ΕΡΓΑΣΙΑ:

ΜΑΘΗΜΑ: ΒΙΟΧΗΜΕΙΑ ΚΑΙ ΣΤΟΙΧΕΙΑ ΒΙΟΠΛΗΡΟΦΟΡΙΚΗΣ

ΟΝΟΜΑΤΕΠΩΝΥΜΟ: ΔΙΟΝΥΣΙΑ ΚΑΚΟΛΥΡΗ

Α.Ε.Μ.: 8312

ΠΡΩΤΕΙΝΗ: 1RNM

FASTA:

```
>sp|P61823|RNAS1_BOVIN Ribonuclease pancreatic
OS=Bos taurus GN=RNASE1 PE=1 SV=1

MALKSLVLLSLLVLVLLLVRVQPSLGKETAAAKFERQHMDSSTSAASSSNYCNQMMKSRN
LTKDRCKPVNTFVHESLADVQAVCSQKNVACKNGQTNCYQSYSTMSITDCRETGSSKYPN
CAYKTTQANKHIIVACEGNPYVPVHFDASV
```

ProtParam

ProtParam

User-provided sequence:

```
        10         20         30         40         50         60
MALKSLVLLS LLVLVLLLVR VQPSLGKETA AAKFERQHMD SSTSAASSSN YCNQMMKSRN

        70         80         90        100        110        120
LTKDRCKPVN TFVHESLADV QAVCSQKNVA CKNGQTNCYQ SYSTMSITDC RETGSSKYPN
```

```
       130        140        150
CAYKTTQANK HIIVACEGNP YVPVHFDASV
```

Number of amino acids: 150

Molecular weight: 16460.8

Theoretical pI: 8.93

Amino acid composition: CSV format

```
Ala (A)  13       8.7%
Arg (R)   5       3.3%
Asn (N)  10       6.7%
Asp (D)   5       3.3%
Cys (C)   8       5.3%
Gln (Q)   8       5.3%
Glu (E)   5       3.3%
Gly (G)   4       2.7%
His (H)   4       2.7%
Ile (I)   3       2.0%
Leu (L)  13       8.7%
Lys (K)  11       7.3%
Met (M)   5       3.3%
Phe (F)   3       2.0%
Pro (P)   5       3.3%
Ser (S)  18      12.0%
Thr (T)  10       6.7%
Trp (W)   0       0.0%
Tyr (Y)   6       4.0%
Val (V)  14       9.3%
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): 16

Atomic composition:

