

**NATIONAL INSTITUTE OF MATERIALS PHYSICS
BUCHAREST-MAGURELE**

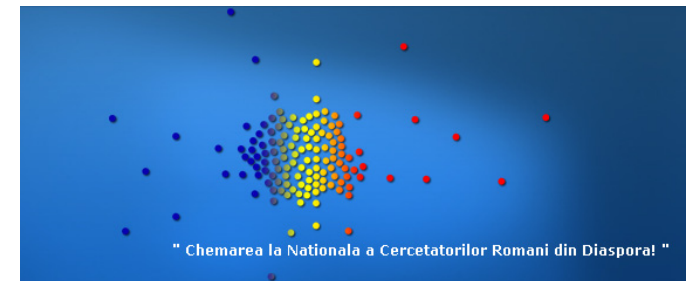
Atomistilor Str. 105 bis, P.O. Box MG-7, 077125 Magurele-Ilfov, Romania

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Regularitati ascunse si corelatii in nano-bio-structuri

M. Popescu, A. Velea

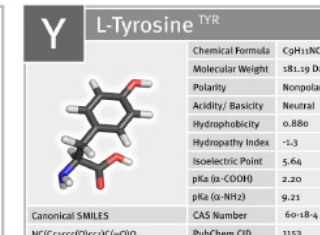
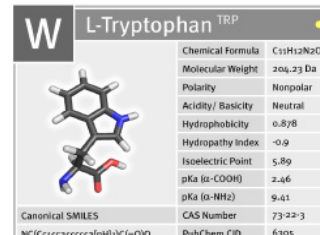
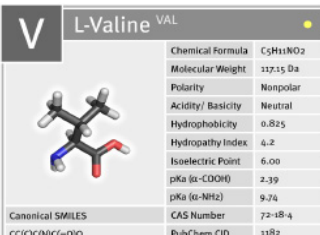
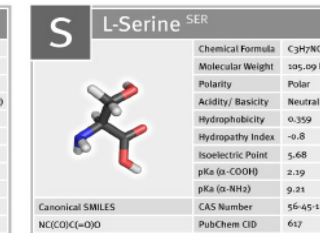
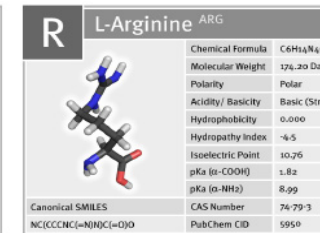
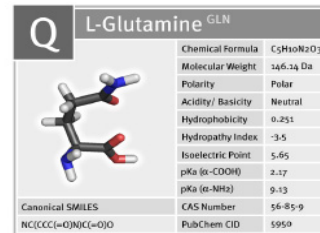
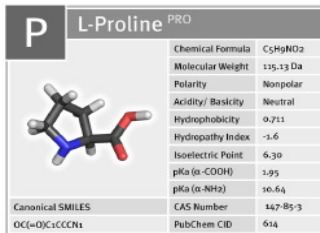
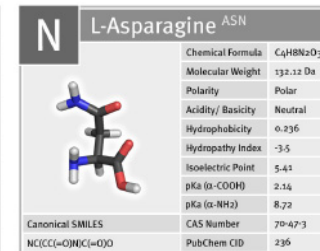
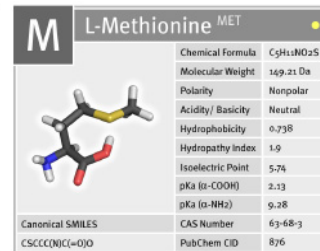
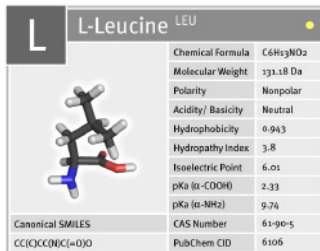
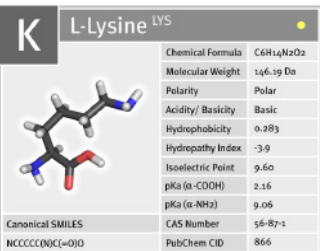
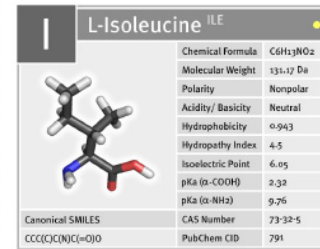
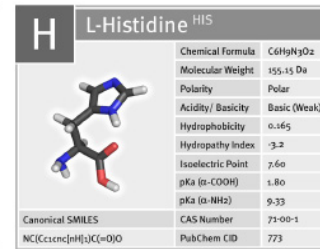
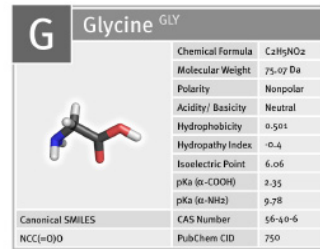
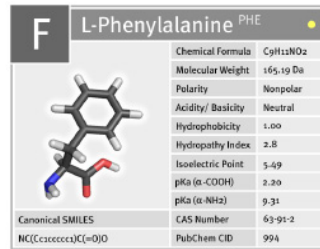
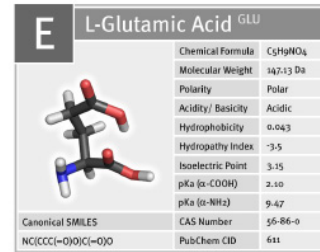
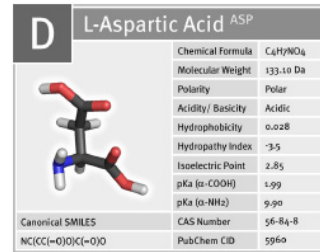
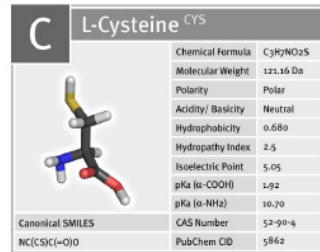
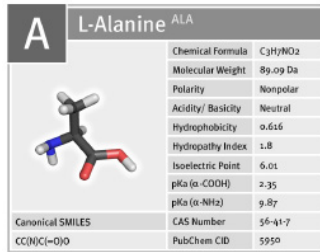
**Workshop Exploratoriu:
"Nano Sisteme Dinamice: de la Concepte la
Aplicatii Senzoristice"
22-23 septembrie 2010, Bucuresti**



