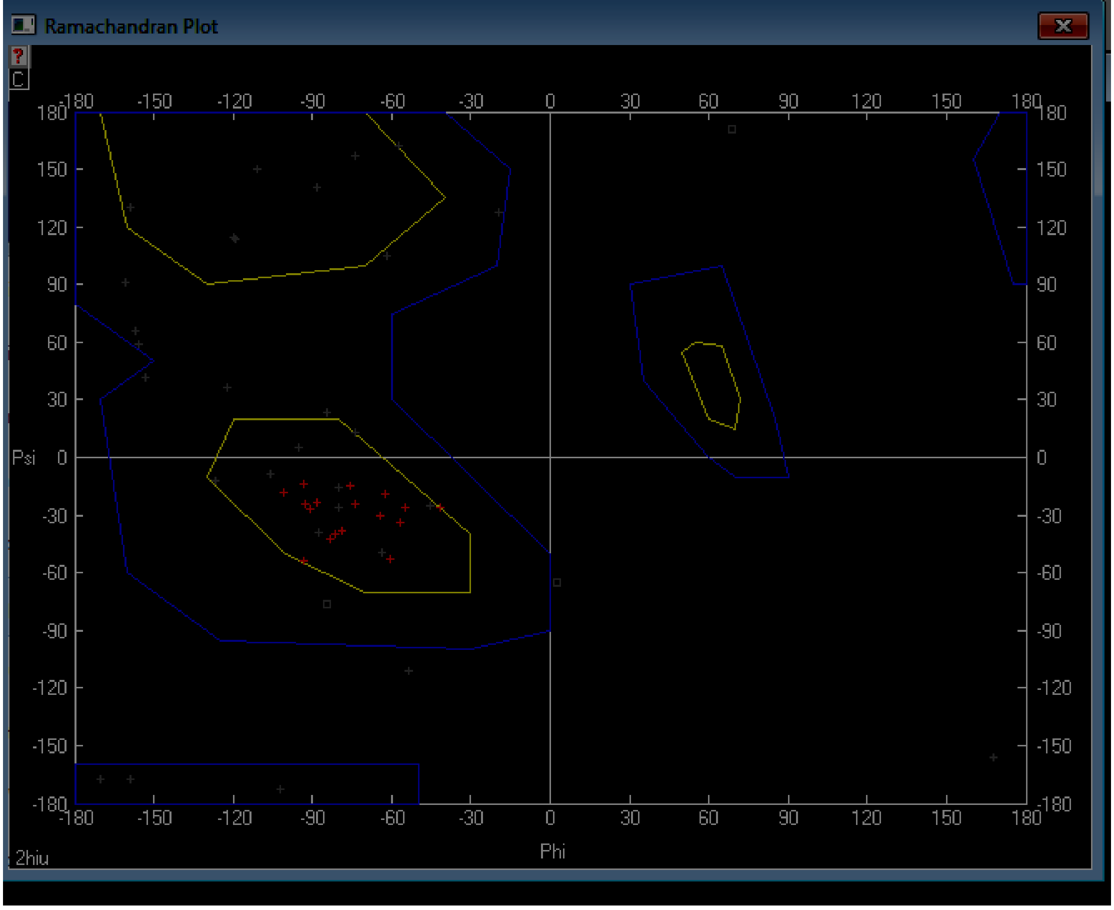


ΟΝΟΜΑΤΕΠΩΝΥΜΟ: ΤΟΠΤΣΗ ΝΤΟΥΙΓΚΟΥ
Α.Ε.Μ: 8391
ΜΑΘΗΜΑ: ΕΡΓΑΣΙΑ ΣΤΗ ΒΙΟΠΛΗΡΟΦΟΡΙΚΗ
►2HIU

2HIU

ISOFORM 1
>sp|P01308|INS_HUMAN Insulin OS=Homo sapiens GN=INS PE=1 SV=1
MALWMRLLPLLALLALWGPDPAAAFVNQHLCGSHLVEALYLVCGERGFFYTPKTRREAED
LQVGQVELGGGPGAGSLQPLALEGSLQKRGIVEQCCTSICSLYQLENYCN

