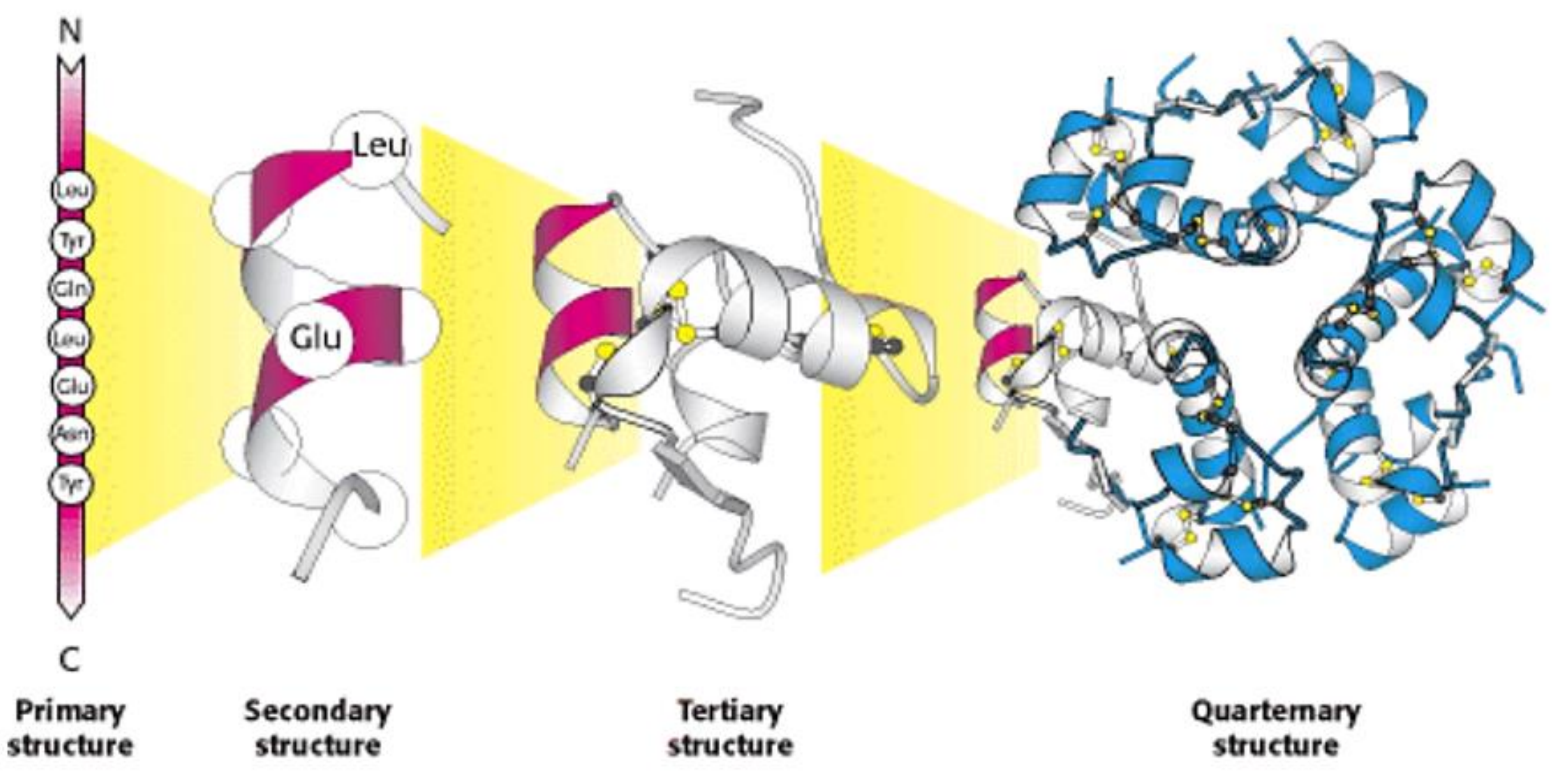
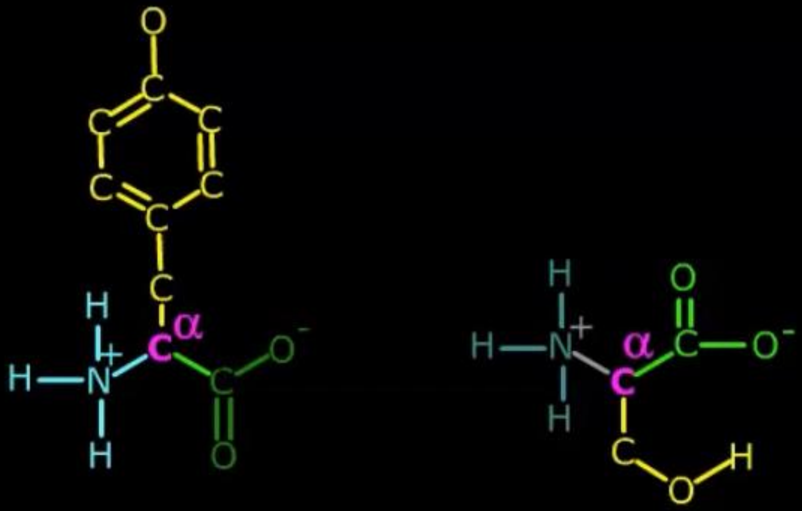
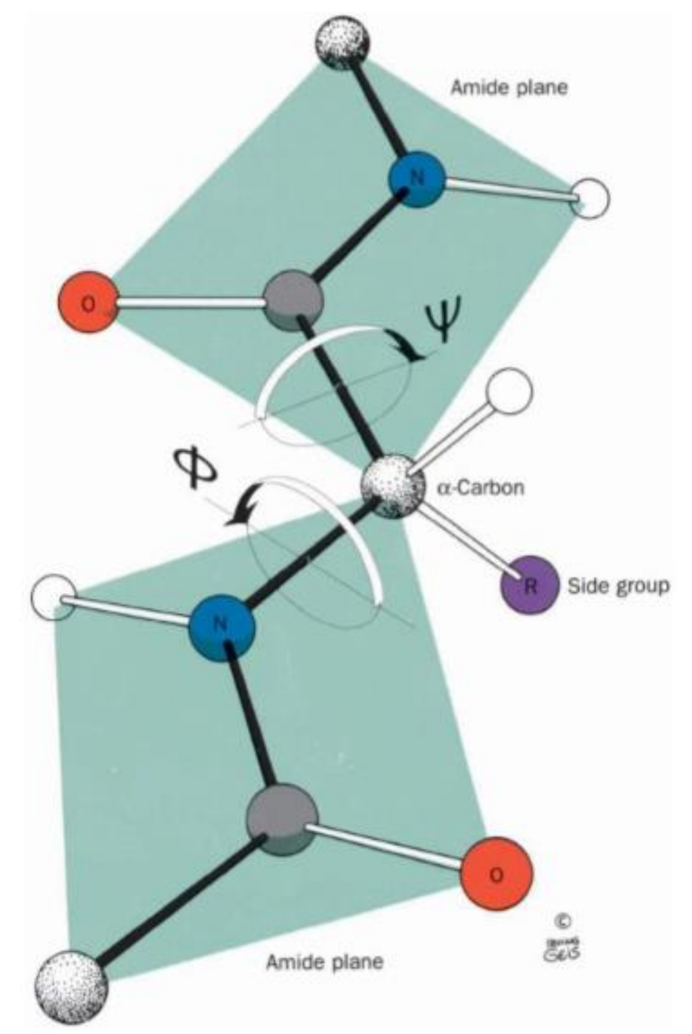
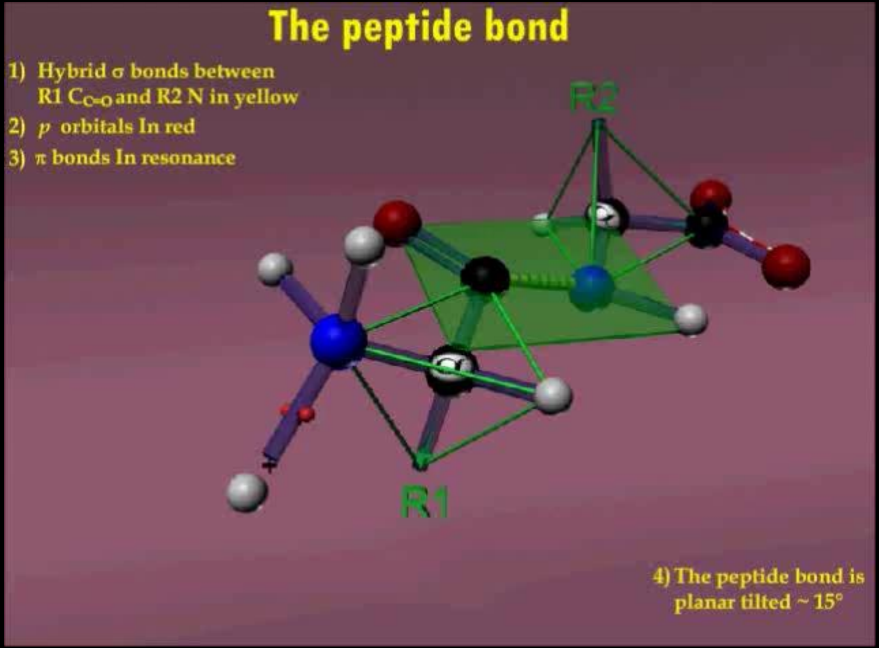
Estrutura de Proteínas

Ronaldo Bento Quaggio


N
Leu
Tyr
Gln
Leu
Glu
Asn
Tyr
C
Leu
Glu
Primary structure
Secondary structure
Tertiary structure
Quarternary structure


α
α



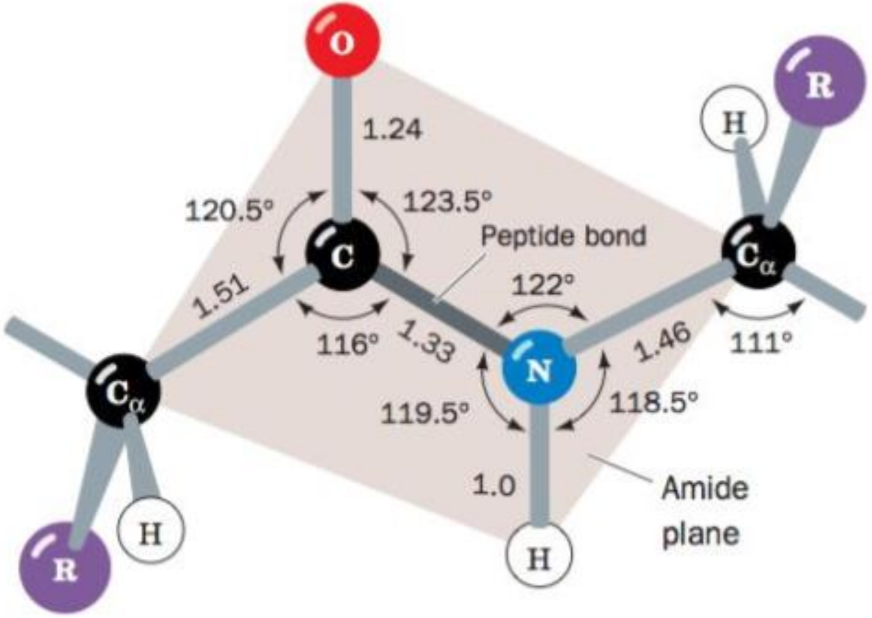


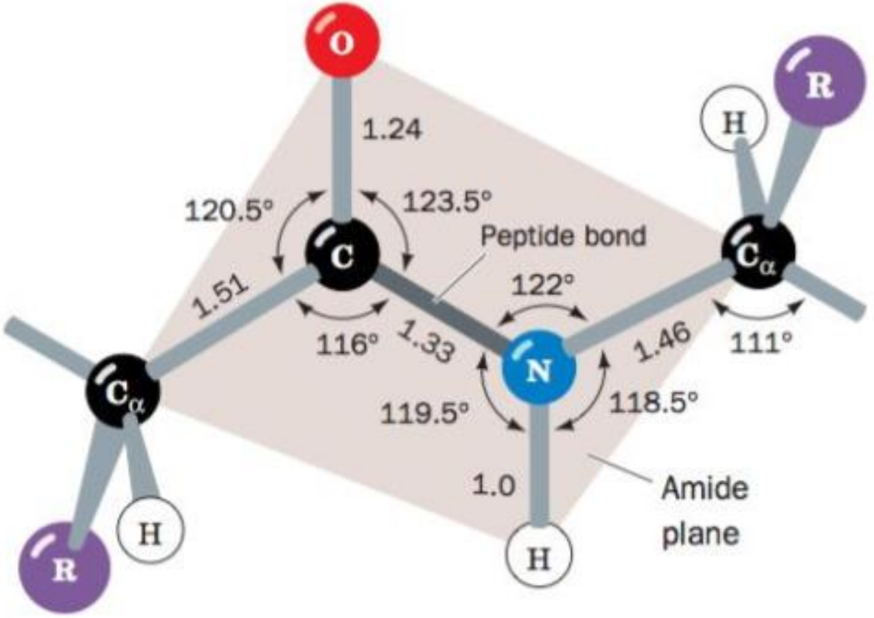
The peptide bond

1) Hybrid σ bonds between R1 $C_{C=O}$ and R2 N in yellow
2) *p* orbitals In red
3) π bonds In resonance

