# 茶尺蠖信息素结合蛋白PBP4功能探究和结构预测

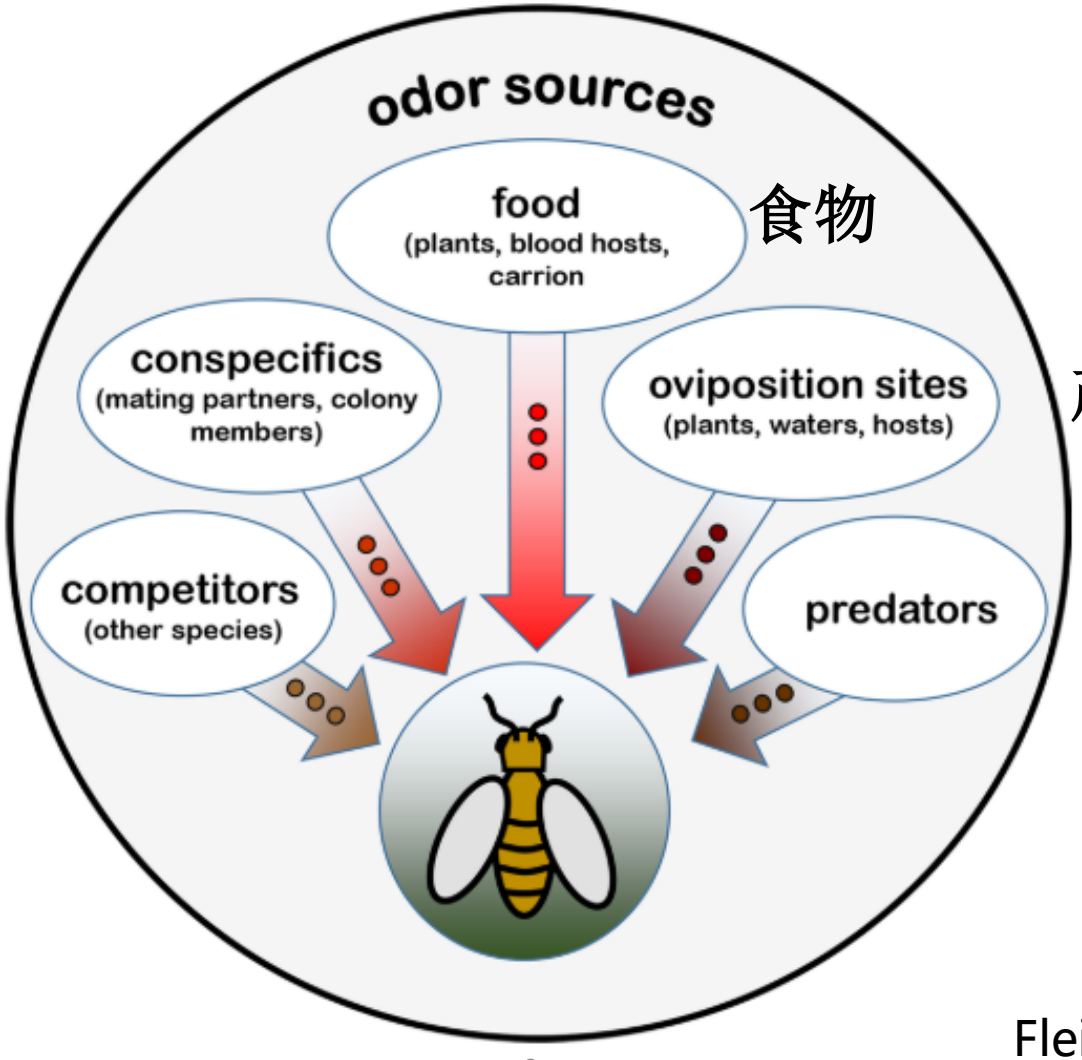
Functional Analysis and Structure Prediction of Pheromone Binding Protein Four in the *Ectropis Obliqua*

汇报人：杨奉水
小组成员：刘毓婕、杨奉水、张政、刘浩然

# Background

同种昆虫

竞争者




食物

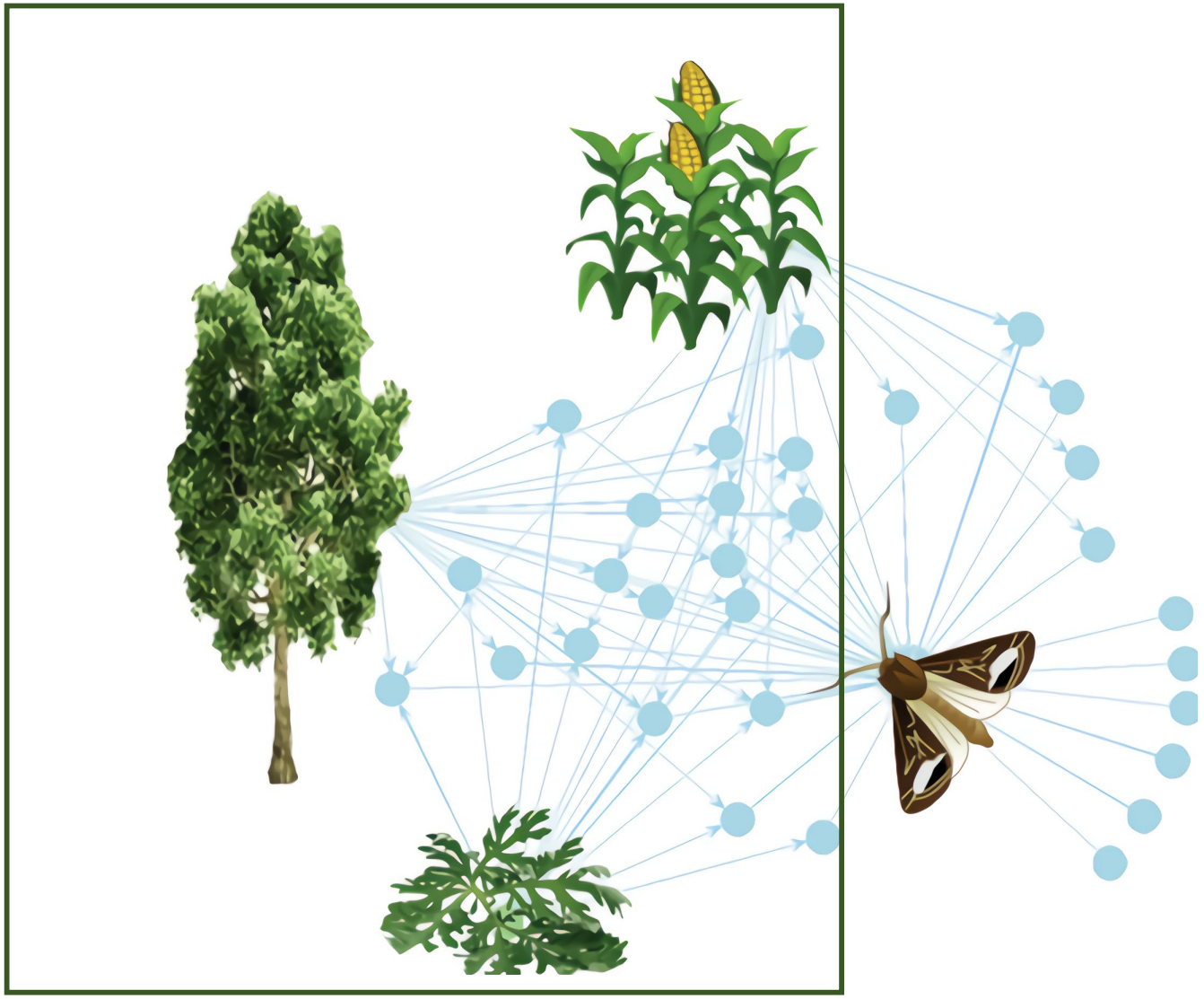
产卵地点

捕食者

Fleischer, J. *Cellular and molecular life sciences* (2018).

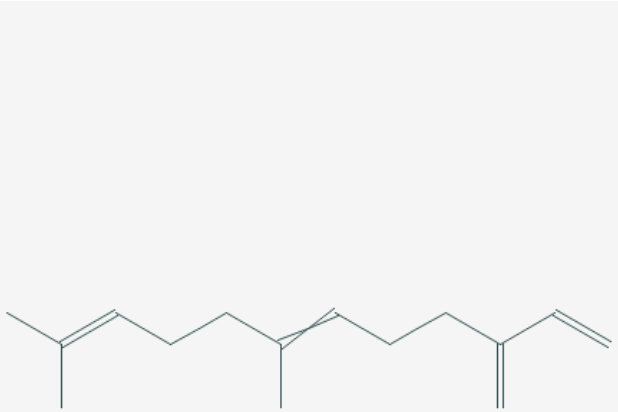
萜类
醇类
酚类
酮类
芳香性物质等

释放

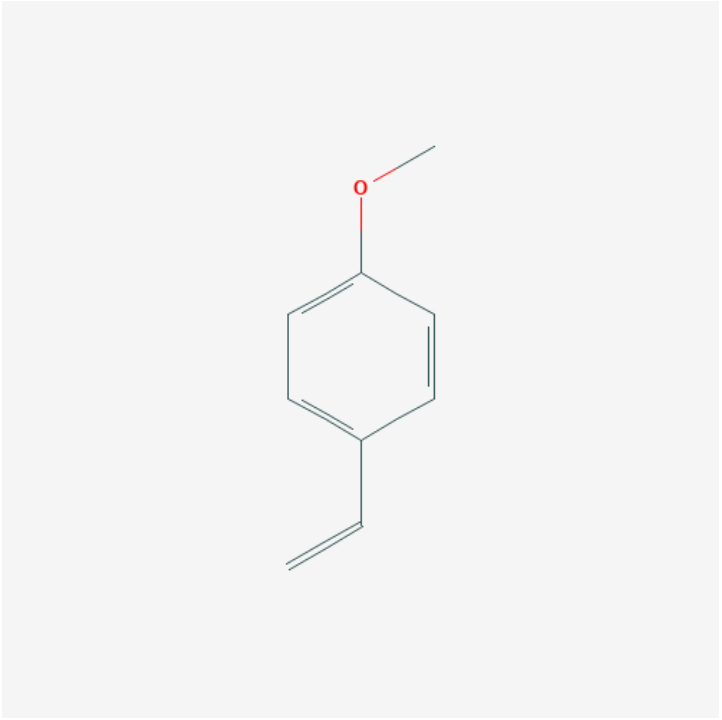


Conchou, L. *et al. Frontiers in physiology* (2019).

