桃热激蛋白101（Hsp101）基因和蛋白序列预测与结构分析

CAAS五组

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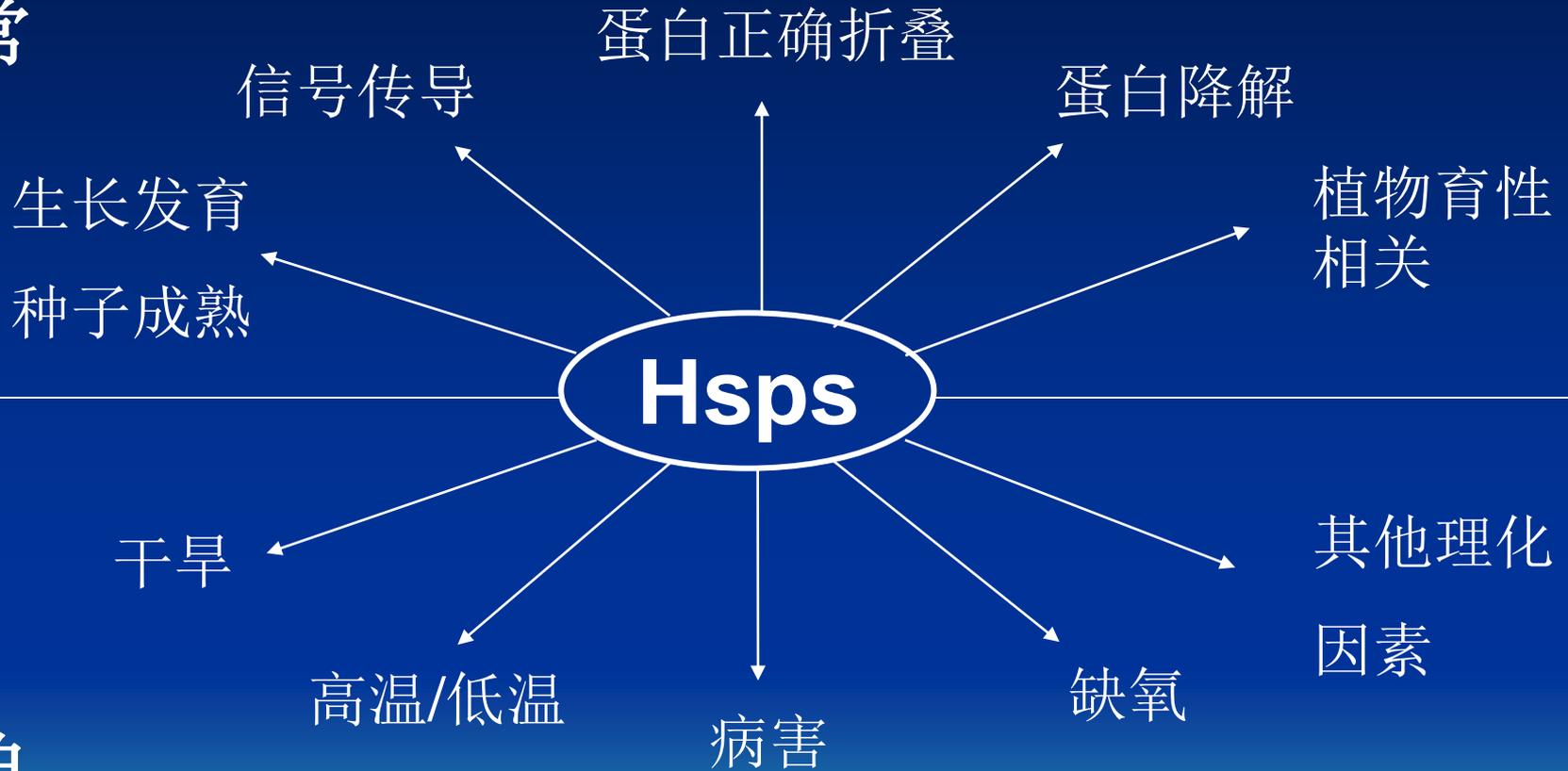
提纲