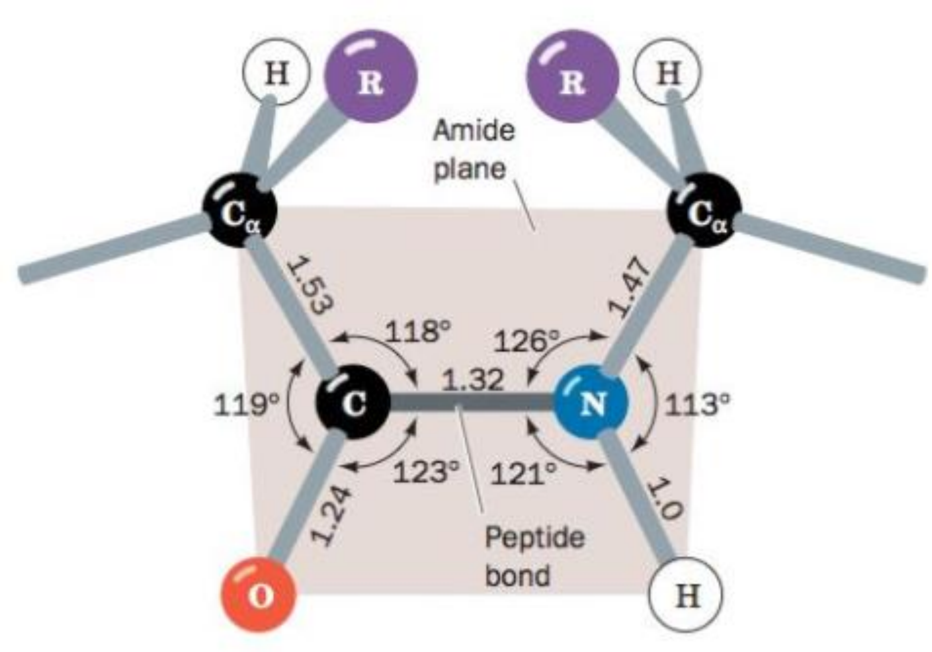
4) The peptide bond is planar tilted ~ 15°