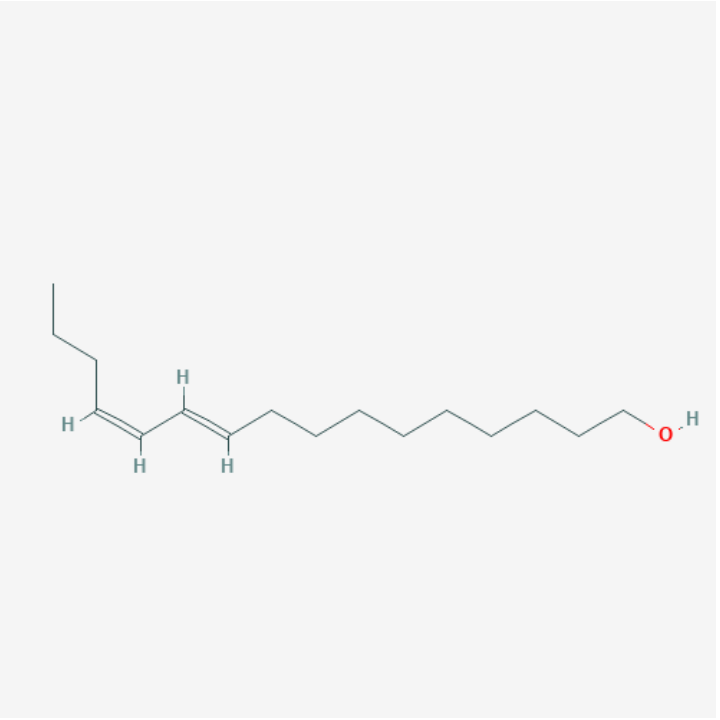
(E)-β-Farnesene
E-β-法呢烯



4-Vinylanisole
4-甲氧基苯乙烯

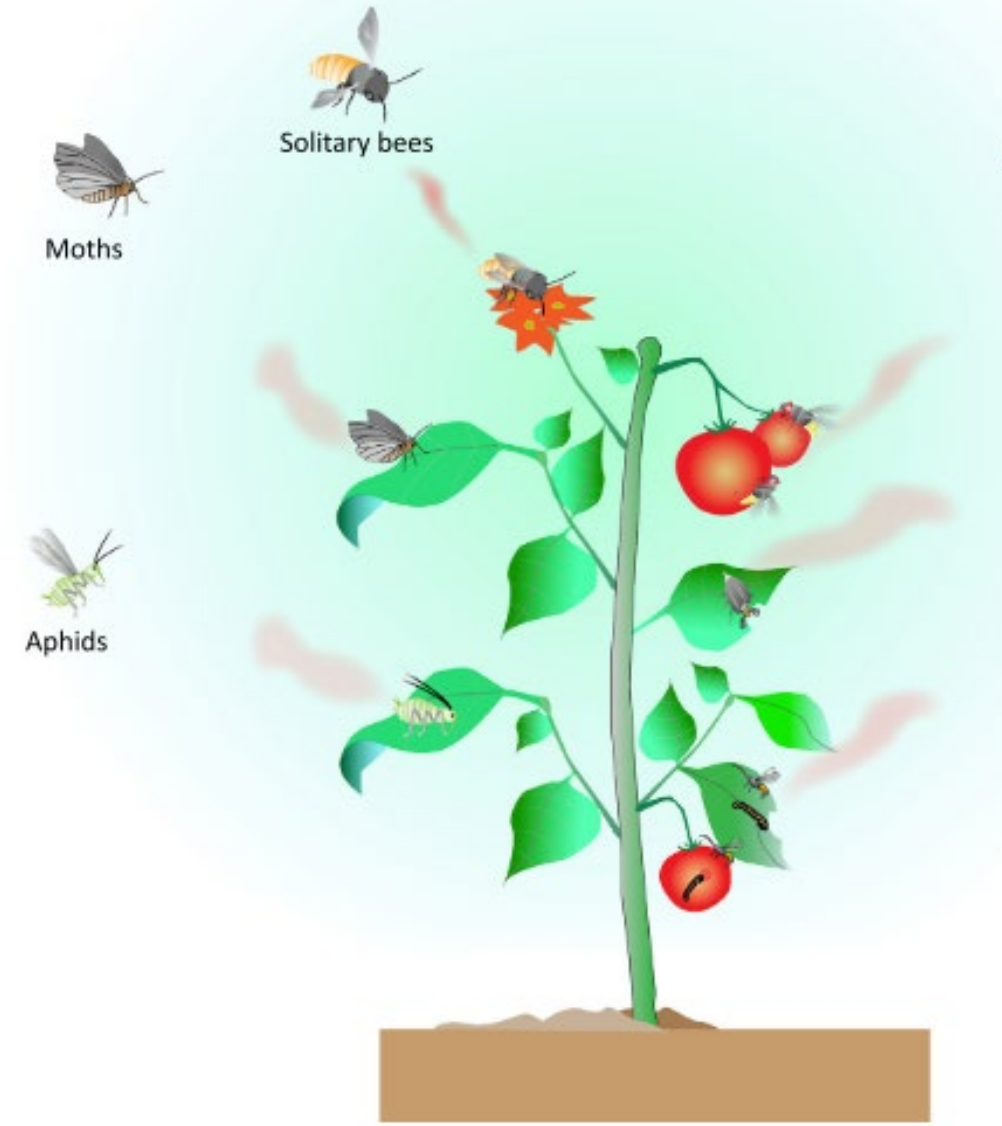



Bombykol
蚕蛾醇



独居蜂

蛾类




果蝇

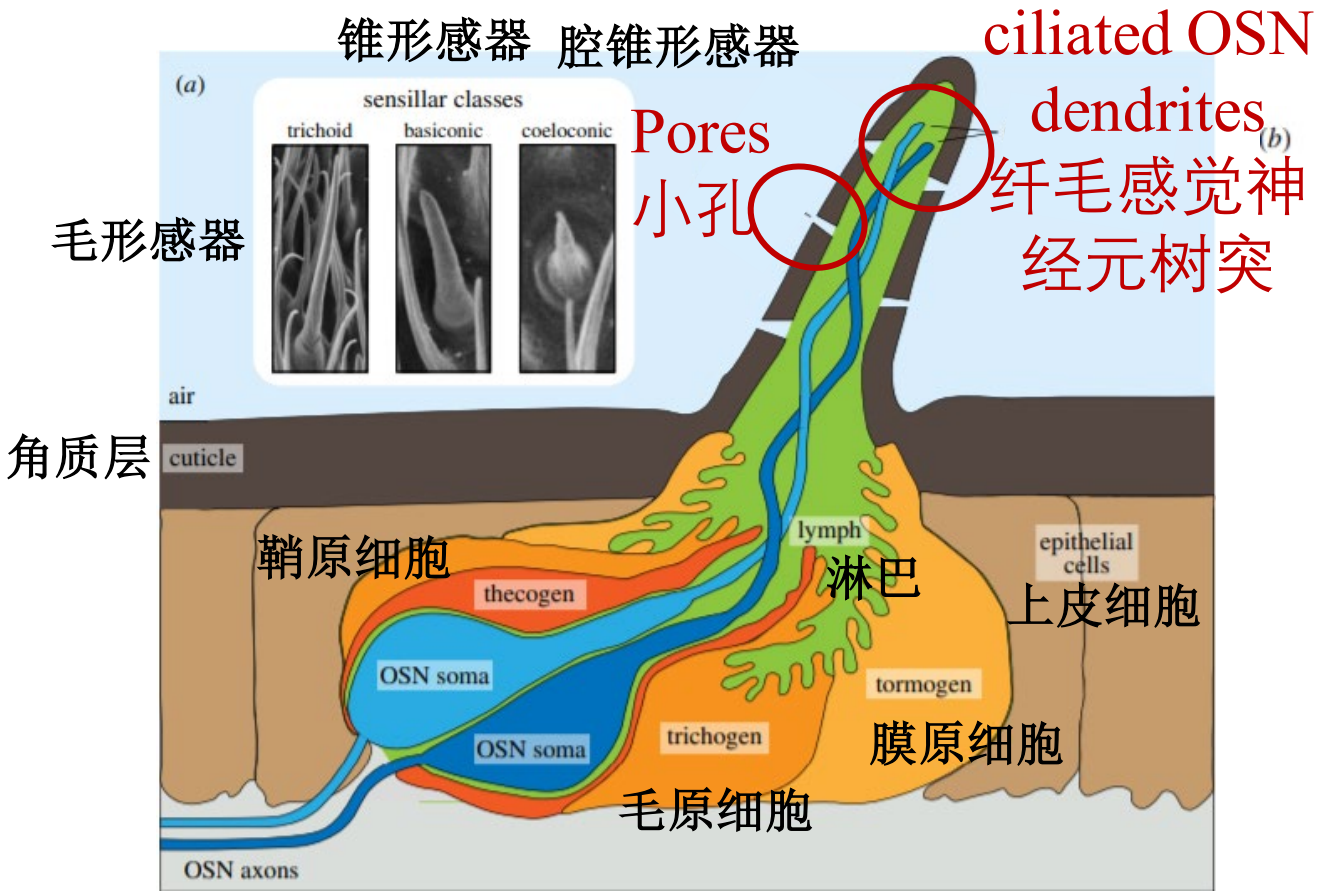
甲虫

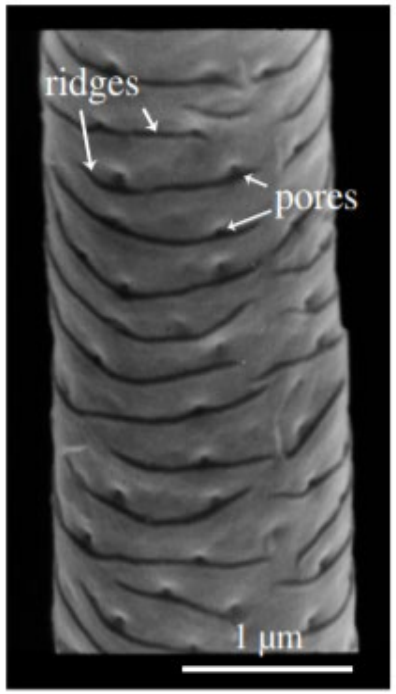
蚜虫

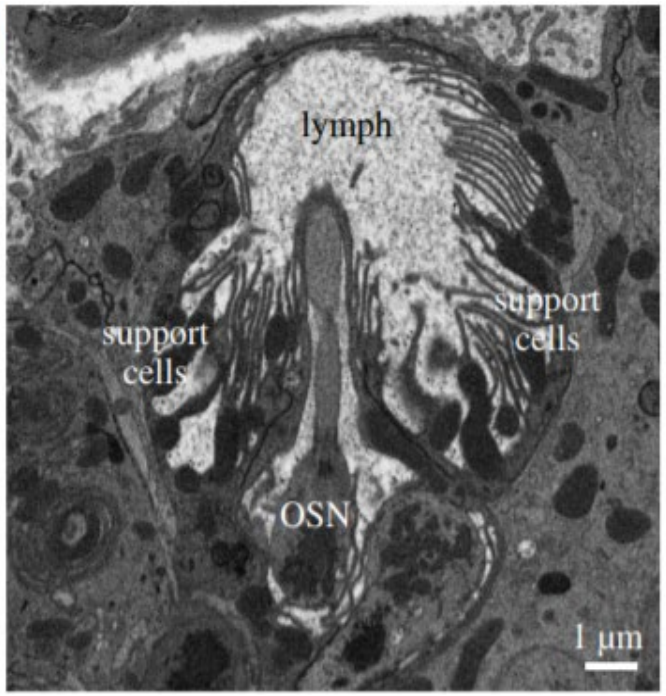
寄生蜂

Xu, H. & Turlings, T. C. J. *Trends in plant science* (2018).

# Peripheral signal system
# 外周信号系统

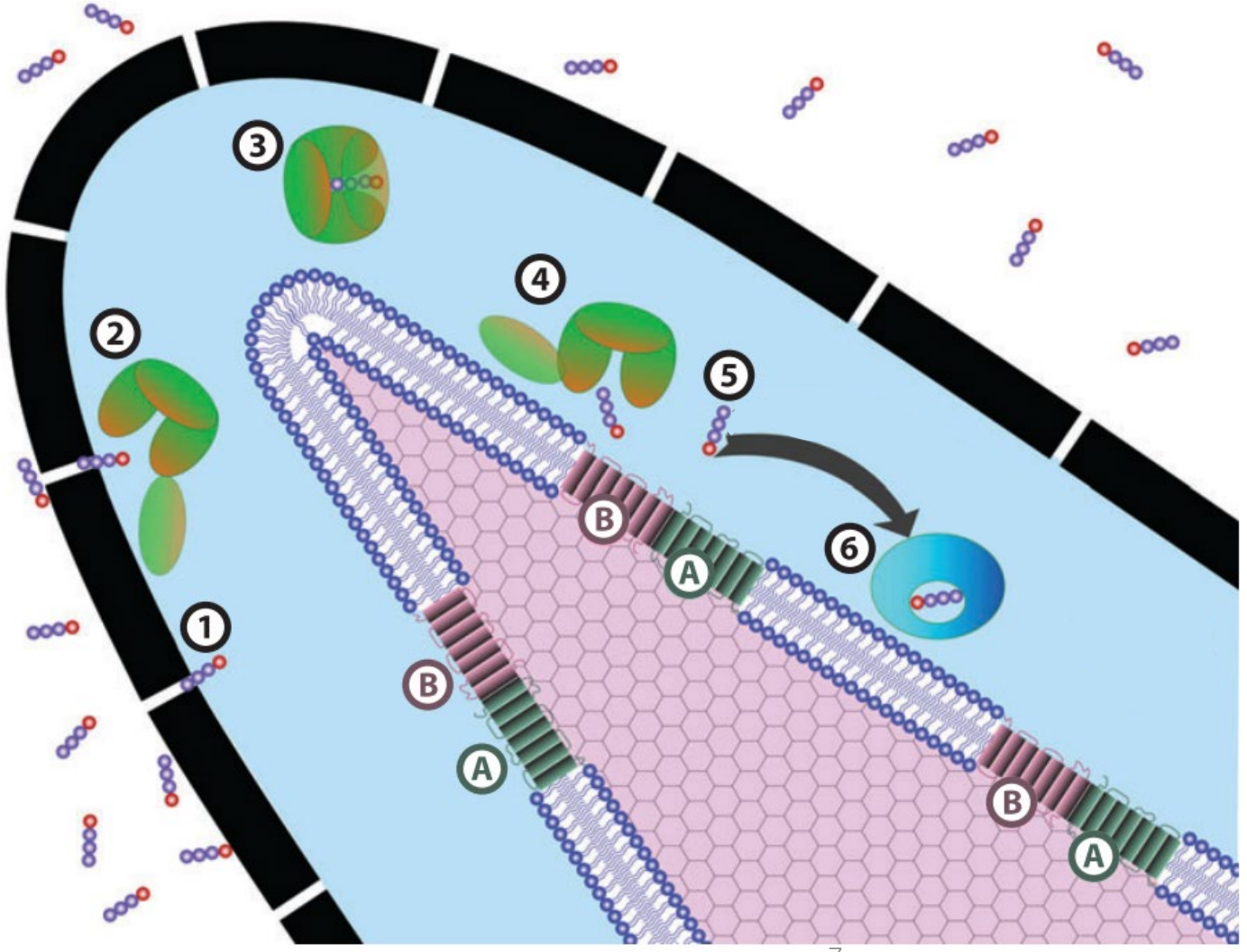



OSN：嗅觉感觉神经元

Schmidt, H. R. & Benton, R. *Open biology* (2020).