```
Carbon      C         707
Hydrogen    H        1146
Nitrogen    N         202
Oxygen      O         223
Sulfur      S          13
```

Formula: $C_{707}H_{1146}N_{202}O_{223}S_{13}$
Total number of atoms: 2291

Extinction coefficients:

This protein does not contain any Trp residues. Experience shows that this could result in more than 10% error in the computed extinction coefficient.

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

Ext. coefficient 9440
Abs 0.1% (=1 g/l) 0.573, assuming all pairs of Cys residues form cystines

Ext. coefficient 8940
Abs 0.1% (=1 g/l) 0.543, assuming all Cys residues are reduced

Estimated half-life:

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

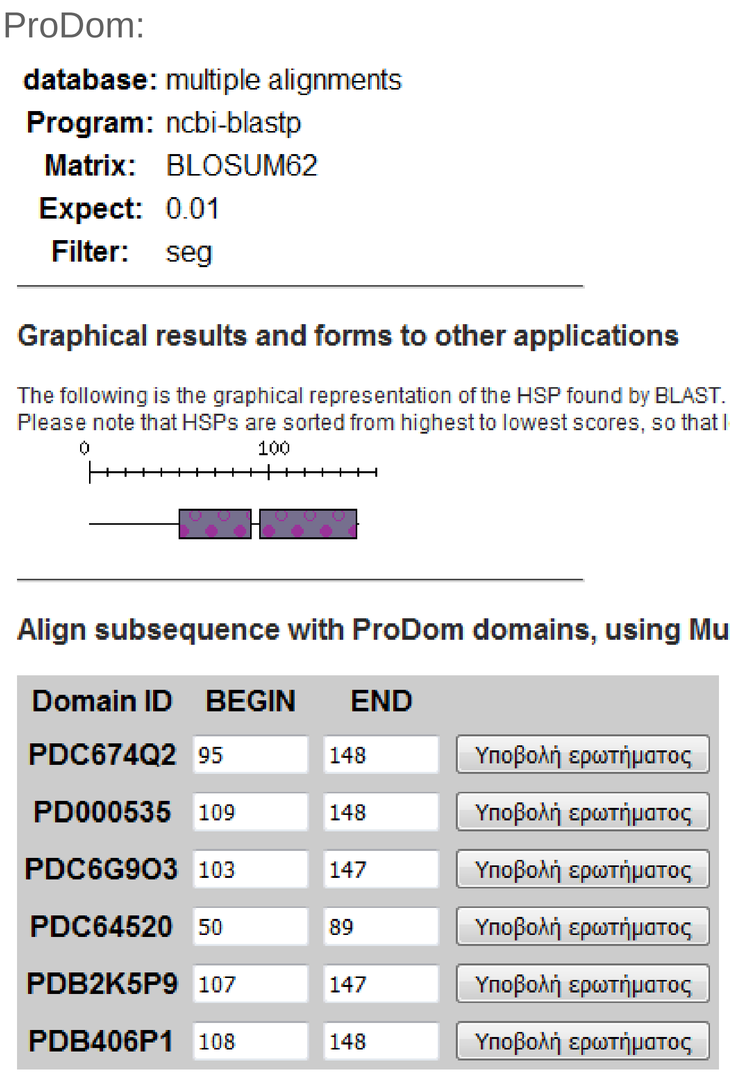
The estimated half-life is: 30 hours (mammalian reticulocytes, in vitro).
