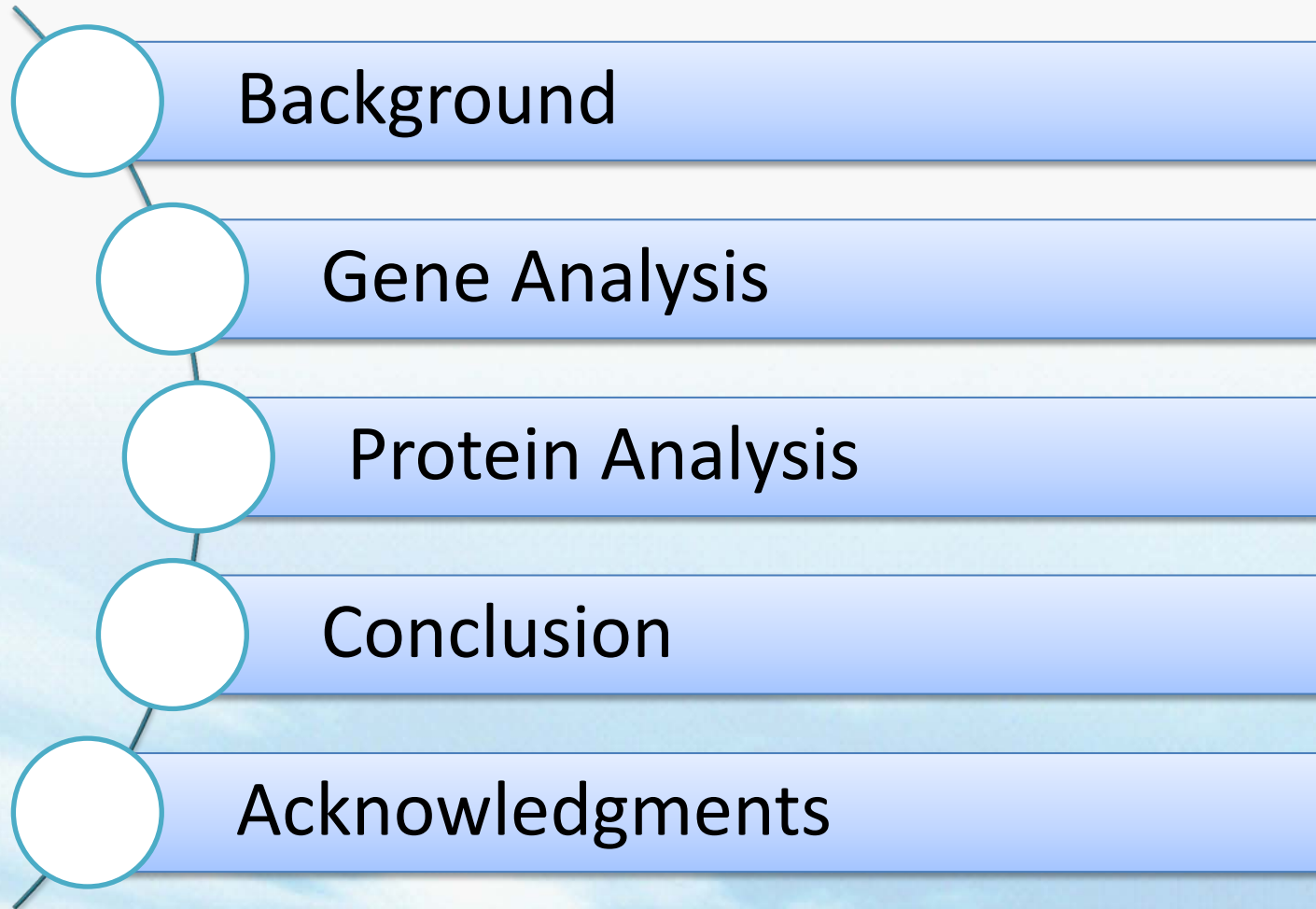


# 小麦中COMT蛋白的结构预测及功能分析

The structural and functional analysis of  
COMT in wheat

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付路平  
张 宁  
报 告 人：方 俐  
2014.01.12

# Outline



# Background

- ◆ 木质素是构成细胞次生壁的成分之一，参与细胞壁木质化
- ◆ 木质素在植物体内含量仅次于纤维素的第二大有机物，也是最大的一类次生物质。
- ◆ 木质素加大了细胞壁的硬度或抗压强度，对植物的抗倒伏、抗病和抗逆性有重要影响。