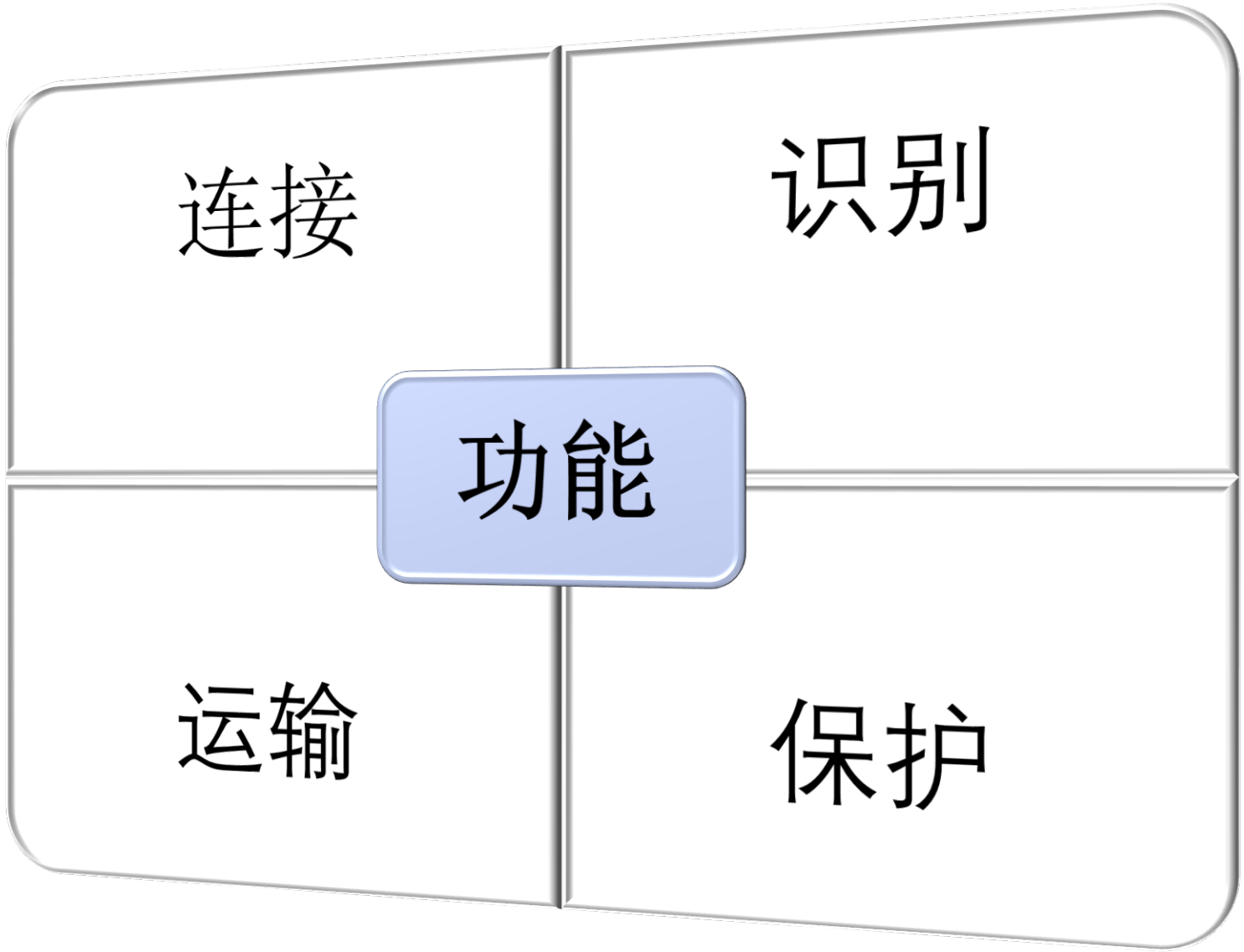

气味分子

气味结合蛋白

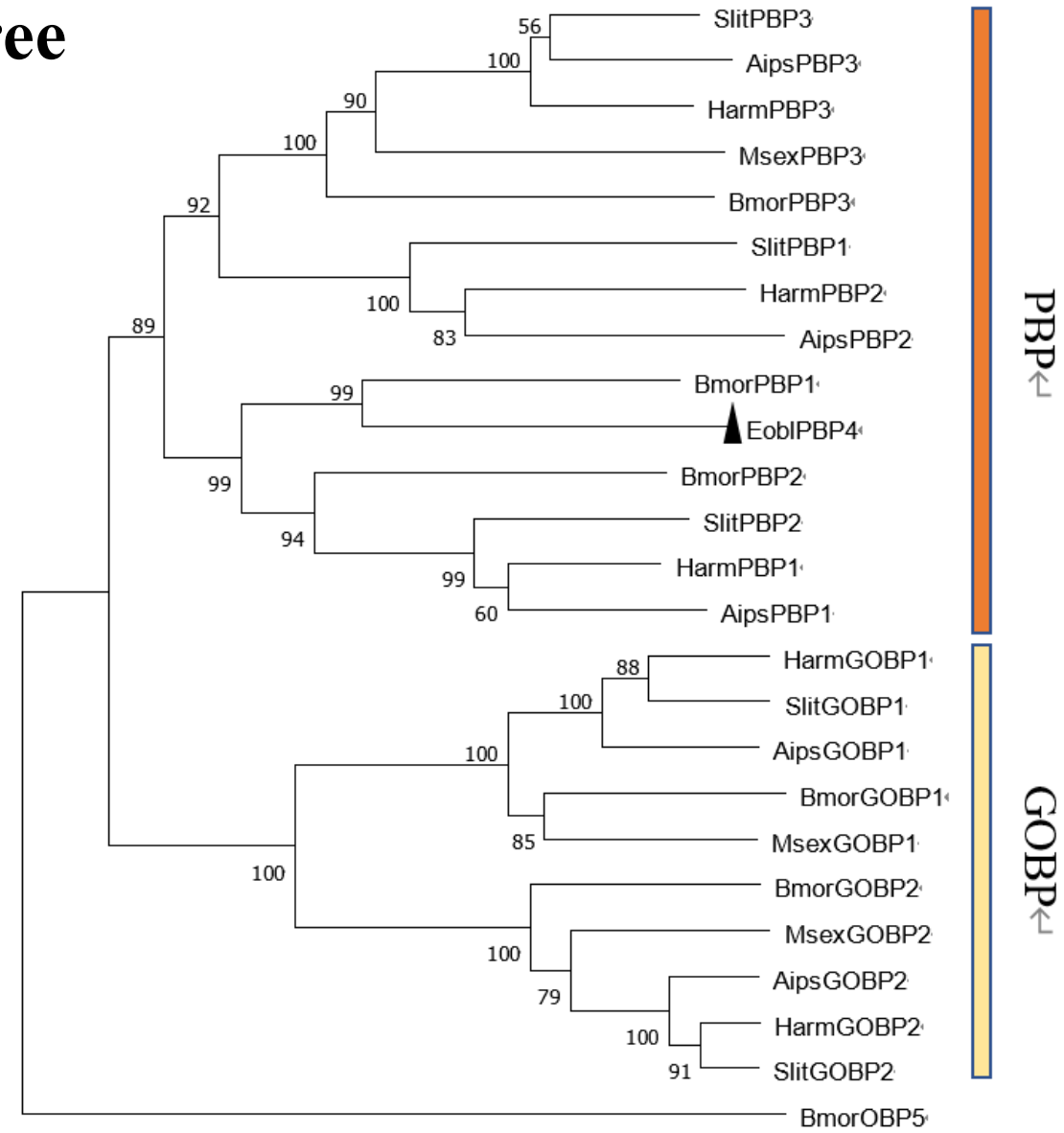
气味降解酶

气味受体

Leal, W. S. *Annual review of entomology* (2013).


连接
识别
功能
运输
保护

# Phylogenetic Tree



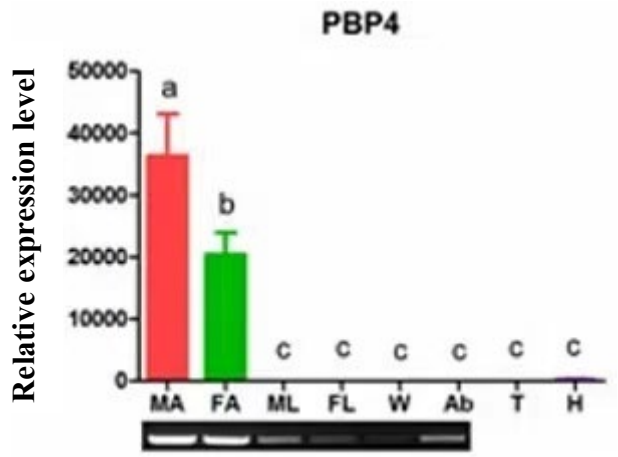

**Pheromone binding protein**
**信息素结合蛋白**

**General odorant binding protein**
**普通气味结合蛋白**

RESEARCH ARTICLE

# Identification and Comparative Study of Chemosensory Genes Related to Host Selection by Legs Transcriptome Analysis in the Tea Geometrid *Ectropis obliqua*

**Long Ma[1☯], Zhao-Qun Li[1☯], Lei Bian[1], Xiao-Ming Cai[1], Zong-Xiu Luo[1], Yong-Jun Zhang[2]*, Zong-Mao Chen[1]***

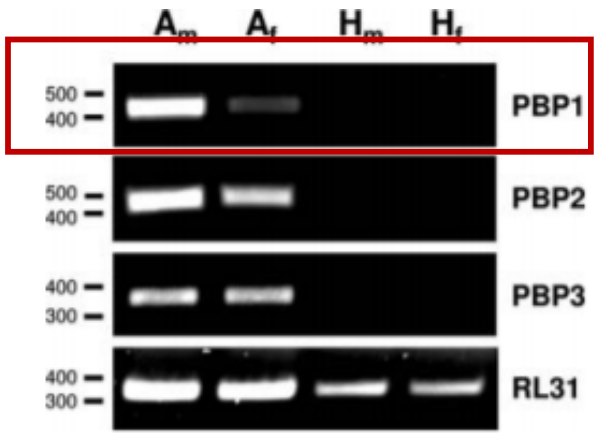


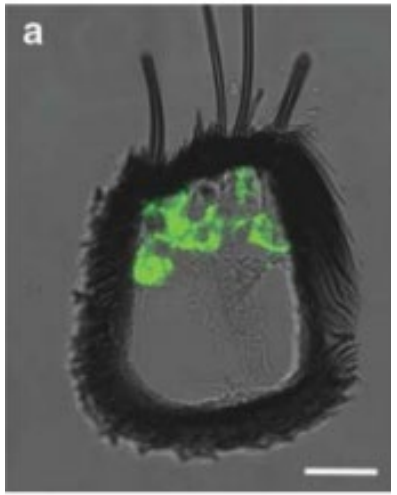

Invert Neurosci (2006) 6:177–187
DOI 10.1007/s10158-006-0032-0

ORIGINAL PAPER

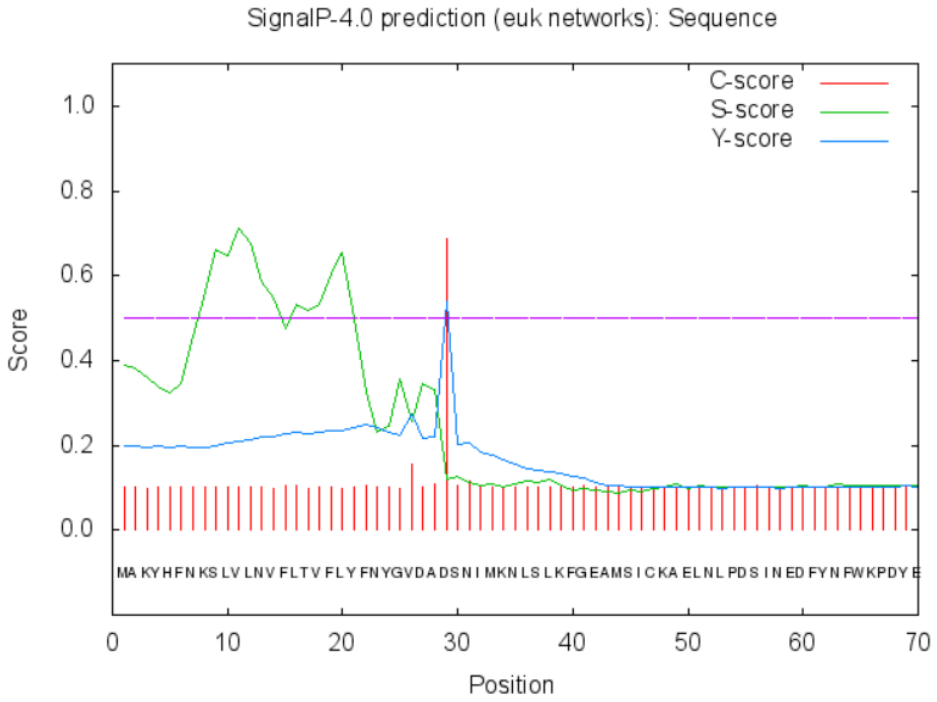
# Candidate pheromone binding proteins of the silkmoth *Bombyx mori*