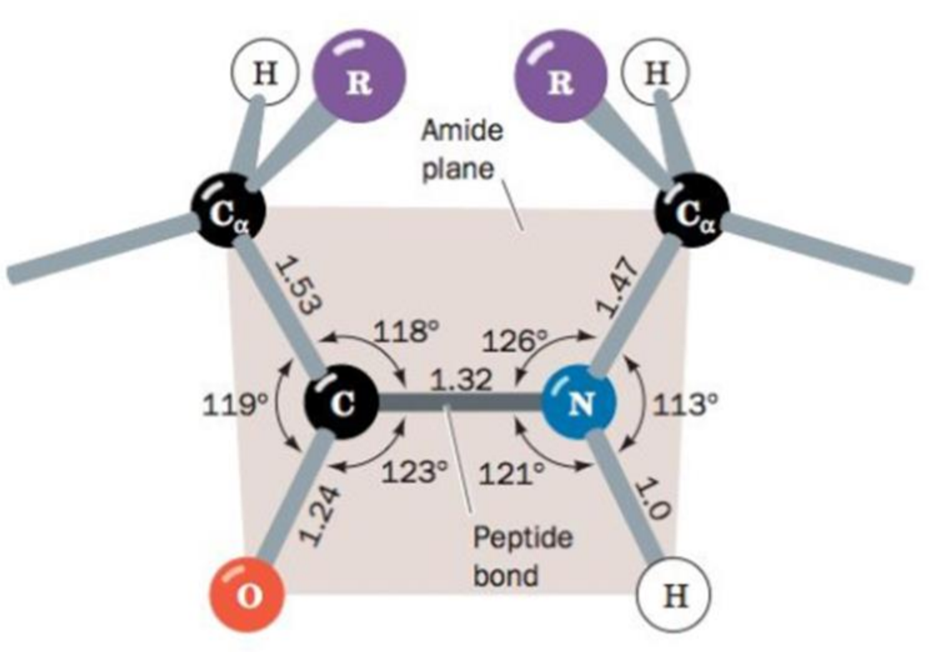
Ligação peptídica trans



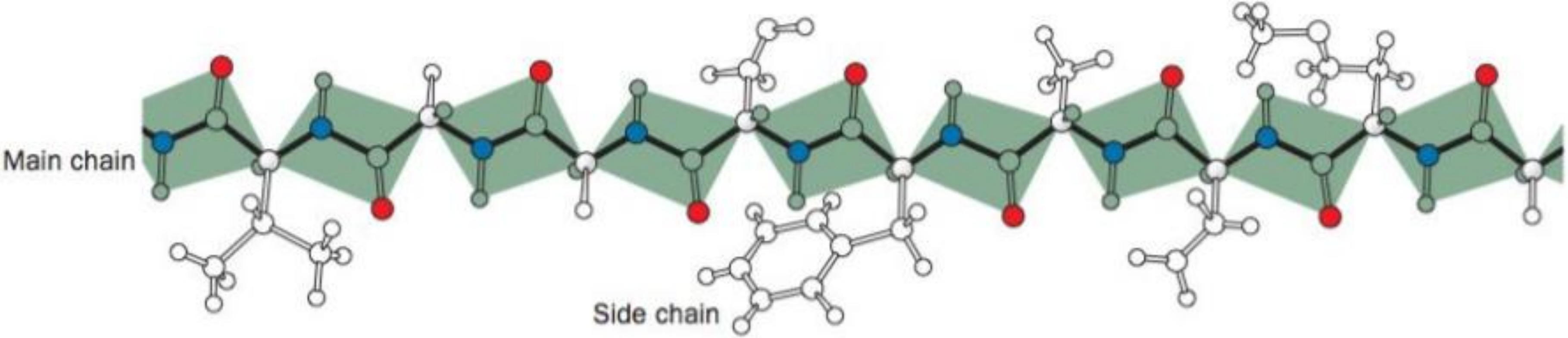


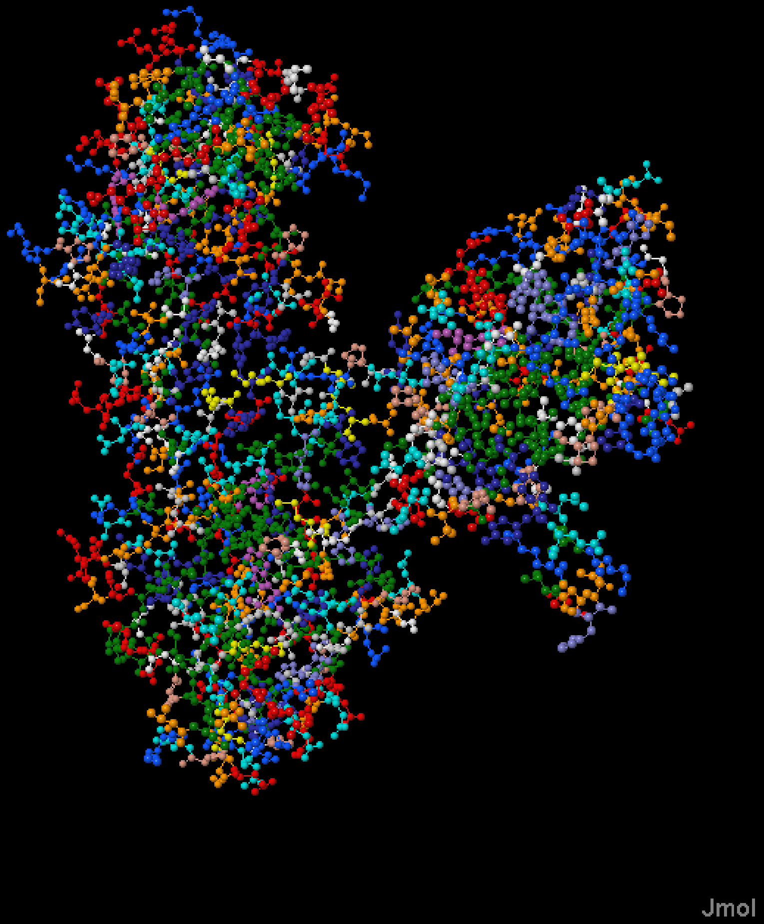
Ligação peptídica cis





Estrutura primária

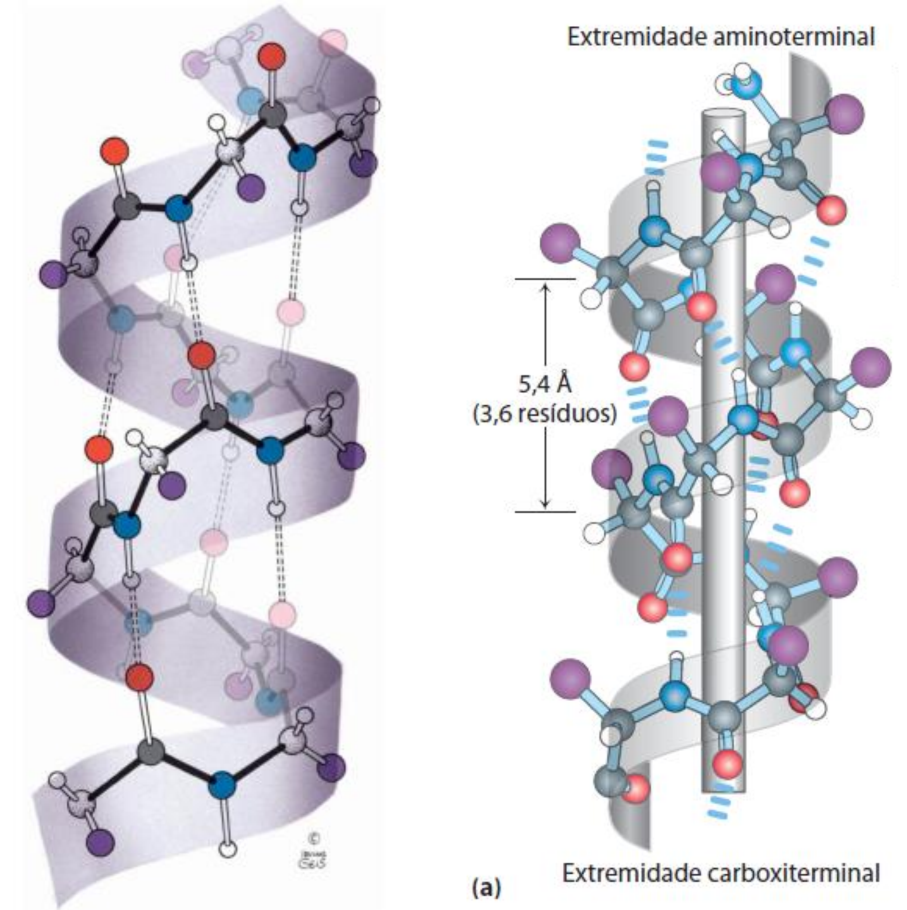


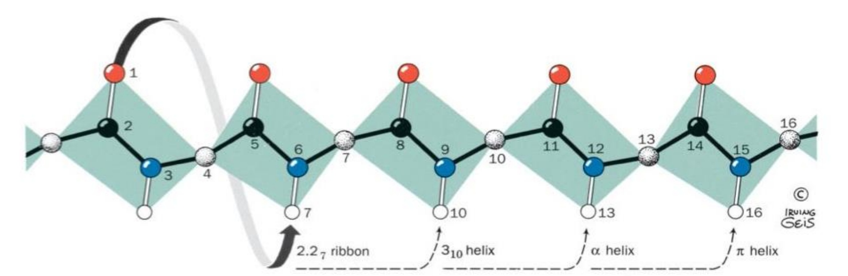


>>Estrutura primária

A estrutura primária é a **seqüência linear** de aminoácidos unidos pela ligação peptídica que constitui uma proteína. Abaixo temos a estrutura primária da difteri
toxina, com seus 535 aminoácidos.
Os aminoácidos estão escritos no código de 3 letras.

```
  1  GLY ALA ASP ASP VAL VAL ASP SER SER LYS   10
 11  SER PHE VAL MET GLU ASN PHE SER SER TYR   20
 21  HIS GLY THR LYS PRO GLY TYR VAL ASP SER   30
 31  ILE GLN LYS GLY ILE GLN LYS PRO LYS SER   40
 41  GLY THR GLN GLY ASN TYR ASP ASP ASP TRP   50
 51  LYS GLY PHE TYR SER THR ASP ASN LYS TYR   60
 61  ASP ALA ALA GLY TYR SER VAL ASP ASN GLU   70
 71  ASN PRO LEU SER GLY LYS ALA GLY GLY VAL   80
 81  VAL LYS VAL THR TYR PRO GLY LEU THR LYS   90
 91  VAL LEU ALA LEU LYS VAL ASP ASN ALA GLU  100
101  THR ILE LYS LYS GLU LEU GLY LEU SER LEU  110
111  THR GLU PRO LEU MET GLU GLN VAL GLY THR  120
121  GLU GLU PHE ILE LYS ARG PHE GLY ASP GLY  130
131  ALA SER ARG VAL VAL LEU SER LEU PRO PHE  140
141  ALA GLU GLY SER SER SER VAL GLU TYR ILE  150
151  ASN ASN TRP GLU GLN ALA LYS ALA LEU SER  160
161  VAL GLU LEU GLU ILE ASN PHE GLU THR ARG  170
171  GLY LYS ARG GLY GLN ASP ALA MET TYR GLU  180
181  TYR MET ALA GLN ALA CYS ALA GLY ASN ARG  190
191  VAL ARG ARG SER VAL GLY SER SER LEU SER  200
201  CYS ILE ASN LEU ASP TRP ASP VAL ILE ARG  210
211  ASP LYS THR LYS THR LYS ILE GLU SER LEU  220
221  LYS GLU HIS GLY PRO ILE LYS ASN LYS MET  230
231  SER GLU SER PRO ASN LYS THR VAL SER GLU  240
241  GLU LYS ALA LYS GLN TYR LEU GLU GLU PHE  250
251  HIS GLN THR ALA LEU GLU HIS PRO GLU LEU  260
261  SER GLU LEU LYS THR VAL THR GLY THR ASN  270
271  PRO VAL PHE ALA GLY ALA ASN TYR ALA ALA  280
281  TRP ALA VAL ASN VAL ALA GLN VAL ILE ASP  290
291  SER GLU THR ALA ASP ASN LEU GLU LYS THR  300
301  THR ALA ALA LEU SER ILE LEU PRO GLY ILE  310
311  GLY SER VAL MET GLY ILE ALA ASP GLY ALA  320
321  VAL HIS HIS ASN THR GLU GLU ILE VAL ALA  330
331  GLN SER ILE ALA LEU SER SER LEU MET VAL  340
341  ALA GLN ALA ILE PRO LEU VAL GLY GLU LEU  350
351  VAL ASP ILE GLY PHE ALA ALA TYR ASN PHE  360
361  VAL GLU SER ILE ILE ASN LEU PHE GLN VAL  370
371  VAL HIS ASN SER TYR ASN ARG PRO ALA TYR  380
381  SER PRO GLY HIS LYS THR GLN PRO PHE LEU  390
391  HIS ASP GLY TYR ALA VAL SER TRP ASN THR  400
401  VAL GLU ASP SER ILE ILE ARG THR GLY PHE  410
411  GLN GLY GLU SER GLY HIS ASP ILE LYS ILE  420
421  THR ALA GLU ASN THR PRO LEU PRO ILE ALA  430
431  GLY VAL LEU LEU PRO THR ILE PRO GLY LYS  440
441  LEU ASP VAL ASN LYS SER LYS THR HIS ILE  450
451  SER VAL ASN GLY ARG LYS ILE ARG MET ARG  460
461  CYS ARG ALA ILE ASP GLY ASP VAL THR PHE  470
471  CYS ARG PRO LYS SER PRO VAL TYR VAL GLY  480
481  ASN GLY VAL HIS ALA ASN LEU HIS VAL ALA  490
491  PHE HIS ARG SER SER SER GLU LYS ILE HIS  500
501  SER ASN GLU ILE SER SER ASP SER ILE GLY  510
511  VAL LEU GLY TYR GLN LYS THR VAL ASP HIS  520
521  THR LYS VAL ASN SER LYS LEU SER LEU PHE  530
531  PHE GLU ILE LYS                          535
```