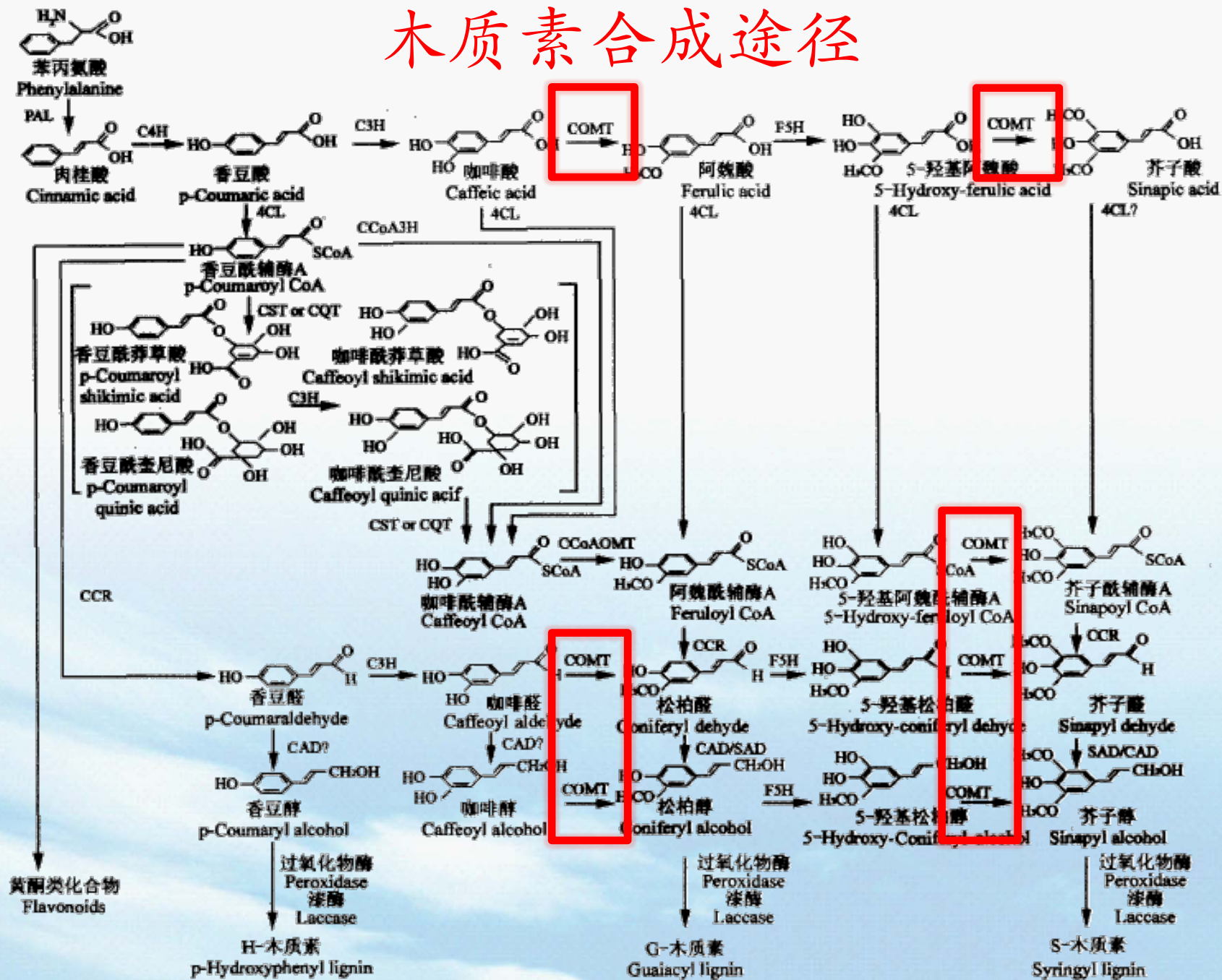
About lignin

# Background

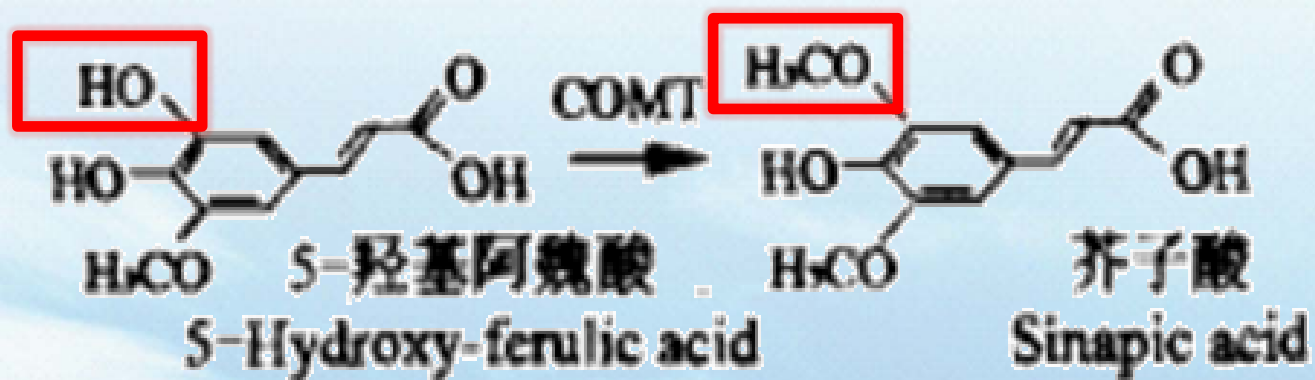
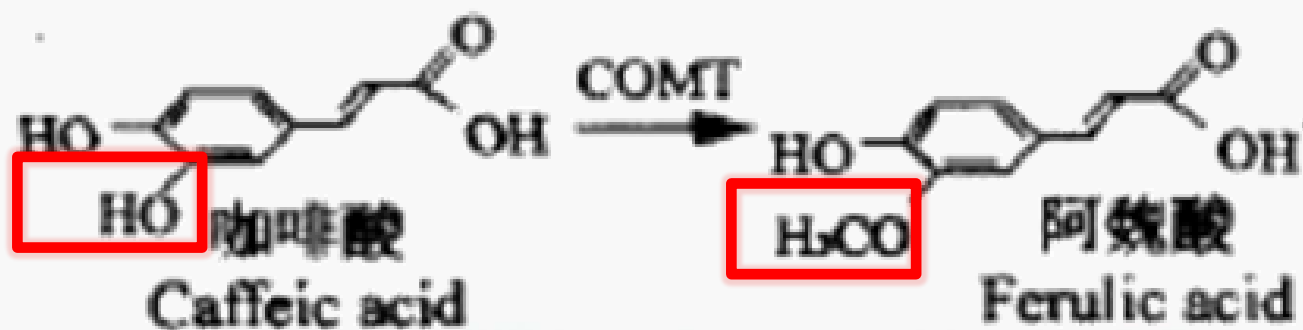
- ◆ 咖啡酸-O-甲基转移酶 (COMT) 是木质素特异的途径中的一个甲基化酶。
- ◆ 不同的甲基转移酶，以S-腺苷蛋氨酸、甜菜碱和二甲基嘧啶作为甲基的供体，把氨基、羟基、巯基甲基化。



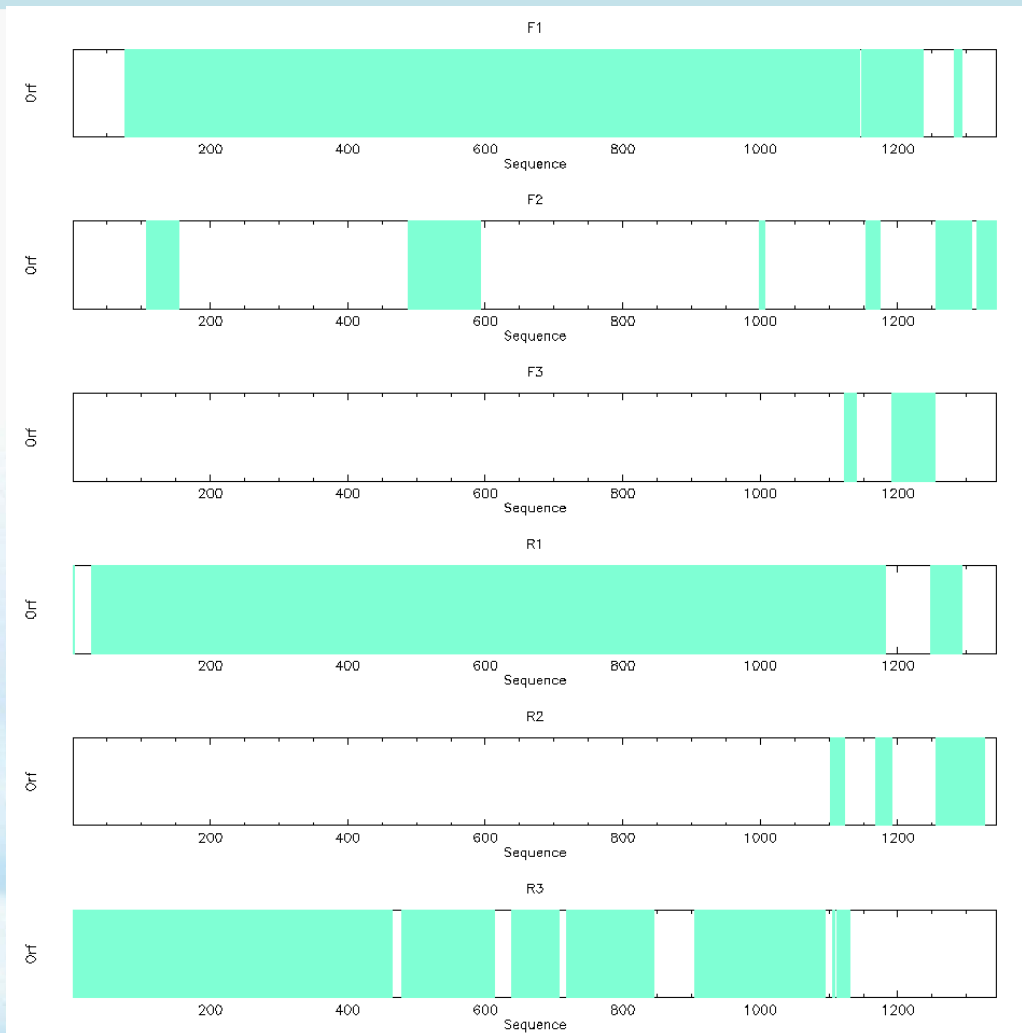
# 木质素合成途径



# Background



# ORF Analysis



# ORF Analysis

>EF413031\_3 [76 - 1143]

MGSIAAGADEDACMYALQLVSSSILPMTLKNAIELGLLETLMAGGKFLTPAEVAAKLPS  
AANPEAPDMVDRMLRLLASYNVVSCRTEEGKDGRLSRRYGAAPVCKYLTPNEDGVSMSAL  
ALMNQDKVLMESWYYLKDAVLDGGIPFNKAYGMSAFEYHGTDPRFNRFNEG MKNHSII I  
TKKLLESYKGFEGGLGTLVDVGGGVGATVAAITAHYPTIKGINFDLPHVISEAPPFPGVTH  
VGGDMFQKVPSADAILMKWILHDWSDEHCATLLKNCYDALPAHGKVVLVECILPVNPEAT  
PKAQGVFHVDMIMLAHNPGGRERYEREF EALAKGAGFAAMKTTYIYANAWAIEFTK



# Phylogenetic Analysis

用于构建系统进化树的序列信息

subject ID	Identity (%)	E-value	bit score	Organism
ABP63535	100	0	738	TaCOMT (ABP63535) 小麦
EMS55685	97.75	0	723	TuOMT (EMS55685) 乌拉尔图小麦
AAK68907	90.08	0	674	FrCOMT (AAK68907) 高羊茅 (Festuca arundinacea)
AAD10255	90.4	0	666	LoCOMT (AAD10255) 黑麦草 (Lolium perenne)
EMT25448	92.78	0	656	AgCOMT (EMT25448) 粗山羊草 (Aegilops tauschii)
ABS18316	87.21	0	638	BaCOMT (ABS18316) 绿竹 (Bambusa oldhamii)
AGS49216	78.89	0	586	ZmCOMT (AGS49216) 玉米 (Zea mays)
AFO69477	78.24	0	580	SbCOMT (AFO69477) 高粱 (Sorghum bicolor)