**Maike Forstner · Thomas Gohl · Heinz Breer · Jürgen Krieger**

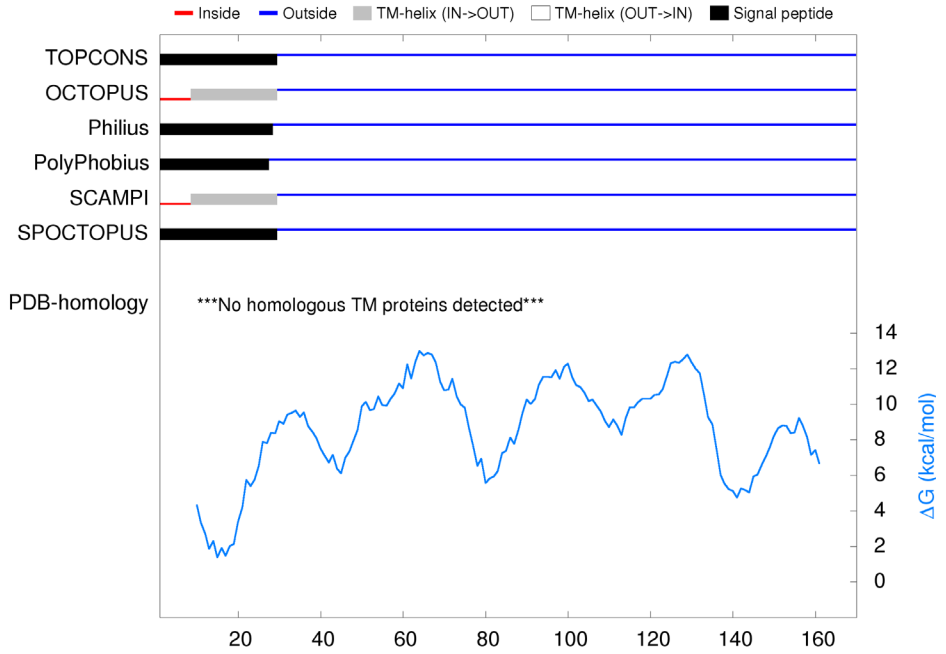


# Signal Peptide Prediction



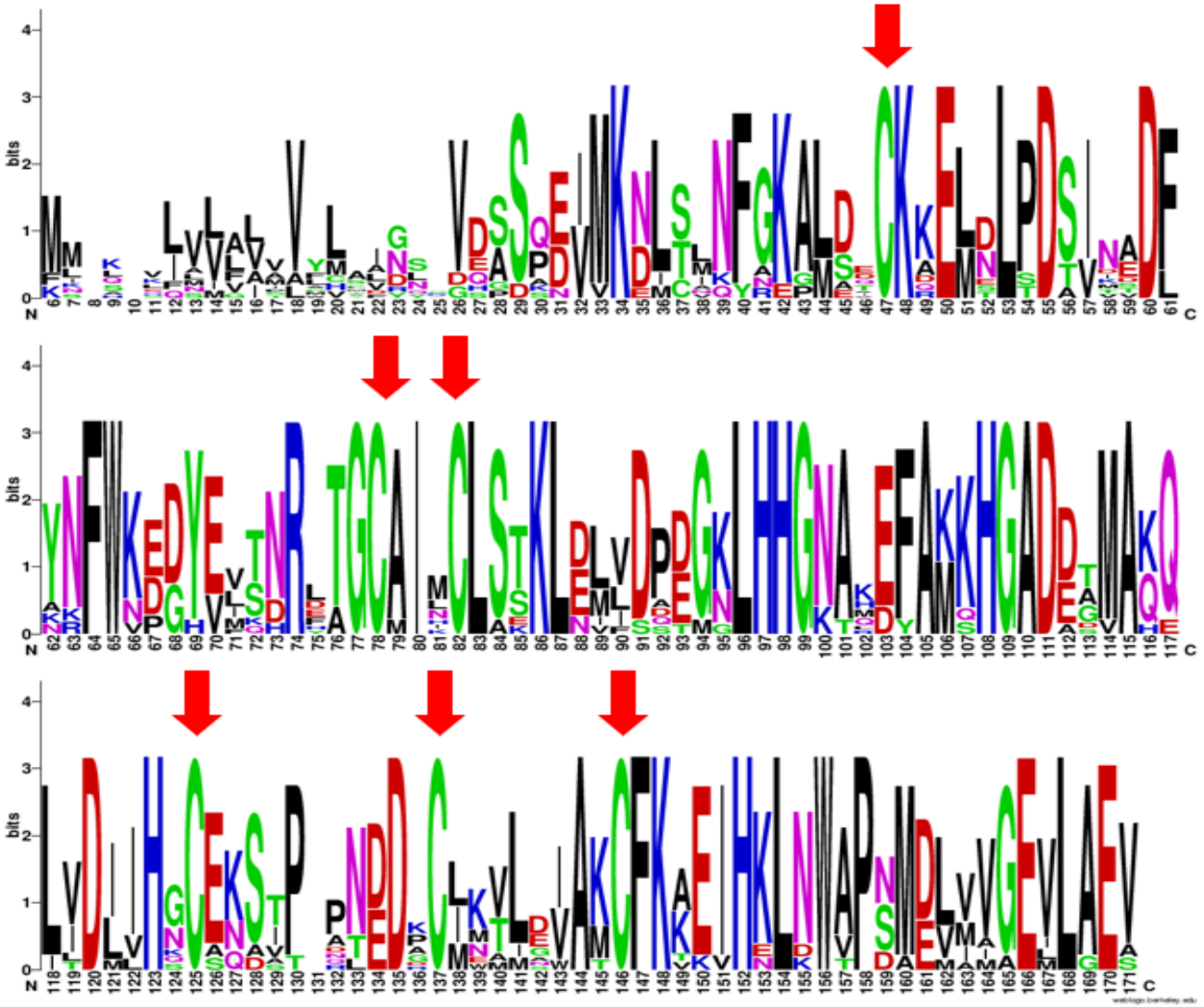

http://www.cbs.dtu.dk/services/SignalP-4.0/



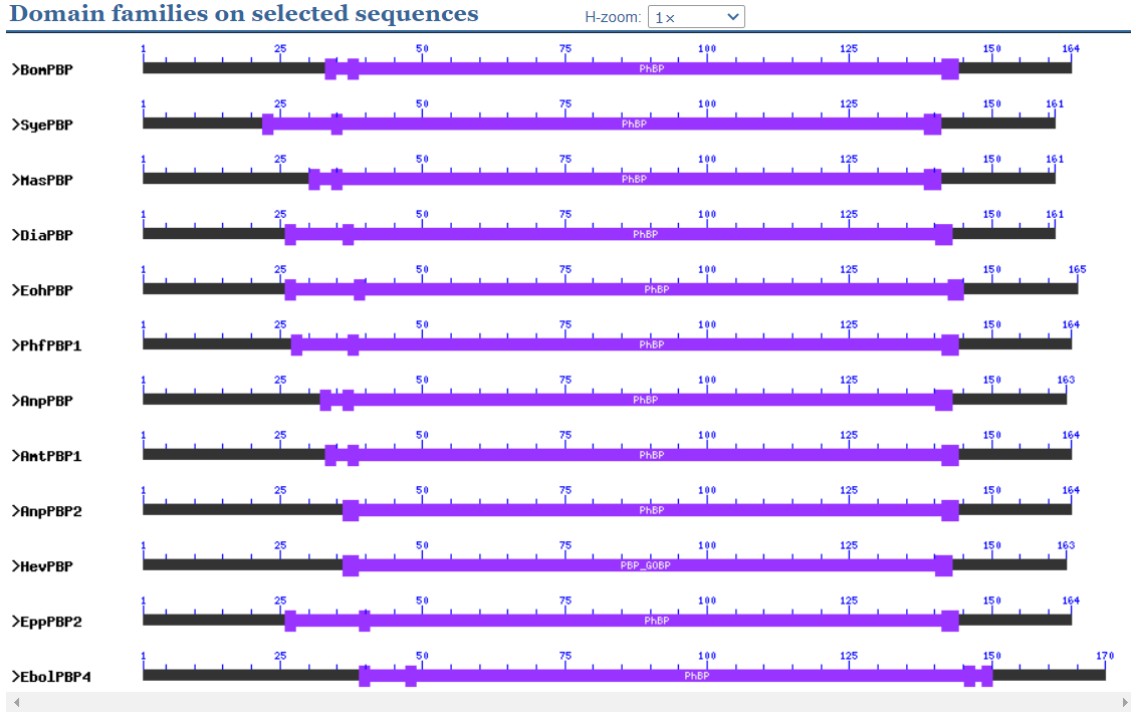

https://topcons.net/pred/

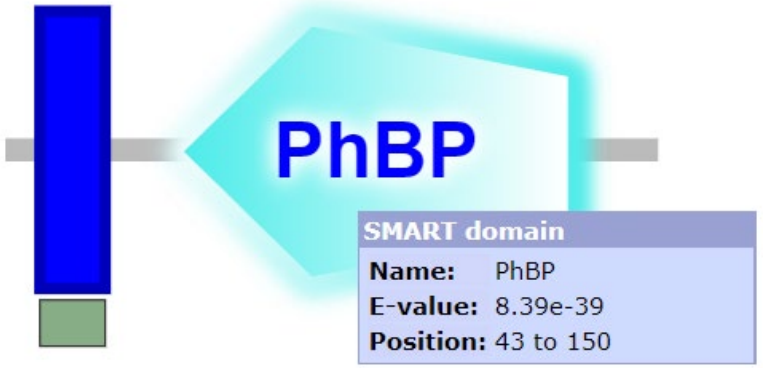
# Conserved Site Analysis

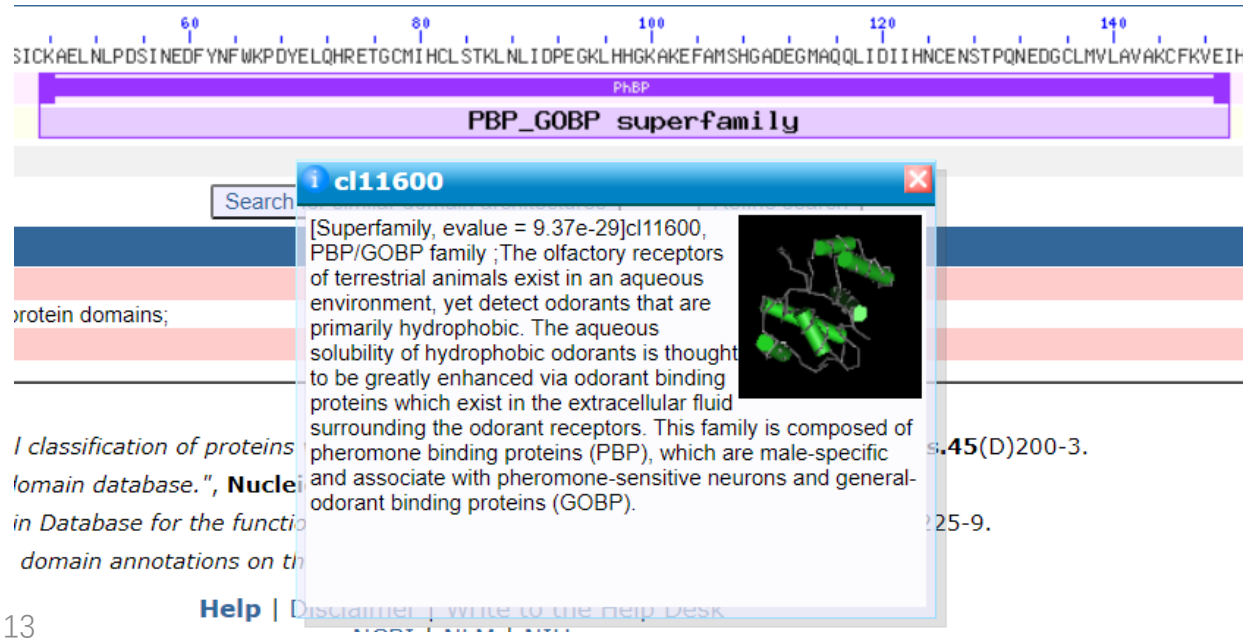
```
CLUSTAL multiple sequence alignment by MUSCLE (3.8)

EppPBP2         -----MMNHKELVLFAVVCLSLYQAVEPSQ-DVVKDMSLNFRKGLDACKKELNLPDTINS
Ebo1PBP4        MAKYHFNKSLVLNVFLTVFLYFNYGVDADS-NIMKNLSLKFGEAMSICKAELNLPDSINE
AnpPBP          ------MLRKISLLLLPVFVAINL-VHSSP-EIMKNLSNNFGKAMDCCKDELSLPDSVVA
AnpPBP2         -----MIRKVLLSVLLAVLMTINL-GQASP-EVMKNLCMNYGKAMDCCKQELNLPDSVIA
HevPBP          ------MMSVRLMLVVAVWLCLR--VDASQ-DVMKNLSMNFAKPLEDCKKEMDLPDSVTT
AmtPBP1         ------MKMHLFVQVIAASVMLMAGVDSSP-EIMKDLSINFGKALDTCKKELDLPDSINE
PhfPBP1         ------MRKFLILVGIVVLHVDNNRVQGSQ-DIMKDLTIQFGKALSICKKELDLPDTIMA
DiaPBP          -----MSLSVLVLAVVAACLA---GVDSSSADIMKDLTANFGKALSECKKELDLPDSINA
BomPBP          -----MSIQGQIALALMVYMAVGS-VDASQ-EVMKNLSLNFGKALDECKKEMTLTDAINE
MasPBP          --------MKVAVVAIVVYLAVGN-VDSSP-EVMKNLCLNFGKALDECKAEMNLSDSIKD
SyePBP          ---------MKFVMVVMLYLSIDSGVDSSQ-EVMKNLTMNFNKALDVCKKELDLPDSINA
EohPBP          -----MLTQTKIVVLVIVYLAIDSRVESSK-EIMKEITVNFGKALAICKREMELPDSIDV
                                              .  :::*::  :: : :  ** *: *.*::

EppPBP2         DFNRFWNDDHVVTNRDTGCAINCLSSKLELVSDTG-LHHGNTLEYAKQHGADDTVAQQIV
Ebo1PBP4        DFYNFWKPDYELQHRETGCMIHCLSTKLNLIDPEGKLHHGKAKEFAMSHGADEGMAQQLI
AnpPBP          DLYNFWKDDYVMTDRLAGCAINCLATKLDVVDPDGNLHHGNAKDFAMKHGADETMAQQLV
AnpPBP2         DLYNFWKDDYVMTDRLAGCAINCLSTKLDIVDPDGNLHHGNAKEFAMKHGADDGMAHELV
HevPBP          DFYNFWKEGYEFTNRHTGCAIICLSSKLELLDQEMKLHHGKAQEFAKKHGADDAMAKQLV
AmtPBP1         DFYKFWKEDYEITNRLTGCAIHCLSEKLEMVDADGKLHHGNAREFAMKHGADDAMAKQLV
PhfPBP1         DFKNFWNDGYELSNRFTGCAINCLSSKLDLLDPEGKLHHGNAQEFAMKHGADATMAKQLT
DiaPBP          DFYNFWKEDYELSNRFTGCAINCLSTKLELVDSEGKLHHGNAHDFAKKHGADDDMAKQLV
BomPBP          DFYNFWKEGYEIKNRETGCAINCLSTKLNMLDPEGNLHHGNAMEFAKKHGADETMAQQLI
MasPBP          DFANFWVEGYEVSNRDTGCAIICLSKKLDMIDPDGKLHHGNAMEFAKKHGADEAMAKQLL
SyePBP          DFYNFWKPDYEVTNRLTGCAINCLSTKLELFDPDGKLHHGNAKEFAMKHGADDSMAQQLV
EohPBP          DFYNFWKEDYEVSNRYTGCAIICLSTKLDLVDPDGGLHHGNAHEFAKKHGADDGMAKQLI
                *: .**  .: .  * :** * **: **::..    ****:: ::* .****  :*:::

EppPBP2         DLLHSCAQAVPD-LEDPCLKVLEWAKCFKAEIHKLNWAPSAEVMAAEMLAEV