Cuprins

- Introducere
- Metode
- Colagen $\alpha 1(I)$ uman
- Interferon β
- Concluzii

Introducere



Metode

- *Pair correlation*

- Se calculeaza numarul de perechi de aminoacizi de acelasi fel situati la anumite distante unul de celalalt
- Se determina functia de corelare de perechi

- *Fast Fourier Transform*

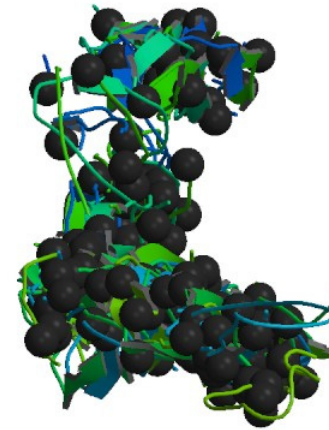
$$X(t) = \frac{A_0}{2} + \sum_{n=1}^{\infty} A_n \cos(n\omega_0 t) + \sum_{n=1}^{\infty} B_n \sin(n\omega_0 t) \quad \omega_0 = \frac{2\pi}{T}$$

$$G(f) = \frac{1}{2}(A_n + iB_n) = \frac{1}{T} \int_{-T/2}^{+T/2} X(t) e^{in\omega_0 t} dt \quad f = n\omega_0$$

