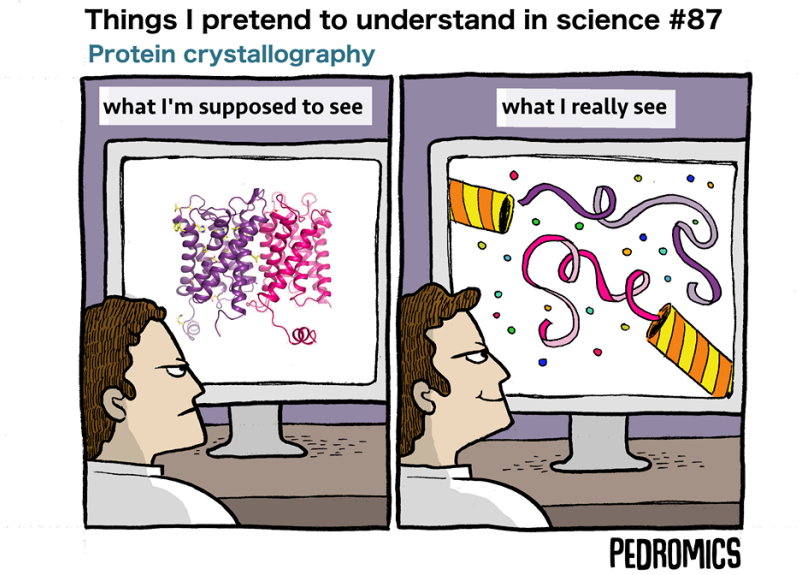
1. Kabsch, W., and C. Sander. "Secondary structure definition by the program DSSP." Biopolymers 22 (1983): 2577-2637.

2. Cock, Peter JA, et al. "Biopython: freely available Python tools for computational molecular biology and bioinformatics." Bioinformatics 25.11 (2009): 1422-1423.

3. Lubienski, Michael J., et al. "Three-dimensional solution structure and 13C assignments of barstar using nuclear magnetic resonance spectroscopy." Biochemistry 33.30 (1994): 8866-8877.

4. Cha, Hyunju, et al. "Structural basis of the adaptive molecular recognition by MMP9." Journal of molecular biology 320.5 (2002): 1065-1079.

5. DeLano, Warren Lyford. "PyMOL." (2002): 700.



6 Annexe

```
./dssp.py -h
Usage: dssp.py [options]

Options:
--version             show program's version number and exit
-h, --help            show this help message and exit
-i FILE, --input=FILE
                      the file name of a PDB formatted file containing the
                      protein structure data
-o FILE, --output=FILE
                      the file name of a DSSP file to create

./dssp.py -i data/1bta.pdb
==== Secondary Structure Assignment using DSSP method ====
DATE          2018-09-17
REFERENCE     W. KABSCH AND C.SANDER, BIOPOLYMERS 22 (1983) 2577-2637
HEADER        RIBONUCLEASE INHIBITOR                  1994-05-09
COMPND        MOL_ID: 1; MOLECULE: BARSTAR; CHAIN: A; ENGINEERED: YES;
SOURCE        MOL_ID: 1; ORGANISM_SCIENTIFIC: BACILLUS AMYLOLIQUEFACIENS; ORGANISM_TAXID: 1390;
AUTHOR        M.J.LUBIENSKI,M.BYCROFT,S.M.V.FREUND,A.R.FERSHT
  #  RESIDUE AA STRUCTURE BP1 BP2    TCO  KAPPA ALPHA   PHI   PSI    X-CA   Y-CA   Z-CA
    1    1 A K              0   0  0.000 360.0 360.0 360.0-171.7   -7.5    5.2    9.2
    2    2 A K   E      -a   50   0 -0.957 360.0-169.5-133.8 153.7   -3.8    5.5    8.5
    3    3 A A   E      -a   51   0 -0.933   5.4-159.9-134.7 157.3   -1.1    3.4    6.8
    4    4 A V   E      -a   52   0 -0.926   5.9-160.1-144.5 118.6    2.7    3.8    6.8
    5    5 A I   E      -a   53   0 -0.740  11.7-170.1-100.1  93.0    5.1    2.2    4.2
    6    6 A N   E >>    -a   54   0 -0.684   4.7-172.9 -83.5 104.2    8.5    2.2    5.9