Ebo1PBP4        DIIHNCENSTPQ-NEDGCLMVLAVAKCFKVEIHKLNWTPSMDMVVGEVLAES
AnpPBP          DIIHGCEKSAPP-NDDKCMKTIDVAMCFKKEIHKLNWVPNMDLVIGEVLAEV
AnpPBP2         DIIHGCEKSSPP-NDDKCIKTMDIAMCFKKEIHKLNWVPNMDLVVGEVLAEV
HevPBP          DMIHGCSQSTPDATDDPCMKALNVAKCFKAKIHELNWAPSMELVVGEVLAEV
AmtPBP1         DLIHGCEKSIPP-NDDRCMEVLSIAMCFKKEIHNLKWAPNMEVVVGEVLAEV
PhfPBP1         DLIHNCEKSITP-TEDDCINVLEVAKCFKAEIHKLNWAPNMDLIVGELLAEA
DiaPBP          DLIHGCEKSVPP-NEDACLNVLEIAKCFKKEIHKLNWAPDMDLIVGEVLG--
BomPBP          DIVHGCEKSTPA-NDDKCIWTLGVATCFKAEIHKLNWAPSMDVAVGEILAEV
MasPBP          DIIHNCENSTPP-NDDACLKTLDIAKCFKKEIHKLNWAPNMDLVVGEVLAEV
SyePBP          DIVHKCENDIPN-NEDPCLKVLDIAKCFKTEVHKLNWAPDMELMMGEVLAEV
EohPBP          DIIHGCEKSTPR-NDDGCIMMLGIAKCFKAEIHKLDWAPSMDLMVGEVLAEV
                *::* * :  .   :* *:  :  * *** ::*:*.*.*. ::  .*:*.
```



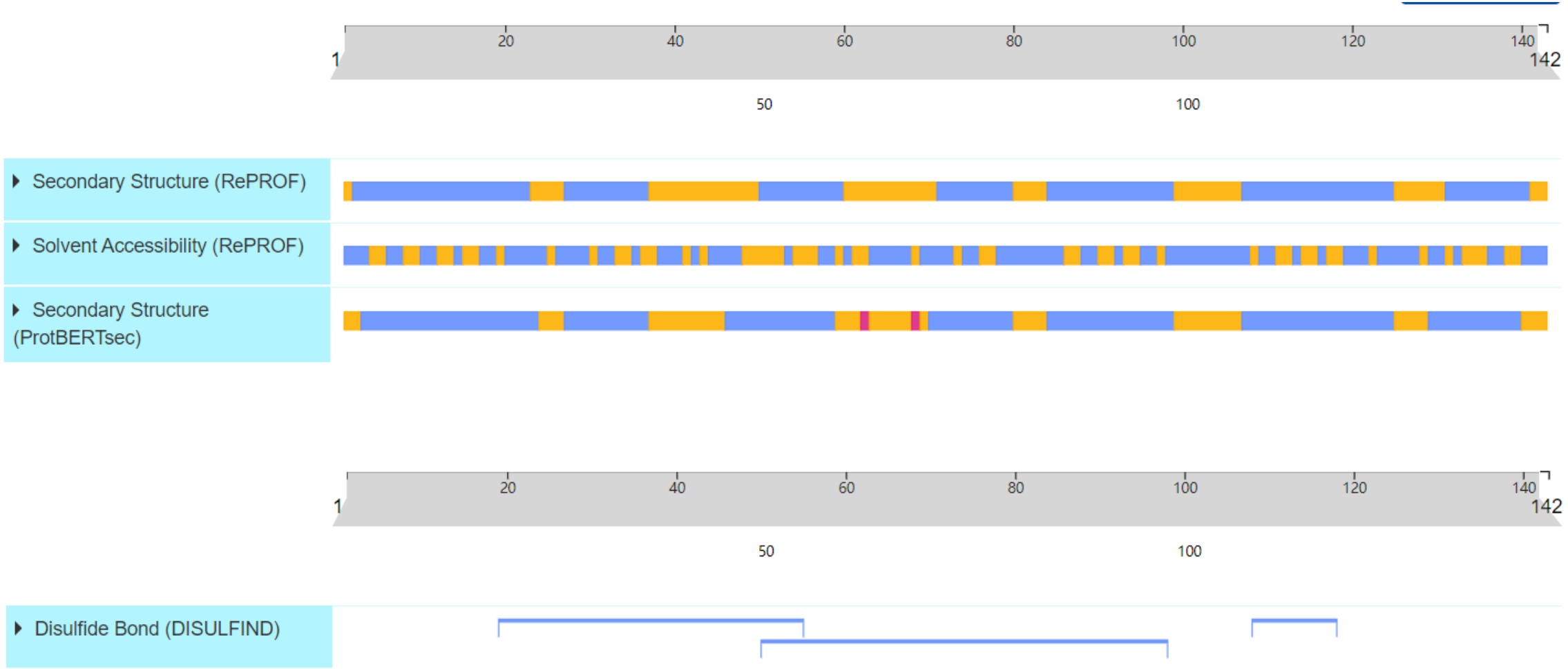
# Motif Prediction



# Prediction Secondary Structure




http://bioinf.cs.ucl.ac.uk/psipred/

**Biological Process Ontology**

| # | GO ID | GO Term | Reliability (%) | |
|---|---|---|---|---|
| 1 | GO:0019236 | response to pheromone | 51 | ☑ |

1/1 | 10

View Biological Process Ontology Tree

**Node color legend**

| | | |
|---|---|---|
| inferred | predicted & selected | predicted & deselected |

**Edge color legend**

| | | |
|---|---|---|
| is_a | part_of | regulates |
| negatively_regulates | positively_regulates | occurs_in |
| | capable_of | |

**Molecular Function Ontology**

| # | GO ID | GO Term | Reliability (%) | |
|---|---|---|---|---|
| 1 | GO:0005550 | pheromone binding | 51 | ☑ |

1/1 | 10

View Molecular Function Ontology Tree

**Node color legend**

| | | |
|---|---|---|
| inferred | predicted & selected | predicted & deselected |

**Edge color legend**

| | | |
|---|---|---|
| is_a | part_of | regulates |
| negatively_regulates | positively_regulates | occurs_in |
| | capable_of | |

**Cellular Component Ontology**

| # | GO ID | GO Term | Reliability (%) | |
|---|---|---|---|---|
| 1 | GO:0005576 | extracellular region | 44 | ☑ |

1/1 | 10

View Cellular Component Ontology Tree

**Node color legend**

| | | |
|---|---|---|
| inferred | predicted & selected | predicted & deselected |

**Edge color legend**

| | | |
|---|---|---|
| is_a | part_of | regulates |
| negatively_regulates | positively_regulates | occurs_in |
| | capable_of | |

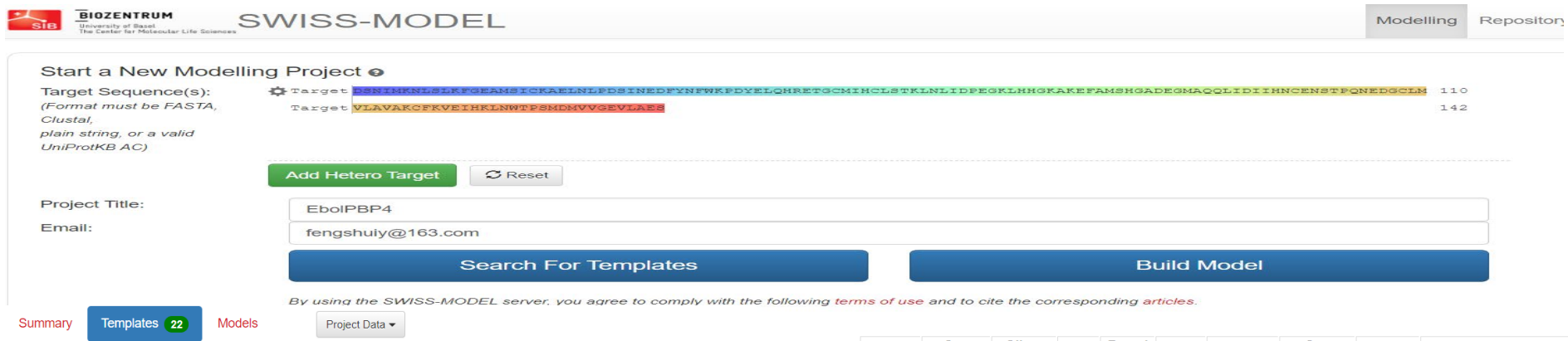
Predicted localization for the Eukarya domain: Secreted (GO term ID: GO:0005576) Prediction confidence 91

