

The analysis of and prediction of the structure of Phytoene synthase in *Daucus carota*

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outline

- 1 Background of the research
- 2 Construction of evolutionary tree
- 3 Analysis of the PSY structure
- 4 Prediction of the 3D structure
- 5 Acknowledgements





1 Background



About in the 13th century, carrots were introduced to China from Iran and developed into the Chinese ecotypes .

The carrot contains a lot of nutrients, including carotenoids、 Ca、 Fe、 Vitamin B1 、 Vitamin B2 、 Vitamin C.

In addition, carrots contain plant fiber , which can promote intestinal peristalsis

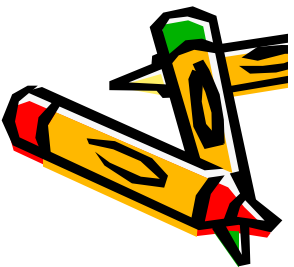
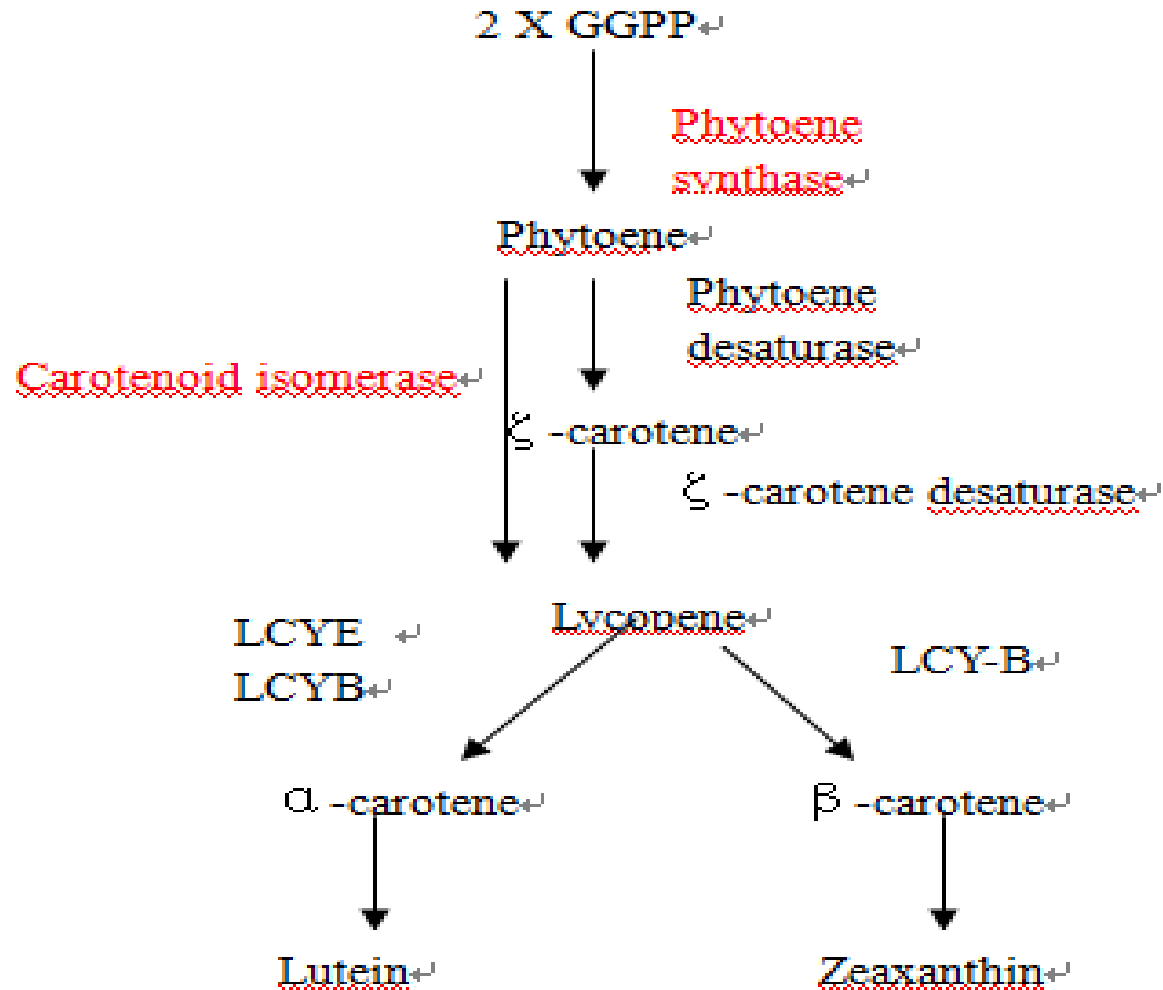


The functions of β -carotene

- 1 Protect eyesight
- 2 Enhance immunity
- 3 Antioxidant
- 4 Cancer prevention
- 5 Prevention of cardiovascular disease



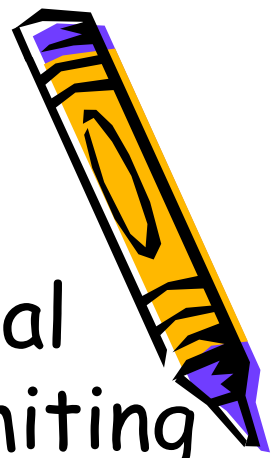
The biosynthetic pathway of β -carotene



- Phytoene synthase (PSY) catalyzes the first committed and rate-limiting step of carotenoid biosynthesis , As the first pathway-specific enzyme in carotenoid biosynthesis, phytoene synthase (PSY) is a prime regulatory target.it is important for us to study the PSY on the way to improve the content of b-carotene in vegetables.



Analysis



- Carotene have important nutritional value, PSY is an important rate-limiting enzyme in carotene synthesis process, having an important significance for improving the carotene content. But there are not enough research on PSY in carrots , so our group are aimed to structure prediction and analysis of the PSY in carrots .