- ➤ 研究背景
- ➤ 基因序列与结构预测
- ➤ 蛋白序列与结构分析

研究背景

正常

胁迫

蛋白正确折叠

信号传导

蛋白降解

生长发育

植物育性相关

种子成熟

Hsps

干旱

其他理化因素

高温/低温

病害

缺氧

稳定蛋白质和膜结构，防止变性蛋白聚合及帮助其再折叠

主要的**Hsp**家族

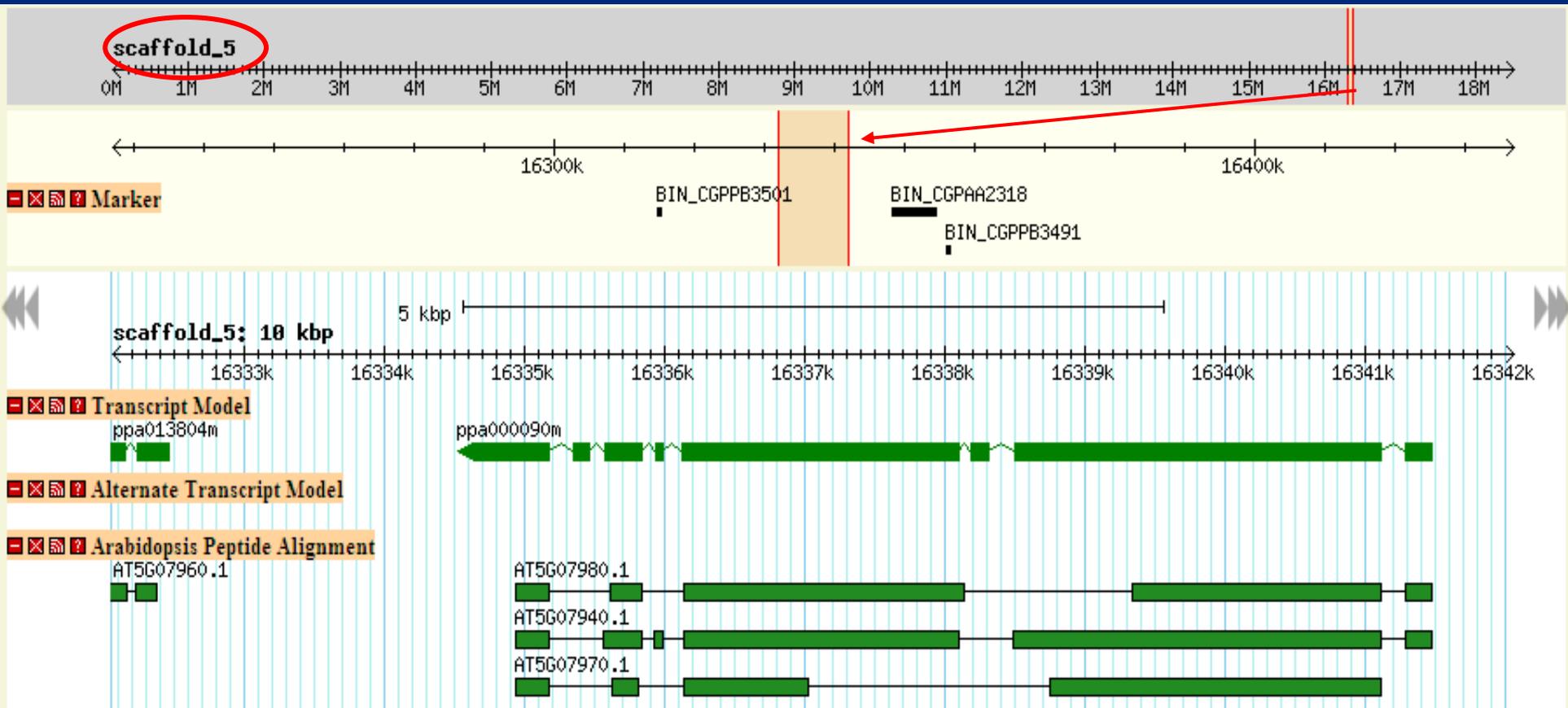| Chaperone families	Major functions of chaperone families
Small heat shock proteins (e.g. Hsp27*)	Prevent the aggregation of other proteins, by collecting protein "garbage", act as "dustmen" of cells
Hsp60 family	Assistance in protein folding and re-folding
Hsp70 family	Assistance in protein folding and re-folding
Hsp90 family	Stabilize substrate proteins and maintain their active, or inactive state, prevent the aggregation of other proteins, by collecting protein "garbage", act as "dustmen" of cells
Hsp100 family	Deseggregation of proteins

(P. Csermely & I. Yahara, 2002)