>20 hours (yeast, in vivo).
>10 hours (Escherichia coli, in vivo).

Instability index:

The instability index (II) is computed to be 38.81
This classifies the protein as stable.

Aliphatic index: 77.33

Grand average of hydropathicity (GRAVY): -0.213



ProDom:

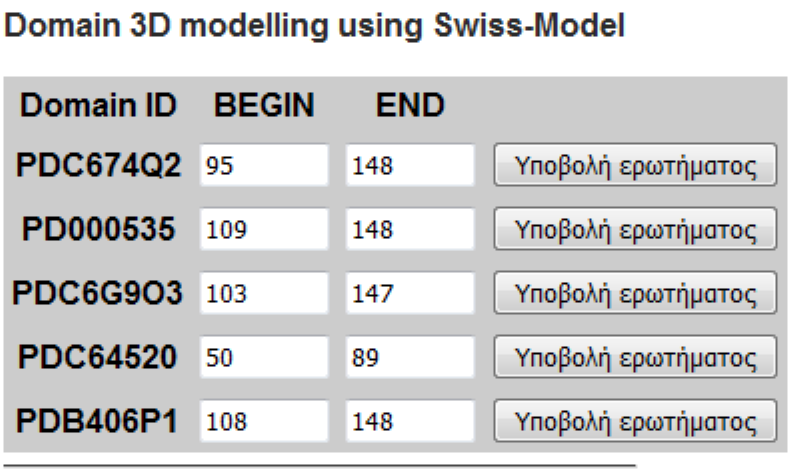
database: multiple alignments
Program: ncbi-blastp
Matrix: BLOSUM62
Expect: 0.01
Filter: seg

Graphical results and forms to other applications

The following is the graphical representation of the HSP found by BLAST.
Please note that HSPs are sorted from highest to lowest scores, so that lower scoring HSPs may be hidden.

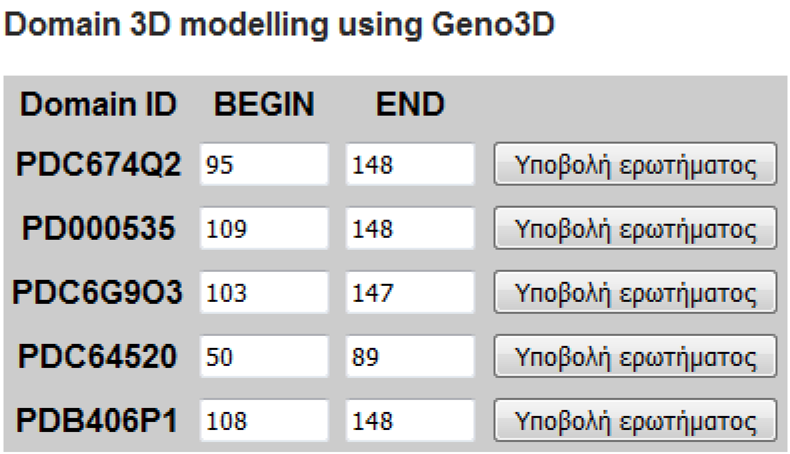
Align subsequence with ProDom domains, using Multalin

Domain ID	BEGIN	END	
PDC674Q2	95	148	Υποβολή ερωτήματος
PD000535	109	148	Υποβολή ερωτήματος