# Model Building

**Sequences producing significant alignments** Download New Select columns Show 1000

select all *12 sequences selected* GenPept Graphics Distance tree of results Multiple alignment New MSA Viewer

| Description | Scientific Name | Max Score | Total Score | Query Cover | E value | Per. Ident | Acc. Len | Accession |
|---|---|---|---|---|---|---|---|---|
| Gypsy Moth Pheromone-binding protein 1 (LdisPBP1) NMR Structure at pH 4.5 [Lymantria dispar] | Lymantria dispar | 167 | 167 | 81% | 3e-53 | 52.86% | 143 | 6UM9_A |
| Crystal Structure of B-form Bombyx mori Pheromone Binding Protein [Bombyx mori] | Bombyx mori | 213 | 213 | 81% | 1e-71 | 69.57% | 142 | 2FJY_A |
| A Form of the Pheromone-Binding Protein from Bombyx mori [Bombyx mori] | Bombyx mori | 213 | 213 | 81% | 2e-71 | 69.57% | 142 | 1GM0_A |
| NMR Structure of AtraPBP1 at pH 4.5 [Amyelois transitella] | Amyelois transitella | 201 | 201 | 81% | 1e-66 | 64.49% | 142 | 2KPH_A |
| Solution structure of Antheraea polyphemus pheromone binding protein (ApolPBP) [Antheraea polyphemus] | Antheraea polyphemus | 199 | 199 | 81% | 6e-66 | 65.22% | 142 | 1QWV_A |
| Crystal Structure of Epiphyas postvittana Pheromone Binding Protein 3 [Epiphyas postvittana] | Epiphyas postvittana | 154 | 154 | 81% | 5e-48 | 50.00% | 159 | 6VQ5_A |
| Structure of Pheromone-binding protein 1 in complex with (11Z,13Z)-hexadecadienal [Amyelois transitella] | Amyelois transitella | 199 | 199 | 80% | 5e-66 | 64.23% | 140 | 4INW_A |
| Bombyx Mori Pheromone Binding Protein [Bombyx mori] | Bombyx mori | 206 | 206 | 78% | 4e-69 | 69.40% | 137 | 1DQE_A |
| Structure of BMori GOBP2 (General Odorant Binding Protein 2) [Bombyx mori] | Bombyx mori | 97.1 | 97.1 | 78% | 9e-26 | 33.08% | 142 | 2WC5_A |
| Structure of BMori GOBP2 (General Odorant Binding Protein 2) with bombykol and water to Arg 110 [Bombyx mori] | Bombyx mori | 97.1 | 97.1 | 78% | 9e-26 | 33.08% | 141 | 2WC6_A |
| Bombyx mori pheromone binding protein bound to bell pepper odorant [Bombyx mori] | Bombyx mori | 200 | 200 | 75% | 1e-66 | 69.77% | 132 | 2P70_A |
| Solution structure of the Bombyx mori pheromone-binding protein fragment BmPBP(1-128) at pH 6.5 [Bombyx m… | Bombyx mori | 191 | 191 | 72% | 4e-63 | 69.35% | 128 | 1XFR_A |

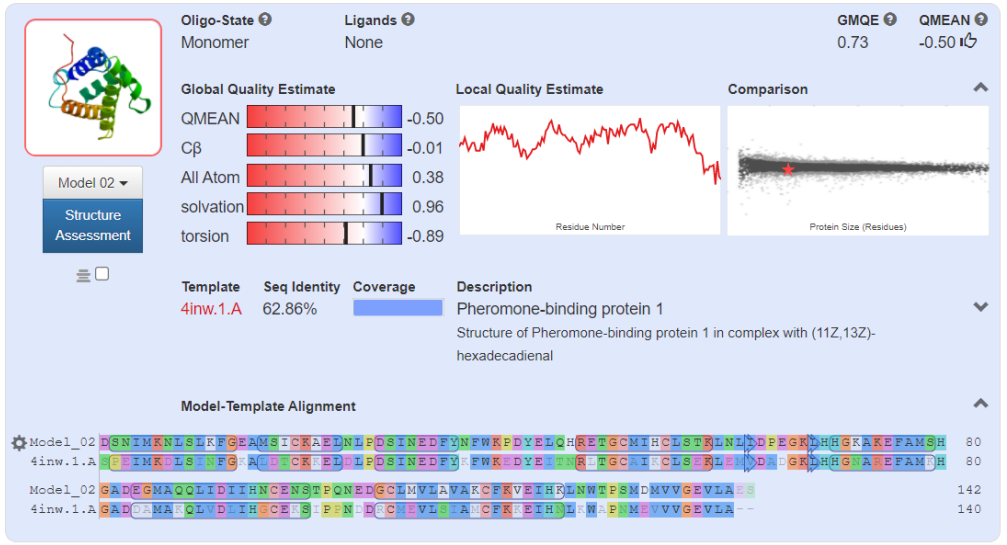


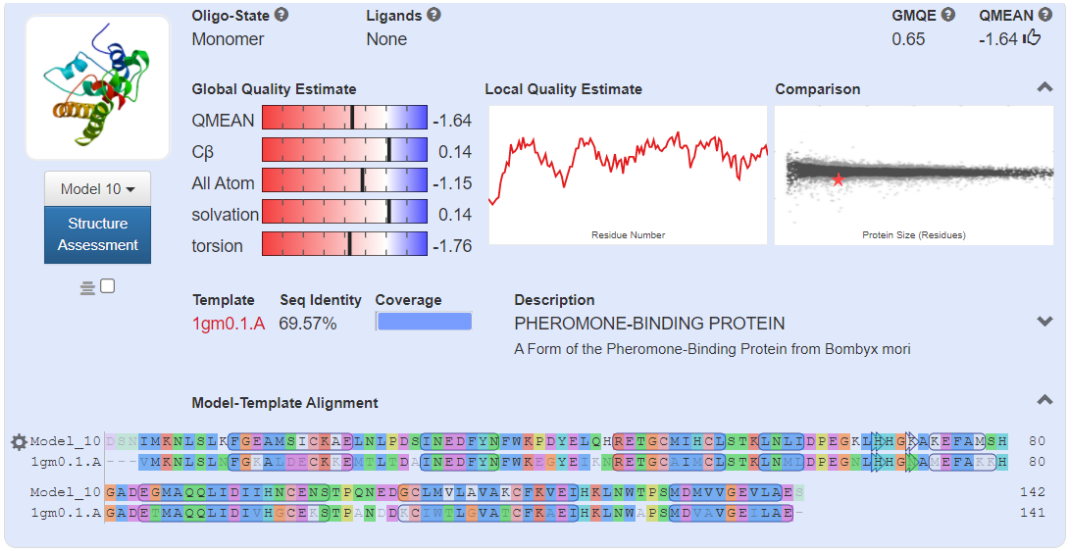

## Template Results

Templates | Quaternary Structure | Sequence Similarity | Alignment | More

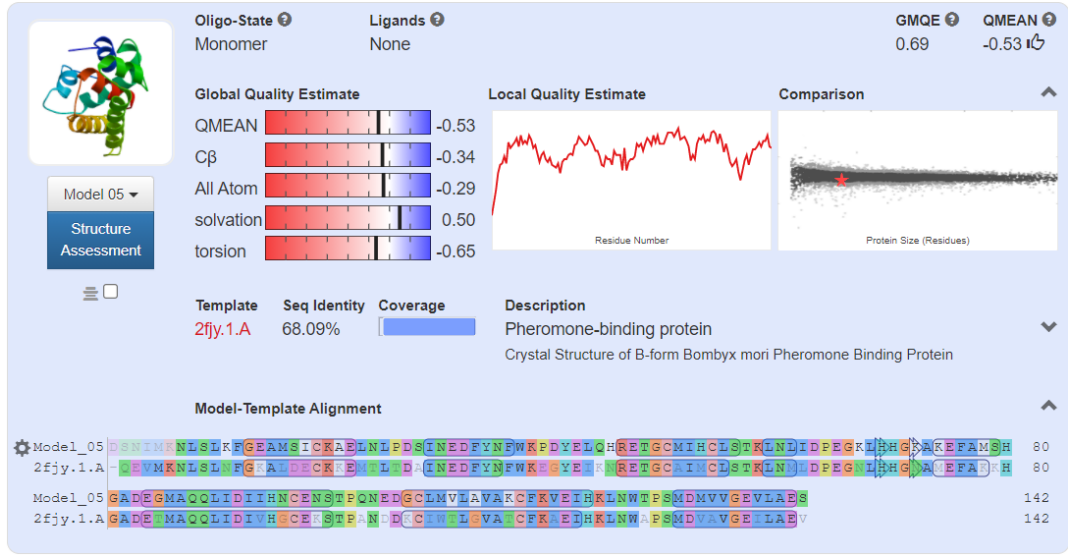
| Sort | Coverage | GMQE | QSQE | Identity | Method | Oligo State | Ligands |
|---|---|---|---|---|---|---|---|
| | 1dqe.1.A PHEROMONE-BINDING PROTEIN *BOMBYX MORI PHEROMONE BINDING PROTEIN* | | | | | | |
| | | 0.76 | 0.58 | 68.38 | X-ray, 1.8Å | homo-dimer ⚠ | 2 x BOM |
| | 4inw.1.A Pheromone-binding protein 1 *Structure of Pheromone-binding protein 1 in complex with (11Z,13Z)-hexadecadienal* | | | | | | |
| | | 0.75 | - | 62.86 | X-ray, 1.1Å | monomer ✓ | 1 x 1EY |
| | 1dqe.1.B PHEROMONE-BINDING PROTEIN *BOMBYX MORI PHEROMONE BINDING PROTEIN* | | | | | | |
| | | 0.74 | 0.58 | 68.38 | X-ray, 1.8Å | homo-dimer ⚠ | 2 x BOM |
| | 4inw.1.A Pheromone-binding protein 1 *Structure of Pheromone-binding protein 1 in complex with (11Z,13Z)-hexadecadienal* | | | | | | |
| | | 0.74 | - | 64.23 | X-ray, 1.1Å | monomer ✓ | 1 x 1EY |
| | 2fjy.1.A Pheromone-binding protein *Crystal Structure of B-form Bombyx mori Pheromone Binding Protein* | | | | | | |
| | | 0.71 | - | 68.09 | X-ray, 2.3Å | monomer ✓ | None |
| | 2fjy.1.A Pheromone-binding protein *Crystal Structure of B-form Bombyx mori Pheromone Binding Protein* | | | | | | |
| | | 0.71 | - | 69.57 | X-ray, 2.3Å | monomer ✓ | None |
| | 2jpo.1.A Pheromone-binding protein | | | | | | |

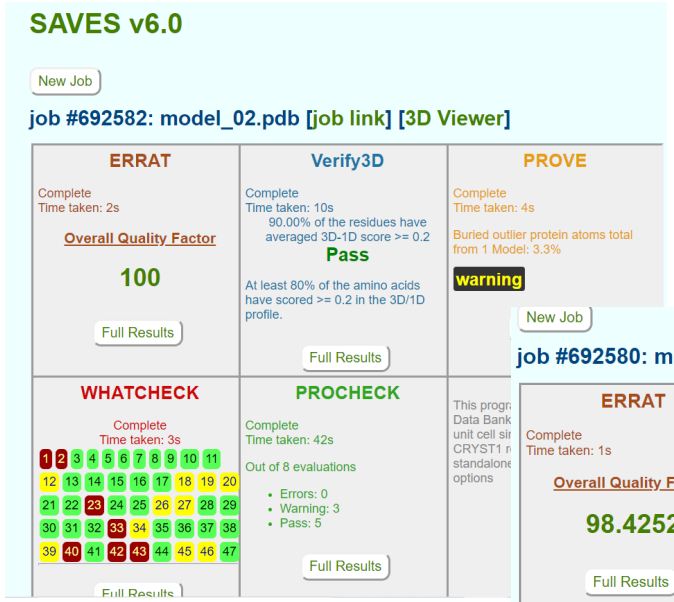
| Template | Seq Identity | Oligo-state | QSQE | Found by | Method | Resolution | Seq Similarity | Coverage | Description |
|---|---|---|---|---|---|---|---|---|---|
| 1dqe.1.A | 68.38 | homo-dimer | 0.58 | HHblits | X-ray | 1.80Å | 0.53 | 0.96 | PHEROMONE-BINDING PROTEIN |
| 4inw.1.A | 62.86 | monomer | - | HHblits | X-ray | 1.14Å | 0.51 | 0.99 | Pheromone-binding protein 1 |
| 1dqe.1.B | 68.38 | homo-dimer | 0.58 | HHblits | X-ray | 1.80Å | 0.53 | 0.96 | PHEROMONE-BINDING PROTEIN |
| 4inw.1.A | 64.23 | monomer | - | BLAST | X-ray | 1.14Å | 0.51 | 0.96 | Pheromone-binding protein 1 |
| 2fjy.1.A | 68.09 | monomer | - | HHblits | X-ray | 2.30Å | 0.52 | 0.99 | Pheromone-binding protein |
| 2fjy.1.A | 69.57 | monomer | - | BLAST | X-ray | 2.30Å | 0.53 | 0.97 | Pheromone-binding protein |
| 2jpo.1.A | 63.38 | monomer | - | HHblits | NMR | NA | 0.50 | 1.00 | Pheromone-binding protein |
| 1gm0.1.A | 68.09 | monomer | - | HHblits | NMR | NA | 0.52 | 0.99 | PHEROMONE-BINDING PROTEIN |
| 2jpo.1.A | 65.22 | monomer | - | BLAST | NMR | NA | 0.51 | 0.97 | Pheromone-binding protein |
| 1gm0.1.A | 69.57 | monomer | - | BLAST | NMR | NA | 0.53 | 0.97 | PHEROMONE-BINDING PROTEIN |
| 1ls8.1.A | 68.09 | monomer | - | HHblits | NMR | NA | 0.52 | 0.99 | pheromone binding protein |
| 2kph.1.A | 62.68 | monomer | - | HHblits | NMR | NA | 0.51 | 1.00 | Pheromone binding protein |
| 1ls8.1.A | 69.57 | monomer | - | BLAST | NMR | NA | 0.53 | 0.97 | pheromone binding protein |
| 2kph.1.A | 64.49 | monomer | - | BLAST | NMR | NA | 0.52 | 0.97 | Pheromone binding protein |
| 6um9.1.A | 52.14 | monomer | - | HHblits | NMR | NA | 0.47 | 0.99 | Pheromone binding protein 1 |
| 6um9.1.A | 53.24 | monomer | - | BLAST | NMR | NA | 0.48 | 0.98 | Pheromone binding protein 1 |
| 1qwv.1.A | 63.38 | monomer | - | HHblits | NMR | NA | 0.50 | 1.00 | Pheromone-binding protein |
| 6vq5.1.A | 48.59 | monomer | - | HHblits | X-ray | 2.60Å | 0.45 | 1.00 | Pheromome Binding Protein |
| 6vq5.1.A | 50.00 | monomer | - | BLAST | X-ray | 2.60Å | 0.46 | 0.97 | Pheromome Binding Protein |
| 1two.1.A | 63.38 | monomer | - | HHblits | NMR | NA | 0.50 | 1.00 | Pheromone-binding protein |
| 1qwv.1.A | 65.22 | monomer | - | BLAST | NMR | NA | 0.51 | 0.97 | Pheromone-binding protein |
| 1two.1.A | 65.22 | monomer | - | BLAST | NMR | NA | 0.51 | 0.97 | Pheromone-binding protein |