Colagen $\alpha 1(I)$ uman

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1464 aminoacizi



A	139
R	71
N	28
D	66
C	18
Q	49
E	75
G	391
H	9
I	24
L	48
K	57
M	13
F	27
P	278
S	60
T	45
W	6
Y	13
V	47

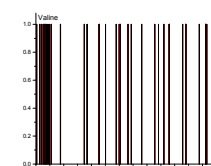
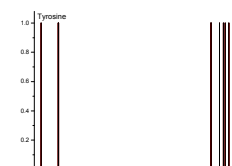
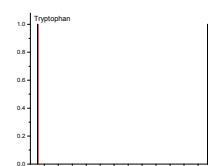
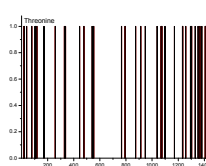
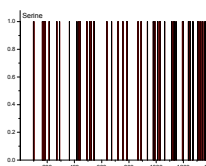
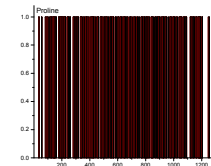
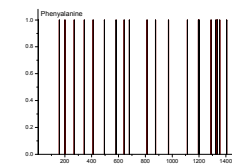
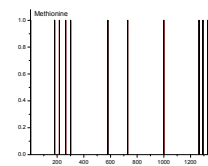
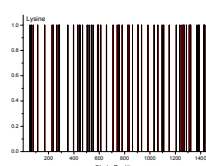
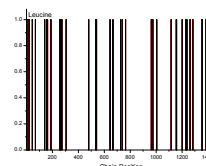
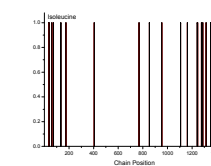
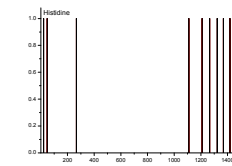
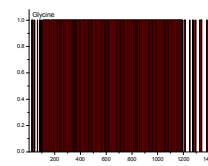
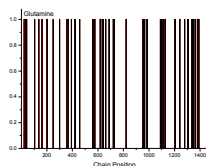
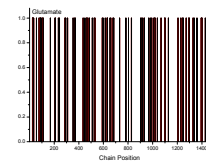
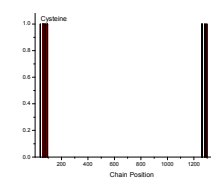
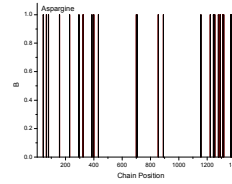
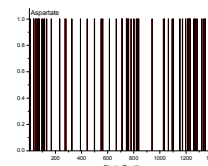
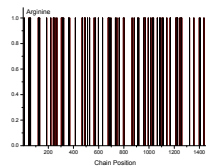
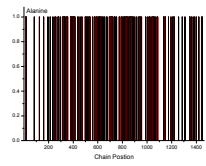