PDC6G9O3	103	147	Υποβολή ερωτήματος
PDC64520	50	89	Υποβολή ερωτήματος
PDB2K5P9	107	147	Υποβολή ερωτήματος
PDB406P1	108	148	Υποβολή ερωτήματος



Domain 3D modelling using Swiss-Model

Domain ID	BEGIN	END	
PDC674Q2	95	148	Υποβολή ερωτήματος
PD000535	109	148	Υποβολή ερωτήματος
PDC6G9O3	103	147	Υποβολή ερωτήματος
PDC64520	50	89	Υποβολή ερωτήματος
PDB406P1	108	148	Υποβολή ερωτήματος



Domain 3D modelling using Geno3D

Domain ID	BEGIN	END	
PDC674Q2	95	148	Υποβολή ερωτήματος
PD000535	109	148	Υποβολή ερωτήματος
PDC6G9O3	103	147	Υποβολή ερωτήματος
PDC64520	50	89	Υποβολή ερωτήματος
PDB406P1	108	148	Υποβολή ερωτήματος

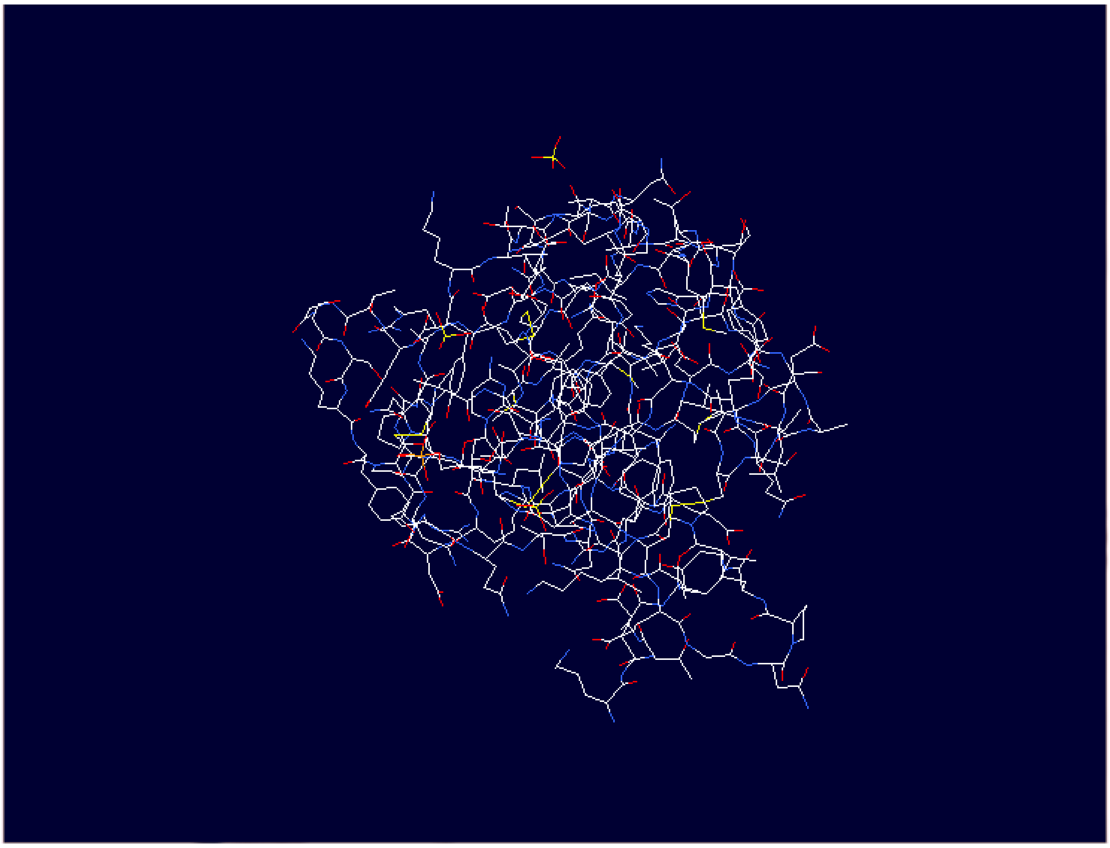
HSP Results

Warning: Original output has been filtered to yield non-redundant similarities

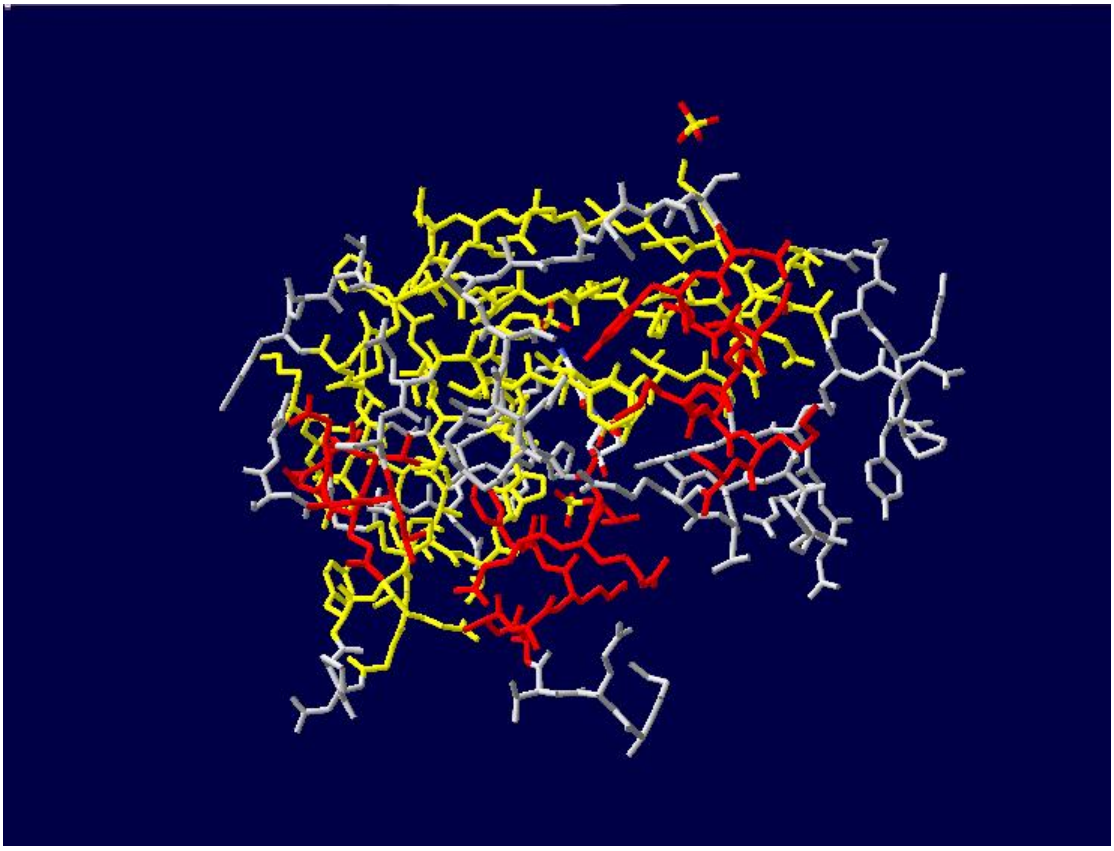
```
blastp 2.2.26 [Sep-21-2011]