2 Construction of evolutionary tree



Amino acid sequence

- >sp|Q9SSU8|PSY_DAUCA Phytoene synthase, chloroplastic
OS=Daucus carota GN=PSY PE=2 SV=1
MACNFAVRVIYYPKEIHGVSVLNTNRSRKS RF SCRVMKLSTG
VSAVAANPVRTSEERVYE
VVLKQAALVREEKRSSRGLCLDTKRTGSKSFDKSEND DAGMK
SWNLLNEAYDRCGEVCAE
YAKTFYLG TLLMTPERRRAVWAIYVWCRRTDELVDGPNASHI
TPKALDRWEKRLNDFDG
QPYDMYDAALADTVSTYPVDIQPFKDMIDGMRMDLKK SRYQ
TFDELYLYCYV VAGTVGLM
SVPVMGIAPESKATTESVYSAALALGIANQLTNILRDVGEDA
RRGRIYLPQEELKLAGIT
PEYIFKGVTDKWR SFMKGQIKRARMFFDEAEKGVAELSSAS
RWPVWASLLLYKQILDAI
EANDYDNFTKRAYVGKAKKLVSLPLAYSRALFAPSTVR



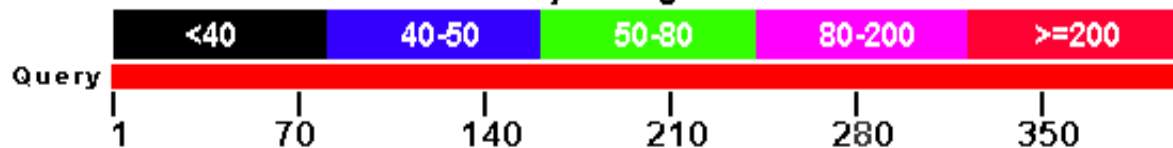
blast



Distribution of 100 Blast Hits on the Query Sequence

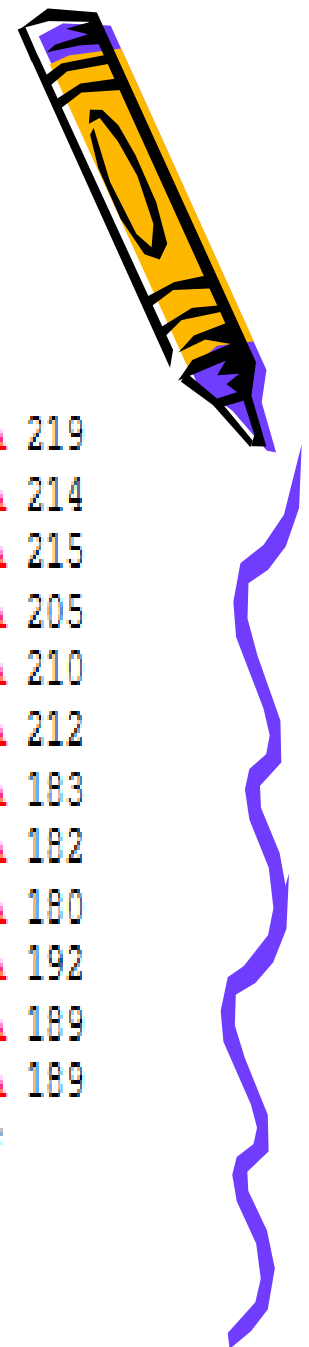
XP_003545292 PREDICTED: phytoene synthase, chloroplastic-like [Glyci.. S=540 E=0

Color key for alignment scores



Q9SSU8.1	RecName: Full=Phytoene synthase, chloroplastic; Flags: Precursor >
ACR61392.1	phytoene synthase protein [Fragaria x ananassa]
XP_002306754.1	predicted protein [Populus trichocarpa] >qb EEE93750.1 predicted
XP_002283193.1	PREDICTED: phytoene synthase, chloroplastic isoform 1 [Vitis vinifer:
CAN70878.1	hypothetical protein VITISV_032970 [Vitis vinifera]
XP_003633261.1	PREDICTED: phytoene synthase, chloroplastic isoform 2 [Vitis vinifer:
XP_003532084.1	PREDICTED: phytoene synthase, chloroplastic-like [Glycine max]
NP_001239926.1	uncharacterized protein LOC100776503 [Glycine max] >qb ACU1853:
XP_003519534.1	PREDICTED: phytoene synthase, chloroplastic-like [Glycine max]
XP_003545292.1	PREDICTED: phytoene synthase, chloroplastic-like [Glycine max]
XP_002442578.1	hypothetical protein SORBIDRAFT_08g022310 [Sorghum bicolor] >qb
XP_002271575.1	PREDICTED: phytoene synthase, chloroplastic [Vitis vinifera]
CBI27361.3	unnamed protein product [Vitis vinifera]
CBI22078.3	unnamed protein product [Vitis vinifera]





Conserved sites : predicted by clustw2

Populus	LLMTPERRRAIWAIYVWCRRTDELVDGPNASHITPTALDRWEARLEDLFQGRPFDMMDAA	219
Manihot	LLMTPERRRAIWAIYVWCRRTDELVDGPNASHITPTALDRWEARLEDMFRGRPFDMLDAA	214
Cucumis	MLMTPERQKAIWAIYVWCRRTDELVDGPNASHITPTALDRWEARLEELFQGRPFDMLDAA	215
Salicornia	QLMTPTRRKAIWAIYVWCRRTDELVDGPNASHITPTALDRWEARLEDLFSGRPFDMLDAA	205
Arabidopsis	LLMTPERRKAIWAIYVWCRRTDELVDGPNASHITPMALDRWEARLEDLFRGRPFDMLDAA	210
Brassica	LLMTPERRKAIWAIYVWCRRTDELVDGPNASHITPMALDRWEARLEDLFRGRPFDMLDAA	212
Fragaria	LLMTPERRRAVWAIYVWCRRTDELVDGPNASYITPKALDRWEKRLTDLFEGRPYDMYDAA	183
Vitis	LLMTPERRRAVWAIYVWCRRTDELVDGPNASHMSPKALDRWEQRLIDLFEHGPYDMYDAA	182
Glycine	QLMTQERRKAIWAIYVWCRRTDELVDGPNASHITPKALDRWEQRLYDVFEGRPYDMYDAA	180
Sorghum	QLMTPERRKAVWAIYVWCRRTDELVDGPNASYITPTALDRWEKRLLEDLFEGRPYDMYDAA	192
Zea	QLMTPERRKAVWAIYVWCRRTDELVDGPNASYITPTALDRWEKRLLEDLFEGRPYDMYDAA	189
Daucus	LLMTPERRRAVWAIYVWCRRTDELVDGPNASHITPKALDRWEKRLNDLFDGQPYDMYDAA	189