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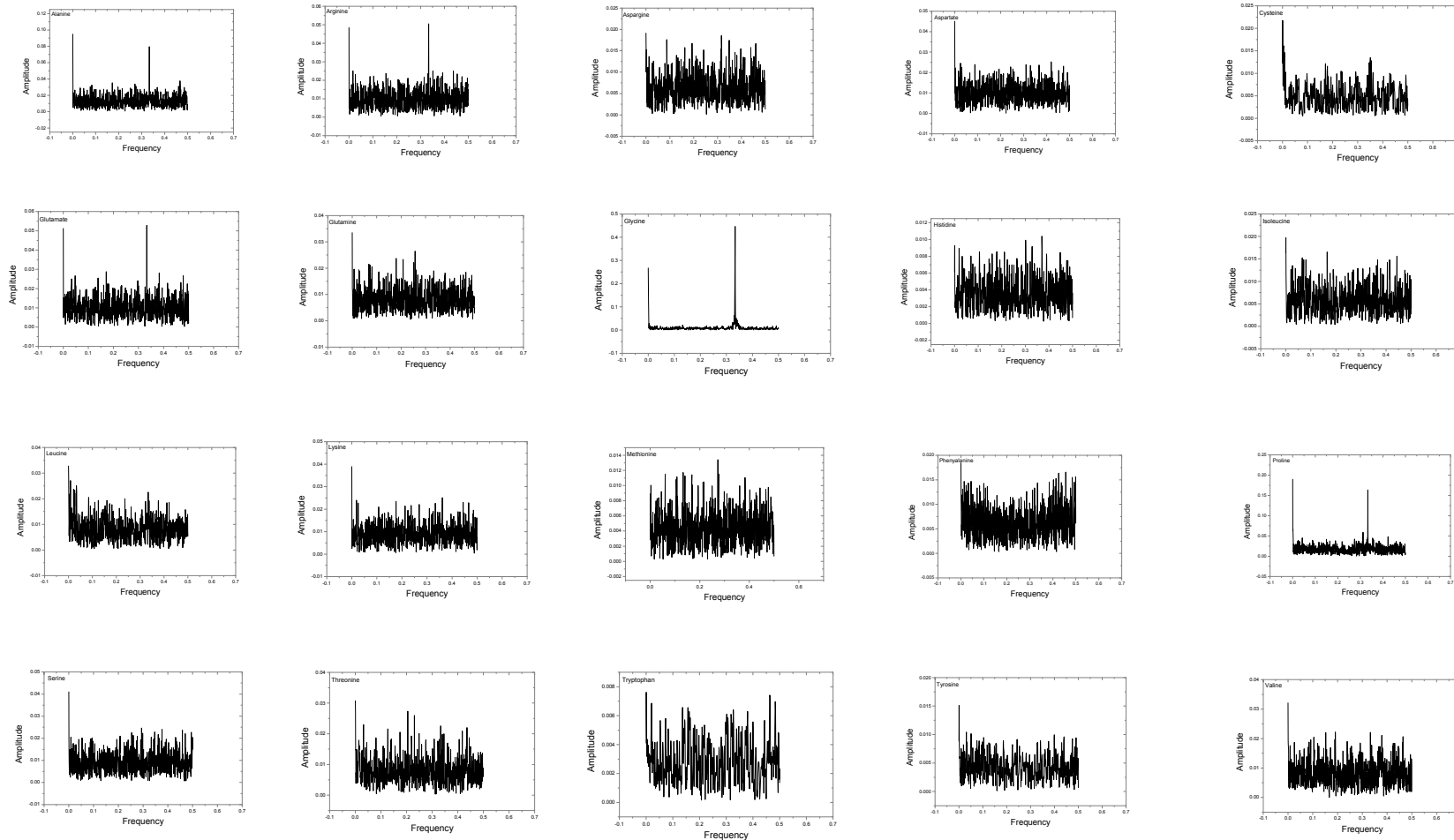
Colagen $\alpha 1(I)$ uman

Pozitionari in lant:



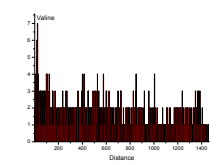
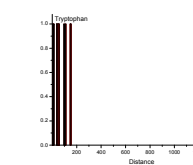
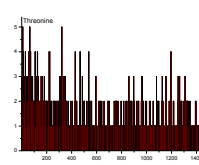
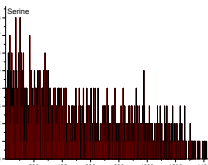
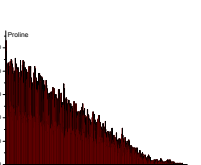
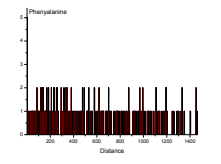
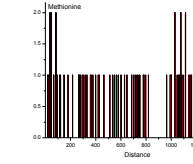
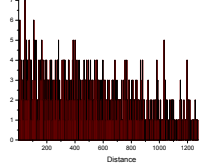
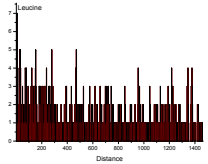
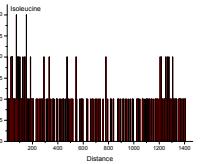
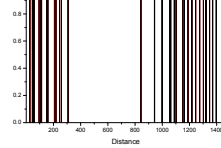
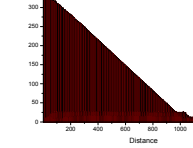
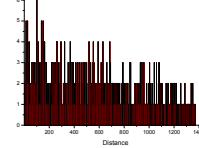
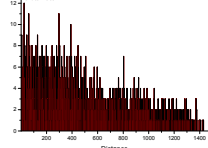
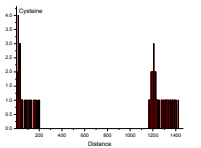
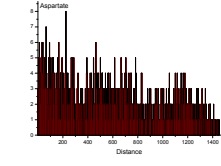
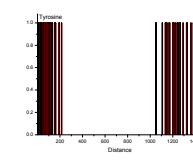
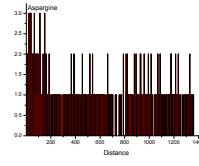
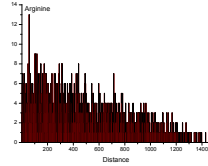
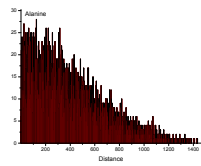
Colagen $\alpha 1(I)$ uman