# Hydrophobicity

Kyte & Doolittle Scale Mean Hydrophobicity Profile  
Scan-window size = 13



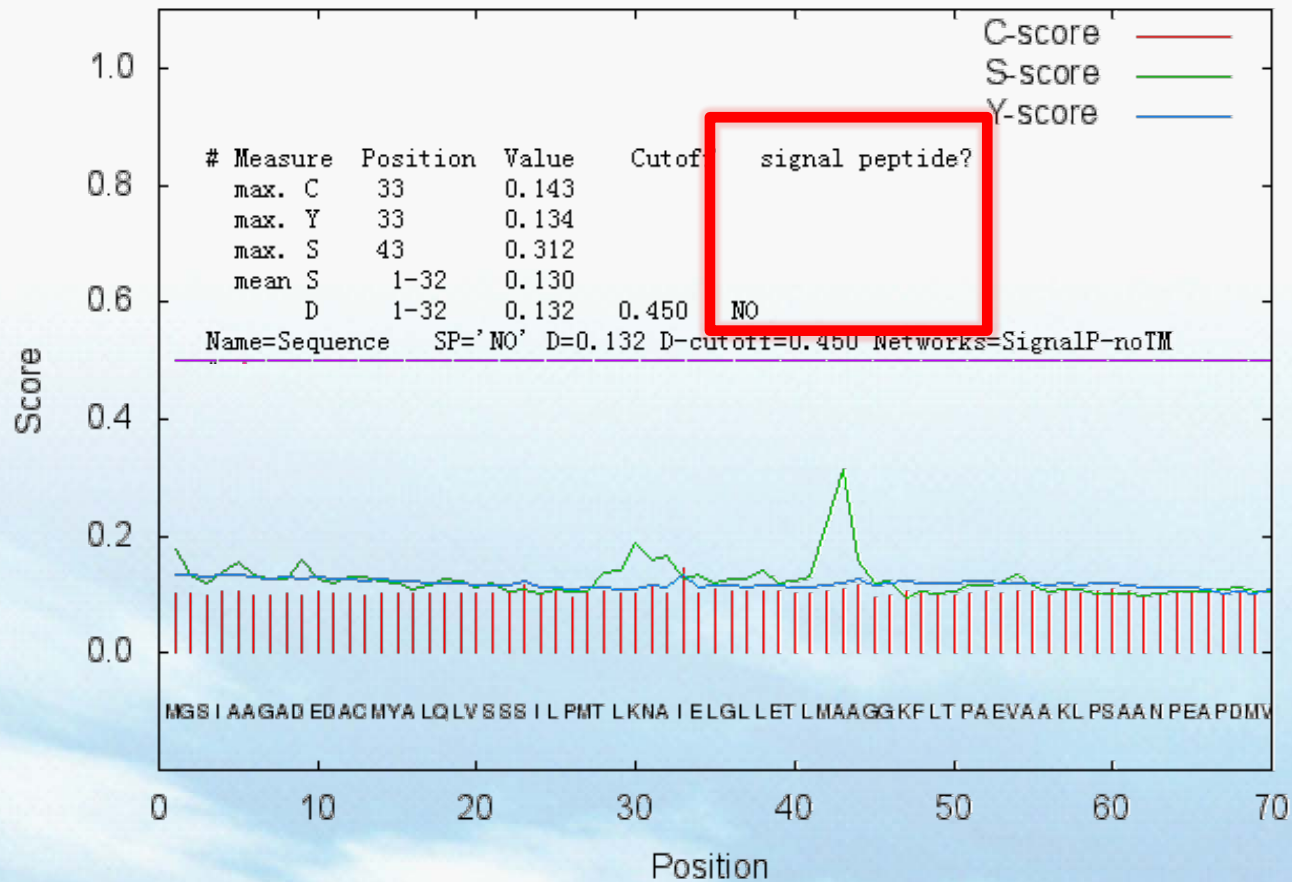
MH < 0: 亲水

MH > 0: 疏水

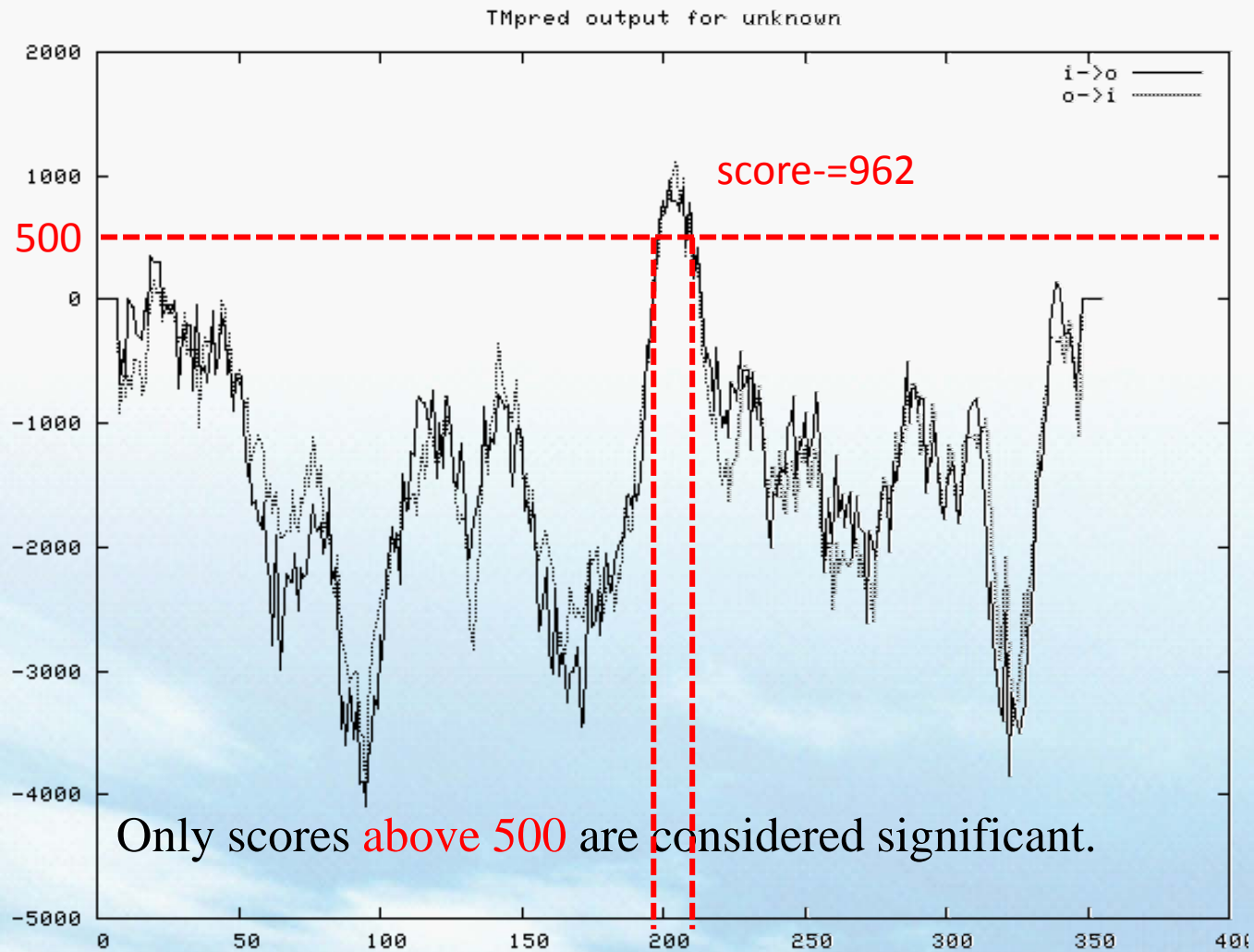


# Signal peptide

SignalP-4.1 prediction (euk networks): Sequence



# TM Regions



区间：193-211

[ch.EMBNef.org](http://ch.EMBNef.org)

[Home](#)

[Services](#)