    7    7 A G   B 34 S+B    9   0  0.931  79.7  70.5 -64.8 -43.3   11.0    1.3    3.1
    8    8 A E   T 34 S+     0   0  0.812 111.2  36.3 -44.5 -25.9   13.9    1.0    5.5
    9    9 A Q   B <4 S+B    7   0  0.868  92.5  99.6 -94.9 -47.2   12.1   -2.1    6.7
   10   10 A I     <  +      0   0 -0.075  41.7 176.6 -41.3 133.7   10.6   -3.4    3.4
   11   11 A R        -      0   0  0.480  64.2 -14.5-119.2 -11.8   12.8   -6.3    2.2
   12   12 A S   S  > S-     0   0 -0.982  82.9 -77.3-174.2 175.9   10.7   -7.3   -0.9
   13   13 A I   H  > S+     0   0  0.951 127.9  57.2 -56.6 -45.7    7.3   -6.8   -2.5
   14   14 A S   H  > S+     0   0  0.940 105.2  51.7 -50.8 -45.4    5.9   -9.3   -0.0
   15   15 A D   H  > S+     0   0  0.933 106.8  54.1 -57.9 -43.3    7.1   -7.0    2.7
   16   16 A L   H  X S+     0   0  0.978 112.3  41.4 -55.2 -56.5    5.3   -4.1    1.0
   17   17 A H   H  X S+     0   0  0.740 110.3  64.2 -64.5 -18.6    2.0   -5.9    0.9
   18   18 A Q   H  X S+     0   0  0.979 107.7  36.0 -70.2 -55.2    2.9   -7.0    4.5
   19   19 A T   H  X S+     0   0  0.935 117.5  53.5 -65.2 -41.3    2.9   -3.6    6.0
   20   20 A L   H  X S+     0   0  0.903 108.1  52.9 -59.0 -35.8   -0.0   -2.6    3.8
   21   21 A K   H  X>S+     0   0  0.915 111.4  44.2 -66.9 -42.1   -1.8   -5.7    5.1
   22   22 A K   H  <5S+     0   0  0.993 120.2  39.8 -67.3 -57.4   -1.2   -4.6    8.7
   23   23 A E   H  <5S+     0   0  0.986 124.9  37.7 -52.3 -66.1   -2.2   -1.0    8.2
   24   24 A L   H  <5S-     0   0  0.680 104.4-138.4 -61.2 -14.8   -5.1   -1.9    5.9
   25   25 A A   T  <5 -      0   0  0.947  32.7-172.8  55.0  47.6   -5.7   -4.9    8.2
   26   26 A L      < -      0   0 -0.276  28.8 -88.3 -69.5 161.1   -6.3   -7.1    5.1
   27   27 A P     >  -      0   0  0.135  42.3 -99.3 -57.4-179.7   -7.5  -10.6    5.5
   28   28 A E   T 3  S+     0   0  0.714 123.6  58.2 -79.9 -18.5   -5.1  -13.5    6.0
   29   29 A Y   T 3  S+     0   0  0.276  71.5 159.2 -93.5  13.8   -5.4  -14.4    2.3
   30   30 A Y     <  -      0   0 -0.088  34.8-151.8 -38.4 105.9   -4.3  -10.9    1.2
   31   31 A G        -      0   0  0.584  14.6-148.0 -64.0  -5.5   -3.2  -11.8   -2.4