FFT:



Colagen $\alpha 1(I)$ uman

Distante intre aminoacizi de acelaasi tip:



Colagen $\alpha 1(I)$ uman

Probabilitati de legare intre doi aminoacizi X si Y in lantul de colagen $\alpha 1(I)$ uman :

$$Pr ob = \frac{LegXY + LegYX}{NrX + NrY}$$

LegXY= nr de legaturi X-Y

LegYX= nr de legaturi Y-X

NrX= numarul de aminoacizi X din lantul colagenului

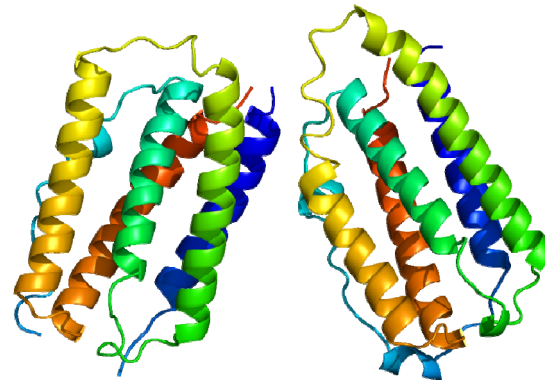
NrY= numarul de aminoacizi Y din lantul colagenului

	A	R	N	D	C	Q	E	G	H	I	L	K	M	F	P	S	T	W	Y	V
A	4.32%	5.71%	2.40%	7.32%	0.00%	1.60%	4.67%	23.02%	0.68%	2.45%	2.14%	6.63%	0.00%	1.20%	13.19%	3.52%	2.72%	0.69%	0.66%	3.76%
R	5.71%	0.00%	0.00%	9.49%	2.25%	1.67%	8.22%	11.90%	3.75%	3.16%	5.04%	2.34%	0.00%	1.02%	4.58%	3.82%	1.72%	0.00%	3.57%	3.39%
N	2.40%	0.00%	0.00%	3.19%	6.52%	3.90%	2.91%	3.82%	0.00%	3.85%	3.95%	7.06%	2.44%	1.82%	1.31%	4.55%	0.00%	2.94%	0.00%	2.67%
D	7.32%	9.49%	3.19%	4.55%	3.57%	4.35%	2.84%	8.10%	2.67%	3.33%	6.14%	5.69%	1.27%	3.23%	1.45%	1.59%	4.50%	1.39%	1.27%	7.96%
C	0.00%	2.25%	6.52%	3.57%	5.56%	0.00%	1.08%	0.49%	7.41%	4.76%	1.52%	1.33%	3.23%	4.44%	1.35%	0.00%	6.35%	0.00%	0.00%	9.23%
Q	1.60%	1.67%	3.90%	4.35%	0.00%	4.08%	6.45%	7.95%	0.00%	2.74%	5.15%	1.89%	1.61%	5.26%	4.59%	2.75%	2.13%	0.00%	0.00%	4.17%
E	4.67%	8.22%	2.91%	2.84%	1.08%	6.45%	2.67%	12.23%	0.00%	5.05%	0.81%	3.03%	1.14%	1.96%	4.25%	4.44%	7.50%	0.00%	3.41%	4.10%
G	23.02%	11.90%	3.82%	8.10%	0.49%	7.95%	12.23%	1.79%	0.75%	1.93%	5.24%	8.93%	1.73%	4.07%	38.42%	8.65%	5.28%	0.25%	0.74%	5.25%
H	0.68%	3.75%	0.00%	2.67%	7.41%	0.00%	0.00%	0.75%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	2.90%	3.70%	0.00%	9.09%	1.79%