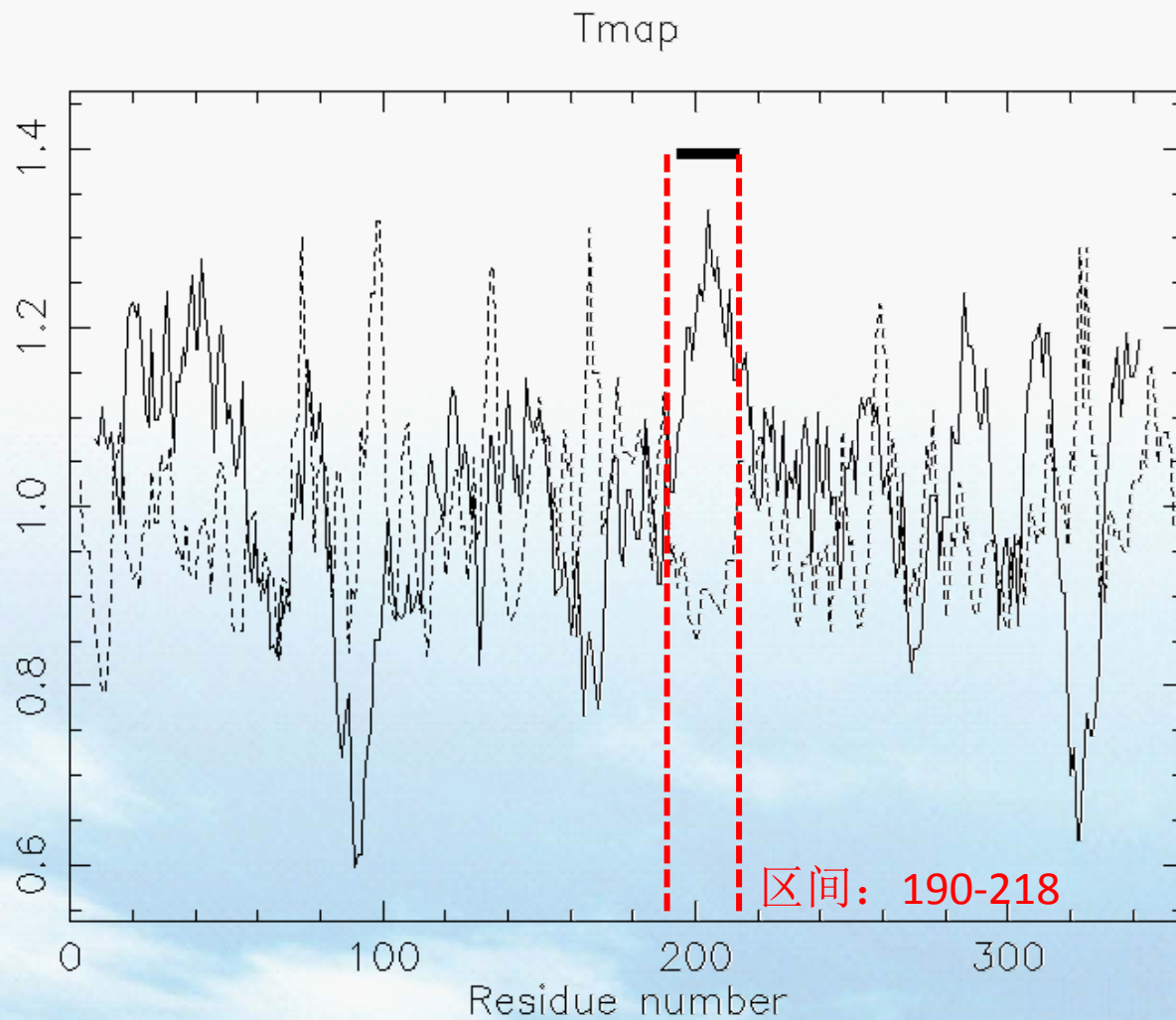
[Courses](#)

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[Contacts](#)

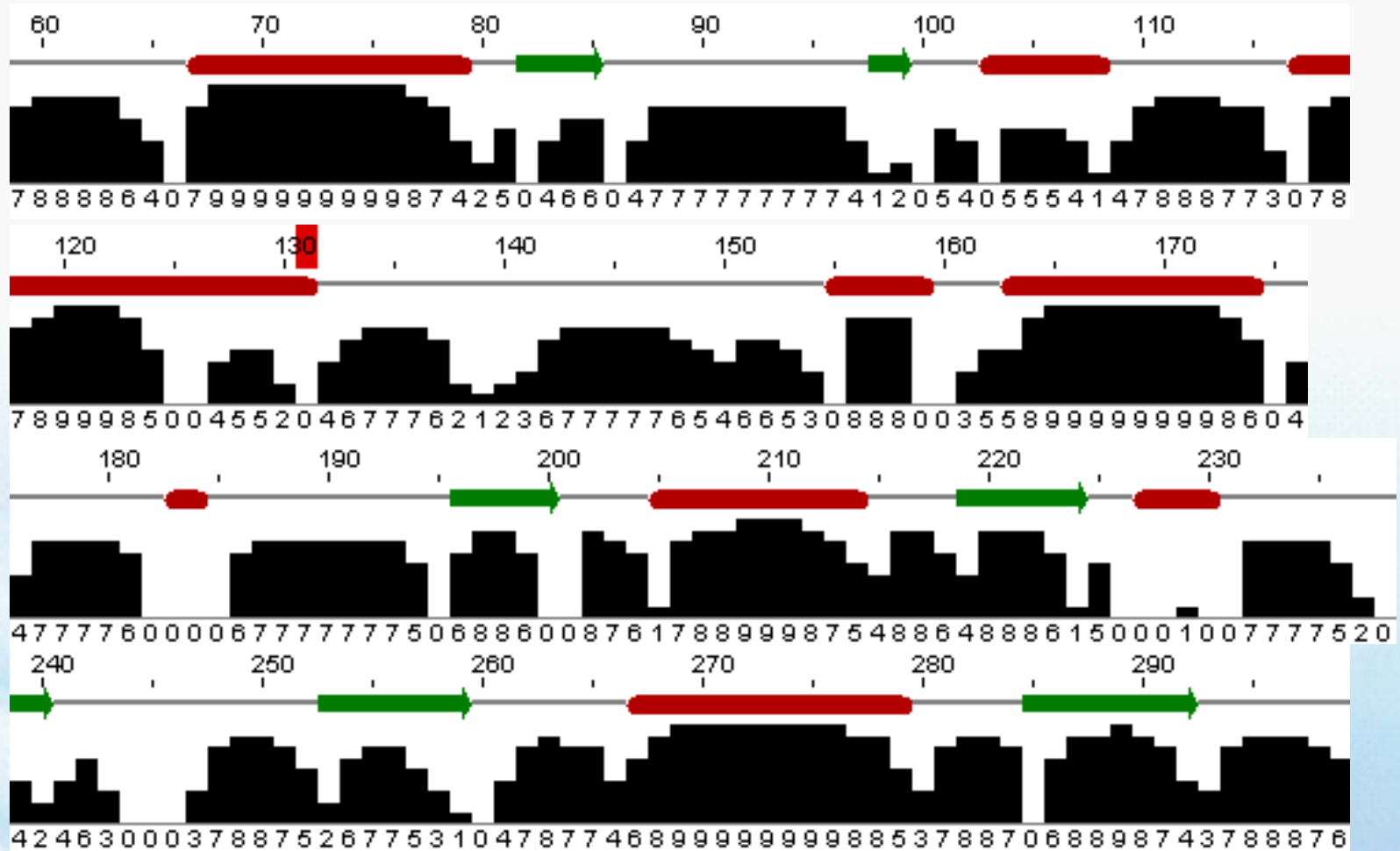
TMpred - Prediction of Transmembrane Regions  
and Orientation

# TM Regions





# Secondary Structure



# Functional sites

Hits for all PROSITE (release 20.98) motifs on sequence sp-Q38J50-FOMT2\_WHEAT :

found: 1 hit in 1 sequence

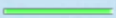
sp-Q38J50-FOMT2\_WHEAT (356 aa)


MGSTAAAGADEDACMYA LQLVSSSILPMTLKNATIELGLLETLM AAGGKFLTPAEVA AKLP SAANPEA  
PDMVDERMLRLLASYNVVS CRTEDGKDGRLSRRYGAAPVCKYLTPNEDGVSMSALALMNQDKVLMES  
WYYLKD AVL DGGIPFNKAYGMSAF EYHGTDPRFN RVFN EG MKNHSIIITKKLLESYKGF EGLGTLV  
DVGGGVGATVAAITAHYPTIKGINF DLPHVISEAPFPFGVTHVGGDMFQKVPSGDAILMKWILHDW  
SDEHCATLLKNCYDALPAHGKVVLVECILPVNPEATPKAQGVFHVDMIMLAHNPGGREYEREFEA  
LAKGAGFAAMKTTYIYANAWAIEFTK