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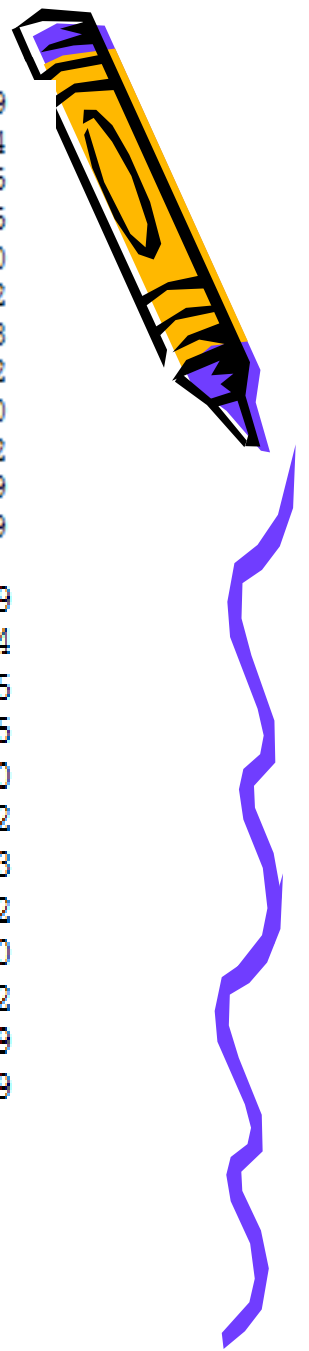


Populus	LADTVGKFPVDIQPFKDMIQGM RMDLRKSRYQNFDELYLYCYVAGTVGLMSVPVMGIAP	279
Manihot	LSDTVTKFPVDIQPFKDMIEGMRMDLKKSRYKNFDELYLYCYVAGTVGLMSVPVMGIAP	274
Cucumis	LADTVTKFPVDIQPFKDMIEGMRMDLRKSRYKNFDELYLYCYVAGTVGLMSVPVMGIAP	275
Salicornia	LCDTVTRFPIDIQPFKDMIEGMRLDLRKSRYKNFDELYLYCYVAGTVGLMSVPVMGIAP	265
Arabidopsis	LADTVARYPVDIQPFRDMIEGMRMDLKKSRYQNFDDLYLYCYVAGTVGLMSVPVMGIDP	270
Brassica	LADTVARYPVDIQPFRDMIEGMRMDLRKSRYKNFDDLYLYCYVAGTVGLMSVPVMGIDP	272
Fragaria	LSDTVTKYPVDIQPFKDMVEGMRLDLRKSRYQNFDELYLYCYVAGTVGLMSVPVMGIAP	243
Vitis	LSDTVAKYPVDVQPFKDMIEGMRLDLRKSRYNSFDELYLYCYVAGTVGLMSVPVMGISP	242
Glycine	LSDTVSKYPVDIQPFKDMIEGMRLDLRKSRYNNFDELYLYCYVAGTVGLMSVPVMGIAP	240
Sorghum	LSDTVSKFPVDIQPFKDMIEGMRLDLWKSRYMTFDELYLYCYVAGTVGLMTPVMGIAP	252
Zea	LSDTVSKFPVDIQPFKDMVQGMRLDLWKSRYMTFDELYLYCYVAGTVGLMTPVMGIAP	249
Daucus	LADTVSTYPVDIQPFKDMIDGM RMDLKKSRYQTFDELYLYCYVAGTVGLMSVPVMGIAP	249

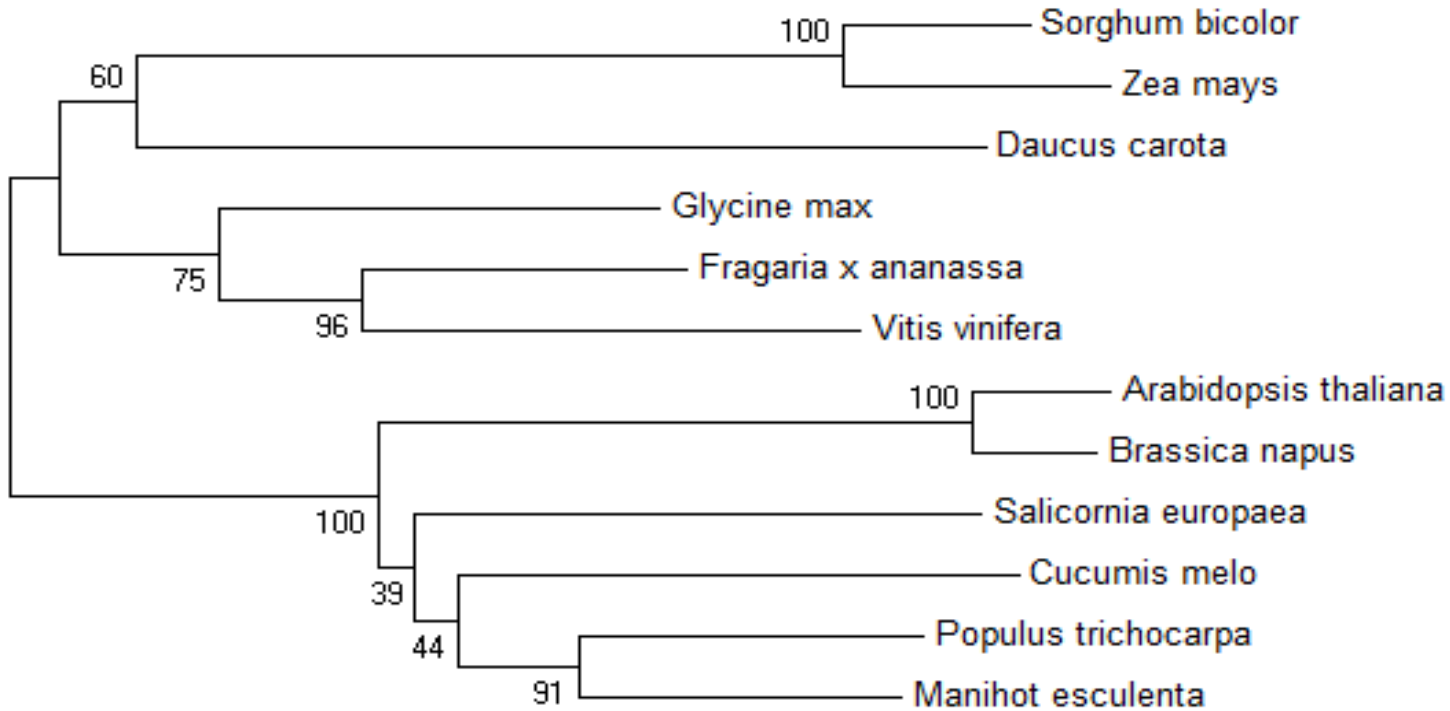
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Populus	ESQASTESVYNAALALGIANQLTNILRDVGEDARRGRVYLPQDELAQAGLSDDDDIFAGKV	339
Manihot	ESQASTESVYNAALALGIANQLTNILRDVGEDARRGRIYLPQDELAQAGLSDDDDIFAGKV	334
Cucumis	ESQASTESVYNAALALGIANQLTNILRDVGEDARRGRIYLPQDELAQAGLSDEDIFAGRV	335
Salicornia	ESKAPTESVYNAALALGIANQLTNILRDVGEDSRRGRVYLPQDELAQAGLSDEDIFAGKV	325
Arabidopsis	KSKATTESVYNAALALGIANQLTNILRDVGEDARRGRVYLPQDELAQAGLSDEDIFAGKV	330
Brassica	KSKATTESVYNAALALGIANQLTNILRDVGEDARRGRVYLPQDELAQAGLSDEDIFAGKV	332
Fragaria	ESKASTESVYNAALALGIANQLTNILRDVGEDARRGRIYLPQDELAQAGLSDDDDIFRGKV	303
Vitis	DSKASTESVYNAALALGIANQLTNILRDVGEDARRGRIYLPQDELERAGLSDDDDILRGKV	302
Glycine	ESKASTESVYNAALALGIANQLTNILRDVGEDARRGRVYLPQDELAQAGLSDDDDIFRGKV	300
Sorghum	DSKASTESVYNAALALGIANQLTNILRDVGEDARRGRIYLPQDELAQAGLTEEDIFRGKV	312
Zea	DSKASTESVYNAALALGIANQLTNILRDVGEDARRGRIYLPQDELAQAGLTEEDIFRGKV	309
Daucus	ESKATTESVYSAALALGIANQLTNILRDVGEDARRGRIYLPQEELKLAGITPEYIFKGV	309