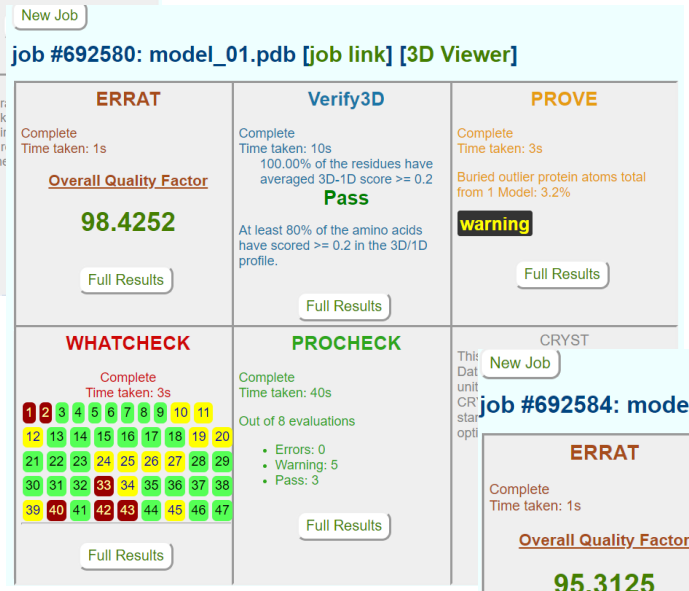

Oligo-State
Monomer
Ligands
None
GMQE
0.73
QMEAN
-0.50
Global Quality Estimate
QMEAN -0.50
Cβ -0.01
All Atom 0.38
solvation 0.96
torsion -0.89
Local Quality Estimate
Residue Number
Comparison
Protein Size (Residues)
Model 02
Structure Assessment
Template
4inw.1.A
Seq Identity
62.86%
Coverage
Description
Pheromone-binding protein 1
Structure of Pheromone-binding protein 1 in complex with (11Z,13Z)-hexadecadienal
Model-Template Alignment
Model_02
4inw.1.A

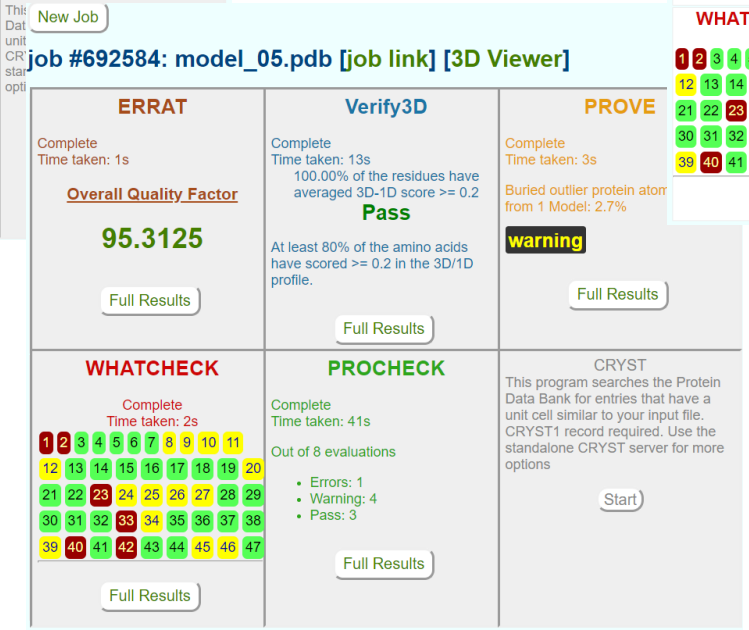

Oligo-State
Monomer
Ligands
None
GMQE
0.65
QMEAN
-1.64
Global Quality Estimate
QMEAN -1.64
Cβ 0.14
All Atom -1.15
solvation 0.14
torsion -1.76
Local Quality Estimate
Residue Number
Comparison
Protein Size (Residues)
Model 10
Structure Assessment
Template
1gm0.1.A
Seq Identity
69.57%
Coverage
Description
PHEROMONE-BINDING PROTEIN
A Form of the Pheromone-Binding Protein from Bombyx mori
Model-Template Alignment
Model_10
1gm0.1.A

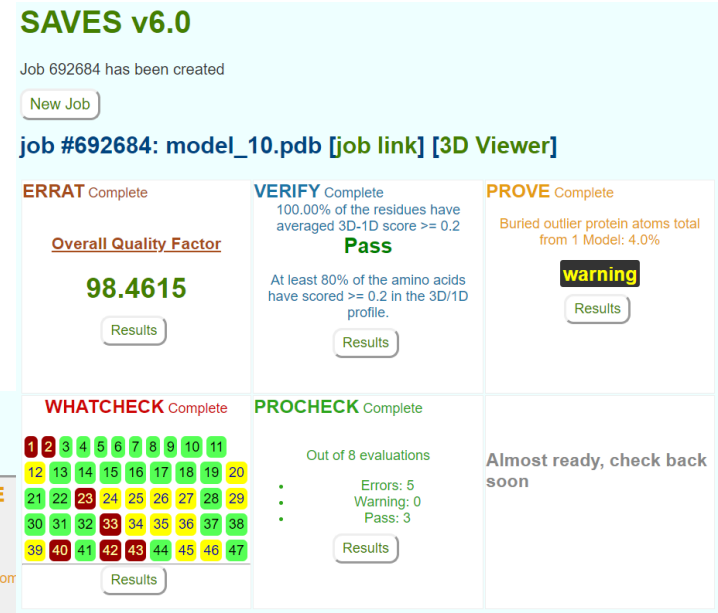

Oligo-State
Monomer (matching prediction)
Ligands
None
GMQE
0.71
QMEAN
-0.55
Global Quality Estimate
QMEAN -0.55
Cβ 0.55
All Atom 0.62
solvation 0.60
torsion -0.94
Local Quality Estimate
Residue Number
Comparison
Protein Size (Residues)
Model 01
Structure Assessment
Template
1dqe.1.A
Seq Identity
68.38%
Coverage
Description
PHEROMONE-BINDING PROTEIN
BOMBYX MORI PHEROMONE BINDING PROTEIN
Model-Template Alignment
Model_01
1dqe.1.A


Oligo-State
Monomer
Ligands
None
GMQE
0.69
QMEAN
-0.53
Global Quality Estimate
QMEAN -0.53
Cβ -0.34
All Atom -0.29
solvation 0.50
torsion -0.65
Local Quality Estimate
Residue Number
Comparison
Protein Size (Residues)
Model 05
Structure Assessment
Template
2fjy.1.A
Seq Identity
68.09%
Coverage
Description
Pheromone-binding protein
Crystal Structure of B-form Bombyx mori Pheromone Binding Protein
Model-Template Alignment
Model_05
2fjy.1.A


SAVES v6.0
New Job
job #692582: model_02.pdb [job link] [3D Viewer]
ERRAT
Complete
Time taken: 2s
Overall Quality Factor
100
Full Results
Verify3D
Complete
Time taken: 10s
90.00% of the residues have averaged 3D-1D score >= 0.2
Pass
At least 80% of the amino acids have scored >= 0.2 in the 3D/1D profile.
Full Results
PROVE
Complete
Time taken: 4s
Buried outlier protein atoms total from 1 Model: 3.3%
warning
WHATCHECK
Complete
Time taken: 3s
PROCHECK
Complete
Time taken: 42s
Out of 8 evaluations
Errors: 0
Warning: 3
Pass: 5
Full Results


New Job
job #692580: model_01.pdb [job link] [3D Viewer]
ERRAT
Complete
Time taken: 1s
Overall Quality Factor
98.4252
Full Results
Verify3D
Complete
Time taken: 10s
100.00% of the residues have averaged 3D-1D score >= 0.2
Pass
At least 80% of the amino acids have scored >= 0.2 in the 3D/1D profile.
Full Results
PROVE
Complete
Time taken: 3s
Buried outlier protein atoms total from 1 Model: 3.2%
warning
Full Results
WHATCHECK
Complete
Time taken: 3s
PROCHECK
Complete
Time taken: 40s
Out of 8 evaluations
Errors: 0
Warning: 5
Pass: 3
Full Results
CRYST

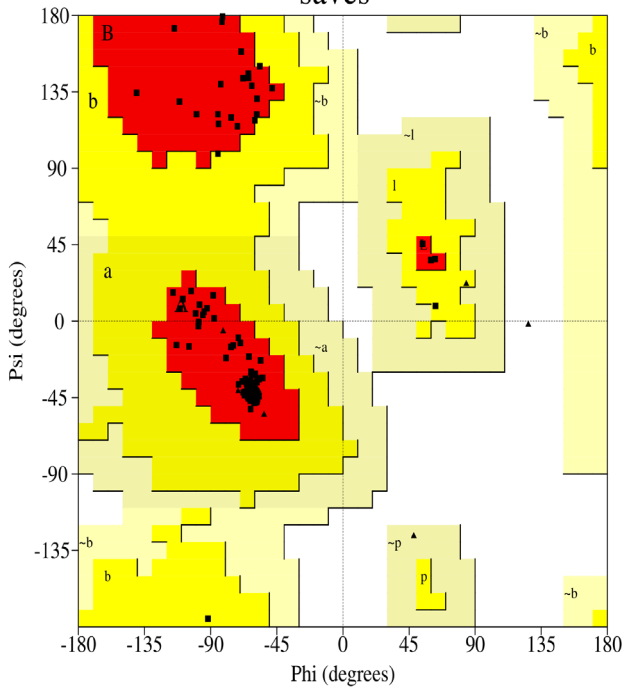

New Job
job #692584: model_05.pdb [job link] [3D Viewer]
ERRAT
Complete
Time taken: 1s
Overall Quality Factor
95.3125
Full Results
Verify3D
Complete
Time taken: 13s
100.00% of the residues have averaged 3D-1D score >= 0.2
Pass
At least 80% of the amino acids have scored >= 0.2 in the 3D/1D profile.
Full Results
PROVE
Complete
Time taken: 3s
warning
Full Results
WHATCHECK
Complete
Time taken: 2s
PROCHECK
Complete
Time taken: 41s
Out of 8 evaluations
Errors: 1
Warning: 4
Pass: 3
Full Results
CRYST
This program searches the Protein Data Bank for entries that have a unit cell similar to your input file. CRYST1 record required. Use the standalone CRYST server for more options
Start


SAVES v6.0
Job 692684 has been created
New Job
job #692684: model_10.pdb [job link] [3D Viewer]
ERRAT Complete
Overall Quality Factor
98.4615
Results
VERIFY Complete
100.00% of the residues have averaged 3D-1D score >= 0.2
Pass
At least 80% of the amino acids have scored >= 0.2 in the 3D/1D profile.
Results
PROVE Complete
Buried outlier protein atoms total from 1 Model: 4.0%
warning
Results
WHATCHECK Complete
PROCHECK Complete
Out of 8 evaluations
Errors: 5
Warning: 0
Pass: 3
Results
Almost ready, check back soon