ISOFORM 2

>sp|F8WCM5|INSR2_HUMAN Insulin, isoform 2 OS=Homo sapiens GN=INS-IGF2 PE=2 SV=1
MALWMRLLPLLALLALWGPDPAAAFVNQHLCGSHLVEALYLVCGERGFFYTPKTRREAED
LQASALSLSSSTSTWPEGLDATARAPPALVVTANIGQAGGSSSRQFRQRALGTSDSPVLF
IHCPGAAGTAQGLEYRGRRVTTELVWEEVDSSPQPQGSESLPAQPPAQPAPQPEPQQARE
PSPEVSCCGLWPRRPQRSQN

Isoform 1

User-provided sequence:

```
        10         20         30         40         50         60
MALWMRLLPL LALLALWGPD PAAAFVNQHL CGSHLVEALY LVCGERGFFY TPKTRREAED

        70         80         90        100        110
LQVGQVELGG GPGAGSLQPL ALEGSLQKRG IVEQCCTSIC SLYQLENYCN
```

Number of amino acids: 110

Molecular weight: 11980.9

Theoretical pI: 5.22

Amino acid composition:

```
Ala (A)  10      9.1%
Arg (R)   5      4.5%
Asn (N)   3      2.7%
Asp (D)   2      1.8%
Cys (C)   6      5.5%
Gln (Q)   7      6.4%
Glu (E)   8      7.3%
Gly (G)  12     10.9%
His (H)   2      1.8%
Ile (I)   2      1.8%
Leu (L)  20     18.2%
Lys (K)   2      1.8%
Met (M)   2      1.8%
Phe (F)   3      2.7%
Pro (P)   6      5.5%
Ser (S)   5      4.5%
Thr (T)   3      2.7%
Trp (W)   2      1.8%
Tyr (Y)   4      3.6%
Val (V)   6      5.5%
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): 10
Total number of positively charged residues (Arg + Lys): 7

Atomic composition:

```
Carbon      C         535
Hydrogen    H         841
Nitrogen    N         143
Oxygen      O         153
Sulfur      S           8
```

Formula: $C_{535}H_{841}N_{143}O_{153}S_8$
Total number of atoms: 1680

Extinction coefficients:

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

Ext. coefficient   17335
Abs 0.1% (=1 g/l)   1.447, assuming all pairs of Cys residues form cystines

Ext. coefficient   16960
Abs 0.1% (=1 g/l)   1.416, 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 40.33
This classifies the protein as unstable.

Aliphatic index: 102.91

Grand average of hydropathicity (GRAVY): 0.193

Isoform 2

User-provided sequence:

```
        10         20         30         40         50         60
MALWMRLLPL LALLALWGPD PAAAFVNQHL CGSHLVEALY LVCGERGFFY TPKTRREAED

        70         80         90        100        110        120
LQASALSLSS STSTWPEGLD ATARAPPALV VTANIGQAGG SSSRQFRQRA LGTSDSPVLF

       130        140        150        160        170        180
IHCPGAAGTA QGLEYRGRRV TTELVWEEVD SSPQPQGSES LPAQPPAQPA PQPEPQQARE

       190        200
PSPEVSCCGL WPRRPQRSQN
```

Number of amino acids: 200

Molecular weight: 21537.2

Theoretical pI: 5.93

Amino acid composition:

```
Ala (A)  24      12.0%
Arg (R)  15       7.5%
Asn (N)   3       1.5%
Asp (D)   5       2.5%
Cys (C)   5       2.5%
Gln (Q)  15       7.5%
Glu (E)  13       6.5%
Gly (G)  15       7.5%
His (H)   3       1.5%
Ile (I)   2       1.0%
Leu (L)  23      11.5%
Lys (K)   1       0.5%
Met (M)   2       1.0%
Phe (F)   5       2.5%
Pro (P)  22      11.0%
Ser (S)  19       9.5%
Thr (T)  10       5.0%
Trp (W)   5       2.5%
Tyr (Y)   3       1.5%
Val (V)  10       5.0%
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): 18
Total number of positively charged residues (Arg + Lys): 16