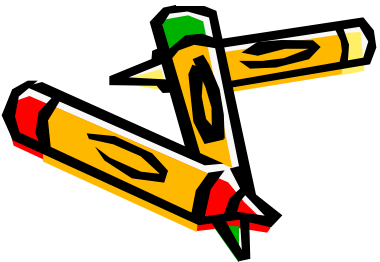
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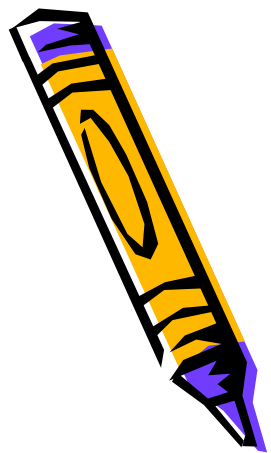
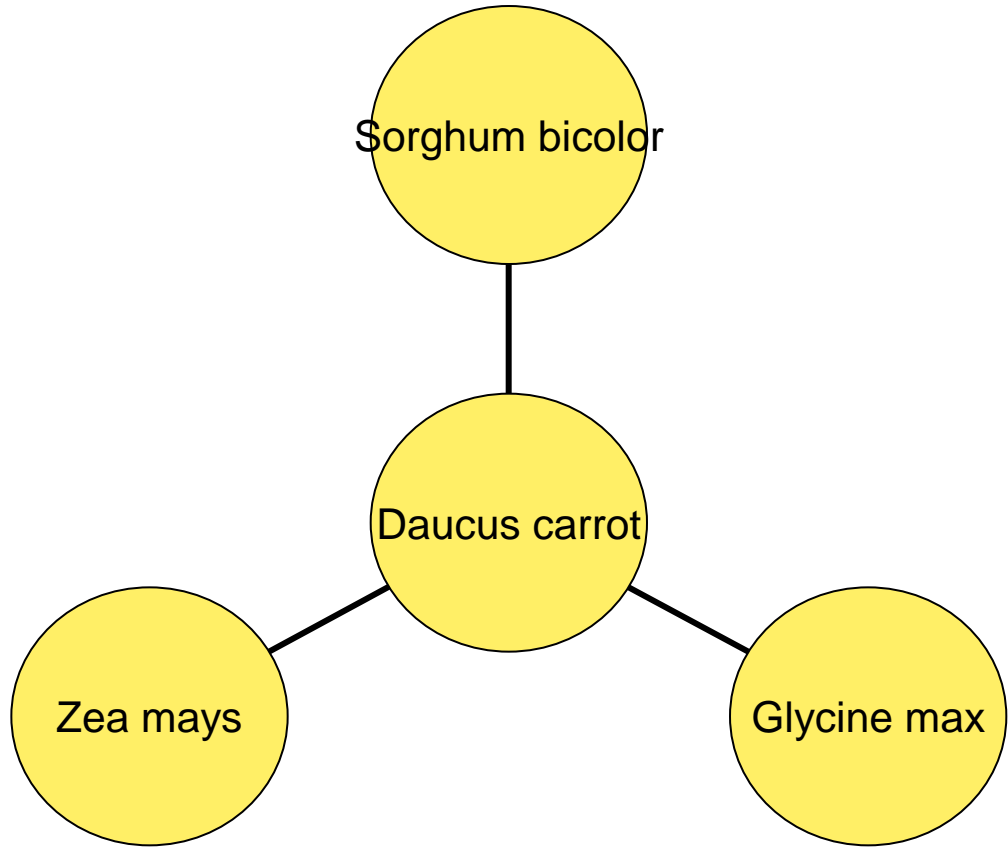


