Εργασία Βιοπληροφορικής

Πρωτεΐνη: 1DHF

Σδούγκου Κωνσταντίνα Α.Ε.Μ. 8373

```
Isoform 1:
>sp|P00374|DYR_HUMAN Dihydrofolate reductase OS=Homo sapiens GN=DHFR
PE=1 SV=2
MVGSLNCIVAVSQNMGIGKNGDLPWPPLRNEFRYFQRMTTTSSVEGKQNLVIMGKKTWFS
IPEKNRPLKGRINLVLSRELKEPPQGAHFLSRSLDDALKLTEQPELANKVDMVWIVGGSS
VYKEAMNHPGHLKLFVTRIMQDFESDTFFPEIDLEKYKLLPEYPGVLSDVQEEKGIKYKF
EVYEKND
```

ProtParam

User-provided sequence:

```
        10         20         30         40         50         60
MVGSLNCIVA VSQNMGIGKN GDLPWPPLRN EFRYFQRMTT TSSVEGKQNL VIMGKKTWFS

        70         80         90        100        110        120
IPEKNRPLKG RINLVLSREL KEPPQGAHFL SRSLDDALKL TEQPELANKV DMVWIVGGSS

       130        140        150        160        170        180
VYKEAMNHPG HLKLFVTRIM QDFESDTFFP EIDLEKYKLL PEYPGVLSDV QEEKGIKYKF


EVYEKND
```

Number of amino acids: 187

Molecular weight: 21452.7

Theoretical pI: 6.85

Amino acid composition:

```
Ala (A)   5       2.7%
Arg (R)   8       4.3%
Asn (N)  10       5.3%
Asp (D)   9       4.8%
Cys (C)   1       0.5%
Gln (Q)   7       3.7%
Glu (E)  16       8.6%
Gly (G)  13       7.0%
His (H)   3       1.6%
Ile (I)   9       4.8%
Leu (L)  19      10.2%
Lys (K)  17       9.1%
Met (M)   7       3.7%
Phe (F)   9       4.8%
Pro (P)  12       6.4%
Ser (S)  12       6.4%
```

Thr (T)	7	3.7%
Trp (W)	3	1.6%
Tyr (Y)	6	3.2%
Val (V)	14	7.5%
Pyl (O)	0	0.0%
Sec (U)	0	0.0%
(B)	0	0.0%
(Z)	0	0.0%
(X)	0	0.0%

Total number of negatively charged residues (Asp + Glu): 25
Total number of positively charged residues (Arg + Lys): 25

Atomic composition:

Carbon	C	968
Hydrogen	H	1520
Nitrogen	N	254
Oxygen	O	280
Sulfur	S	8

Formula: $C_{968}H_{1520}N_{254}O_{280}S_8$
Total number of atoms: 3030

Extinction coefficients:

Extinction coefficients are in units of M^{-1} cm^{-1}, at 280 nm measured in water.

Ext. coefficient 25440
Abs 0.1% (=1 g/l) 1.186, assuming all pairs of Cys residues form cystines

Ext. coefficient 25440
Abs 0.1% (=1 g/l) 1.186, assuming all Cys residues are reduced

Estimated half-life:

The N-terminal of the sequence considered is M (Met).

The estimated half-life is: 30 hours (mammalian reticulocytes, in vitro).
>20 hours (yeast, in vivo).
>10 hours (Escherichia coli, in vivo).

Instability index:

The instability index (II) is computed to be 27.16
This classifies the protein as stable.

Aliphatic index: 82.78

Grand average of hydropathicity (GRAVY): -0.464

Isoform 2:

```
>sp|P00374-2|DYR_HUMAN Isoform 2 of Dihydrofolate reductase OS=Homo
sapiens GN=DHFR
MGKKTWFSIPEKNRPLKGRINLVLSRELKEPPQGAHFLSRSLDDALKLTEQPELANKVDM
VWIVGGSSVYKEAMNHPGHLKLFVTRIMQDFESDTFFPEIDLEKYKLLPEYPGVLSDVQE
EKGIKYKFEVYEKND
```

ProtParam

User-provided sequence:

```
        10         20         30         40         50         60
MGKKTWFSIP EKNRPLKGRI NLVLSRELKE PPQGAHFLSR SLDDALKLTE QPELANKVDM

        70         80         90        100        110        120
VWIVGGSSVY KEAMNHPGHL KLFVTRIMQD FESDTFFPEI DLEKYKLLPE YPGVLSDVQE

       130
EKGIKYKFEV YEKND
```

References and documentation are available.