Atomic composition:

```
Carbon      C         947
Hydrogen    H        1483
Nitrogen    N         275
Oxygen      O         287
Sulfur      S           7
```

Formula: $C_{947}H_{1483}N_{275}O_{287}S_{7}$
Total number of atoms: 2999

Extinction coefficients:

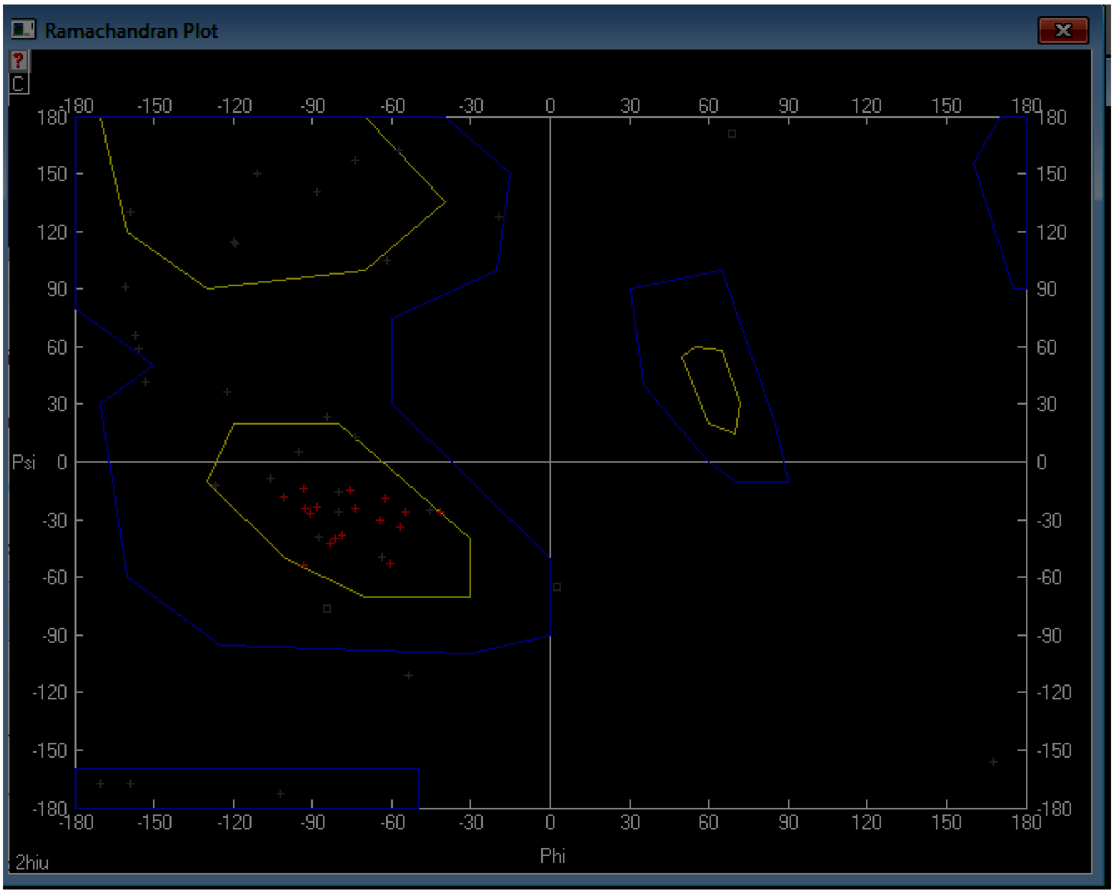
Extinction coefficients are in units of M^{-1} cm^{-1}, at 280 nm measured in water.