Evolutionary tree



0.02



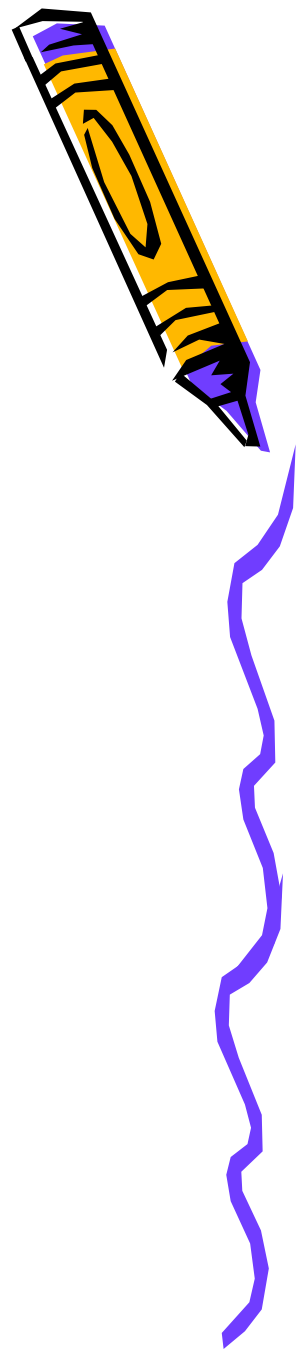


3 Analysis of the PSY structure

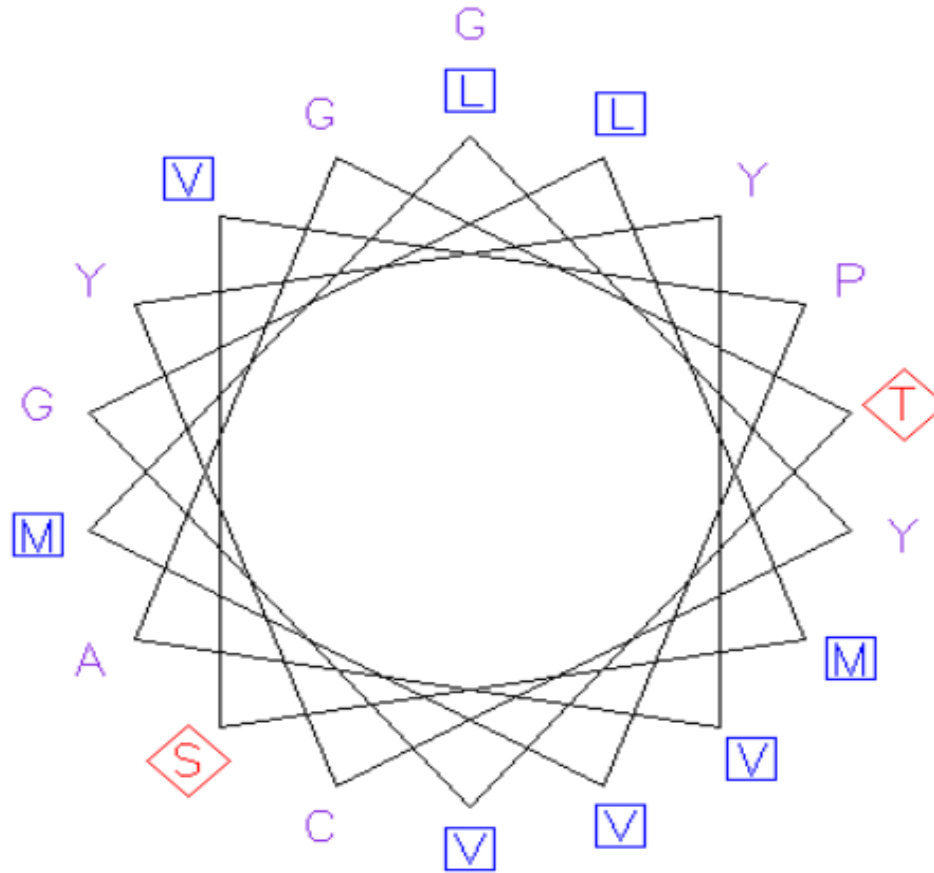
2D Structure

Predicted by [garnier\(v6.0.1\)](#)

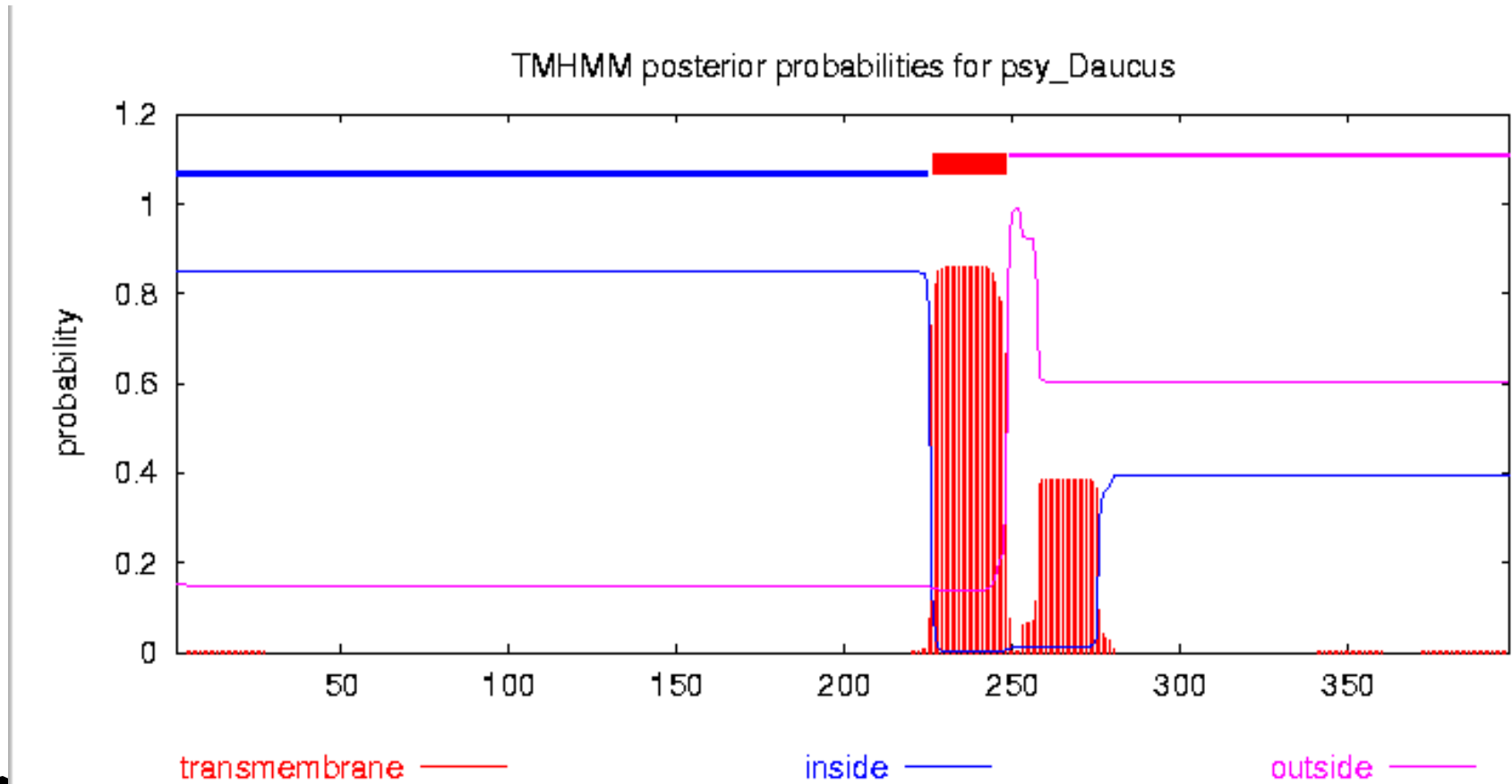
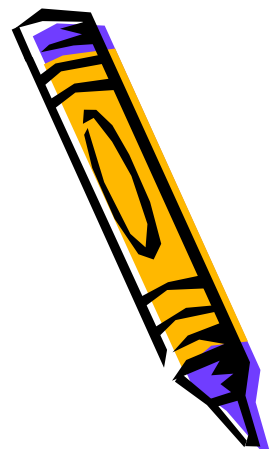
- Helix : 163 42.7%
- Sheet: 100 26.2%
- Turns: 75 19.6%
- Coils : 60 15.7%