Hsp101基因序列与结构预测

EST序列~150bp → **BLAST** → 桃基因组序列

http://www.rosaceae.org/

基因组序列6.7kb

拟南芥和葡萄的Hsp101基因大小在**6.3-6.5kb**

推测该DNA片段包含一个基因

FGENESH基因预测
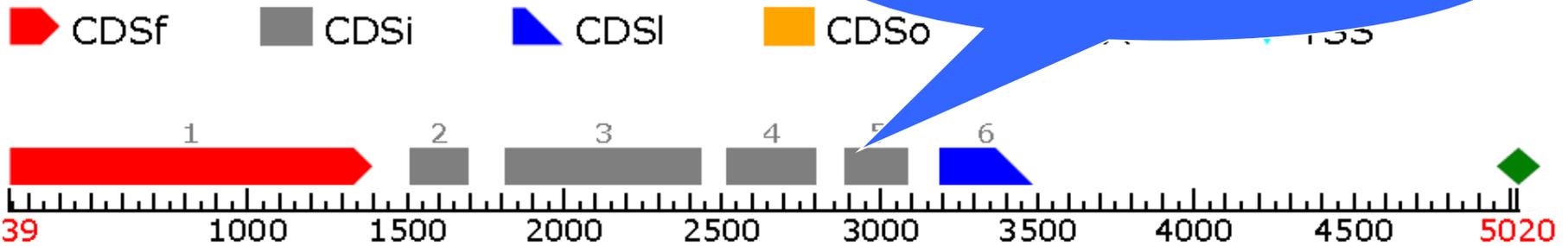
用**DSDS**显示基因结构（http://gsds.cbi.pku.edu.cn）