I	2.45%	3.16%	3.85%	3.33%	4.76%	2.74%	5.05%	1.93%	0.00%	4.17%	0.00%	2.47%	0.00%	0.00%	2.32%	2.38%	2.90%	3.33%	2.70%	2.82%
L	2.14%	5.04%	3.95%	6.14%	1.52%	5.15%	0.81%	5.24%	0.00%	0.00%	14.58%	2.86%	1.64%	4.00%	4.60%	2.78%	5.38%	0.00%	0.00%	1.05%
K	6.63%	2.34%	7.06%	5.69%	1.33%	1.89%	3.03%	8.93%	0.00%	2.47%	2.86%	1.75%	2.86%	0.00%	3.58%	5.13%	5.88%	3.17%	1.43%	1.92%
M	0.00%	0.00%	2.44%	1.27%	3.23%	1.61%	1.14%	1.73%	0.00%	0.00%	1.64%	2.86%	0.00%	2.50%	1.37%	2.74%	1.72%	0.00%	3.85%	1.67%
F	1.20%	1.02%	1.82%	3.23%	4.44%	5.26%	1.96%	4.07%	0.00%	0.00%	4.00%	0.00%	2.50%	0.00%	2.30%	6.90%	2.78%	3.03%	0.00%	2.70%
P	13.19%	4.58%	1.31%	1.45%	1.35%	4.59%	4.25%	38.42%	0.00%	2.32%	4.60%	3.58%	1.37%	2.30%	17.63%	6.80%	2.17%	0.00%	0.34%	3.38%
S	3.52%	3.82%	4.55%	1.59%	0.00%	2.75%	4.44%	8.65%	2.90%	2.38%	2.78%	5.13%	2.74%	6.90%	6.80%	0.00%	3.81%	0.00%	2.74%	3.74%
T	2.72%	1.72%	0.00%	4.50%	6.35%	2.13%	7.50%	5.28%	3.70%	2.90%	5.38%	5.88%	1.72%	2.78%	2.17%	3.81%	6.67%	0.00%	3.45%	3.26%
W	0.69%	0.00%	2.94%	1.39%	0.00%	0.00%	0.00%	0.25%	0.00%	3.33%	0.00%	3.17%	0.00%	3.03%	0.00%	0.00%	0.00%	0.00%	10.53%	3.77%
Y	0.66%	3.57%	0.00%	1.27%	0.00%	0.00%	3.41%	0.74%	9.09%	2.70%	0.00%	1.43%	3.85%	0.00%	0.34%	2.74%	3.45%	10.53%	7.69%	1.67%
V	3.76%	3.39%	2.67%	7.96%	9.23%	4.17%	4.10%	5.25%	1.79%	2.82%	1.05%	1.92%	1.67%	2.70%	3.38%	3.74%	3.26%	3.77%	1.67%	4.26%

Interferon β

MTNKCLLQIALLLCFSTTAL
SMSYNLLGFLQRSSNFQC
QKLLWQLNGRLEYCLKDR
MNFDIPEEIKQLQQFQKED
AALTIYEMLQNIFAIFRQDS
SSTGWNETIVENLLANVY
HQINHLKTVLEEKLEKEDF
TRGKLMSSLHLKRYYYGRIL
HYLKAKEYSHCAWTIVRV
EILRNFYFINRLTGYLRN