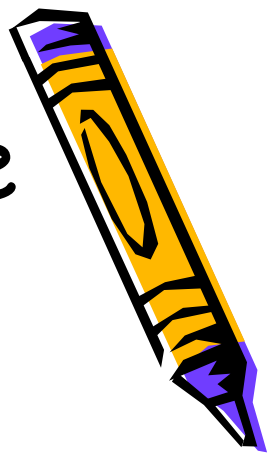
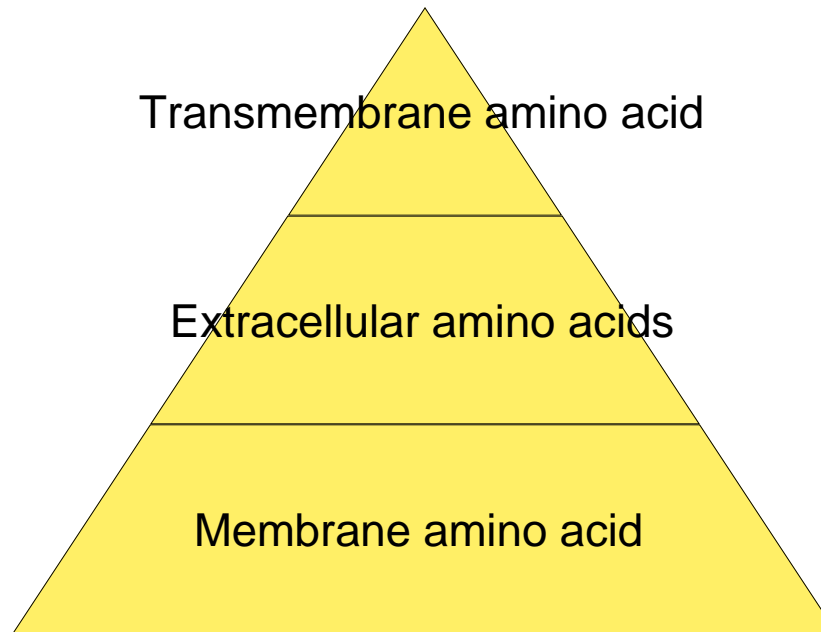
228-246 alpha helix



Transmembrane region prediction



The relationship between the number of three amino acids



对PSY性质进行分析

➤用PEPSTATS软件对psy蛋白进行分析

- PEPSTATS of psy Daucus from 1 to 398

Molecular weight = 45199.79 Residues = 398

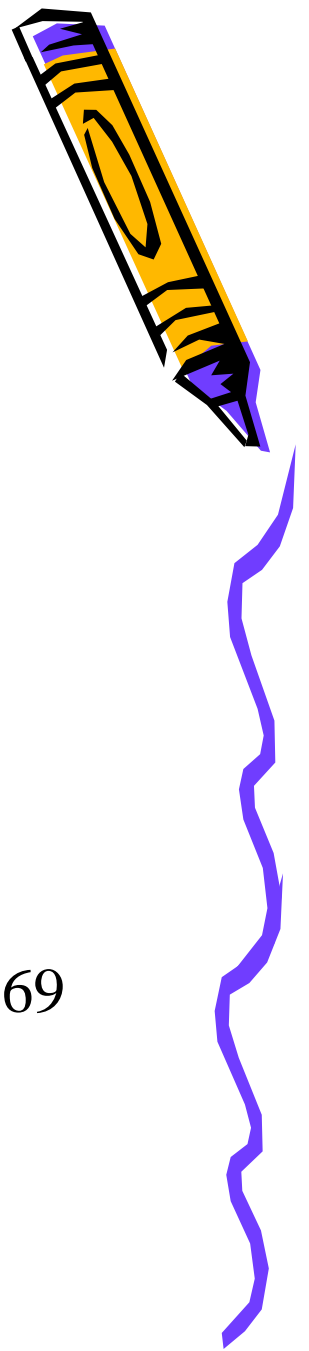
Average Residue Weight = 113.567 Charge = 12.0

Isoelectric Point = 9.3232

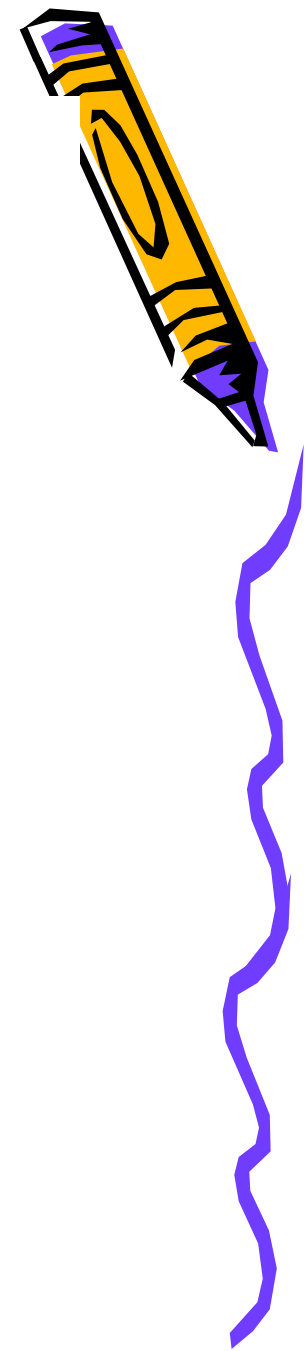
A280 Molar Extinction Coefficient = 67990

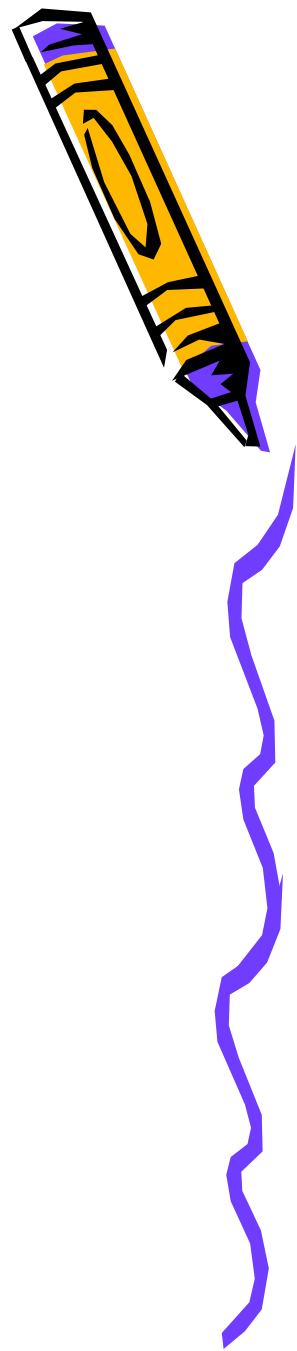
A280 Extinction Coefficient 1mg/ml = 1.50