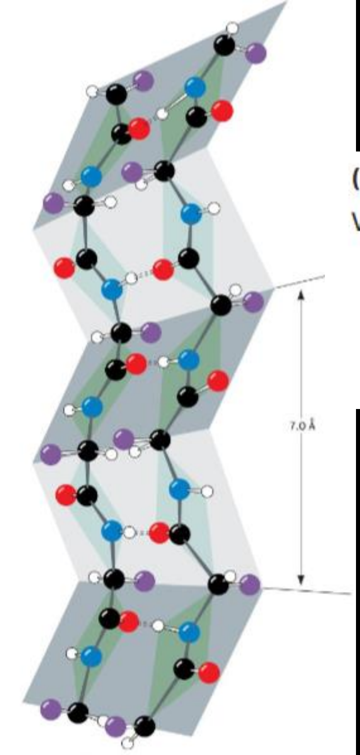


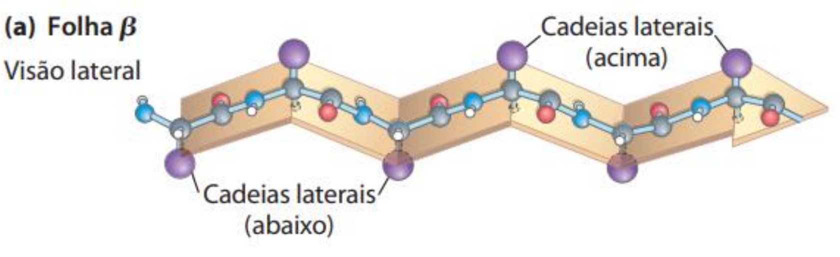


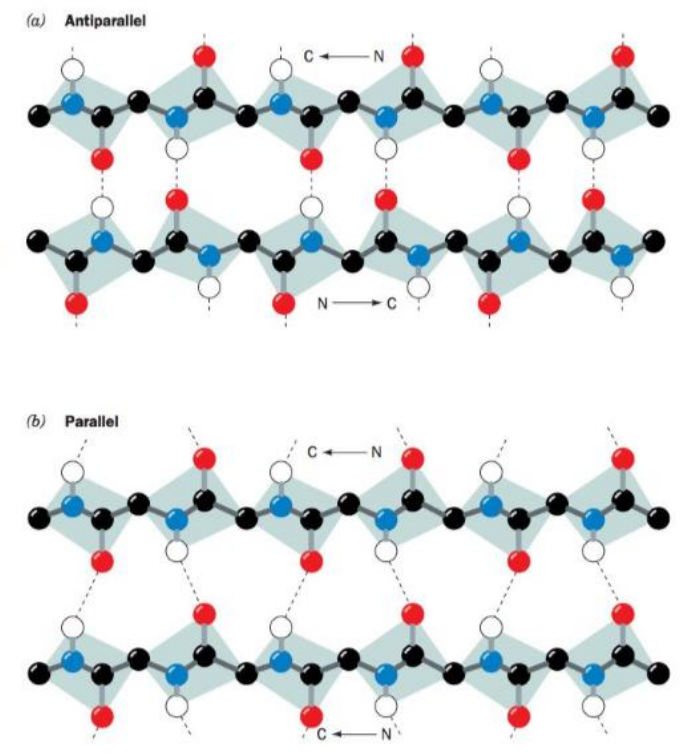
Estrutura Secundária

α-Hélice

Folhas β pregueadas

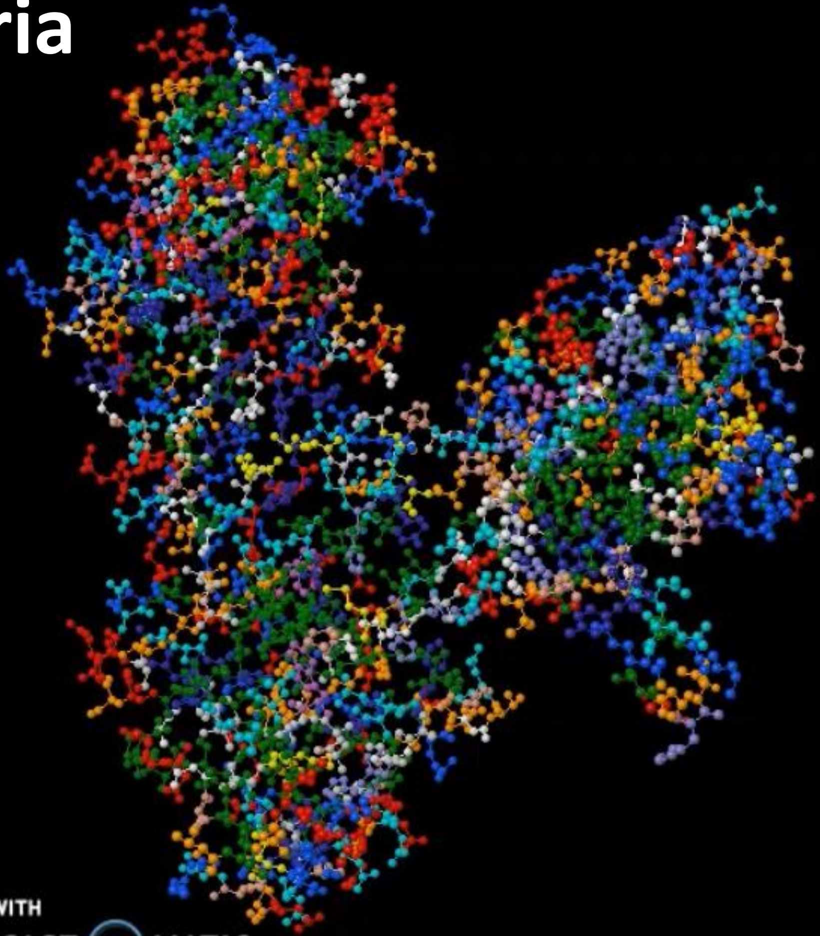


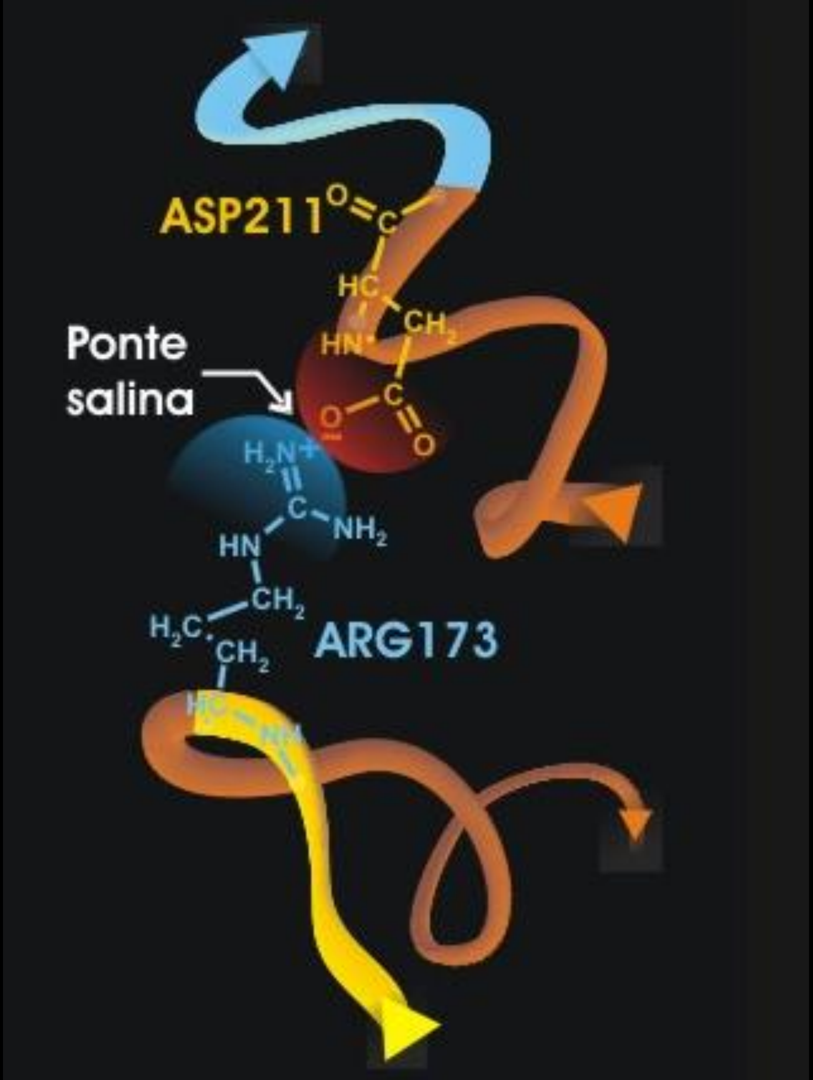




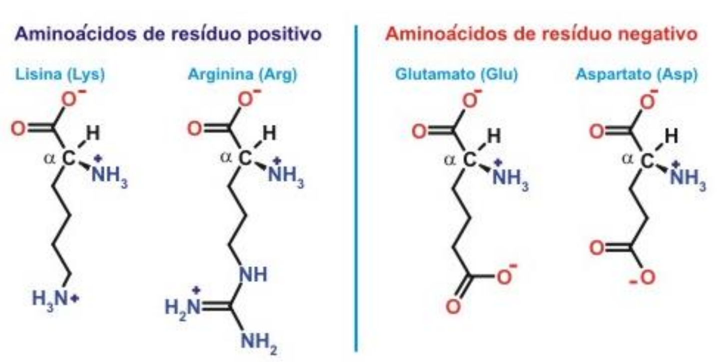

THR386
GL 23

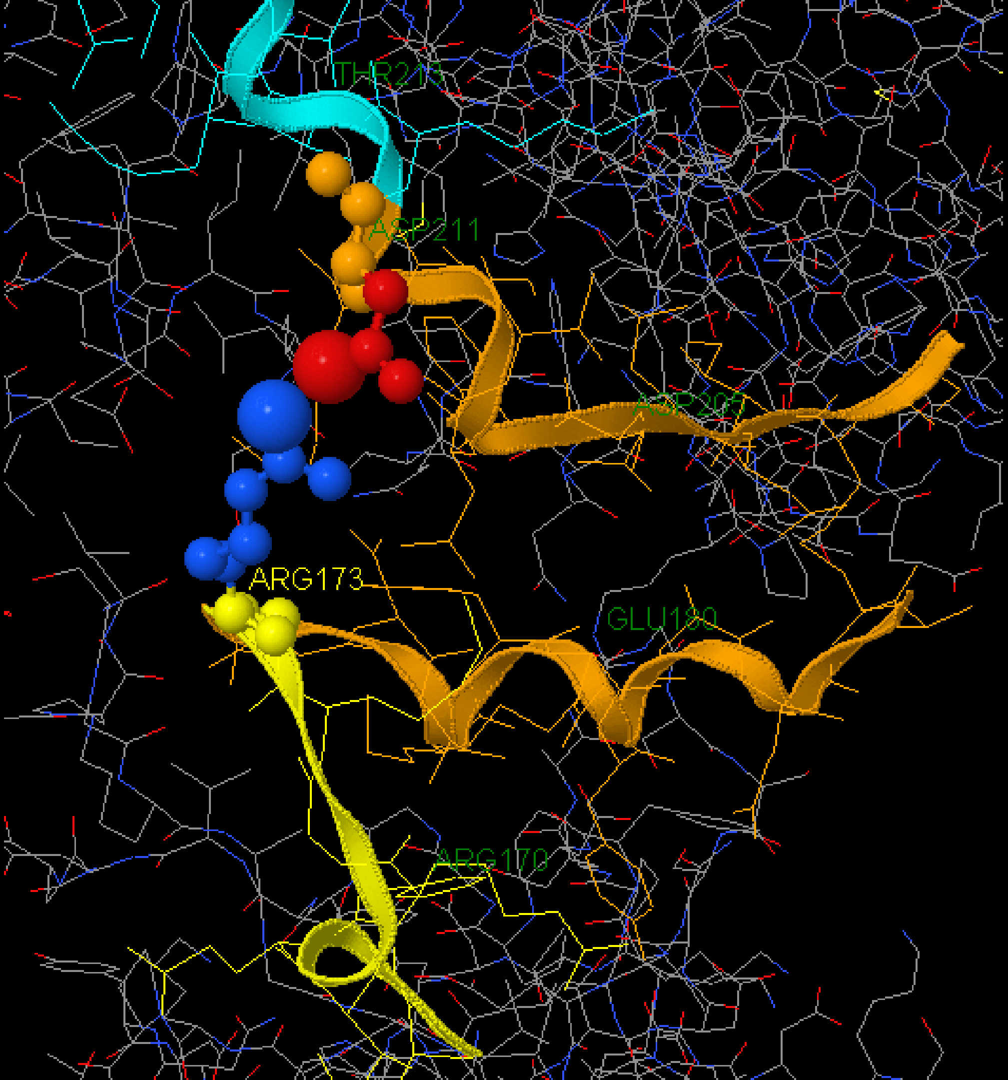