Number of amino acids: 135

Molecular weight: 15672.0

Theoretical pI: 5.95

Amino acid composition:

```
Ala (A)   4         3.0%
Arg (R)   5         3.7%
Asn (N)   5         3.7%
Asp (D)   8         5.9%
Cys (C)   0         0.0%
Gln (Q)   4         3.0%
Glu (E)  14        10.4%
Gly (G)   8         5.9%
His (H)   3         2.2%
Ile (I)   6         4.4%
Leu (L)  15        11.1%
Lys (K)  15        11.1%
Met (M)   4         3.0%
Phe (F)   7         5.2%
Pro (P)   9         6.7%
Ser (S)   8         5.9%
Thr (T)   4         3.0%
Trp (W)   2         1.5%
Tyr (Y)   5         3.7%
Val (V)   9         6.7%
Pyl (O)   0         0.0%
Sec (U)   0         0.0%

 (B)   0            0.0%
```

(Z)	0	0.0%
(X)	0	0.0%

Total number of negatively charged residues (Asp + Glu): 22
Total number of positively charged residues (Arg + Lys): 20

Atomic composition:

Carbon	C	714
Hydrogen	H	1114
Nitrogen	N	182
Oxygen	O	206
Sulfur	S	4

Formula: $C_{714}H_{1114}N_{182}O_{206}S_4$
Total number of atoms: 2220

Extinction coefficients:

Extinction coefficients are in units of M^{-1} cm^{-1}, at 280 nm measured in water.

Ext. coefficient	18450
Abs 0.1% (=1 g/l)	1.177

Estimated half-life:

The N-terminal of the sequence considered is M (Met).

The estimated half-life is: 30 hours (mammalian reticulocytes, in vitro).
>20 hours (yeast, in vivo).
>10 hours (Escherichia coli, in vivo).