Legend:

  
disulfide bridge

  
active site

  
other 'ranges'

  
other sites



Expasy  
Bioinformatics F



# Functional sites

17 - 356: score = 72.612

LQLVSSSILPMTLKNALIELGLLETLMAagGKFLTPAEVAAKLPsaanpEAPDMVDRMLRL  
LASYNVVSCTEDgkdgrLSRRYGAAPVCKYLTPNEDGVsMSALALMNQDKVLMESWYYL  
KDAVLGGGIP-FNKAYGMSAFEYHGTDPFRFNRVFNEMGMKNHSIIITKKLLESYKGFEGLG  
TLVDVGGGVGATVAAITAHYPTIKGINFDLPHVISEA---PPFPGVTHVGGDMFQKVPSP  
DAILMKHLLHDSDEHCATLLKNCYDALPAHGKVVLVCEILPVNPEATPKaaggVFHVDMI  
MLAhnPGGRERYEREFEALAKGAGFAAMKTTYIYANAWALEFTK

## Predicted features:

BINDING	224	S-adenosyl-L-methionine (By similarity)	[condition: [DE]]
ACT_SITE	262	Proton acceptor (By similarity)	[condition: H]

## Absent features:

BINDING	162	S-adenosyl-L-methionine (By similarity)	[condition not true: Y]	
BINDING	177	S-adenosyl-L-methionine (By similarity)	[condition not true: W]	
REGION	243	245	S-adenosyl-L-methionine binding (By similarity)	[condition not true: G-D-F]
BINDING	259	S-adenosyl-L-methionine (By similarity)	[condition not true: [KR]]	

# Function domains



# Function domains



## Significant Pfam-A Matches

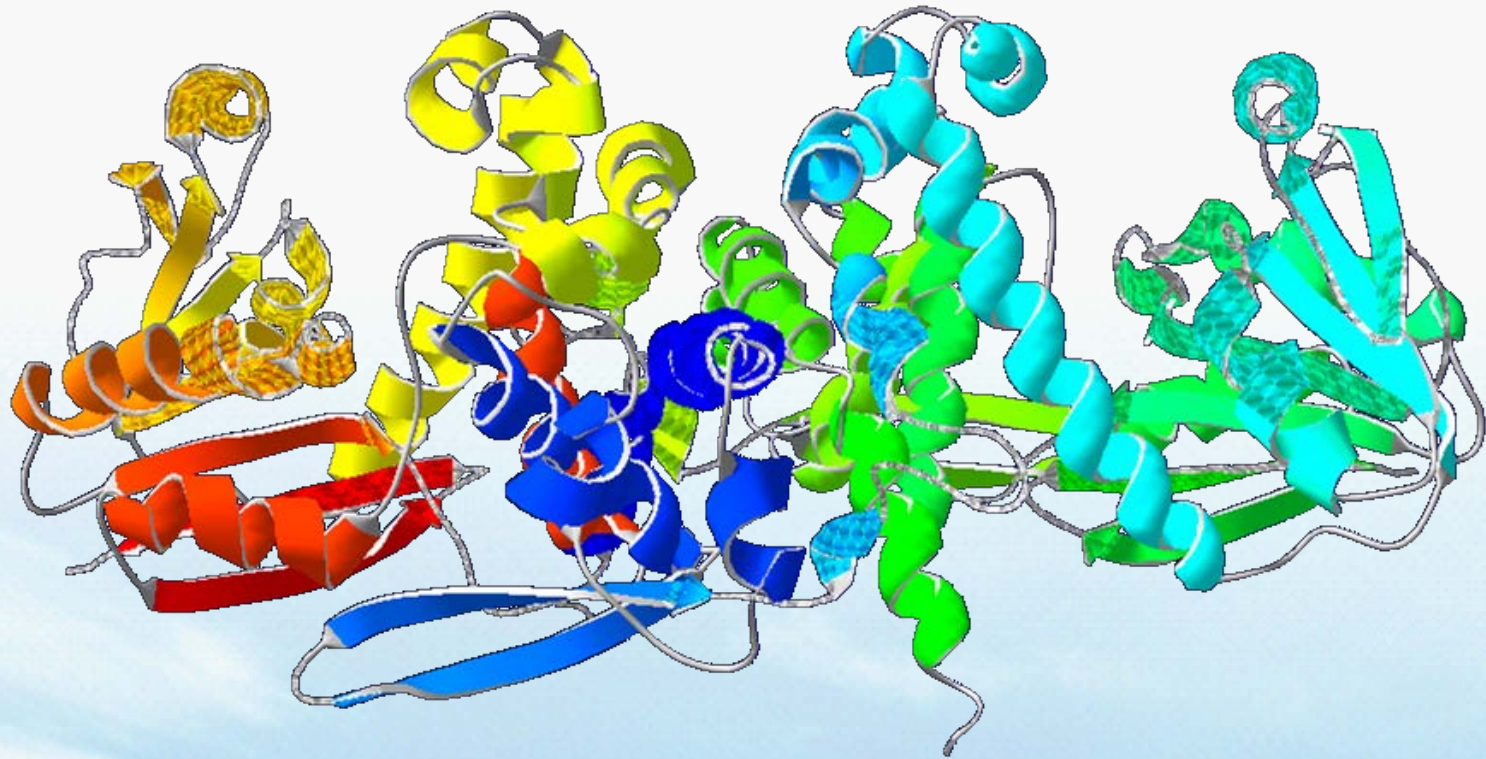
[Show](#) or [hide](#) all alignments.

Family	Description	Entry type	Clan	Envelope		Alignment		HMM		HMM length	Bit score	E-value	Predicted active sites	Show/hide alignment
				Start	End	Start	End	From	To					
<a href="#">Dimerisation</a>	Dimerisation domain	Domain	<a href="#">CL0123</a>	27	78	27	78	1	51	51	77.4	5.1e-22	n/a	<a href="#">Show</a>
<a href="#">Methyltransf_2</a>	O-methyltransferase	Family	<a href="#">CL0063</a>	88	333	97	333	5	242	242	328.8	1.5e-98	262	<a href="#">Show</a>





# 3D Structure

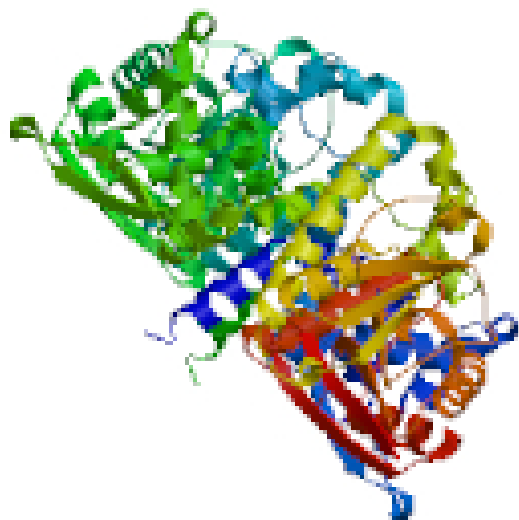


SWISS-MODEL

# 3D Structure

## Model Information

### Model Summary ?



#### Model information:

Modelled residue range: 5 to 356  
Based on template: [3p9cA] (1.80 Å)  
Sequence Identity [%]: 90.06  
Evalue: 0.00e-1