Reference: Altschul, Stephen F., Thomas L. Madden, Alejandro A.
Schaffer,
Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997),
_quot;Gapped BLAST and PSI-BLAST: a new generation of protein
database search
programs_quot;,  Nucleic Acids Res. 25:3389-3402.

Query: unkwown
        (150 letters)

Database: prodom2010.1 multiple alignments
        45,292,438 sequences; 2,147,483,647 total letters



ProDom domains producing High-scoring Segment Pairs:

  Position  ProDom domain                                      Score
E value
```

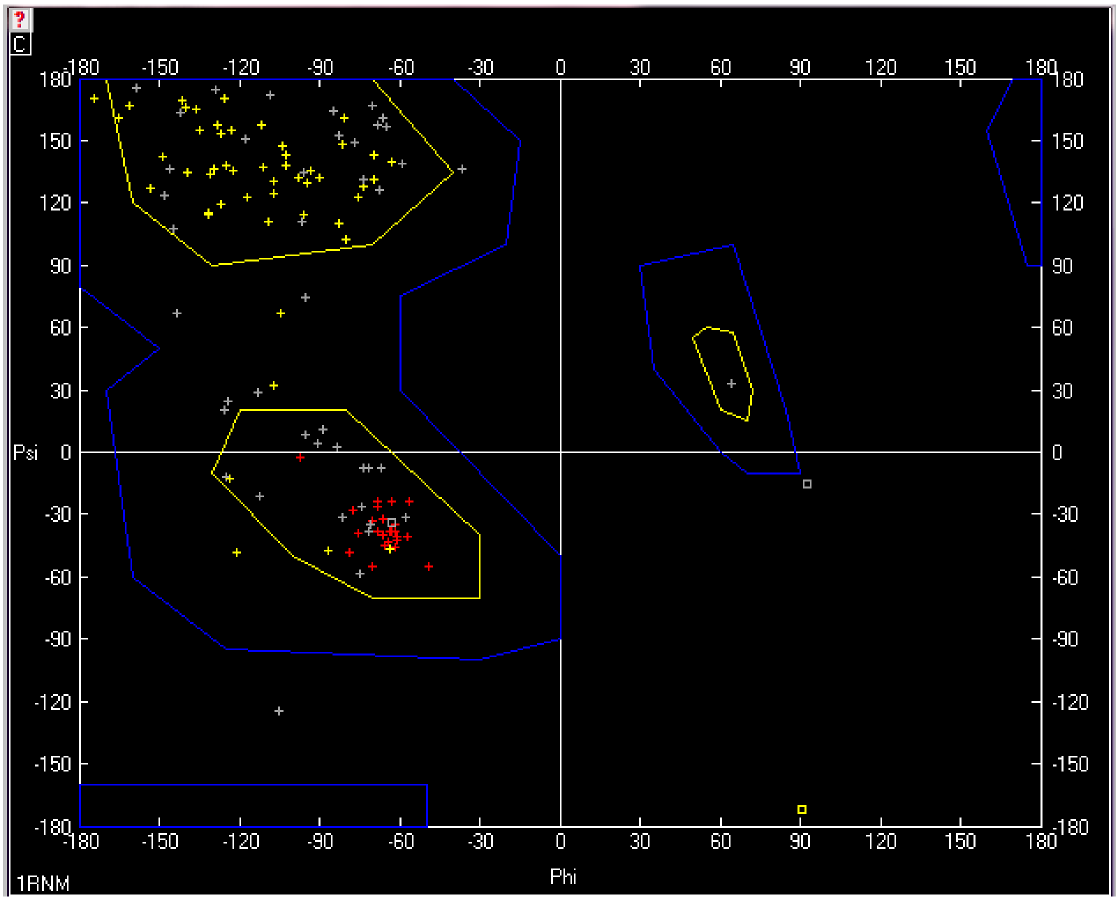
```
     50-89  #PDC64520                                            213
4e-20
    95-148  #PDC674Q2                                            235
2e-23
   103-147  #PDC6G9O3                                            214
2e-20
   107-147  #PDB2K5P9                                            209
1e-19
   108-148  #PDB406P1                                            159
2e-12
   109-148  #PD000535                                            221
2e-21