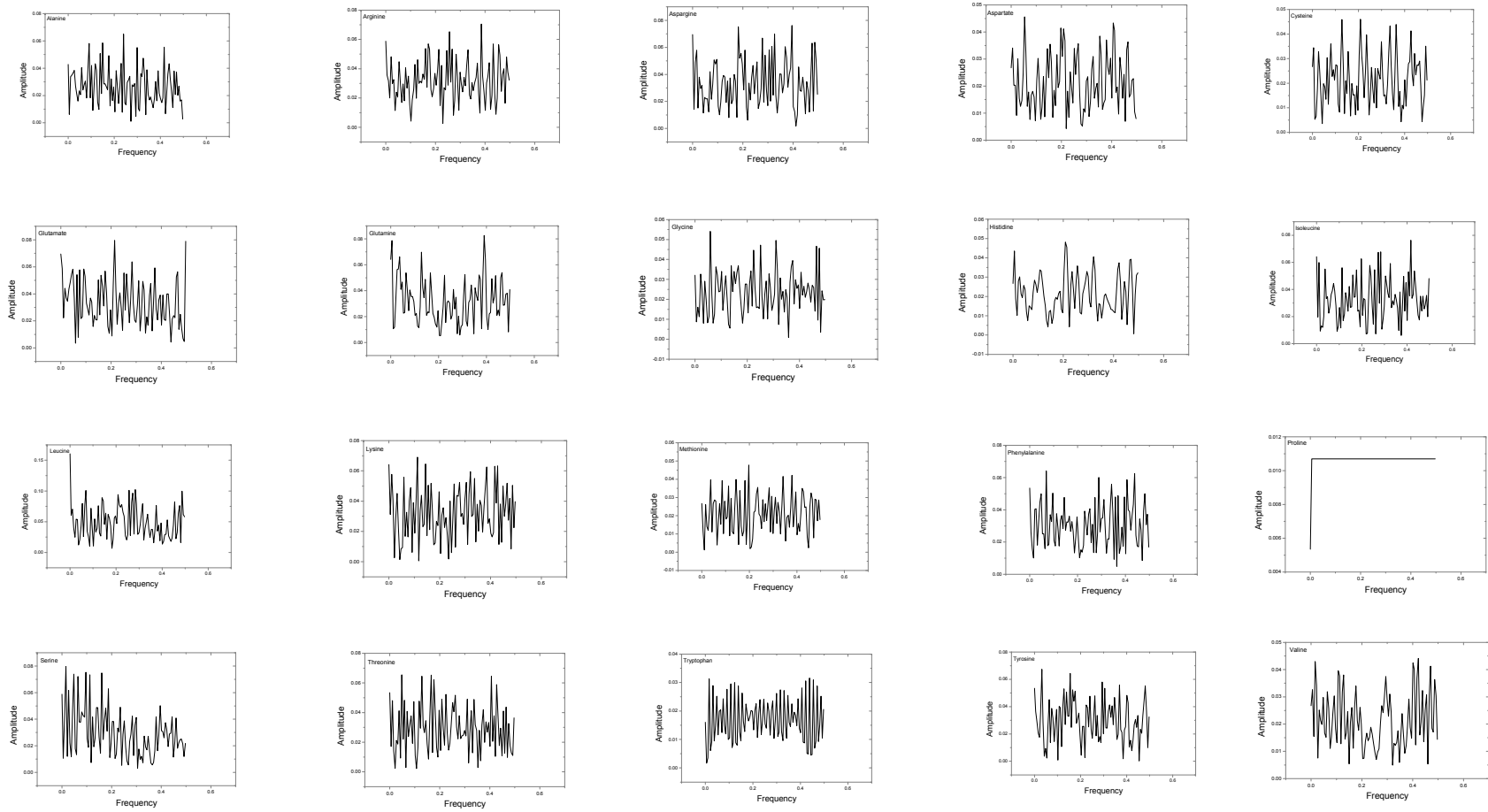
187 aminoacizi



A	8
R	11
N	13
D	5
C	5
Q	12
E	13
G	6
H	5
I	12
L	30
K	12
M	5
F	10
P	1
S	11
T	10
W	3
Y	10
V	5

Interferon β

FFT:



Concluzii

- Aplicarea metodelor statistice in moleculele cu lanturi mari permite obtinerea de argumente pentru ordonarea partiala a aminoacizilor si obtinerea de corelatii intre aminoacizi.
- Atunci cand aminoacizii sunt folositi pentru construirea unor lanturi lungi si complicate metodele statistice sunt eficiente pentru dezvaluirea structurii primare a biomoleculelor.

**Va multumesc
pentru atentie!**