Improbability of expression in inclusion bodies = 0.769



Residue	Number	Mole%	DayhoffStat
A = Ala	39	9.799	1.139
B = Asx	0	0.000	0.000
C = Cys	7	1.759	0.606
D = Asp	25	6.281	1.142
E = Glu	24	6.030	1.005
F = Phe	13	3.266	0.907
G = Gly	21	5.276	0.628
H = His	2	0.503	0.251
I = Ile	15	3.769	0.838
J = ---	0	0.000	0.000
K = Lys	28	7.035	1.066
L = Leu	36	9.045	1.222
M = Met	12	3.015	1.774
N = Asn	13	3.266	0.760
O = ---	0	0.000	0.000
P = Pro	15	3.769	0.725
Q = Gln	8	2.010	0.515
R = Arg	32	8.040	1.641
S = Ser	28	7.035	1.005
T = Thr	21	5.276	0.865
U = ---	0	0.000	0.000
V = Val	30	7.538	1.142
W = Trp	7	1.759	1.353
X = Xaa	0	0.000	0.000
Y = Tyr	22	5.528	1.626
Z = Glx	0	0.000	0.000

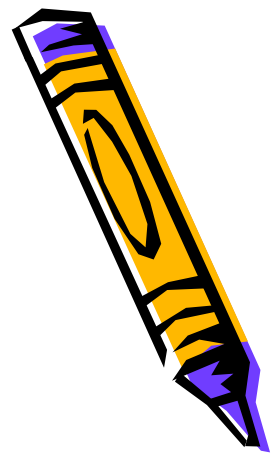
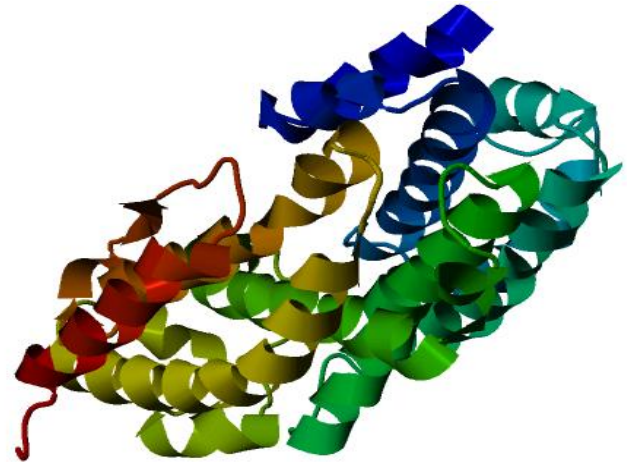
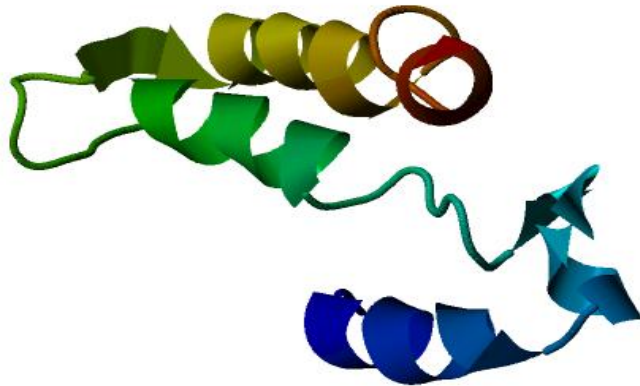




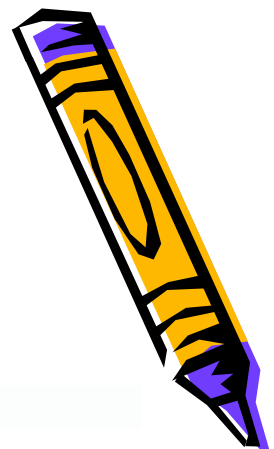
Property Residues Number	Mole%
Tiny (A+C+G+S+T) 116	29.146
Small (A+B+C+D+G+N+P+S+T+V)	199 50.000
Aliphatic (A+I+L+V) 120	30.151
Aromatic (F+H+W+Y) 44	11.055
Non-polar (A+C+F+G+I+L+M+P+V+W+Y)	217 54.523
Polar (D+E+H+K+N+Q+R+S+T+Z) 181	45.477
Charged (B+D+E+H+K+R+Z) 111	27.889
Basic (H+K+R) 62	15.578
Acidic (B+D+E+Z) 49	12.312



4 Prediction of the 3D structure



PSY Structure Blast



Details of selected Models/Structures ?

Your query was: Q9SSU8



Colors: **Query** | **Structures** | **Models** | **Range covered by final alignment**

Analyzed residue range: from 139 to 325

Domain annotation: [**InterPro**] ?

SQS_PSY ?

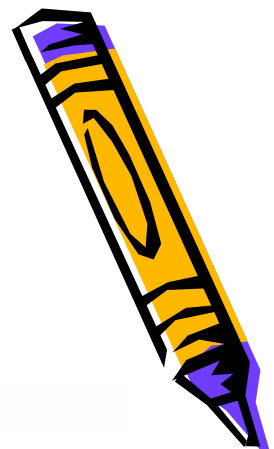
Q9SSU8 ? PSY_DAUCA ; Phytoene synthase, chloroplastic; EC=2.5.1.32; Flags: Precursor; Daucus carota (Carrot).

Models:

Index	Model	Rel.	Provider	Type	Templates	% Seq id	from	to
1	[Show]		NYSGXRC	TC	3ipiA ?	32%	206	273
2	[Show]		MODBASE	SC	1ezfA ?	20%	110	398
3	[Show]		NYSGXRC	TC	3ipiA ?	18%	139	325