Estrutura Terciária

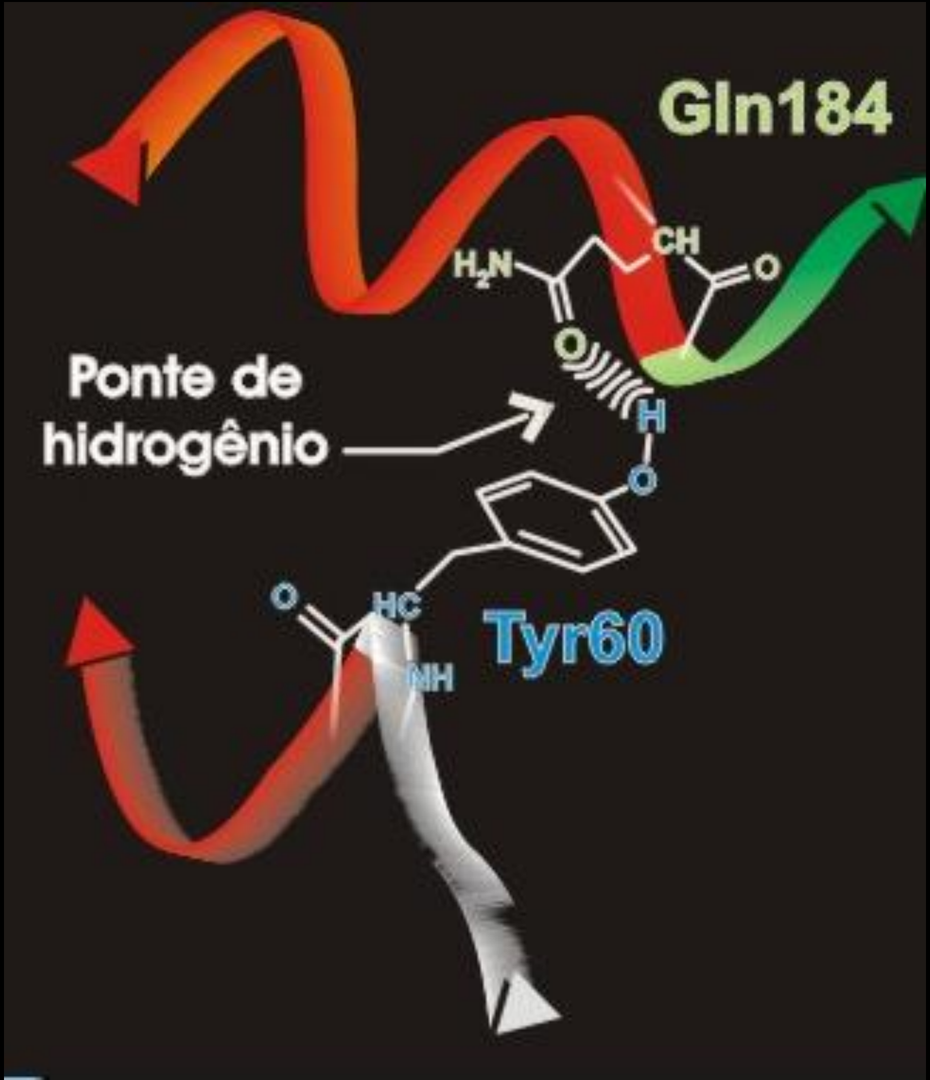




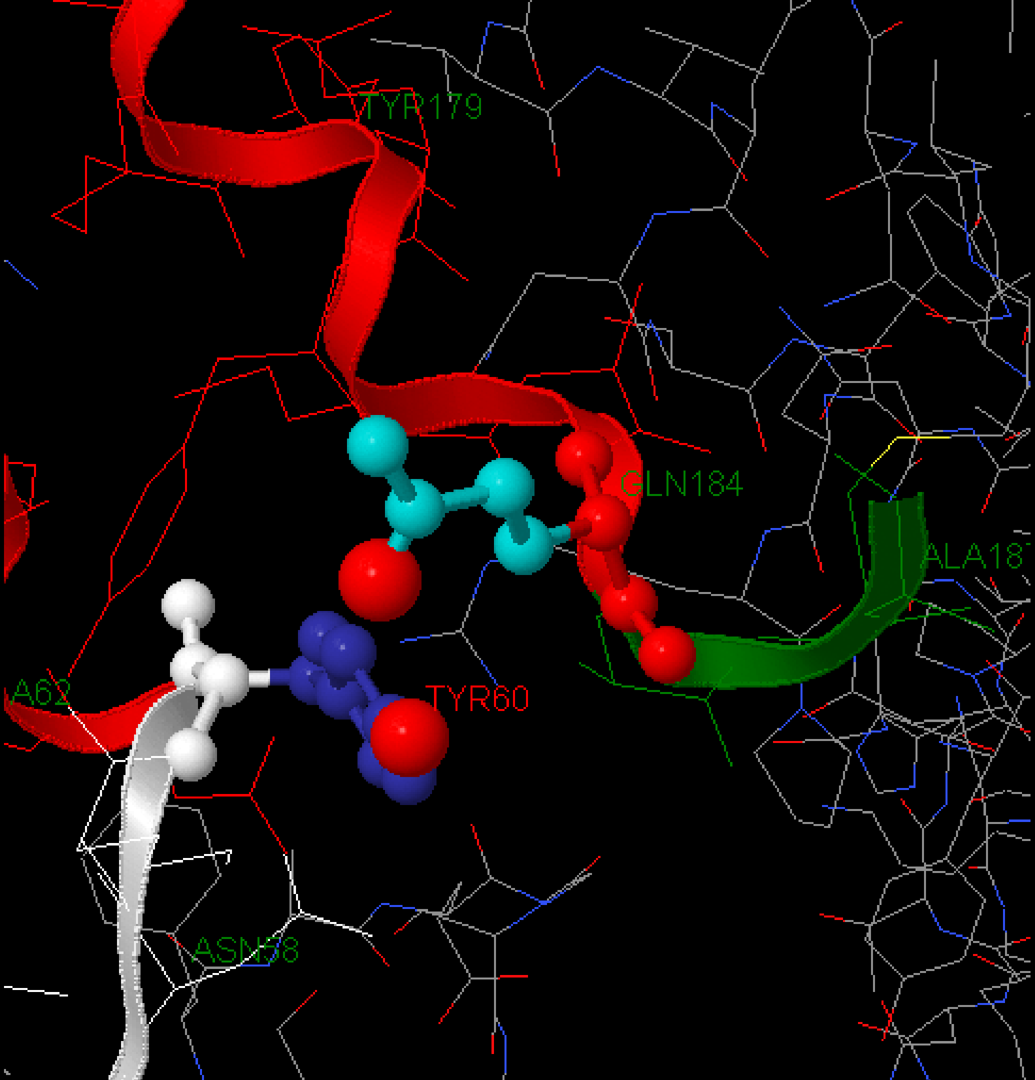
Ponte salina

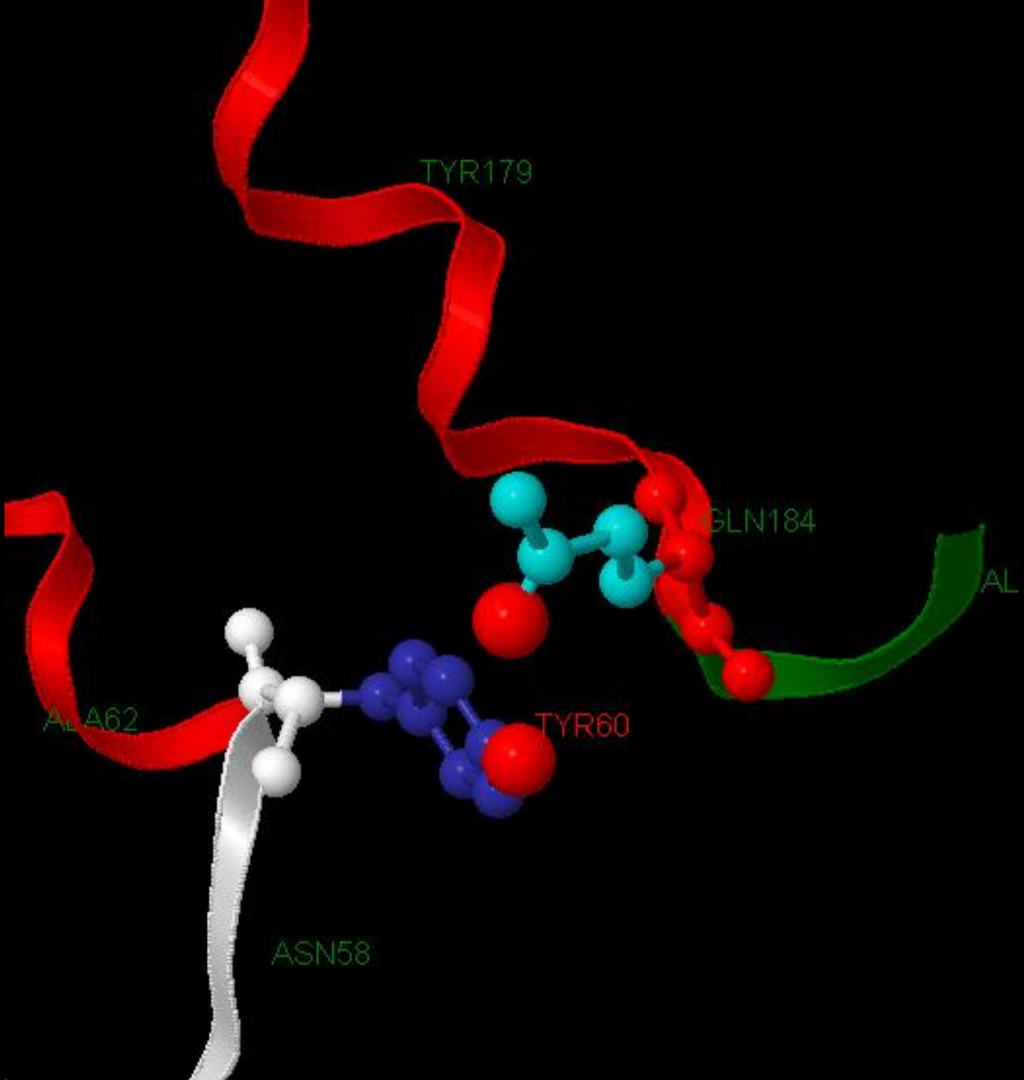


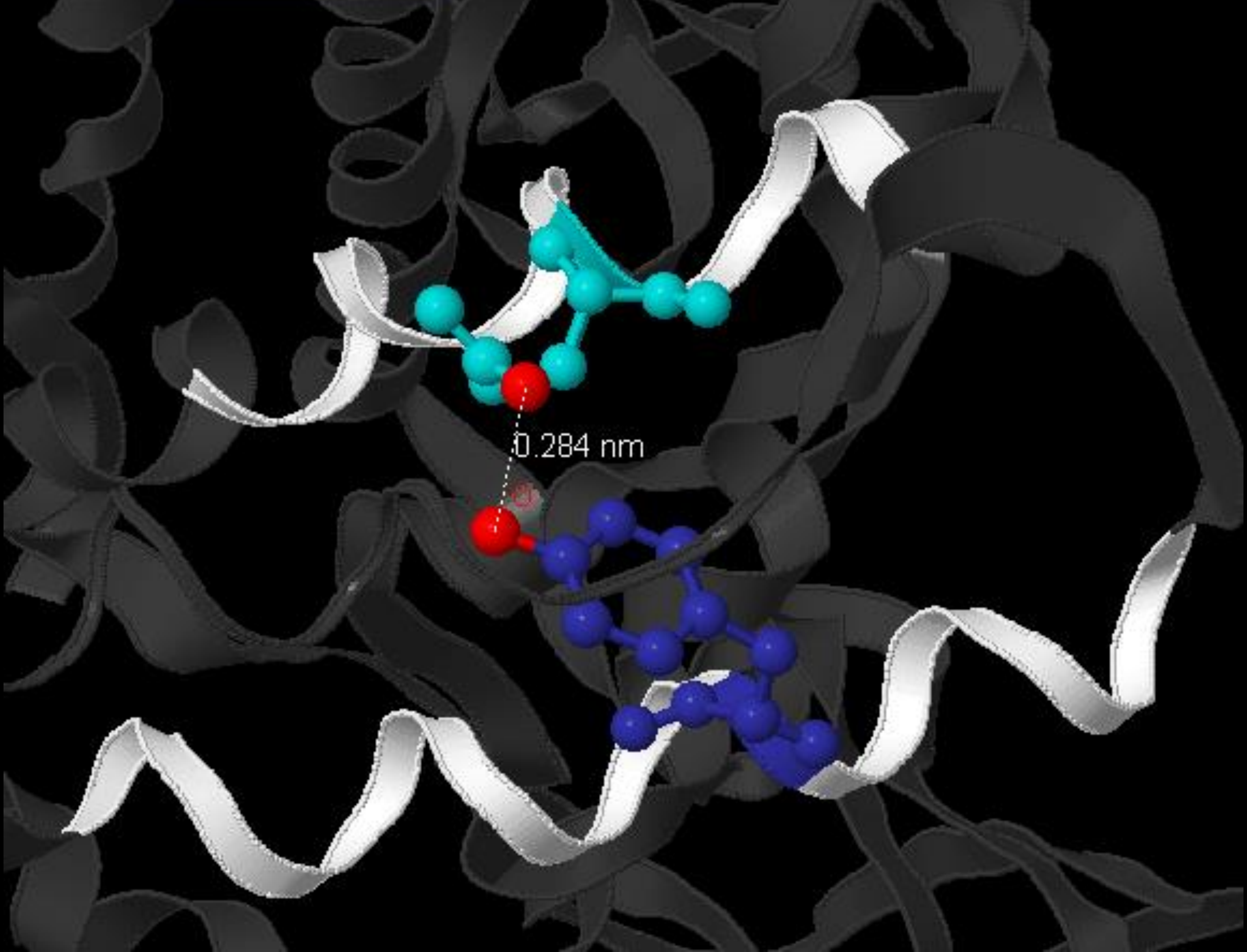

THR213
ASP211
ASP205
ARG173
GLU180
ARG170



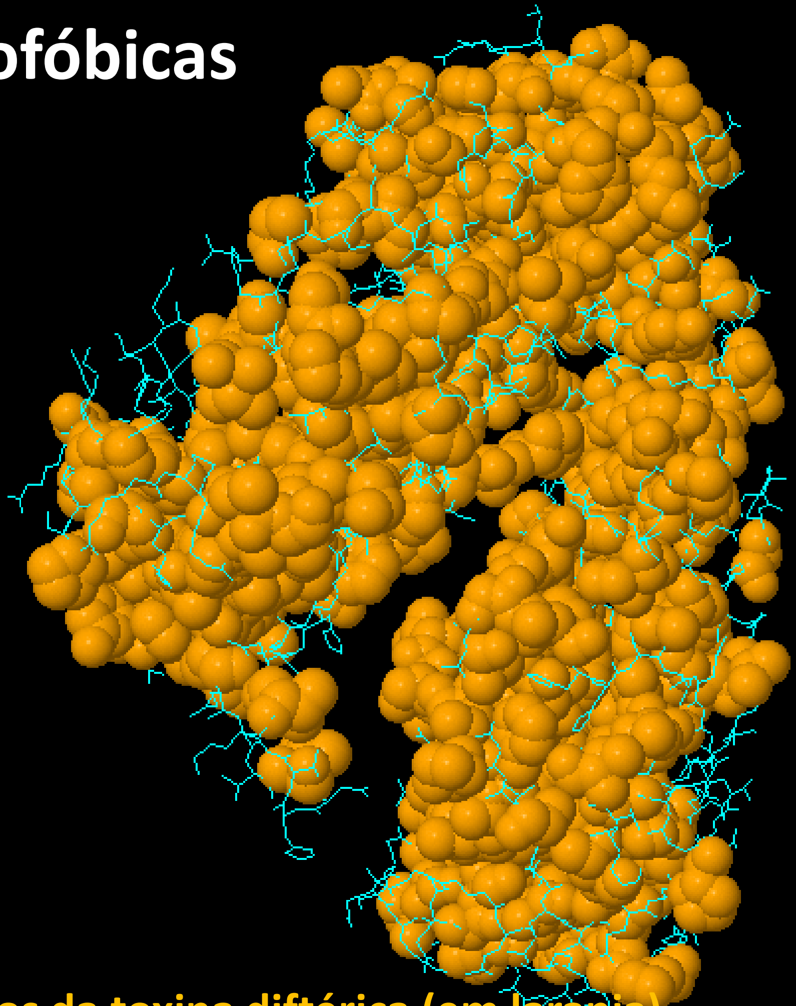
Ponte de hidrogênio


TYR179
GLN184
ALA18
A62
TYR60
ASN58