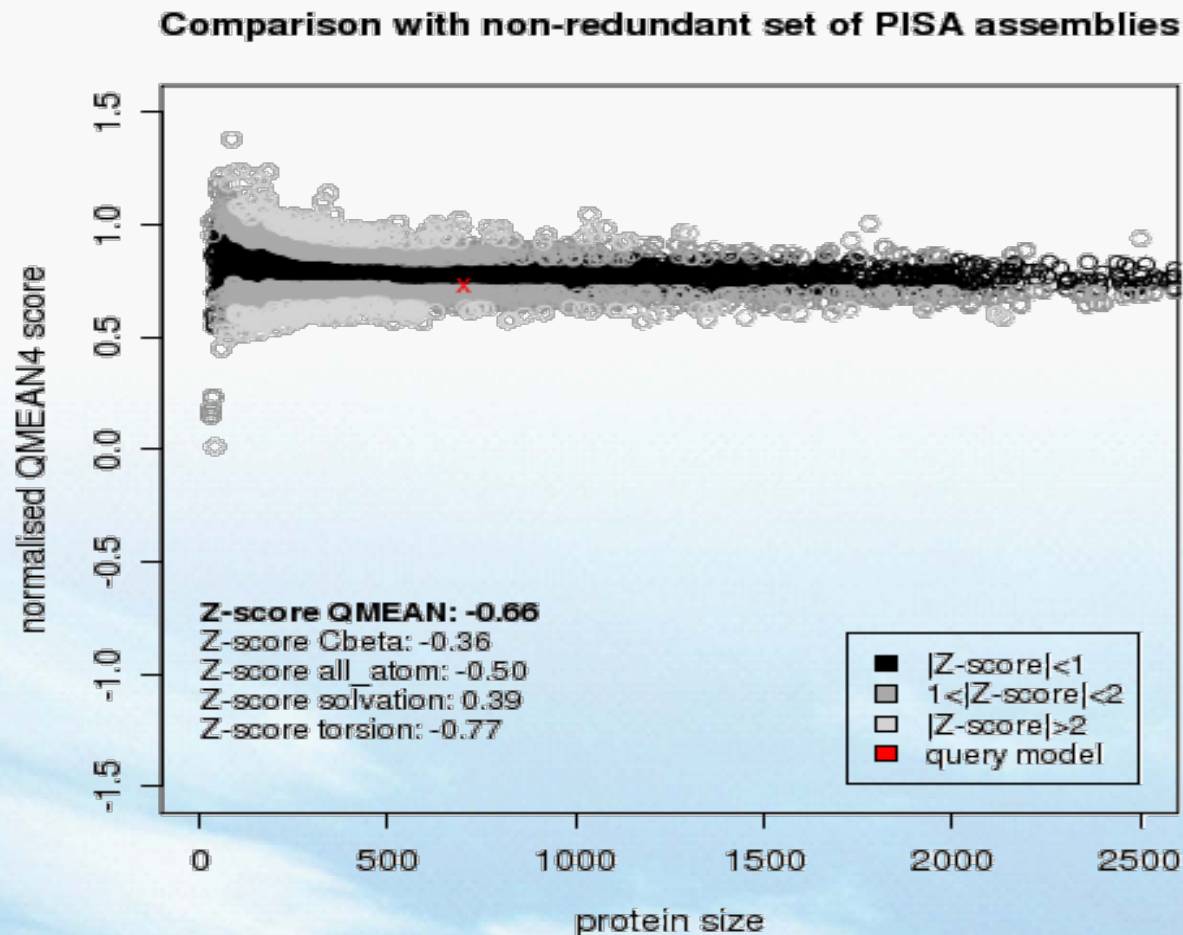
#### Quality information:

QMEAN Z-Score: -0.66

[details] ▾



# 3D Structure

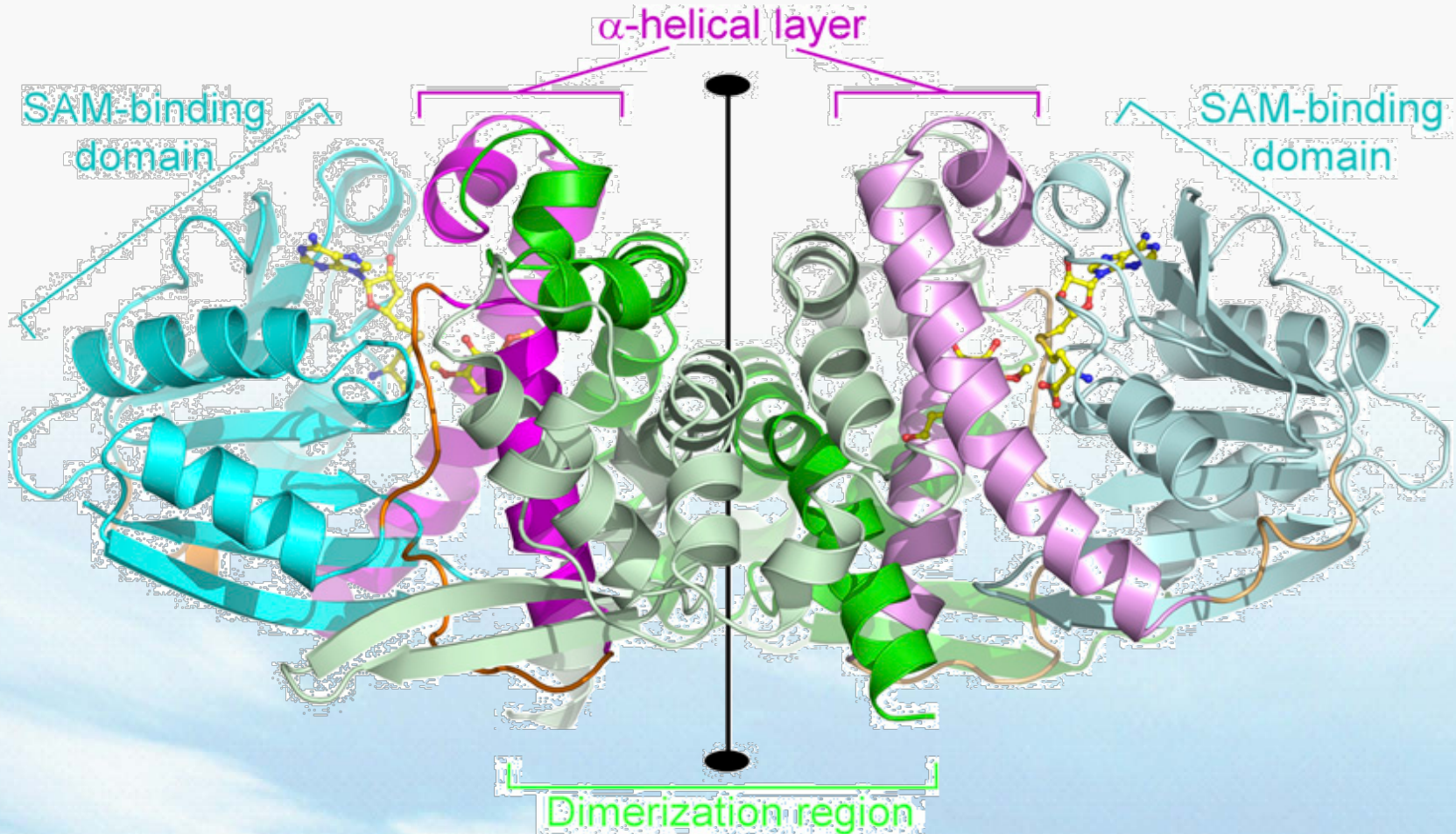


高分辨率的模型  
Z-score为0。

目标蛋白各项  
Z-score都接近  
于0，说明此模  
型比较可靠。

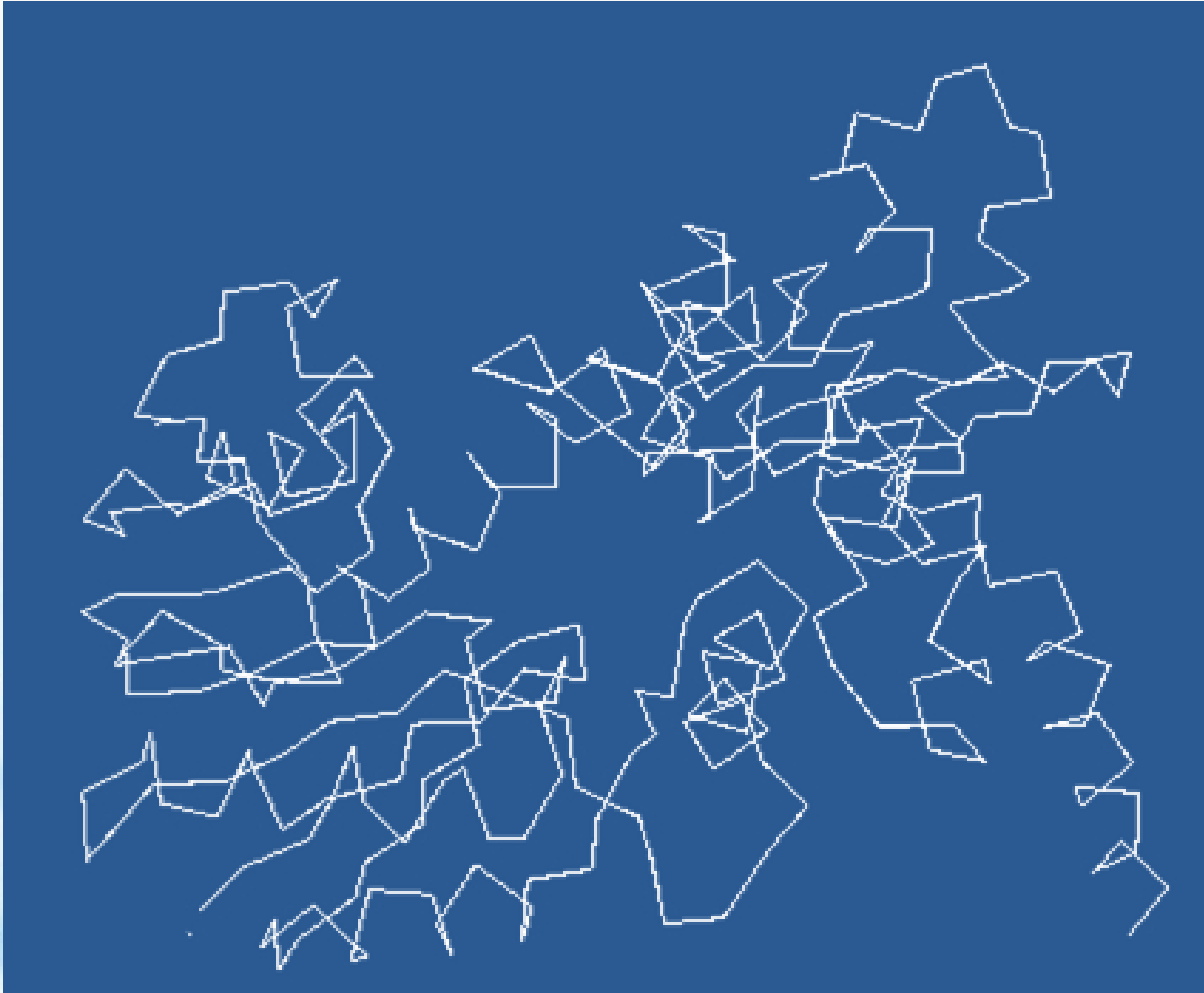


# COMT Structure



Structure-Function Analyses of a Caffeic Acid O-Methyltransferase from Perennial Ryegrass Reveal the Molecular Basis for Substrate Preference

# Protein Analysis

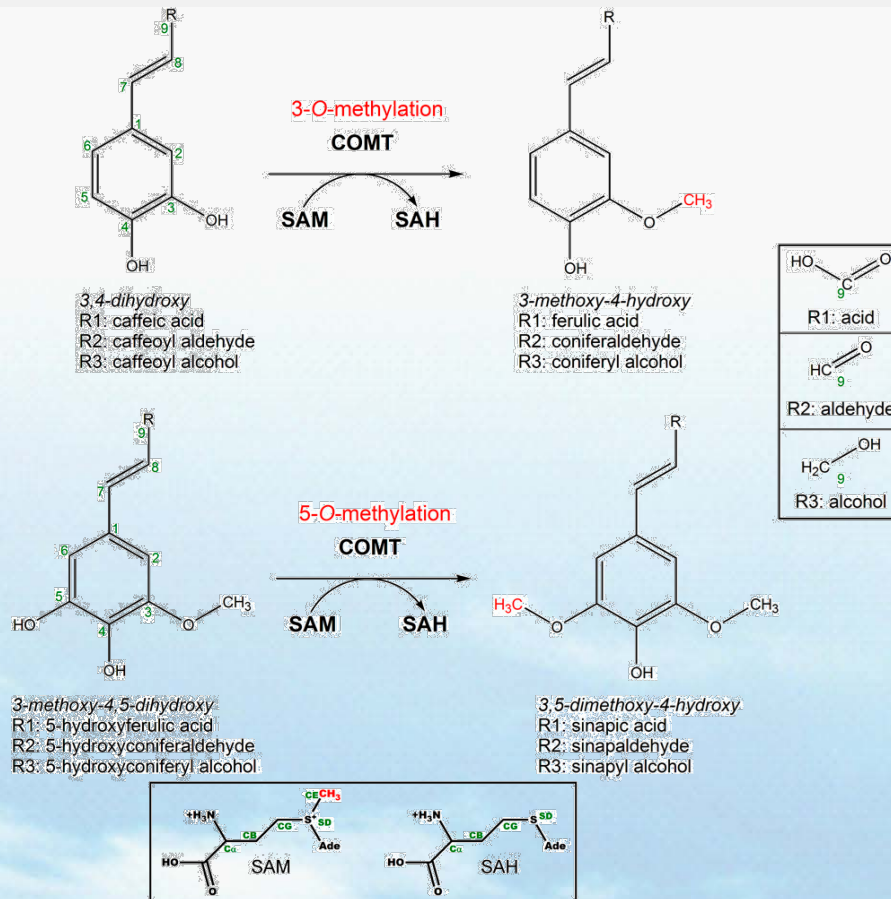


RSMD值为  
0.02,说明目  
标蛋白与模  
板结构高度  
相似



# Protein Analysis

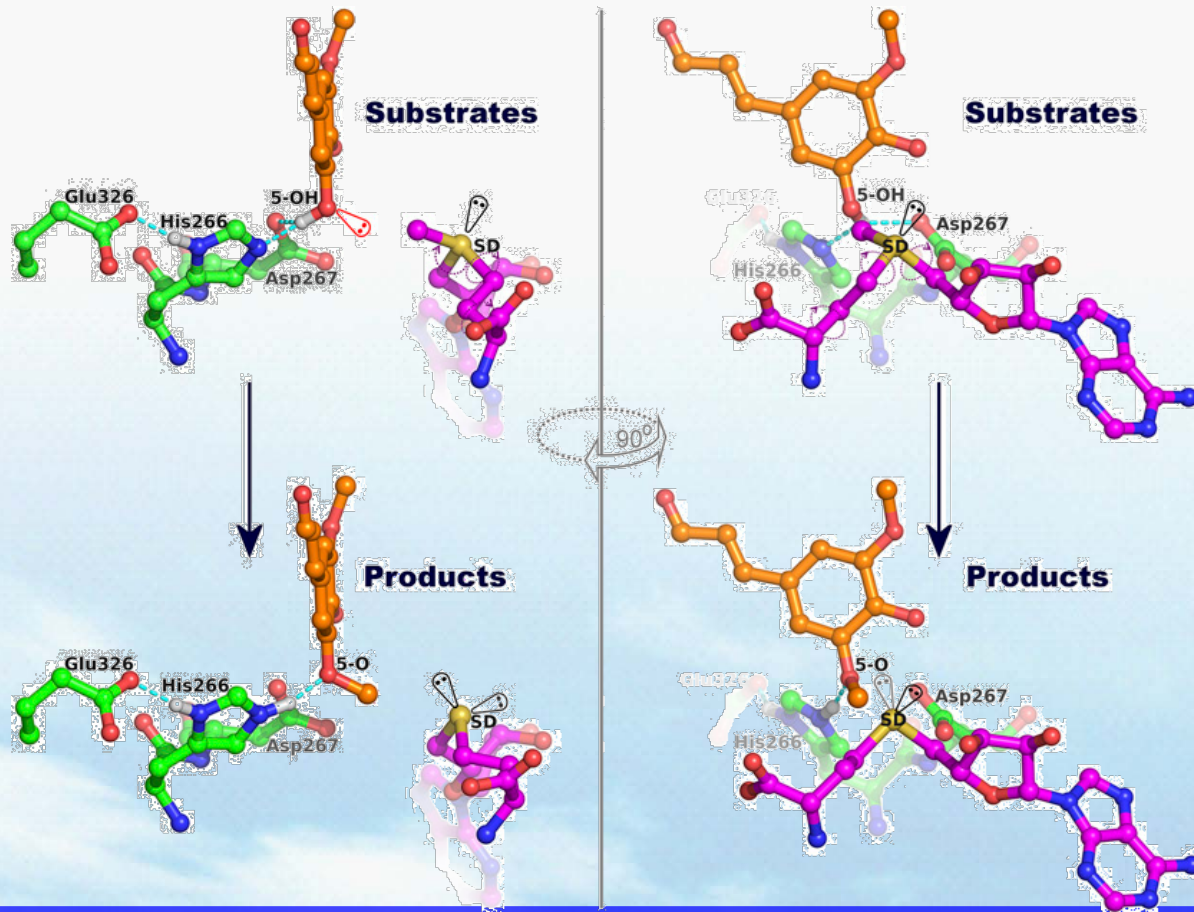
## COMT基因催化的甲基化过程



Structure-Function Analyses of a Caffeic Acid O-Methyltransferase from Perennial Ryegrass Reveal the Molecular Basis for Substrate Preference