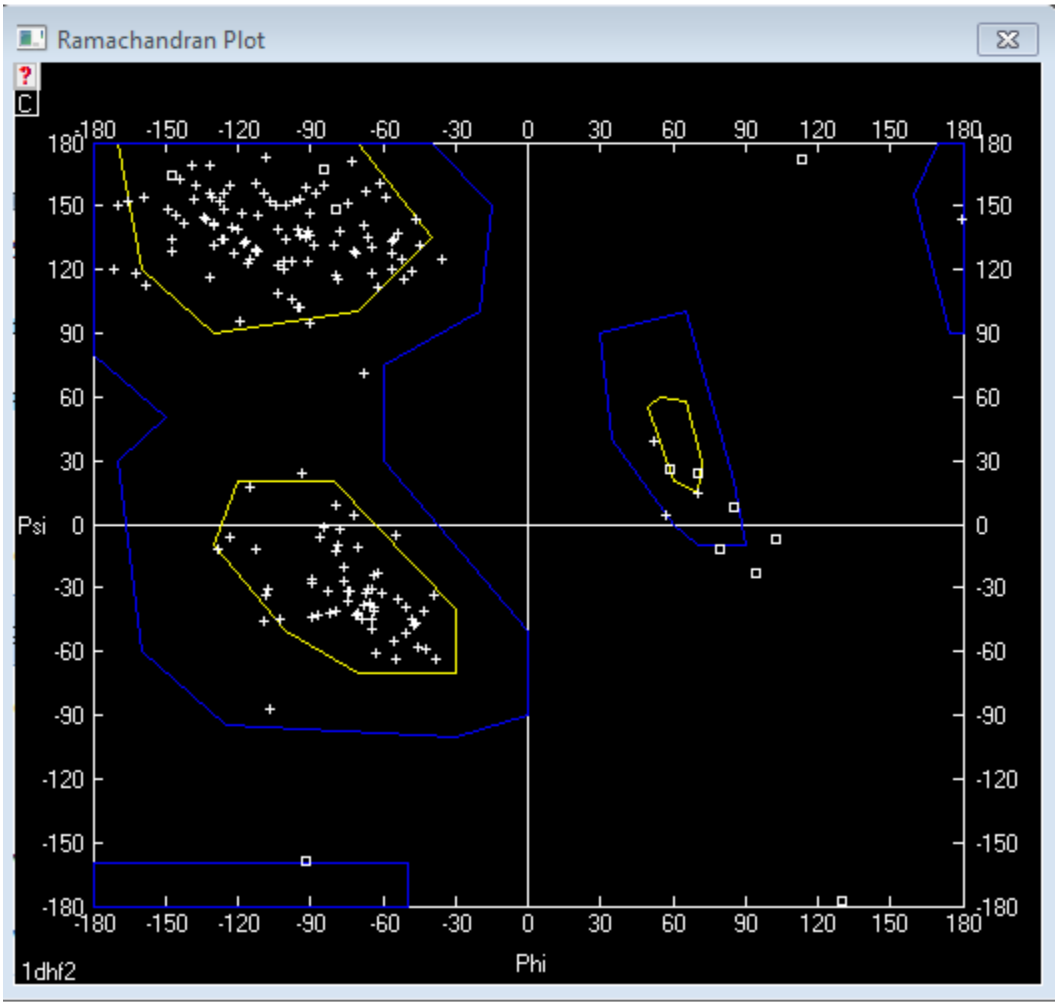
Instability index:

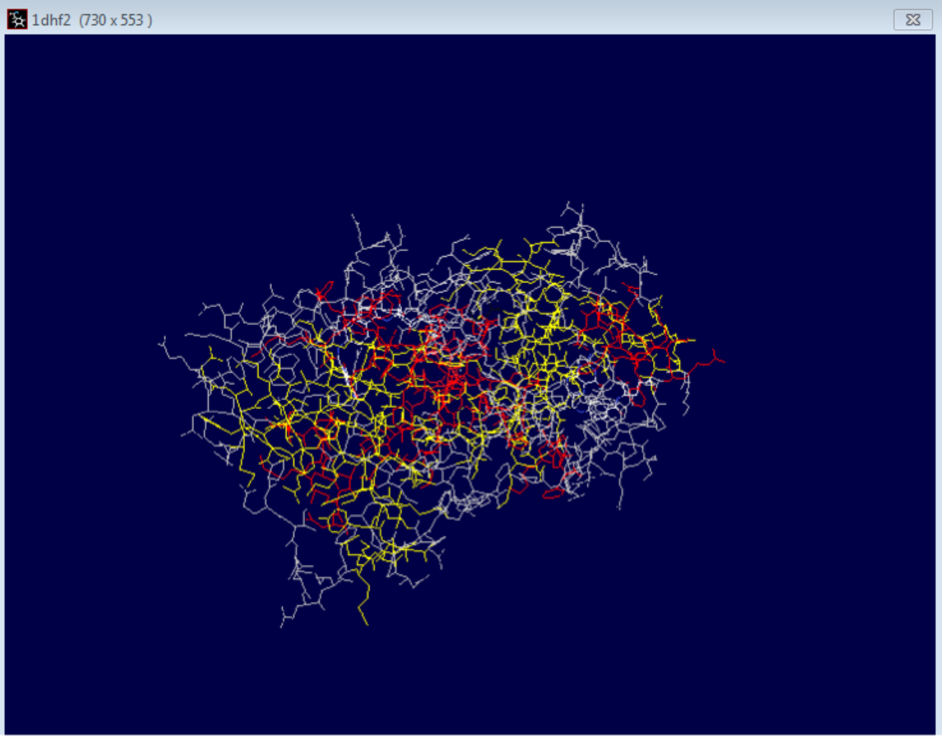
The instability index (II) is computed to be 29.42
This classifies the protein as stable.