   32   32 A E        +      0   0  0.533  59.2 118.6  50.1   3.6   -0.7   -8.9   -2.0
   33   33 A N   S  > S-     0   0 -0.245  83.5-105.6 -84.8-176.0   -1.2   -8.3   -5.8
   34   34 A L   H  > S+     0   0  0.879 122.2  52.6 -76.7 -36.9   -2.6   -5.1   -7.3
   35   35 A D   H  > S+     0   0  0.864 117.0  38.0 -66.2 -36.2   -5.9   -6.9   -8.0
   36   36 A A   H  > S+     0   0  0.958 115.3  50.2 -80.8 -55.9   -6.2   -8.1   -4.4
   37   37 A L   H >X S+     0   0  0.945 117.0  44.5 -45.1 -50.8   -4.8   -5.0   -2.7
   38   38 A W   H 3X S+     0   0  0.981 104.5  59.7 -58.5 -56.4   -7.3   -3.0   -4.8
   39   39 A D   H 3< S+     0   0  0.812 108.4  50.8 -44.0 -26.1  -10.1   -5.5   -4.1
   40   40 A C   H X<>S+     0   0  0.948 110.2  44.4 -79.7 -51.4   -9.4   -4.4   -0.6
   41   41 A L   H 3<5S+     0   0  0.950 117.0  45.6 -58.8 -49.5   -9.5   -0.6   -1.1
   42   42 A T   T 3<5S+     0   0  0.445 137.1  10.0 -75.7   3.9  -12.6   -0.8   -3.2
   43   43 A G   T < 5S+     0   0 -0.002 130.8  26.0-177.1  60.5  -14.3   -3.2   -0.7
   44   44 A W   T   5S+     0   0 -0.122  87.7  83.5 177.1 -66.6  -12.5   -3.8    2.6
   45   45 A V   S   <S-     0   0 -0.236  74.1-125.7 -58.4 149.6  -10.3   -0.9    3.9
   46   46 A E        -      0   0 -0.847  39.5-110.6-102.7 132.4  -12.2    1.8    5.8
   47   47 A Y   S    S+     0   0 -0.696  90.6  61.5-114.5 169.3  -11.7    5.4    4.6
   48   48 A P   S    S+     0   0  0.380  81.4 177.7 -61.4 136.7  -10.9    8.1    4.7
   49   49 A L   E      - c  0  84 -0.825  22.4-142.4-113.2 156.5   -7.5    6.3    4.8
   50   50 A V   E      -ac  2  85 -0.941   5.5-163.5-117.3 138.5   -4.0    7.8    4.9
   51   51 A L   E      -ac  3  86 -0.706   6.7-175.6-120.0  81.8   -1.1    6.2    3.0
   52   52 A E   E      -ac  4  87 -0.526  12.7-169.6 -77.6  83.2    2.0    7.7    4.5
   53   53 A W   E      -ac  5  88 -0.650   2.5-170.5 -79.7 111.4    4.4    6.1    2.1
```

75	54	54	A	R	E	+a	6	0	−0.740	66.4	12.3	−100.4	150.0	8.0	6.6	3.4
76	55	55	A	Q	S	> S+	0	0	0.977	75.3	172.3	49.9	68.7	11.1	5.7	1.3
77	56	56	A	F	T	>4 S+	0	0	0.990	74.6	35.2	−73.9	−66.7	9.0	5.2	−1.9
78	57	57	A	E	T	>> S+	0	0	0.885	118.0	56.0	−56.2	−35.2	11.8	4.8	−4.6