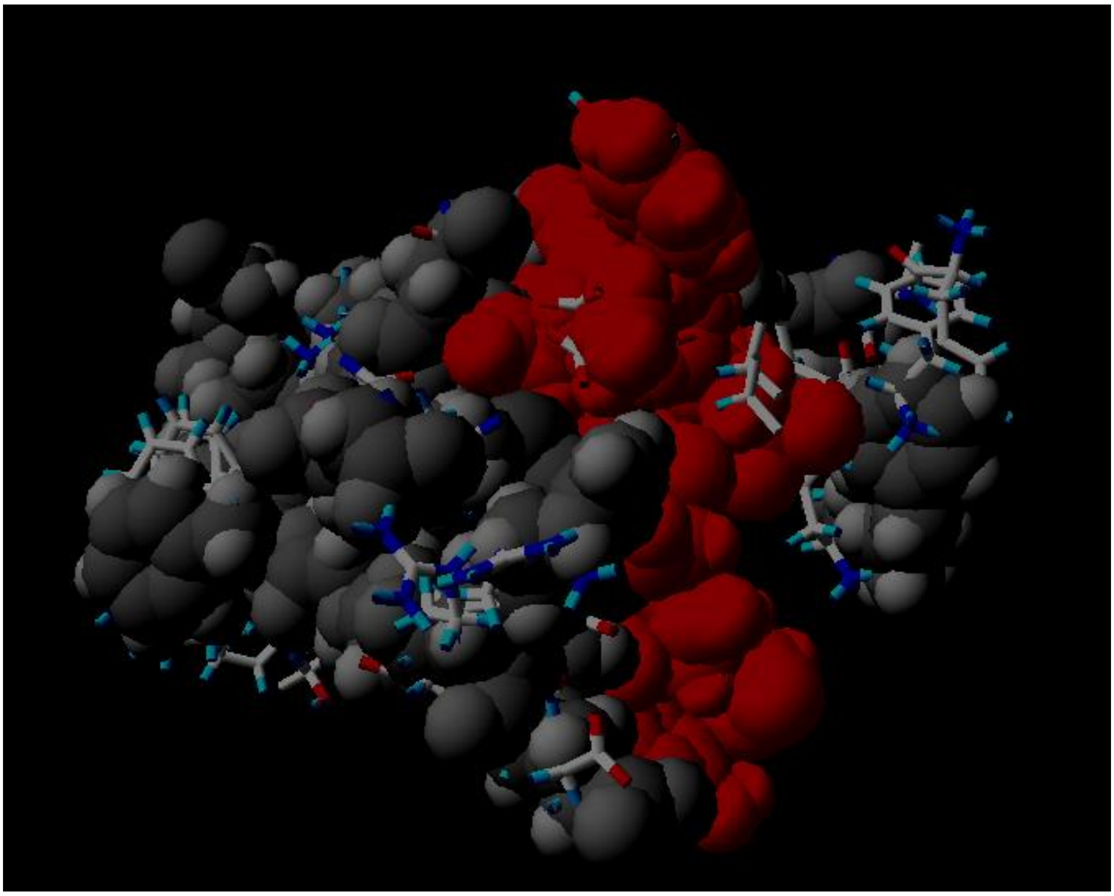
```
Ext. coefficient    32220
Abs 0.1% (=1 g/l)   1.496, assuming all pairs of Cys residues form cystines
```