Deviation score of each Model



Deviation Score of each Model/Structure

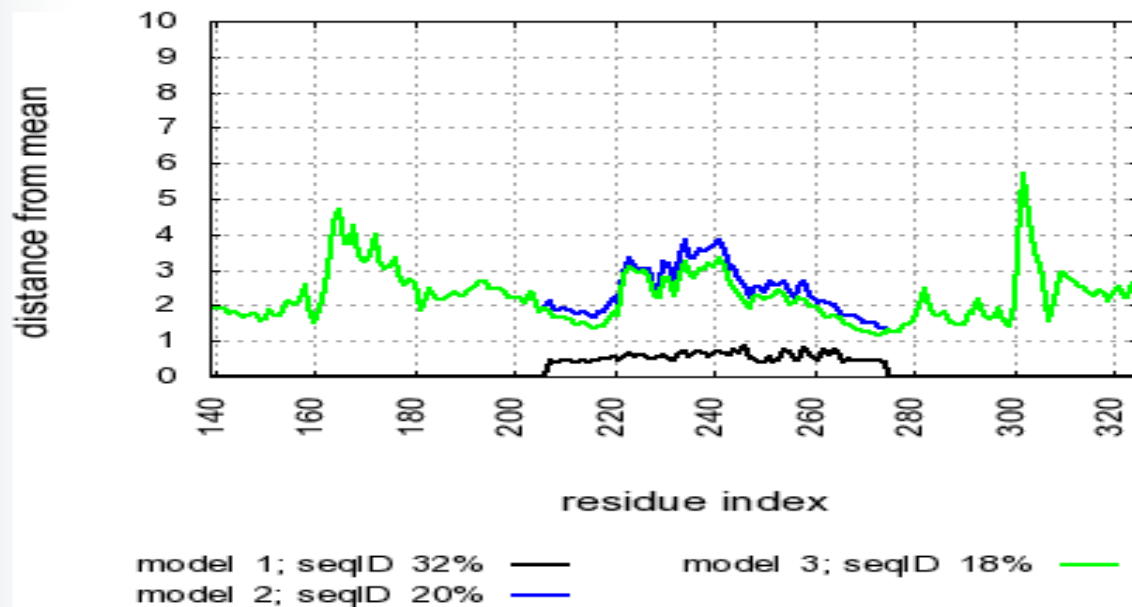



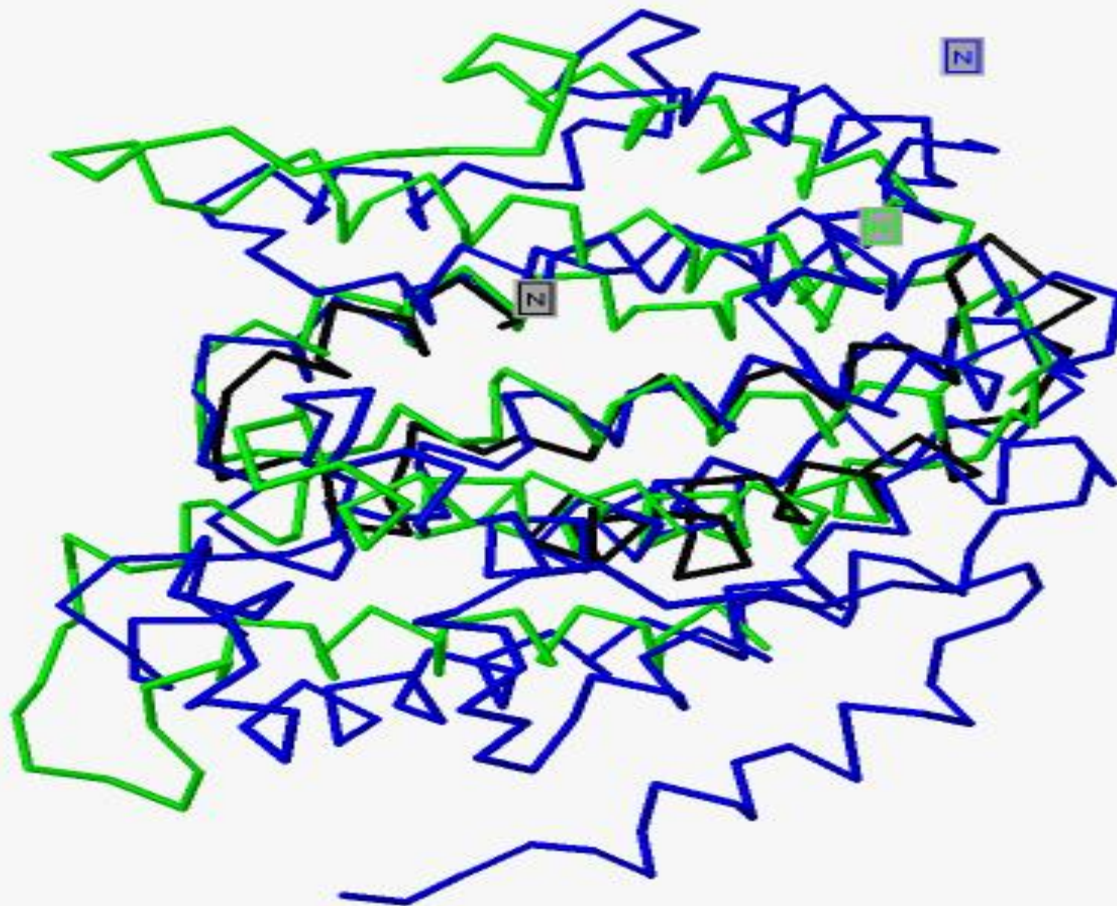
Fig. 2: Local (per residue) deviation of individual models/structures from mean of the ensemble of models/structures based on a distance RMSD (dRMSD). 



The part of 3D structure



PSY 3D Structure



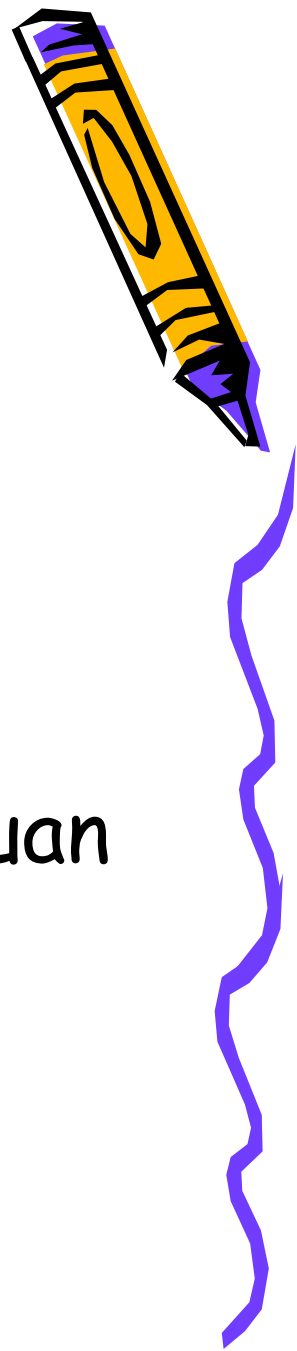
Next step



- We hope the predictions of protein structure can help find its substrate binding domain. By changing the substrate binding domain structure, we can improve its activity to promote the synthesis of carotenoids.



5 Acknowledgements



- 1 Thanks for teacher luo guidance
- 2 Thanks for the help of other members of group 15:wang min、duan mengmeng、 wang hui



The end !



Thanks for your attention