TYR179
GLN184
AL
ALA62
TYR60
ASN58

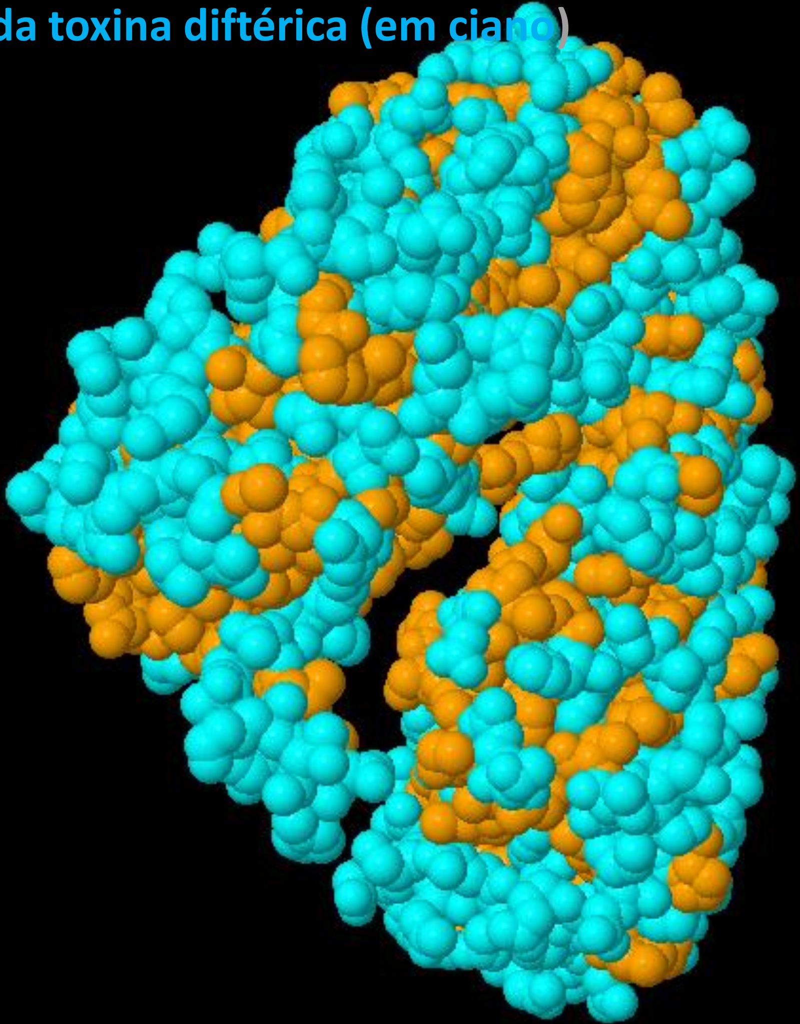

0.284 nm

Interações Hidrofóbicas

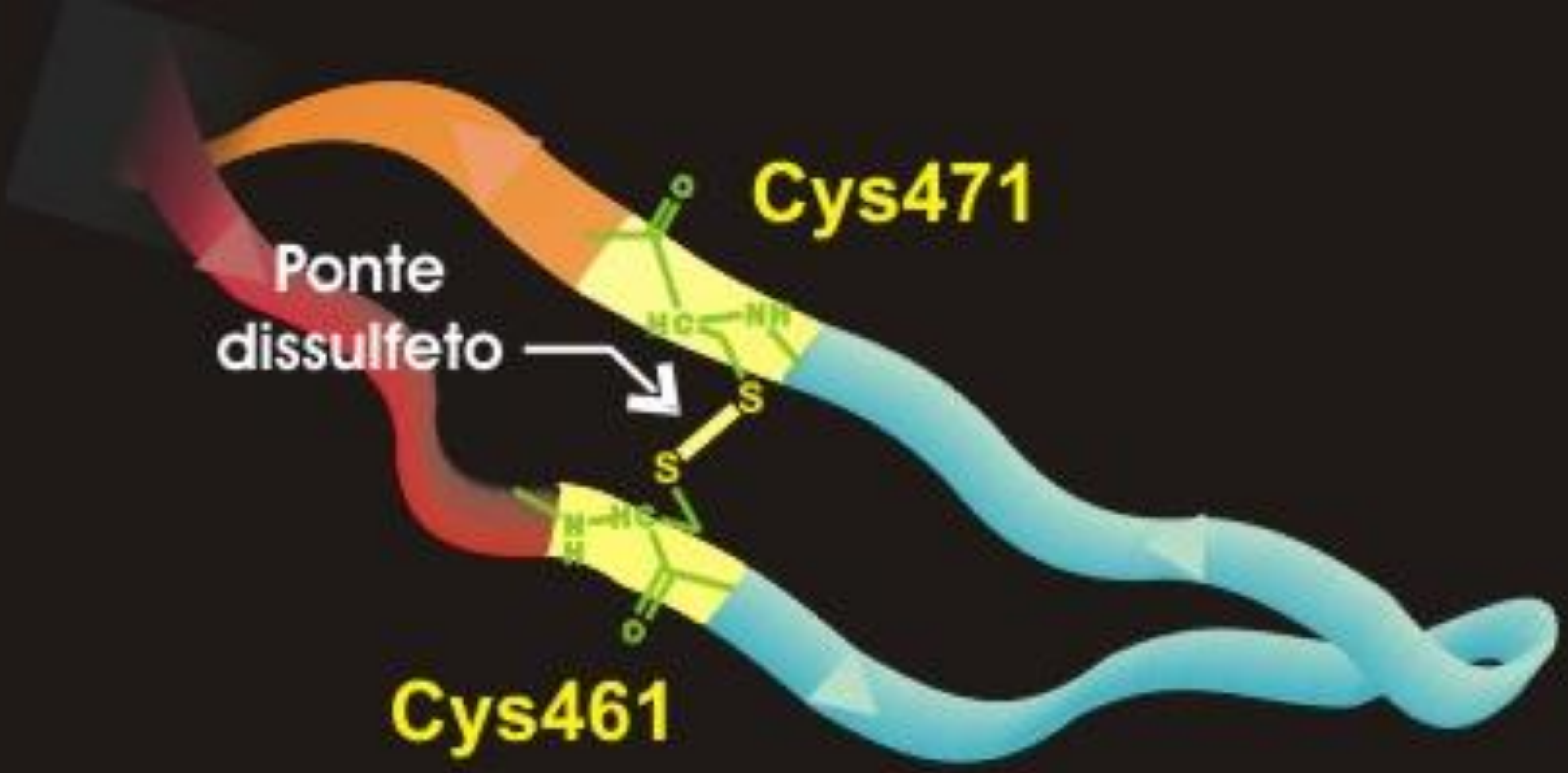


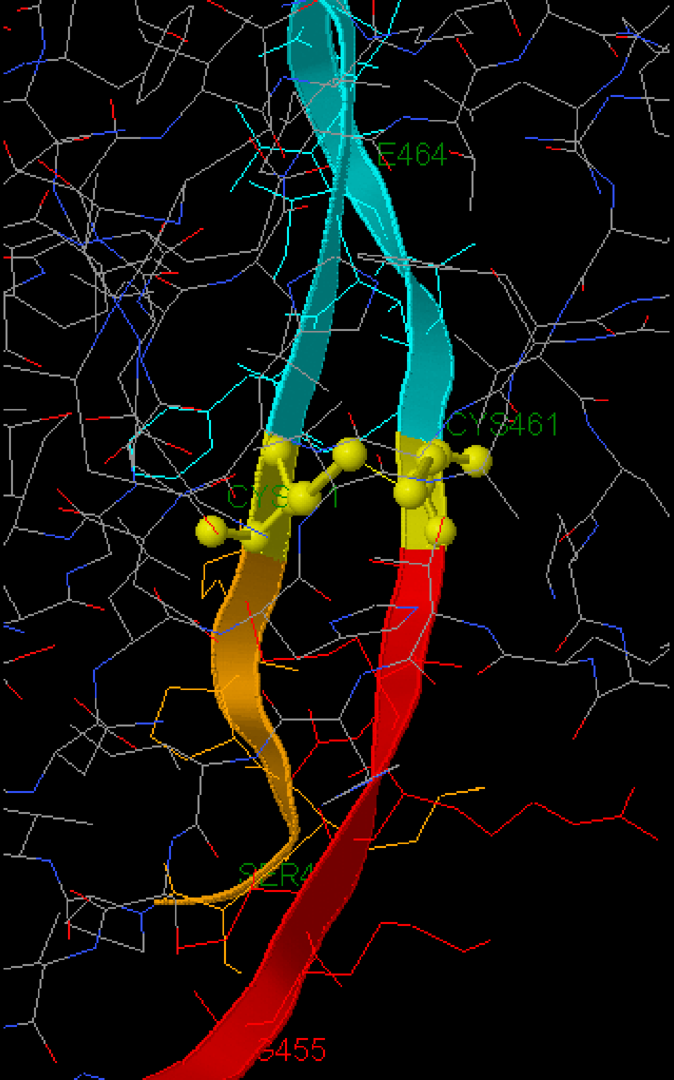
Aminoácidos hidrofóbicos da toxina diftérica (em laranja)

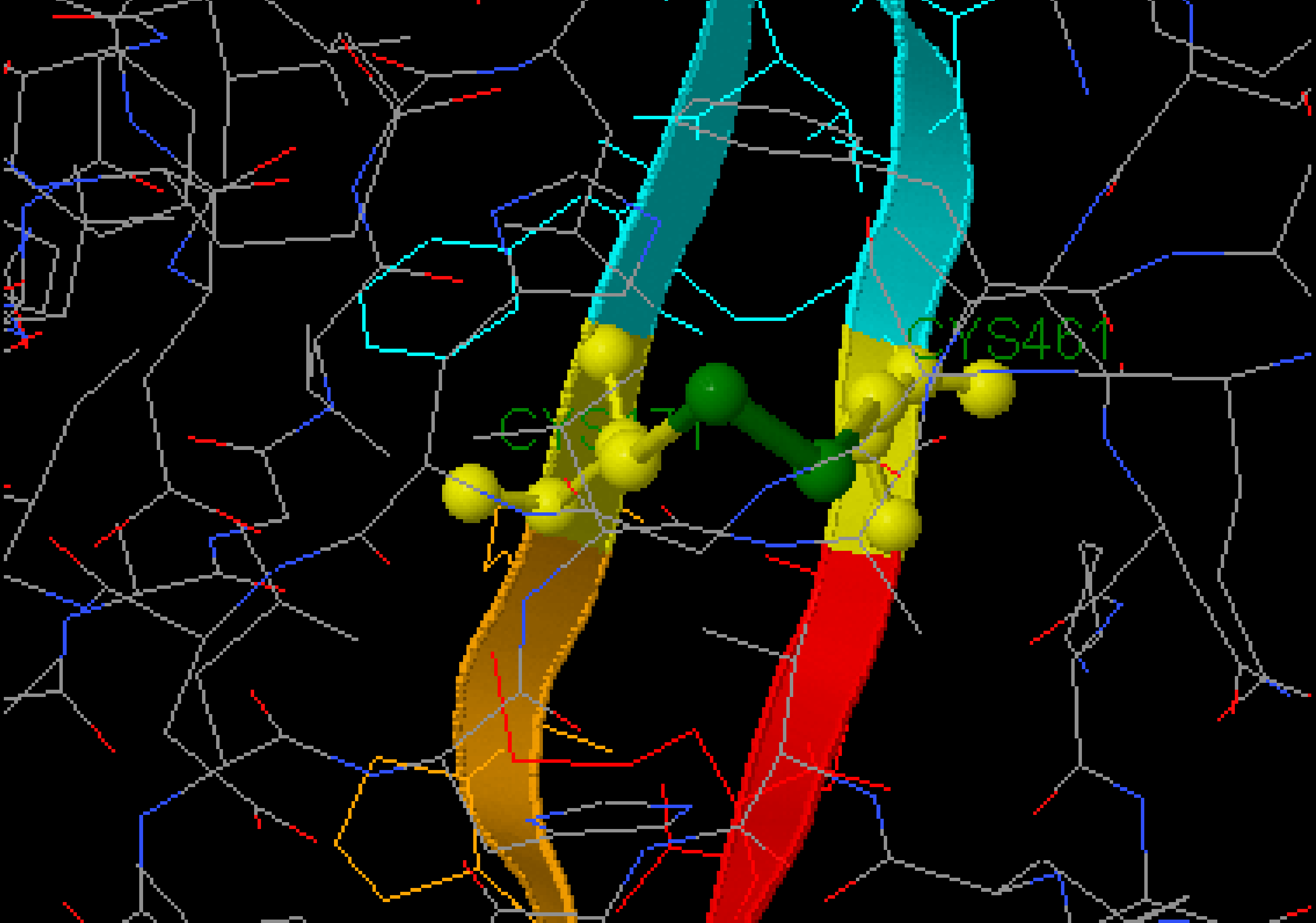
Aminoácidos hidrofílicos da toxina diftérica (em ciano)