得到了**2730bp**的**mRNA**序列

蛋白序列与结构分析

编码蛋白**Hsp101**长**909**个氨基酸残基

Amino Acid Composition hsp101

30%+

Bioedit计算氨基酸组成

氨基酸	数目	百分比%
L	104	11.44
I	47	5.17
V	77	8.47
M	17	1.87
D	64	7.04
E	85	9.35
R	82	9.02
K	51	5.61
A	86	9.46
C	3	0.33
F	17	1.87
G	65	7.15
H	17	1.87
N	25	2.75
P	35	3.85
Q	38	4.18
S	38	4.18
T	38	4.18
W	2	0.22
Y	18	1.98
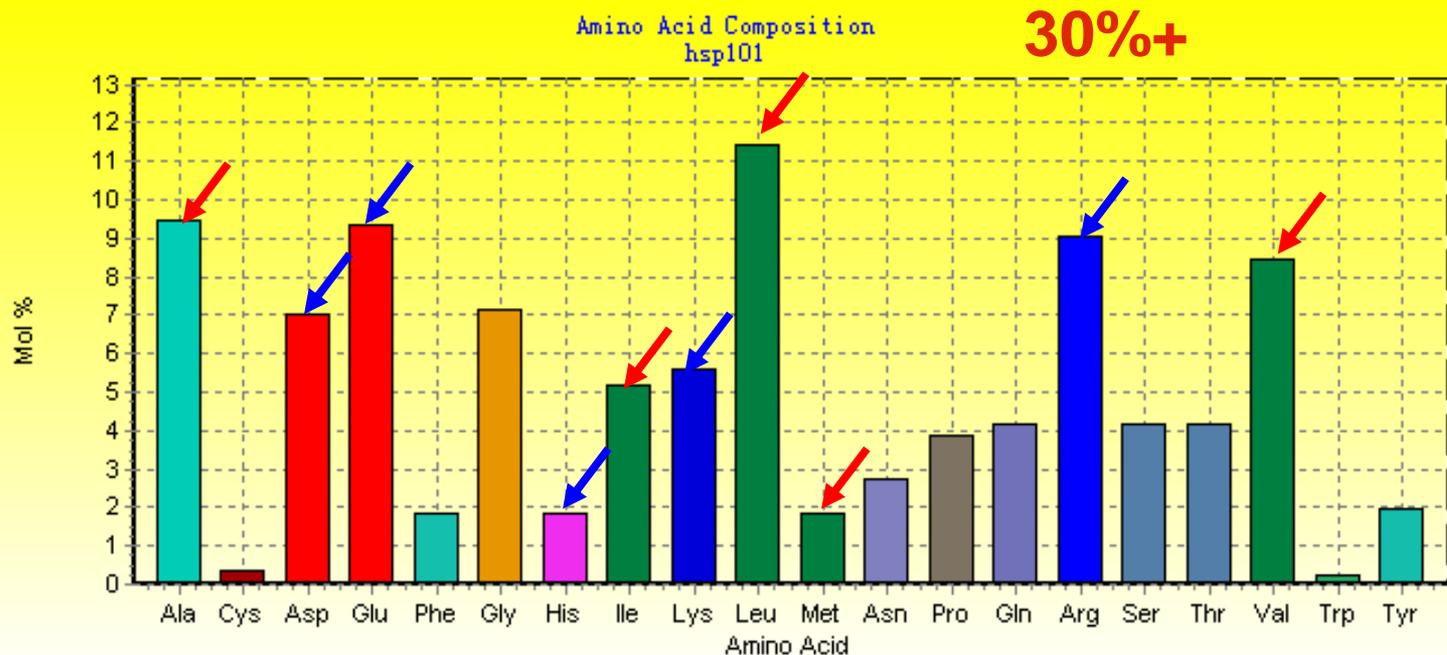
ProtScale疏水性分析
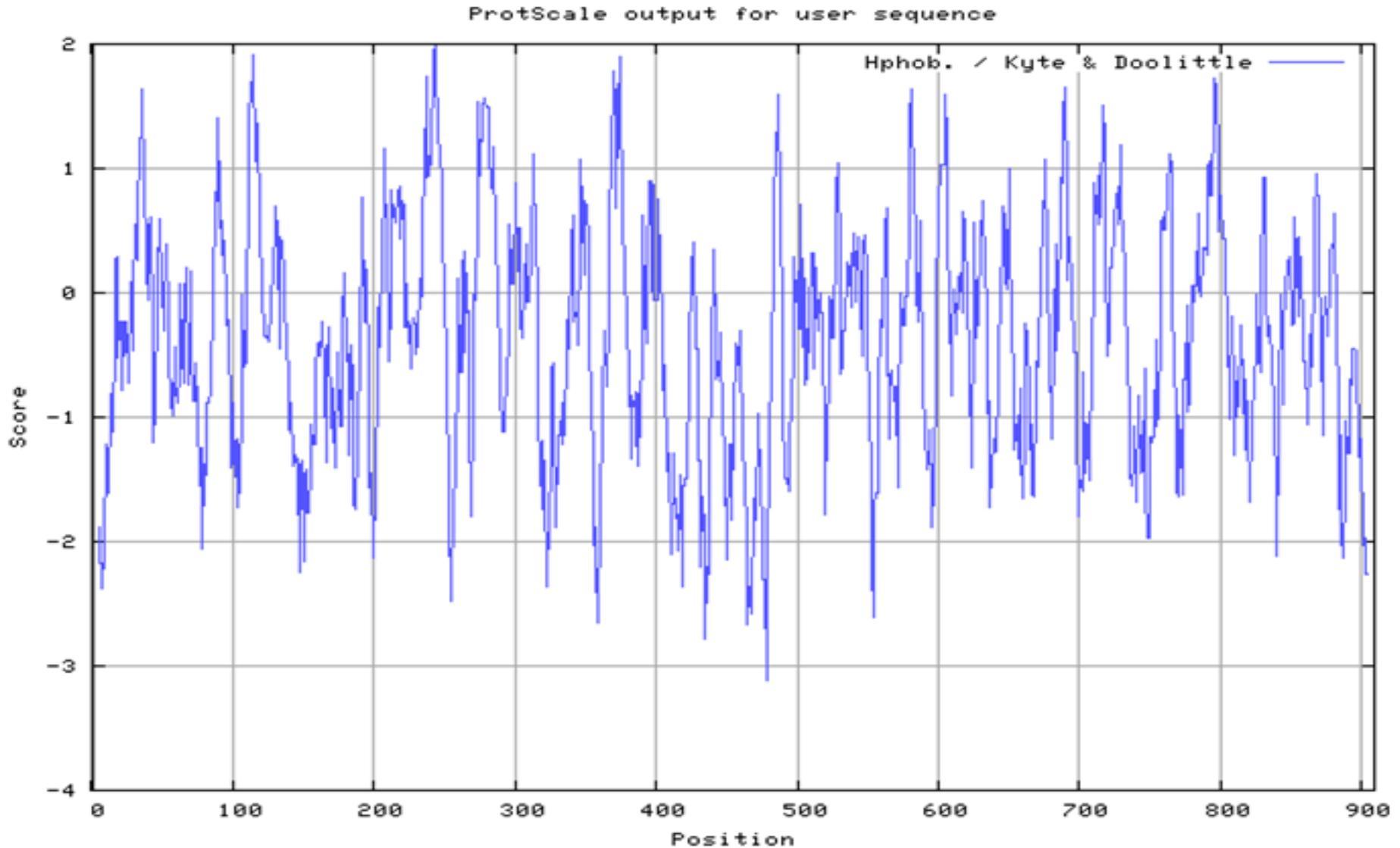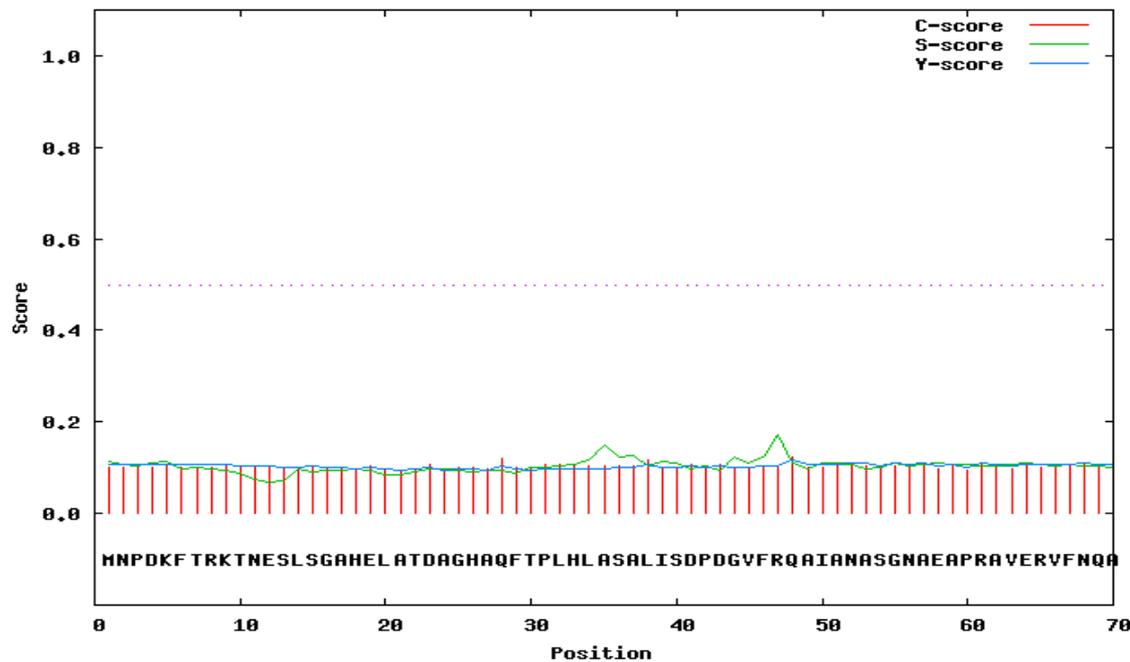
SignalP 4.0 Server