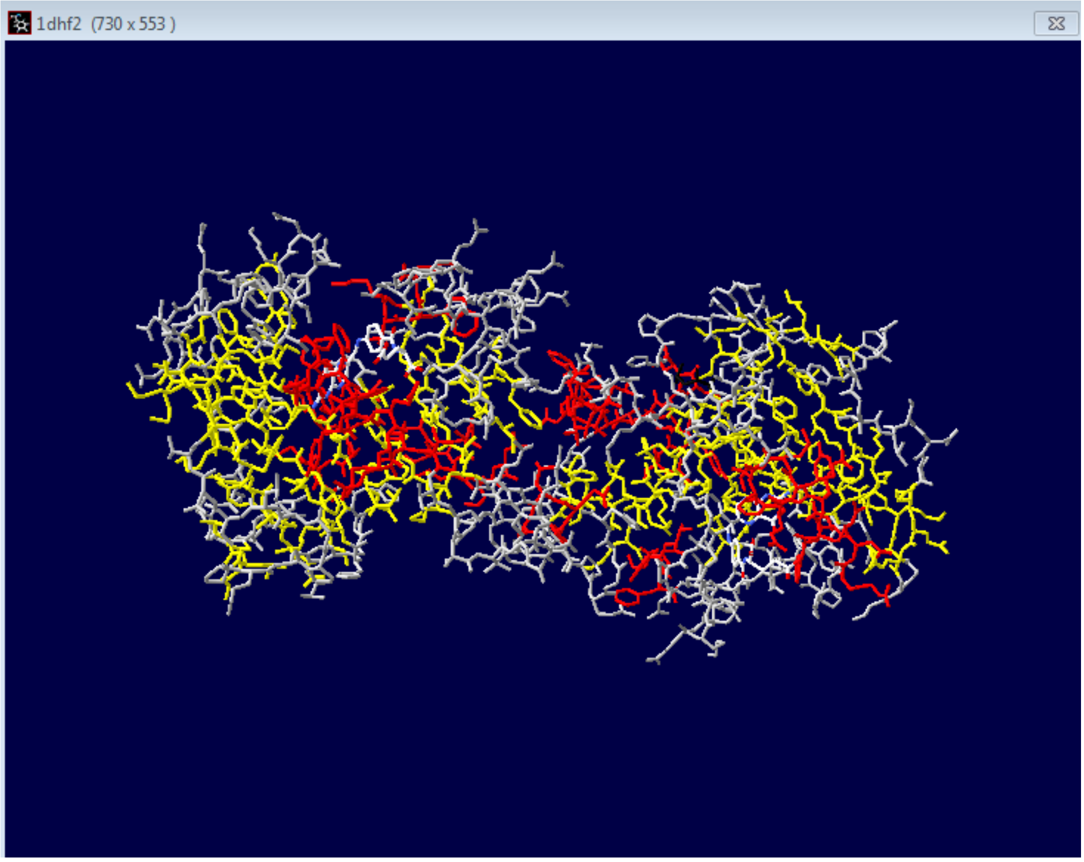
Aliphatic index: 82.96

Grand average of hydropathicity (GRAVY): -0.578

Από το Ramachandran plot βλέπουμε ότι εκτός των μπλε περιοχών είναι τα αμινοξέα GLY 85, GLY 20, GLY 116


Ramachandran Plot
?
C
-180 -150 -120 -90 -60 -30 0 30 60 90 120 150 180
180 150 120 90 60 30 0 -30 -60 -90 -120 -150 -180
Psi
Phi
1dhf2


1dhf2 (730 x 553)



Η γλυκίνη είναι το μικρότερο και το απλούστερο αμινοξύ ως πλευρική αλυσίδα. Η απουσία πλευρικής ομάδας δίνει στον πεπτιδικό σκελετό στα κατάλοιπα της γλυκίνης πολύ μεγαλύτερη διαμορφωτική ευελιξία σε σχέση με τα υπόλοιπα.