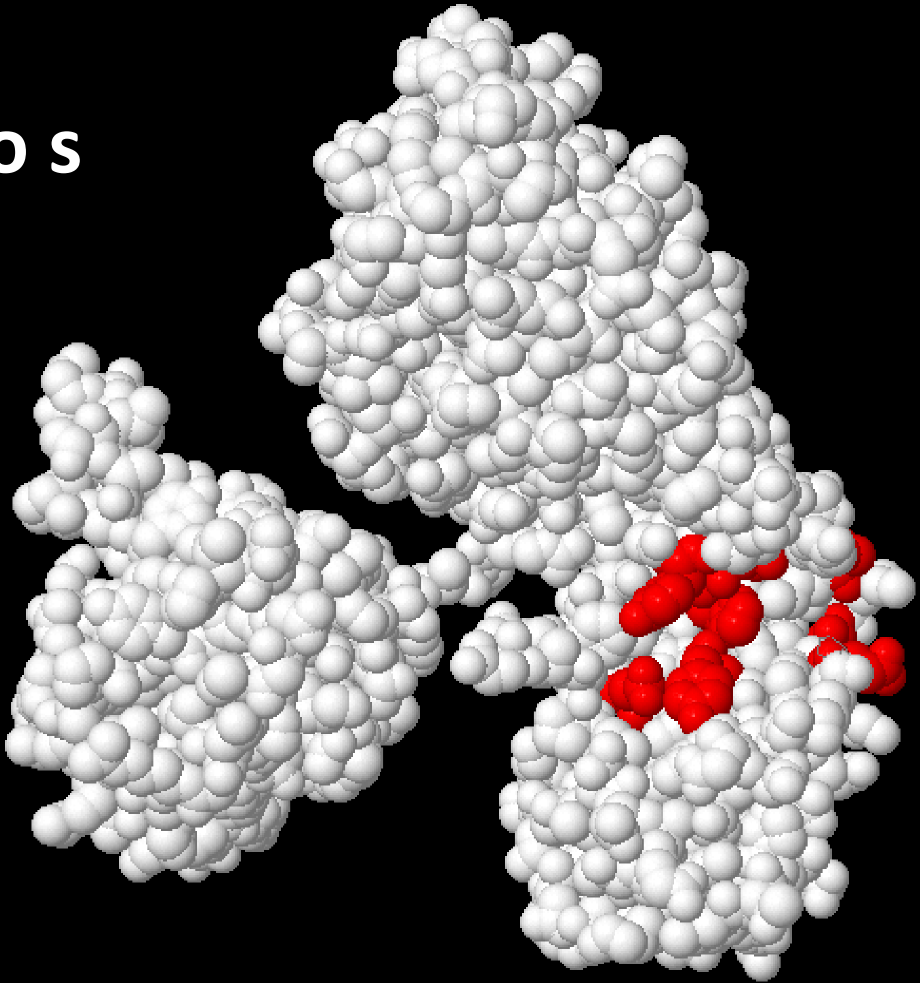
Ponte dissulfeto

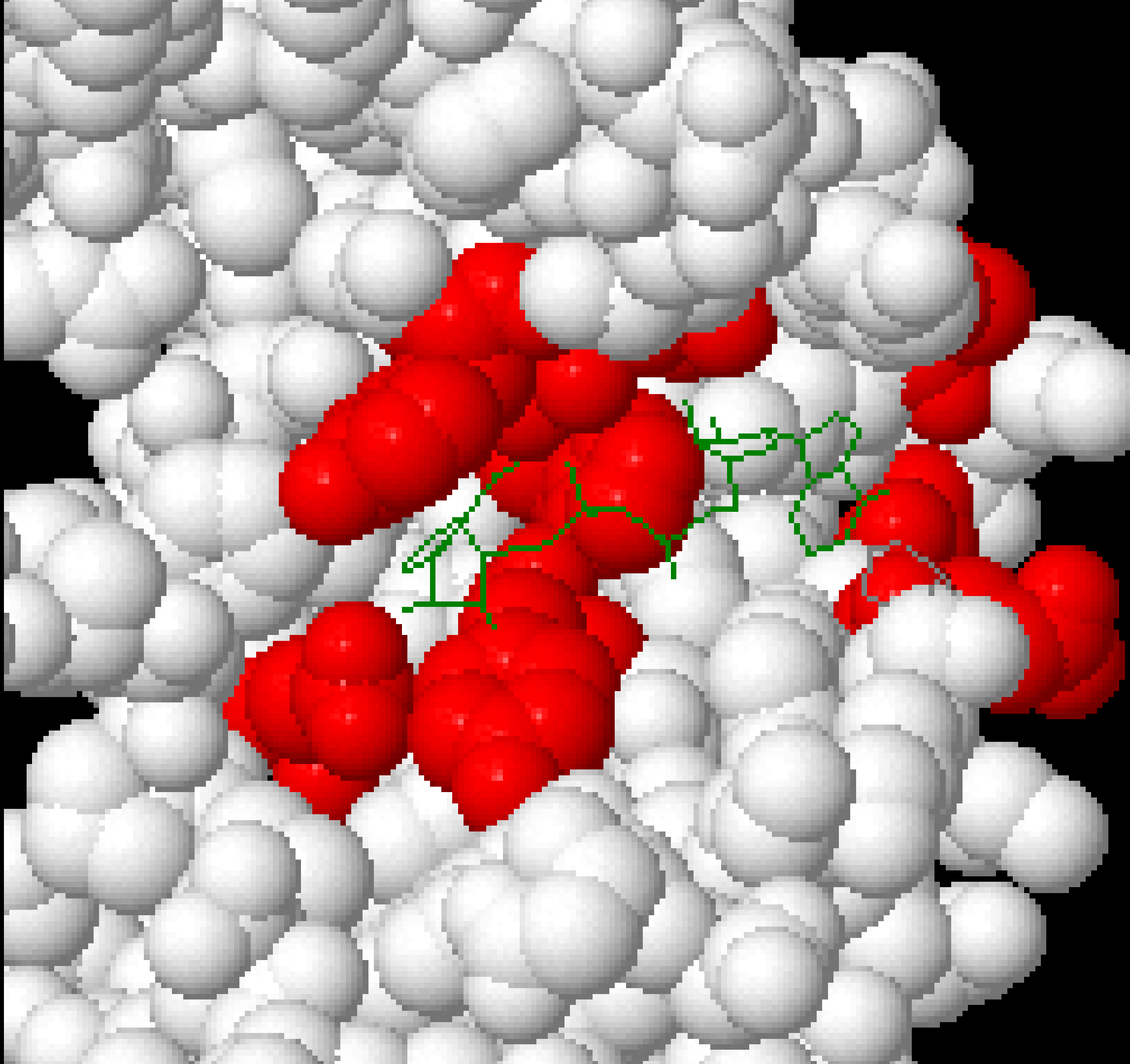



E464
CYS461
CYS 1
SER4
455


CYS461
CYS471

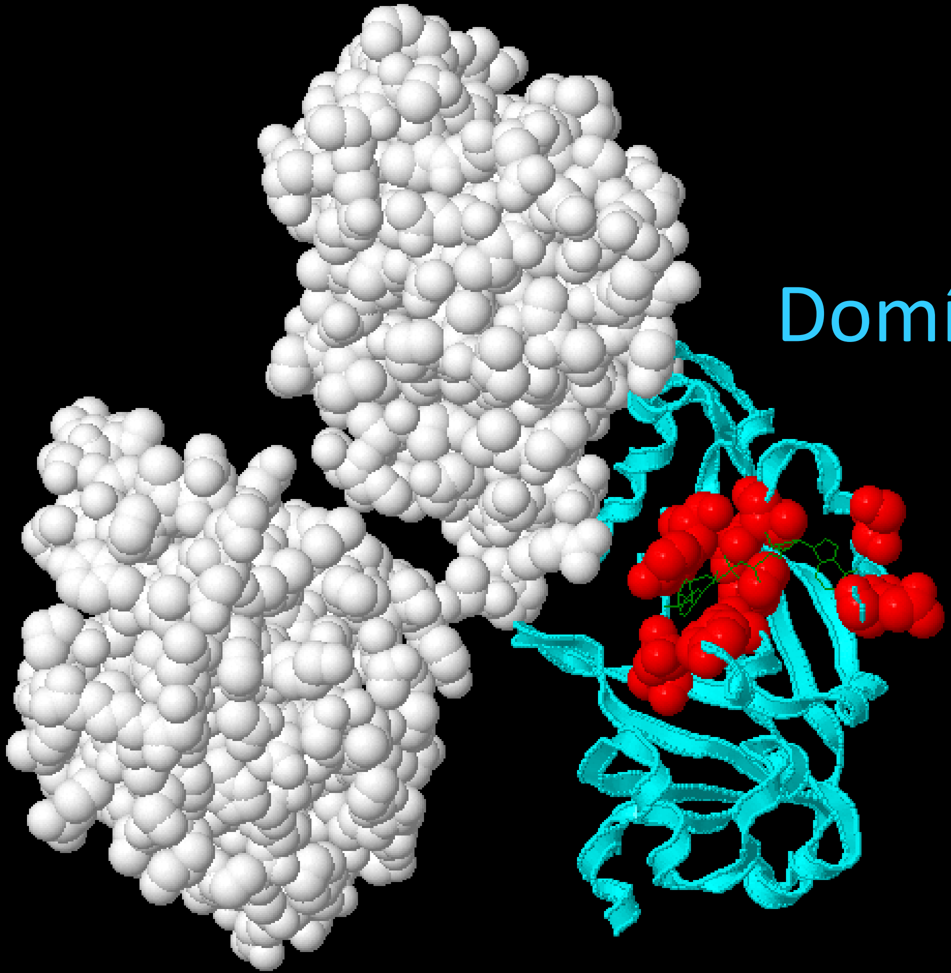
Domínios



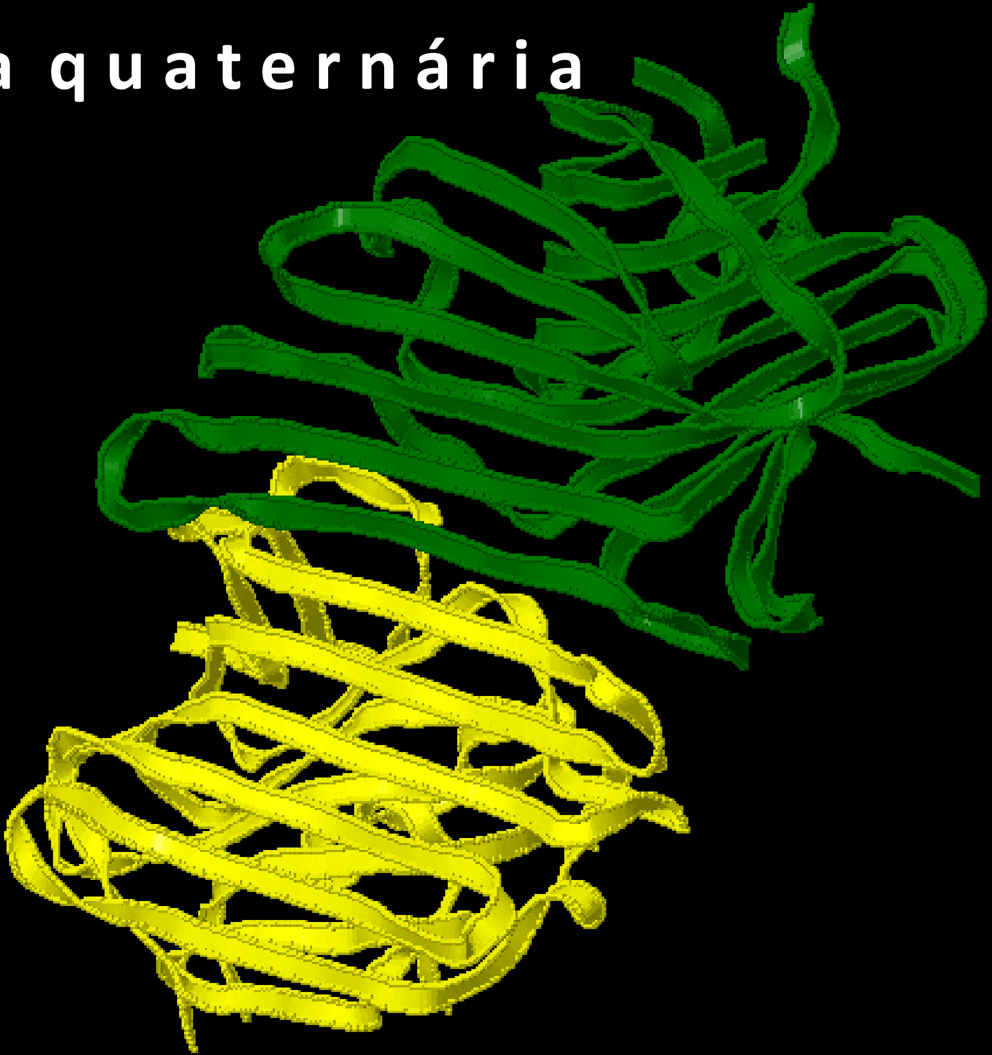


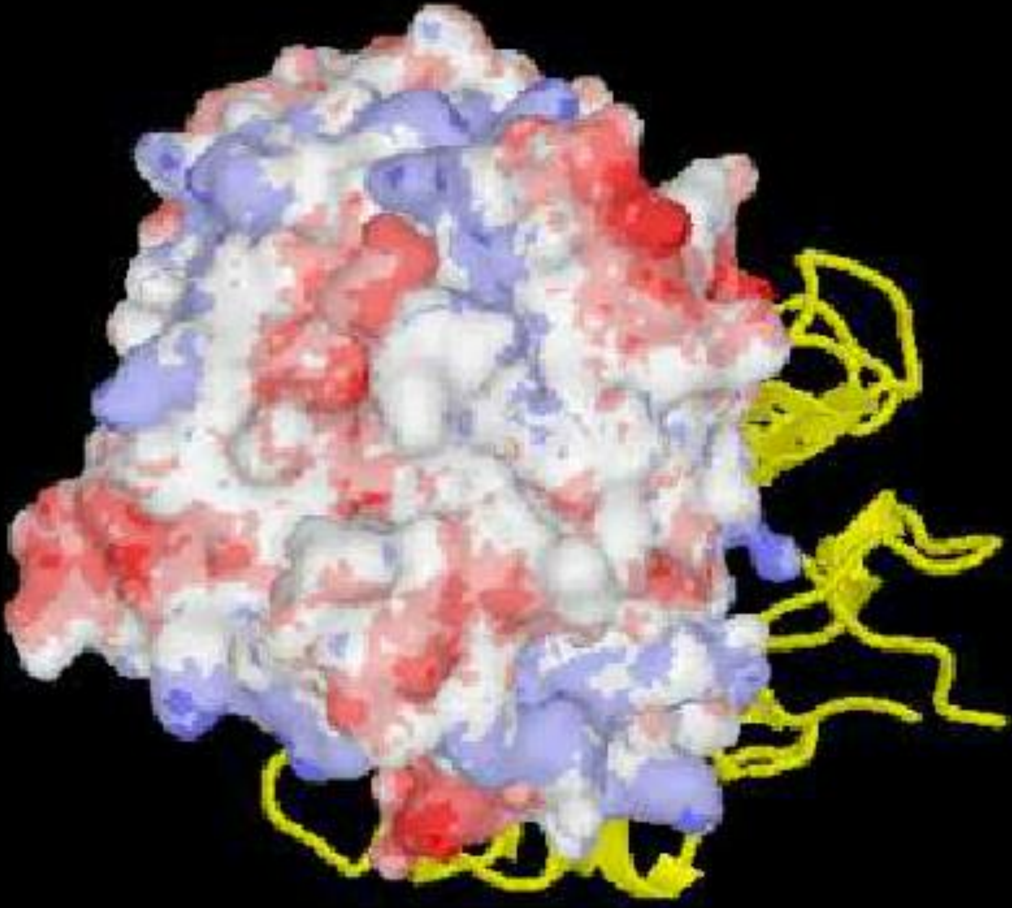
Substrato no sítio ativo

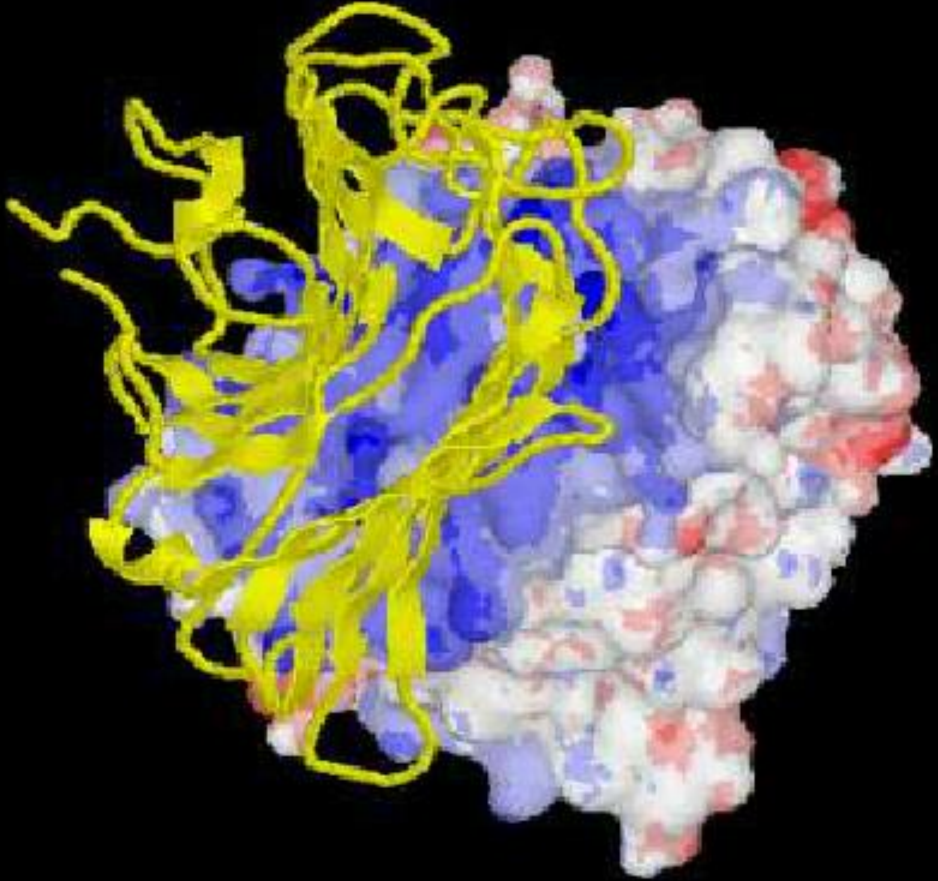