>PDC674Q2 (Closest domain: RNAS1_HORSE 69-122)
Number of domains in family: 86
Commentary (automatic):
DISULFIDE BOND ENDONUCLEASE HYDROLASE NUCLEASE SUBNAME: ALTNAME:
RECNAME: RIBONUCLEASE FULL=RIBONUCLEASE
Length = 54
Score = 235  (95.1 bits), Expect = 2e-23
Identities = 42/54 (77%), Positives = 47/54 (87%)

 Query:     95 QTNCYQSYSTMSITDCRETGSSKYPNCAYKTTQANKHIIVACEGNPYVPVHFDA
148
               Q+NCYQS S+M ITDCR T  SKYPNCAY+T+Q  +HIIVACEGNPYVPVHFDA
 Sbjct:     69 QSNCYQSSSSMHITDCRLTSGSKYPNCAYQTSQKERHIIVACEGNPYVPVHFDA
122




>PD000535 (Closest domain: RNAS1_BOVIN 109-148)
Number of domains in family: 245
Commentary (automatic):
DISULFIDE BOND HYDROLASE ENDONUCLEASE NUCLEASE ALTNAME: FULL=RNASE
SUBNAME: FULL=RIBONUCLEASE RECNAME:
Length = 40
Score = 221  (89.7 bits), Expect = 2e-21
Identities = 40/40 (100%), Positives = 40/40 (100%)

 Query:    109 DCRETGSSKYPNCAYKTTQANKHIIVACEGNPYVPVHFDA 148
               DCRETGSSKYPNCAYKTTQANKHIIVACEGNPYVPVHFDA
 Sbjct:    109 DCRETGSSKYPNCAYKTTQANKHIIVACEGNPYVPVHFDA 148




>PDC6G9O3 (Closest domain: RNAS1_DAMDA 76-121)
Number of domains in family: 31
Commentary (automatic):
SUBNAME: DISULFIDE BOND HYDROLASE ENDONUCLEASE NUCLEASE ALTNAME:
FULL=RIBONUCLEASE RECNAME: FULL=RNASE
Length = 46
Score = 214  (87.0 bits), Expect = 2e-20
Identities = 38/45 (84%), Positives = 40/45 (88%)

 Query:    103 STMSITDCRETGSSKYPNCAYKTTQANKHIIVACEGNPYVPVHFD 147
               S M ITDCRE+G+SKYPNC YK TQA KHIIVACEGNPYVPVHFD
```

```
 Sbjct:     77 SAMHITDCRESGNSKYPNCVYKATQAEKHIIVACEGNPYVPVHFD 121



>PDC64520 (Closest domain: RNAS1_BOVIN 47-89)
Number of domains in family: 244
Commentary (automatic):
DISULFIDE BOND ALTNAME: ENDONUCLEASE HYDROLASE NUCLEASE FULL=RNASE
FULL=RIBONUCLEASE RECNAME: SUBNAME:
Length = 43
Score = 213  (86.7 bits), Expect = 4e-20
Identities = 40/40 (100%), Positives = 40/40 (100%)

 Query:     50 NYCNQMMKSRNLTKDRCKPVNTFVHESLADVQAVCSQKNV 89
               NYCNQMMKSRNLTKDRCKPVNTFVHESLADVQAVCSQKNV
 Sbjct:     50 NYCNQMMKSRNLTKDRCKPVNTFVHESLADVQAVCSQKNV 89



>PDB2K5P9 (Closest domain: RNAS1_CAPCA 81-121)
Number of domains in family: 32
Commentary (automatic):
DISULFIDE BOND ENDONUCLEASE HYDROLASE NUCLEASE SUBNAME: PRECURSOR
FLAGS: RIBONUCLEASE SIGNAL
Length = 41
Score = 209  (85.1 bits), Expect = 1e-19
Identities = 37/41 (90%), Positives = 39/41 (95%)

 Query:    107 ITDCRETGSSKYPNCAYKTTQANKHIIVACEGNPYVPVHFD 147
               ITDCRE+G+SKYPNC YKTTQA KHIIVACEGNPYVPVHFD
 Sbjct:     81 ITDCRESGNSKYPNCVYKTTQAEKHIIVACEGNPYVPVHFD 121