# Protein Analysis

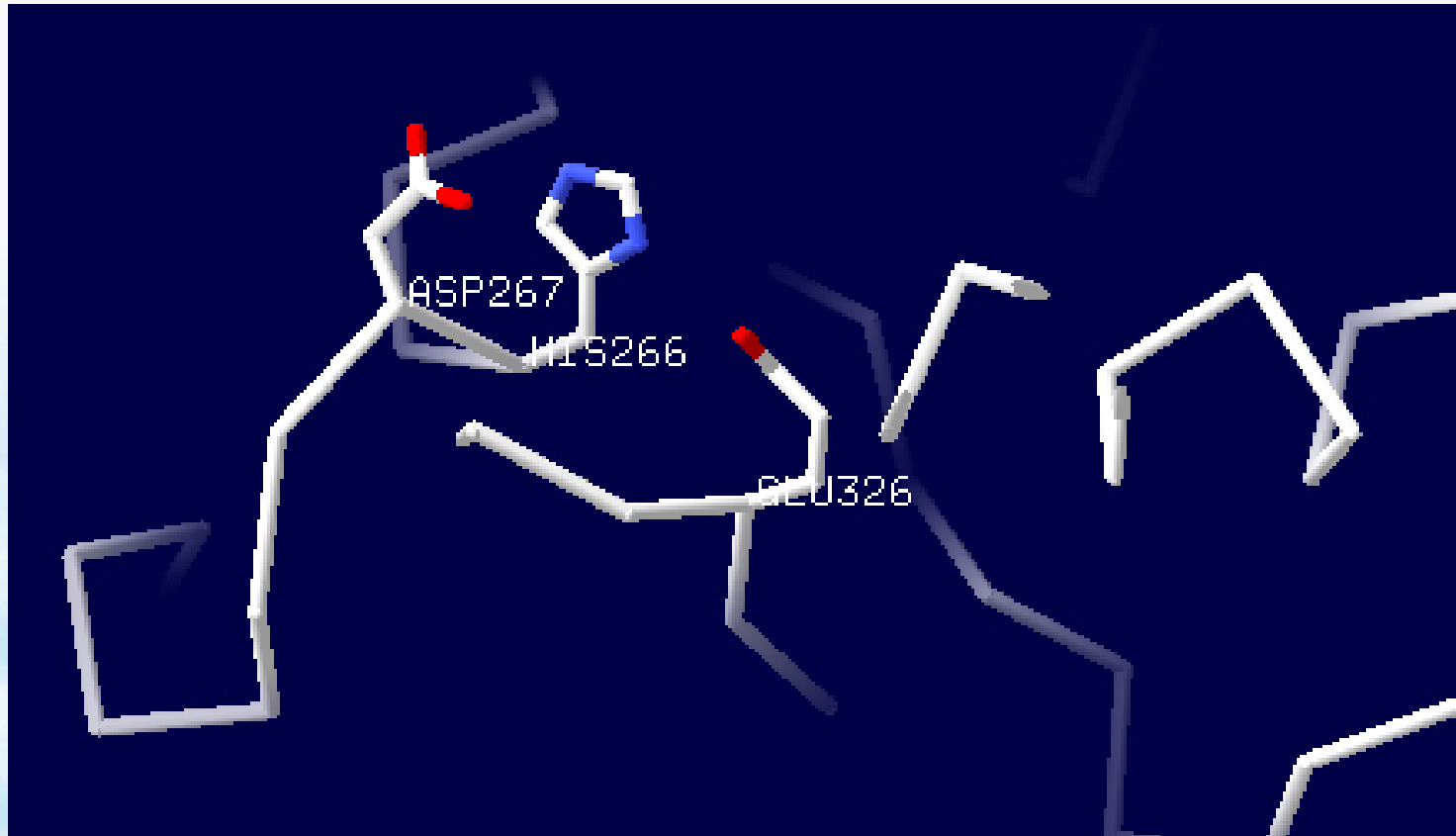
## 黑麦草COMT (3P9C) 催化机制



Structure-Function Analyses of a Caffeic Acid O-Methyltransferase from Perennial Ryegrass Reveal the Molecular Basis for Substrate Preference

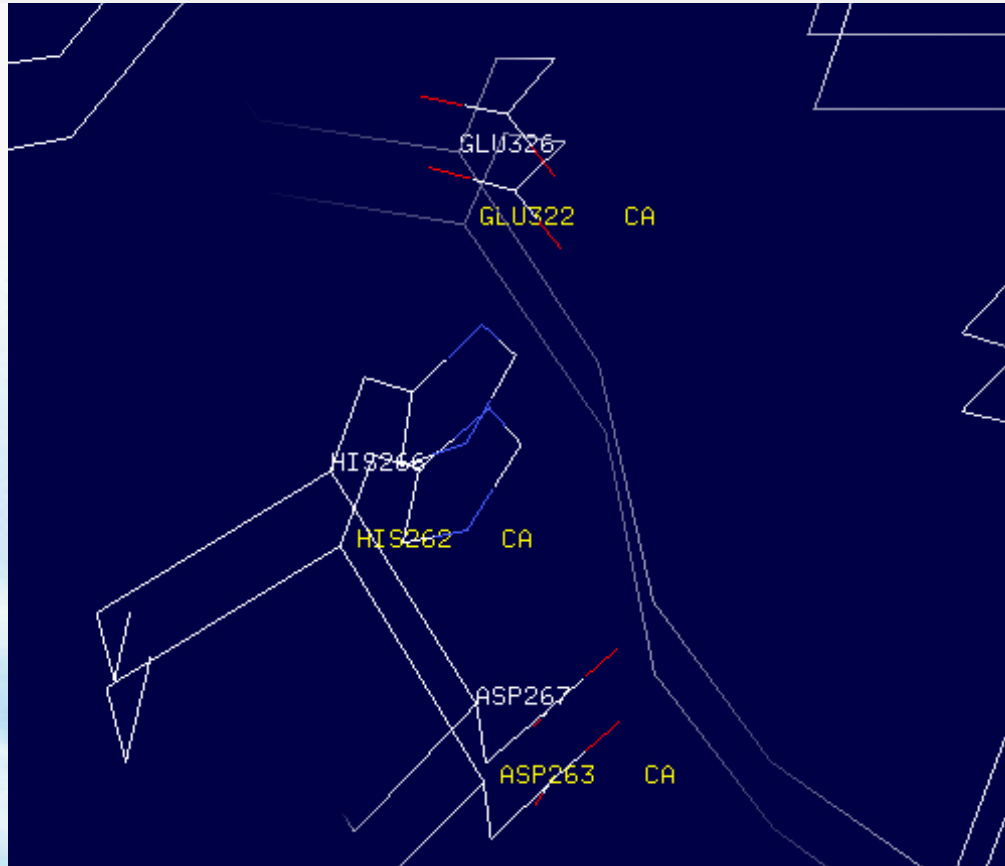
# Protein Analysis

黑麦草COMT蛋白催化活性中心 (S-PdbViewer)



# Protein Analysis

## 目标蛋白与模板活性中心对比



# Conclusion

- ◆通过基因序列分析得到其编码阅读框，并翻译得到蛋白序列；
- ◆通过蛋白基本理化性质、亲疏水性、信号肽、跨膜区等的分析，初步了解该酶的基本特征；
- ◆通过对该酶二级结构、结构域预测、活性位点的分析了解其催化机制；
- ◆通过同源模建，得到与目的蛋白结构十分相似的黑麦草COMT，根据黑麦草COMT的研究进展辅导该酶研究，指导生物学实验。



# Acknowledge

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衷心感谢罗老师一学期以来的耐心指导！

祝愿罗老师身体健康，工作愉快！

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Thanks for  
Your Attention