NAD

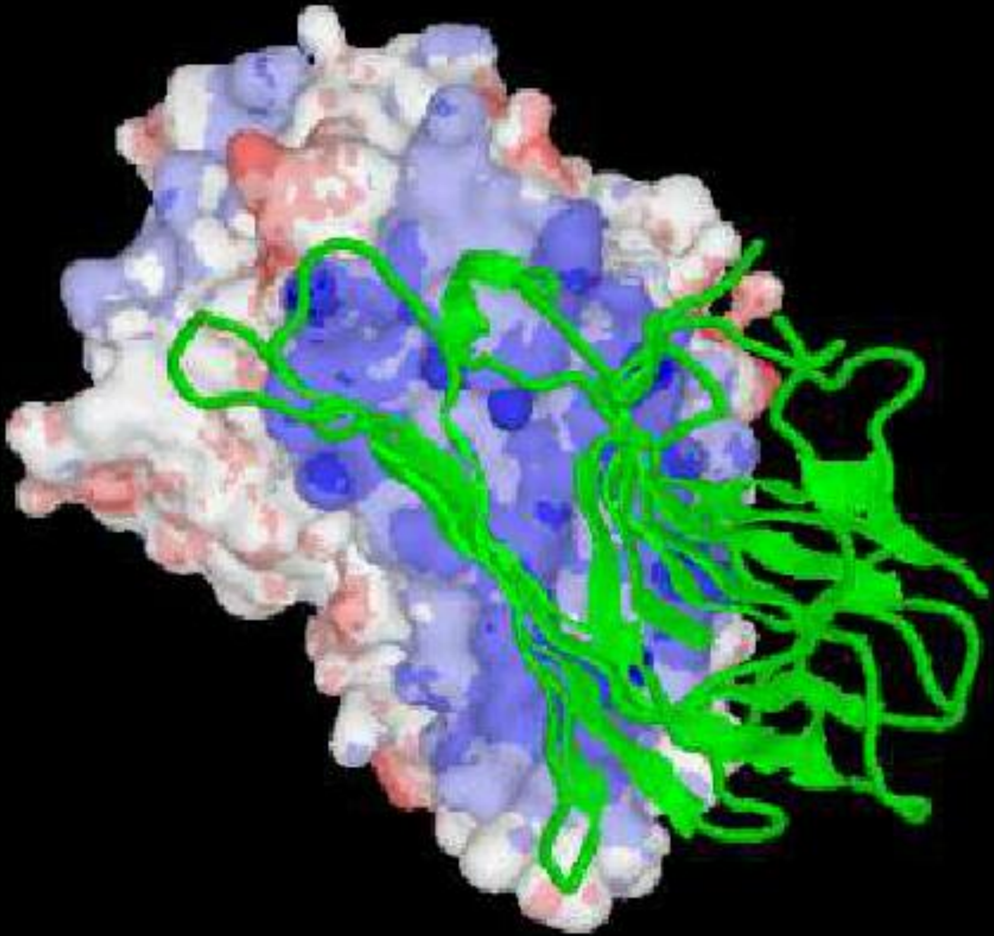

Domínio catalítico

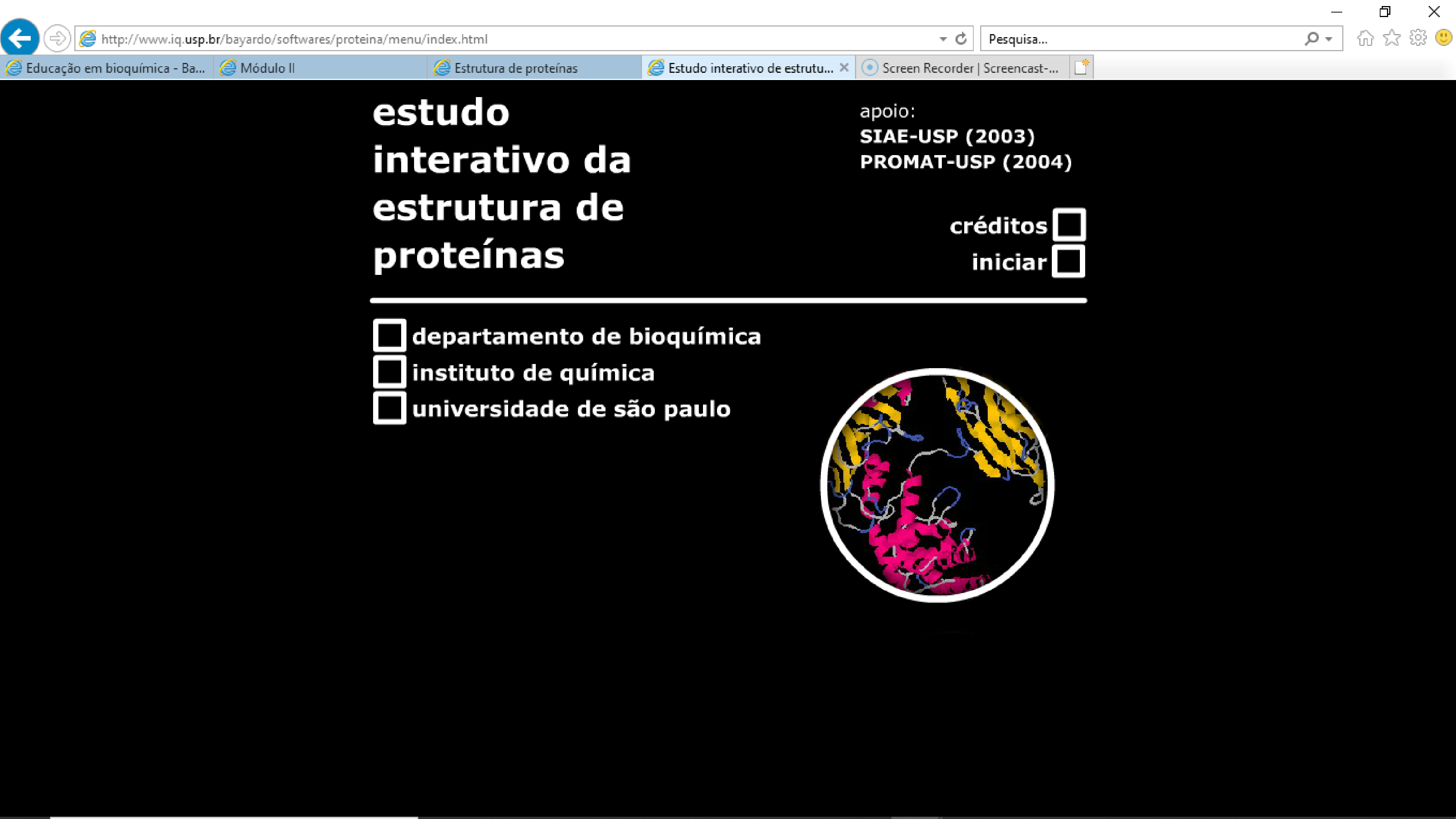
Estrutura quaternária











estudo interativo da estrutura de proteínas

apoio:
SIAE-USP (2003)
PROMAT-USP (2004)

créditos ☐
iniciar ☐

☐ departamento de bioquímica
☐ instituto de química
☐ universidade de são paulo