>PDB406P1 (Closest domain: RNAS4_BOVIN 79-119)
Number of domains in family: 15
Commentary (automatic):
DISULFIDE HYDROLASE BOND ENDONUCLEASE FULL=RIBONUCLEASE NUCLEASE
EC=3.1.27.- RECNAME: PRECURSOR SHORT=RNASE
Length = 41
Score = 159  (65.9 bits), Expect = 2e-12
Identities = 25/41 (60%), Positives = 32/41 (78%)

 Query:    108 TDCRETGSSKYPNCAYKTTQANKHIIVACEGNPYVPVHFDA 148
               TDCRETGSS+ PNC Y+   + + +++ACEGNP VPVHFD
 Sbjct:     79 TDCRETGSSRAPNCRYRAKASTRRVVIACEGNPQVPVHFDG 119
```

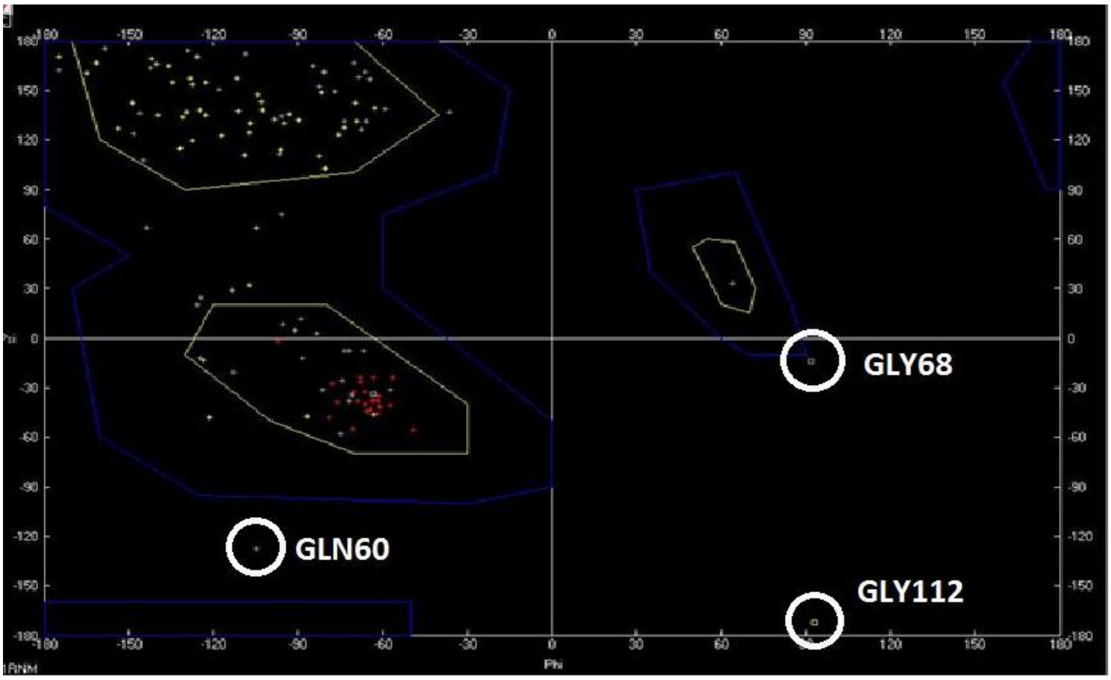


render by 3D/colored by secondary structure:





Τα αμινοξέα που είναι εκτός Ramachandran είναι 3: GLY112, GLN60, GLY68.



Επειδή η πλευρική αλυσίδα της γλυκίνης είναι μόλις ένα άτομο υδρογόνου), η γλυκίνη μπορεί να συμμετέχει σε πολλές διαμορφώσεις μη αποδεκτές για άλλα αμινοξέα. Η γλυκίνη έχει μόνο ένα άτομο υδρογόνου για πλευρική αλυσίδα με μια πολύ μικρότερη ακτίνα van der Waals από τις CH_3, CH_2, ή CH ομάδες που ξεκινούν την πλευρική αλυσίδα όλων των άλλων αμινοξέων και είναι λιγότερο περιορισμένη.

Τα αμινοξέα της γλυκίνης στο πρωτεϊνικό μόριο της 1 RNM (με πορτοκαλί μόνο):