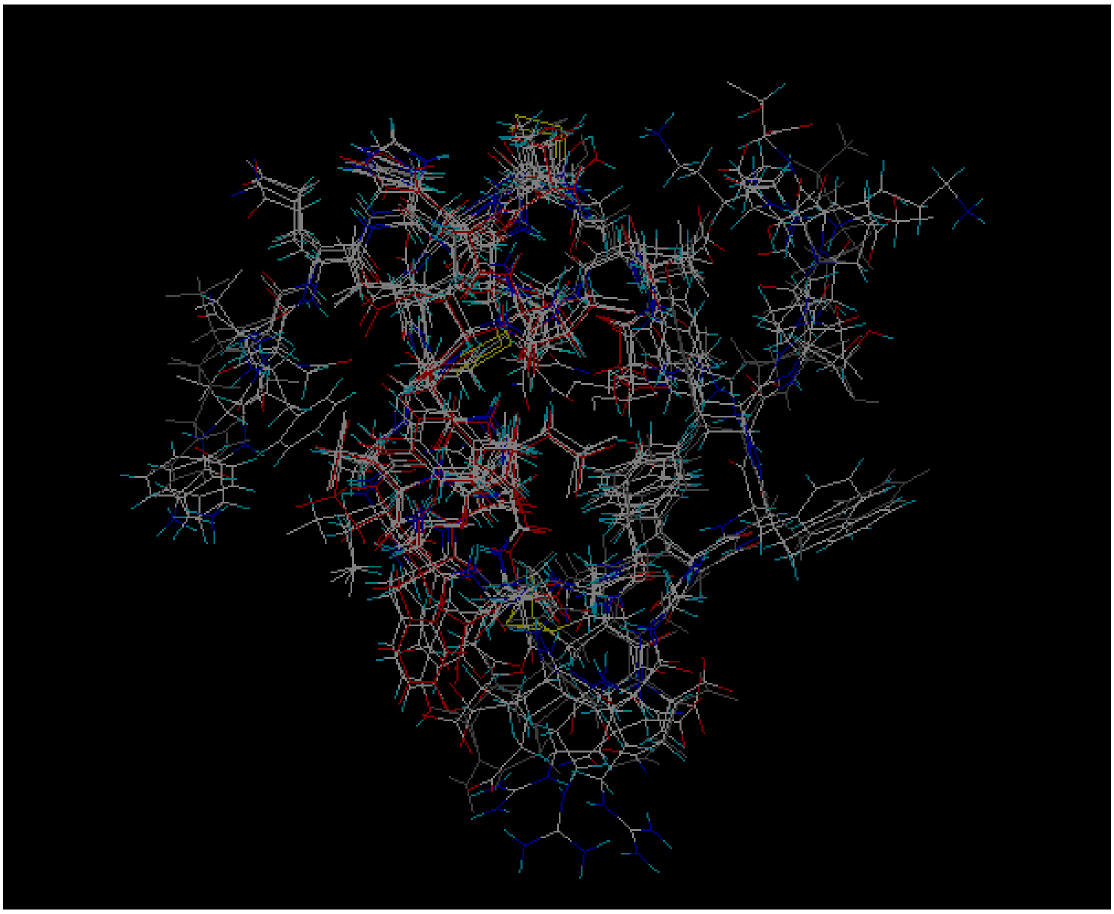
```
Ext. coefficient    31970
Abs 0.1% (=1 g/l)   1.484, assuming all Cys residues are reduced
```

```
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 77.16
This classifies the protein as unstable.



Aliphatic index: 75.25

Grand average of hydropathicity (GRAVY): -0.335
```

Ερμηνεία του Ramachandran Plot:
Οι δύο γωνίες στρέψης μιας πολυπεπτιδικής αλυσίδας περιγράφουν τις περιστροφές του πολυπεπτιδικού σκελετού ανάμεσα στους δεσμούς μεταξύ των ατόμων N-Ca (γωνία φ) και Ca-C (γωνία ψ). Το διάγραμμα Ramachandran παρέχει έναν απλό τρόπο να οπτικοποιηθεί η κατανομή των γωνιών στρέψης μιας πολυπεπτιδικής αλυσίδας.
Κάποιες τιμές των γωνιών φ και ψ είναι απαγορευτικές, επειδή κάποια άτομα πρόκειται να έρθουν πάρα πολύ κοντά , με αποτέλεσμα στερεοχημικής παρεμπόδισης. Σε αυτή την περίπτωση, η ενέργεια του συστήματος αυξάνει υπερβολικά, γεγονός καθόλου ευνοϊκό. Αυτές οι τιμές απαντώνται στα αμινοξέα που βρίσκονται εκτός των επιτρεπτών περιοχών Ramachandran. Τα συγκεκριμένα αμινοξέα αναφέρονται εν συνεχεία.







AMINOACIDS OUTSIDE THE RAMACHANDRAN PLOT

CYS20

PHE24

GLN4

SER12

SER9

GLY23

(IN THE BOX)

GLY8

CYS7

GLY20

THR8

LEU6

THR27

CYS19

LYS29

PHE25

ASN3

ASN21