信号肽预测

TMHMM

跨膜预测
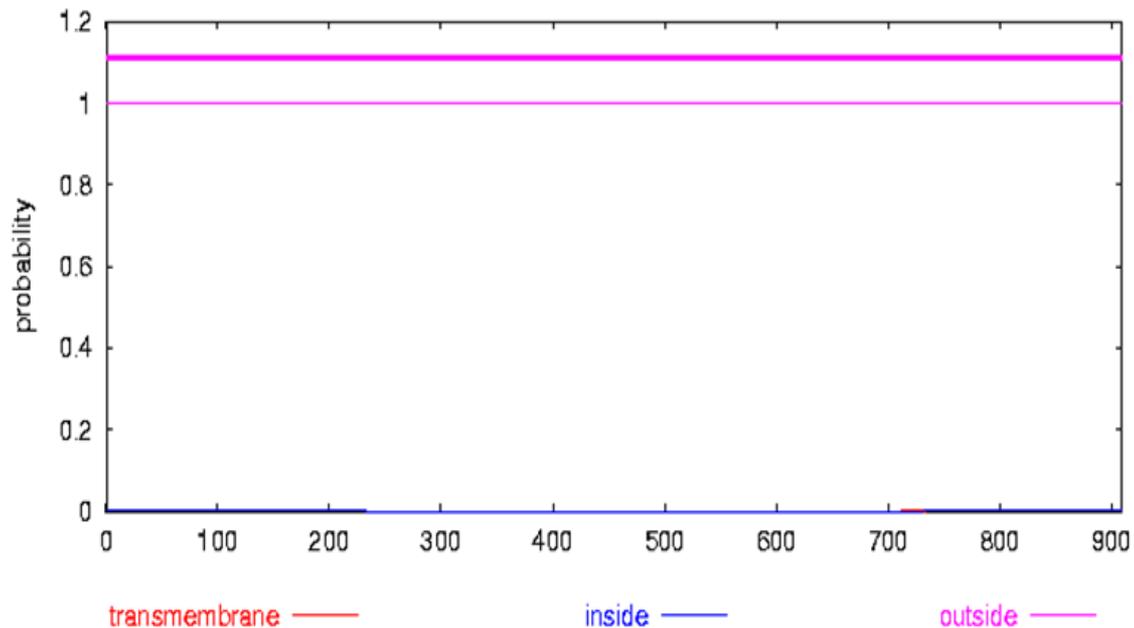
SMART结构域预测

Domains within the query sequence of 909 residues

6个结构域
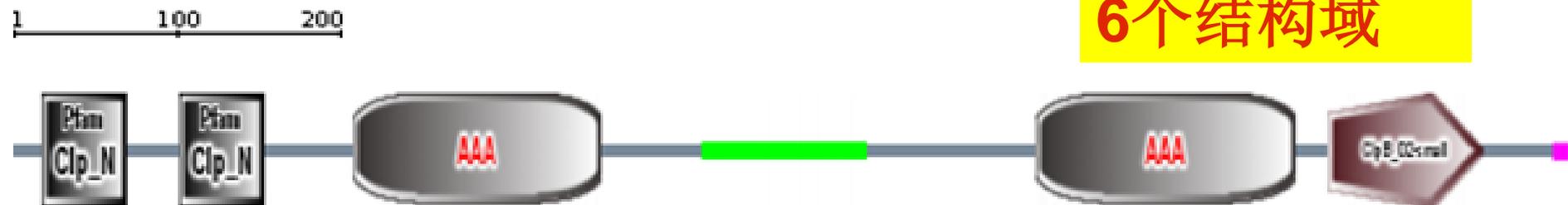
Name	Begin	End	E-value
Pfam:Clp_N	17	67	7.70e-10
Pfam:Clp_N	97	147	1.40e-07
AAA	199	344	2.81e-11
coiled coil	403	500	-
AAA	597	749	4.64e-12
ClpB_D2-small	767	858	3.15e-26
low complexity	899	909	-

与蛋白酶或其他基底结合的结构域

ATP酶结构域，ATP结合与水解

多聚化相关

3D-JIGSAW预测

Hsp101

Domains within the query sequence of 909 residues

Hsp100

Domains within the query sequence of 758 residues
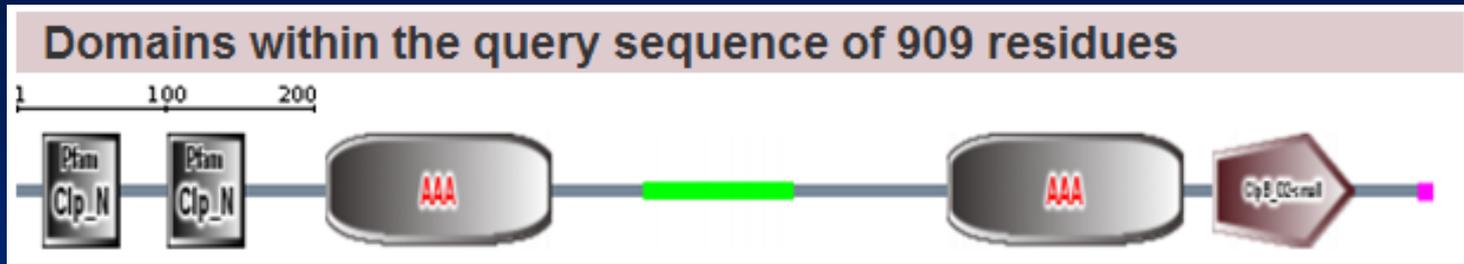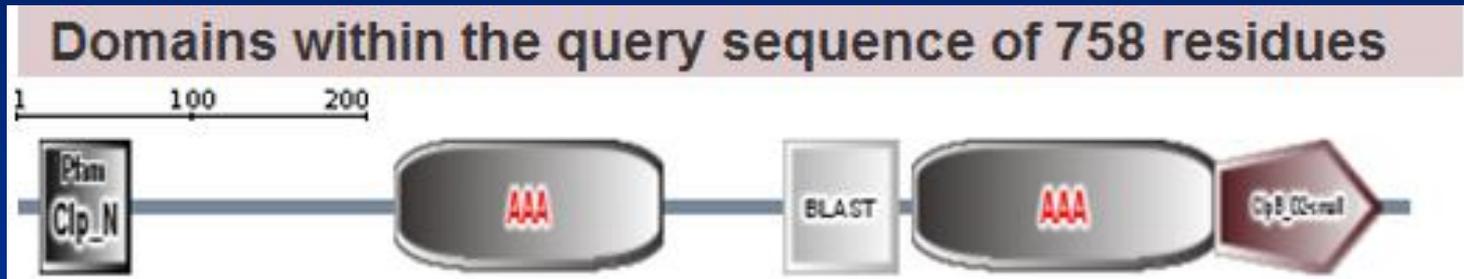
与E. Coli的Hsp100结构极类似（M. Agrawal et al. 2003），其晶体结构以测定，PDB ID为 **1KSF**