79	58	58	A	Q	H	3> S+	0	0	0.870	110.1	44.4	−66.4	−32.2	13.8	2.9	−1.9
80	59	59	A	S	H	<< S+	0	0	0.203	110.8	59.4	−94.7	17.7	10.8	0.6	−1.5
81	60	60	A	K	H	<4>S+	0	0	0.721	102.9	45.3	−111.5	−38.1	10.5	0.3	−5.3
82	61	61	A	Q	H	><5S+	0	0	0.992	101.0	62.9	−70.6	−62.9	14.0	−1.0	−6.3
83	62	62	A	L	T	3<5S+	0	0	0.779	118.8	32.6	−33.5	−32.0	14.4	−3.8	−3.7
84	63	63	A	T	T	3 5S−	0	0	−0.471	103.0	−130.4	−128.6	62.6	11.3	−5.3	−5.4
85	64	64	A	E	T	< 5S+	0	0	0.326	96.9	3.8	−12.4	107.0	11.7	−4.2	−9.0
86	65	65	A	N	T	<S+	0	0	0.874	104.4	124.7	73.7	32.1	8.3	−2.8	−9.8
87	66	66	A	G	T	> S+	0	0	0.939	72.3	21.6	−89.1	−69.2	7.2	−3.3	−6.2
88	67	67	A	A	H	> S+	0	0	0.716	111.9	68.3	−77.8	−21.6	6.0	−0.1	−4.6
89	68	68	A	E	H	> S+	0	0	0.795	103.2	48.0	−71.3	−21.9	5.1	1.9	−7.8
90	69	69	A	S	H	> S+	0	0	0.956	108.6	48.6	−81.4	−55.3	2.2	−0.6	−8.4
91	70	70	A	V	H	X S+	0	0	0.931	112.0	52.4	−52.0	−43.2	0.5	−0.7	−5.0
92	71	71	A	L	H	X S+	0	0	0.949	103.5	56.7	−59.2	−45.3	0.7	3.1	−5.0
93	72	72	A	Q	H	X S+	0	0	0.891	109.3	47.4	−52.7	−38.1	−1.0	3.1	−8.4
94	73	73	A	V	H	X S+	0	0	0.830	110.4	51.0	−75.0	−30.8	−3.8	1.2	−6.8
95	74	74	A	F	H	X S+	0	0	0.881	116.9	39.6	−74.7	−35.0	−4.0	3.5	−3.8
96	75	75	A	R	H	X S+	0	0	0.874	115.3	52.1	−80.2	−37.3	−4.3	6.6	−6.0
97	76	76	A	E	H	X S+	0	0	0.958	112.5	45.1	−63.3	−46.7	−6.5	4.8	−8.5
98	77	77	A	A	H	<>S+	0	0	0.931	109.5	55.9	−62.6	−38.8	−8.8	3.9	−5.6
99	78	78	A	K	H	><5S+	0	0	0.859	107.6	50.2	−58.4	−30.9	−8.4	7.5	−4.5
100	79	79	A	A	H	3<5S+	0	0	0.788	94.7	70.7	−77.3	−28.8	−9.7	8.2	−7.9
101	80	80	A	E	T	3<5S−	0	0	0.585	129.3	−91.6	−65.8	−6.6	−12.6	5.8	−7.4
102	81	81	A	G	T	< 5S+	0	0	0.209	87.8	133.5	113.3	−14.1	−14.0	8.4	−5.0
103	82	82	A	C		< −	0	0	−0.209	60.3	−126.0	−63.9	160.5	−12.3	6.9	−1.9
104	83	83	A	D		+	0	0	−0.492	47.3	152.7	−109.3	65.3	−10.5	9.3	0.4
105	84	84	A	I	E	−c	49	0	−0.688	39.5	−144.7	−94.3	87.9	−7.0	7.7	0.7
106	85	85	A	T	E	−c	50	0	−0.284	15.8	−146.8	−52.9	98.9	−4.8	10.7	1.4
107	86	86	A	I	E	−c	51	0	−0.577	18.1	−174.3	−73.4	114.6	−1.7	9.7	−0.6
108	87	87	A	I	E	−c	52	0	−0.865	2.5	−173.3	−114.2	101.2	1.3	11.0	1.3
109	88	88	A	L	E	c	53	0	−0.800	360.0	360.0	−96.8	106.7	4.6	10.3	−0.7
110	89	89	A	S			0	0	−0.879	360.0	360.0	−109.0	360.0	7.6	11.3	1.4