问题：结构基本相同，为什么同源模建失败？

3D结构预测

RMS: 10.87

AAA

Clp-N

ClpB-D2
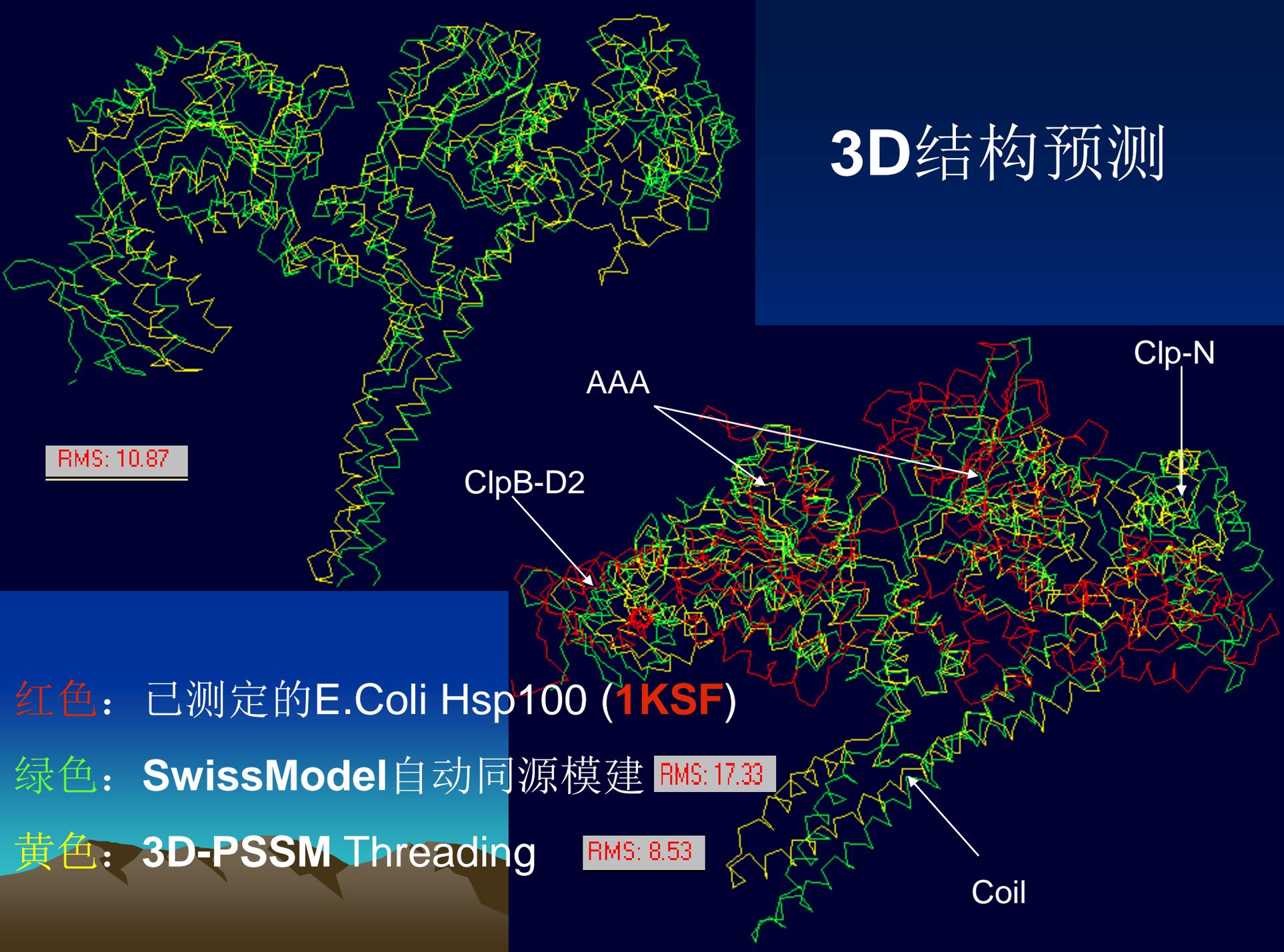
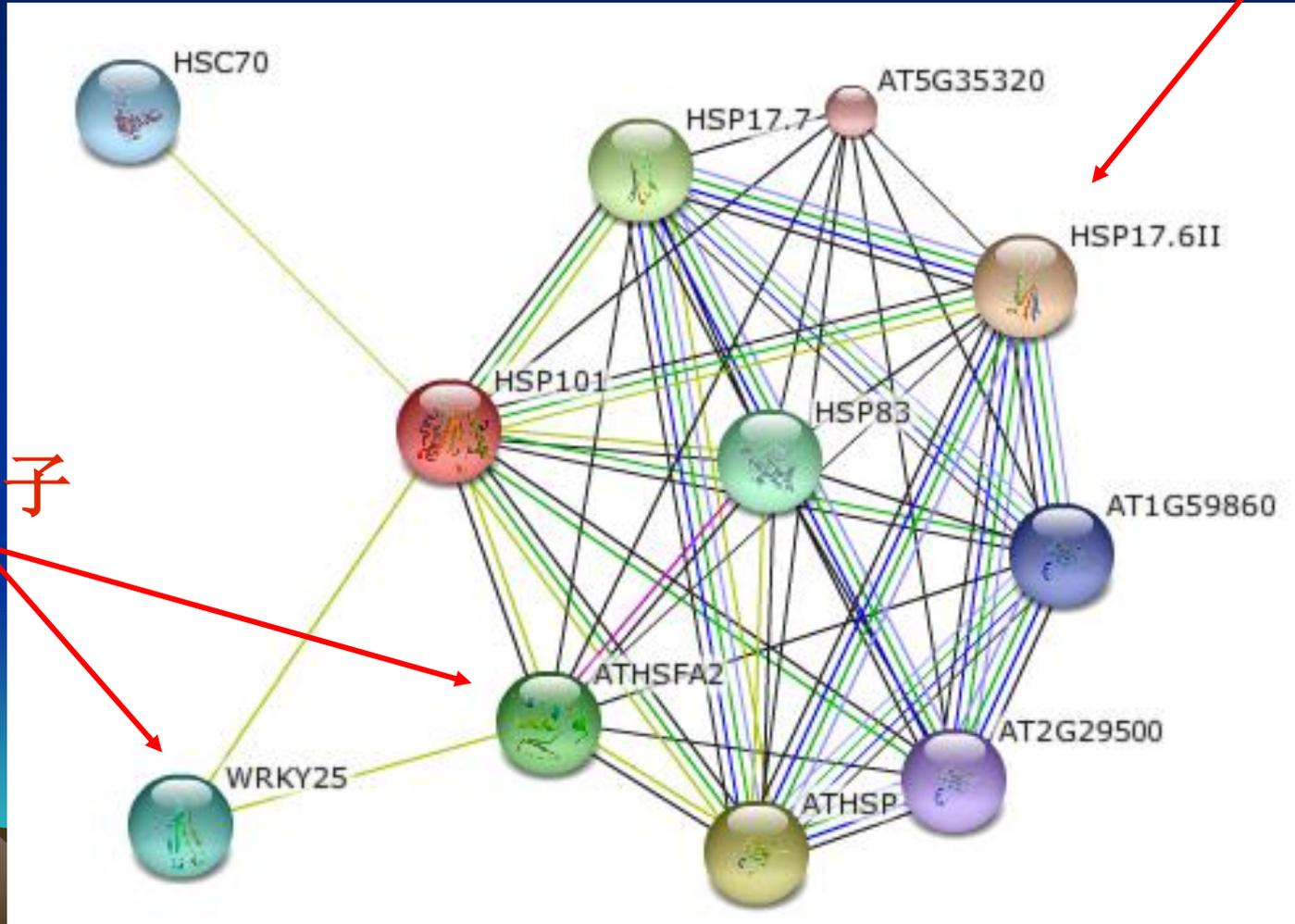红色：已测定的E.Coli Hsp100 (**1KSF**)

绿色：**SwissModel**自动同源模建 RMS: 17.33

黄色：**3D-PSSM** Threading RMS: 8.53

Coil

String蛋白相互作用

A. Thaliana   小热激蛋白家族

转录因子

参考文献

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- M. Agarwal et al. molecular characterization of rice Hsp101

- 陈建南，曲军. 温度，热激蛋白与高粱与性变化

- Guanfeng W. and Xuening W. Molecular analysis of common wheat genes encoding three types of cytosolic heat shock protein 90 (Hsp90): functional involvement of cytosolic Hsp90s in the control of wheat seedling growth and disease resistance

致谢

- 感谢尊敬的罗老师
- 感谢CAAS

谢谢！

请大家批评指正！