PROCHECK

# Ramachandran Plot

## saves




### Plot statistics

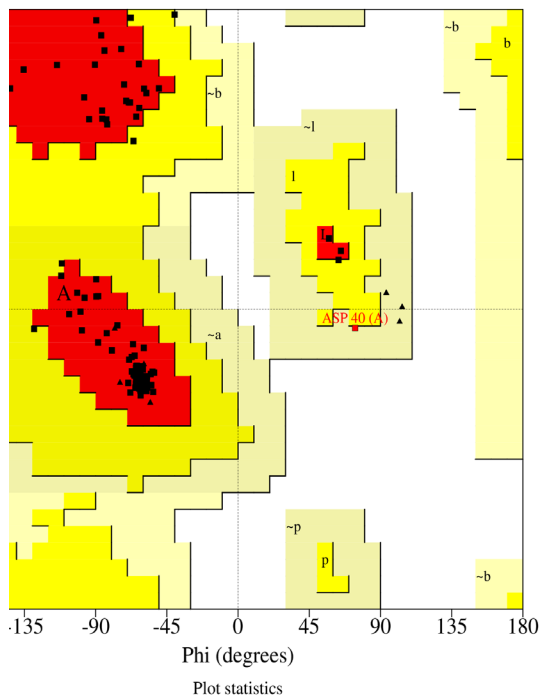
| | | |
|---|---|---|
| Residues in most favoured regions [A,B,L] | 121 | 96.8% |
| Residues in additional allowed regions [a,b,l,p] | 4 | 3.2% |
| Residues in generously allowed regions [~a,~b,~l,~p] | 0 | 0.0% |
| Residues in disallowed regions | 0 | 0.0% |
| Number of non-glycine and non-proline residues | 125 | 100.0% |
| Number of end-residues (excl. Gly and Pro) | 2 | |
| Number of glycine residues (shown as triangles) | 8 | |
| Number of proline residues | 5 | |
| Total number of residues | 140 | |

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

saves_01.ps

# Ramachandran Plot

## saves



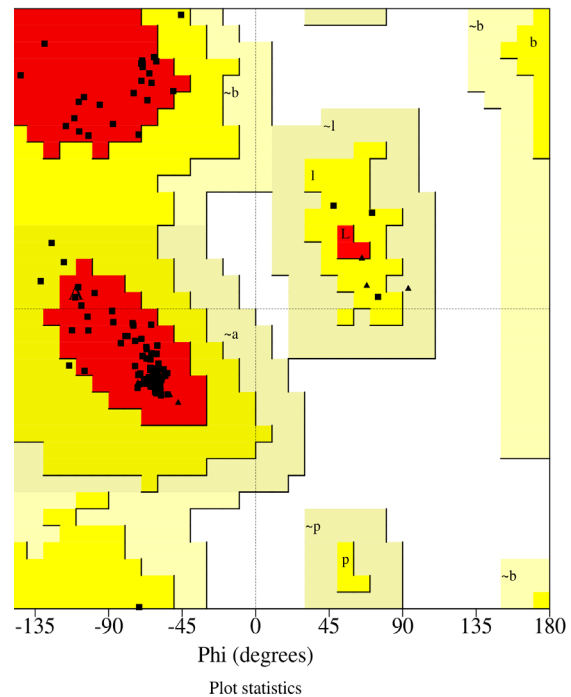

### Plot statistics

| | | |
|---|---|---|
| Residues in most favoured regions [A,B,L] | 114 | 94.2% |
| Residues in additional allowed regions [a,b,l,p] | 6 | 5.0% |
| Residues in generously allowed regions [~a,~b,~l,~p] | 1 | 0.8% |
| Residues in disallowed regions | 0 | 0.0% |
| Number of non-glycine and non-proline residues | 121 | 100.0% |
| Number of end-residues (excl. Gly and Pro) | 2 | |
| Number of glycine residues (shown as triangles) | 8 | |
| Number of proline residues | 5 | |
| Total number of residues | 136 | |

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

# Ramachandran Plot

## saves



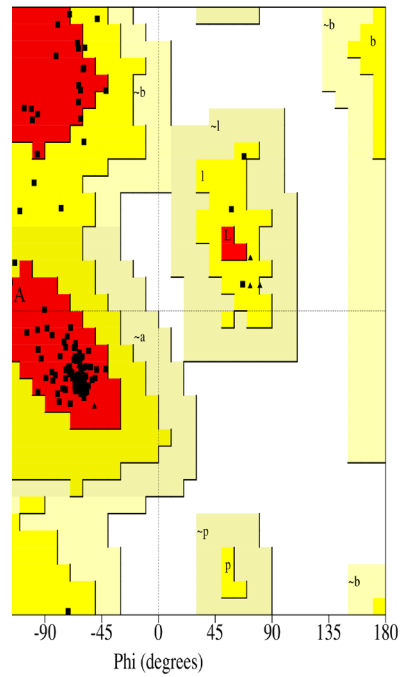

### Plot statistics

| | | |
|---|---|---|
| Residues in most favoured regions [A,B,L] | 111 | 91.7% |
| Residues in additional allowed regions [a,b,l,p] | 10 | 8.3% |
| Residues in generously allowed regions [~a,~b,~l,~p] | 0 | 0.0% |
| Residues in disallowed regions | 0 | 0.0% |
| Number of non-glycine and non-proline residues | 121 | 100.0% |
| Number of end-residues (excl. Gly and Pro) | 2 | |
| Number of glycine residues (shown as triangles) | 8 | |
| Number of proline residues | 5 | |
| Total number of residues | 136 | |

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

# Ramachandran Plot

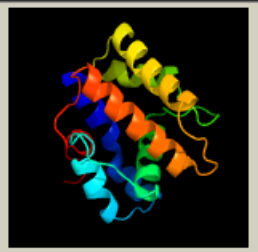
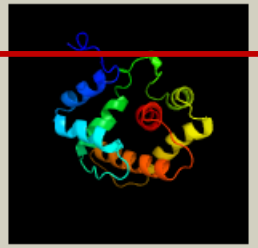
## saves

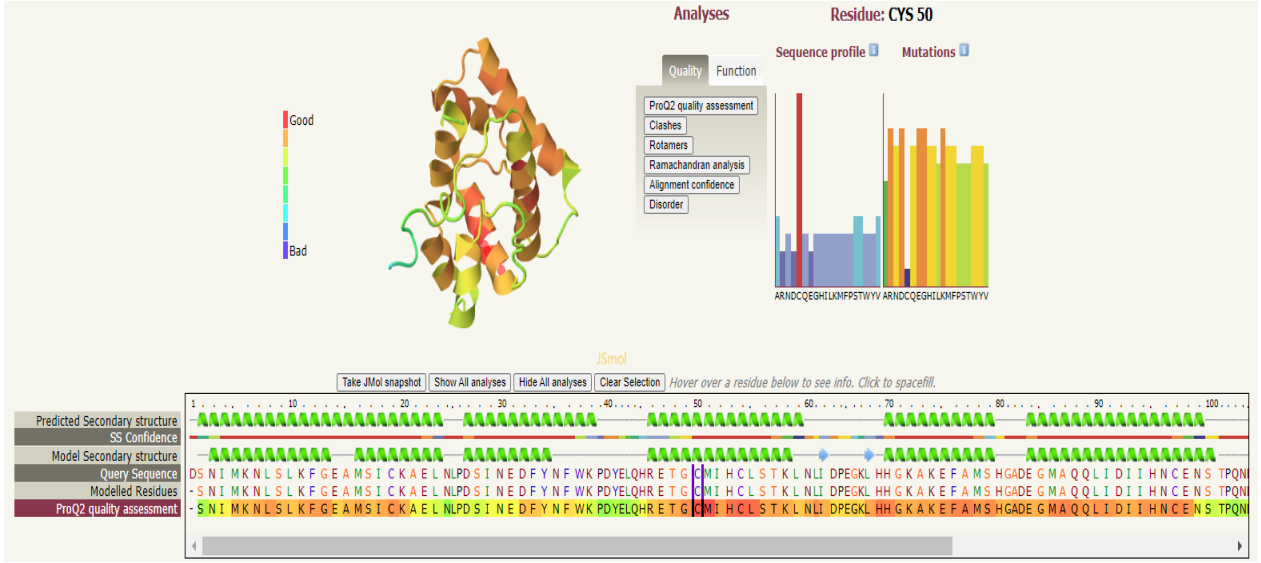


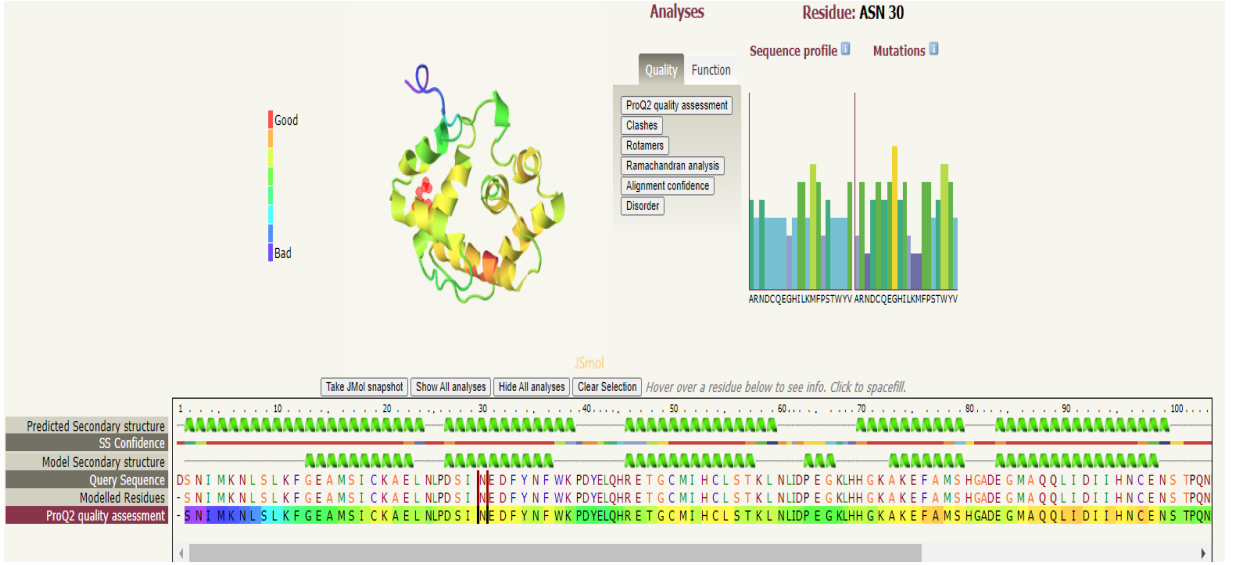

### Plot statistics

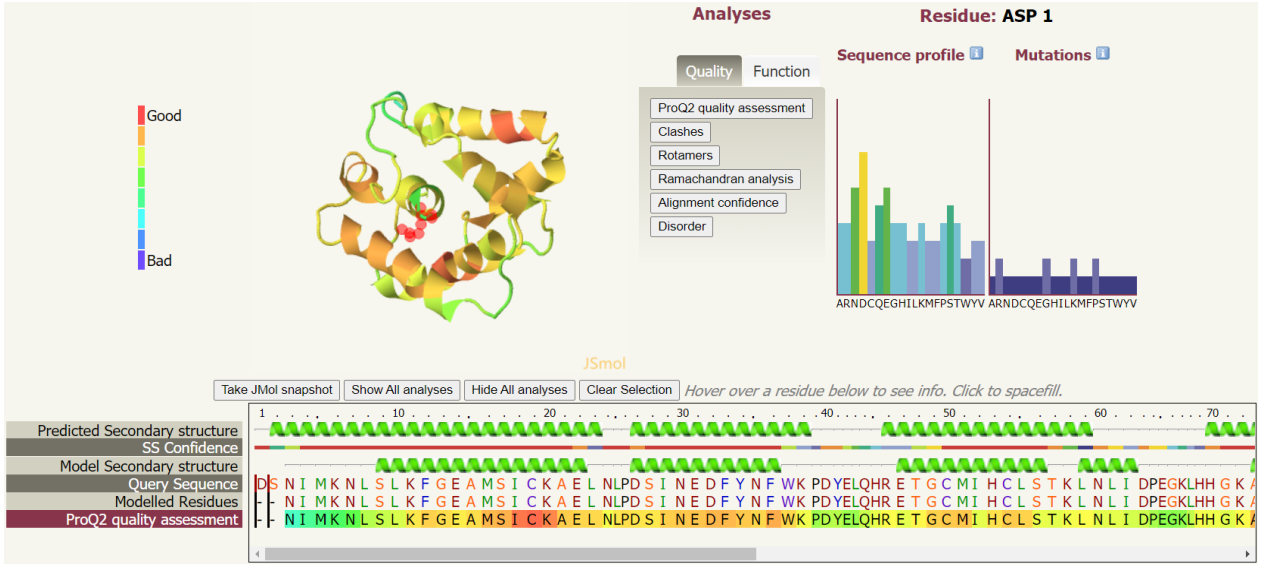
| | | |
|---|---|---|
| aes in most favoured regions [A,B,L] | 111 | 90.2% |
| aes in additional allowed regions [a,b,l,p] | 12 | 9.8% |
| aes in generously allowed regions [~a,~b,~l,~p] | 0 | 0.0% |
| aes in disallowed regions | 0 | 0.0% |
| er of non-glycine and non-proline residues | 123 | 100.0% |
| er of end-residues (excl. Gly and Pro) | 2 | |
| er of glycine residues (shown as triangles) | 8 | |
| er of proline residues | 5 | |
| number of residues | 138 | |

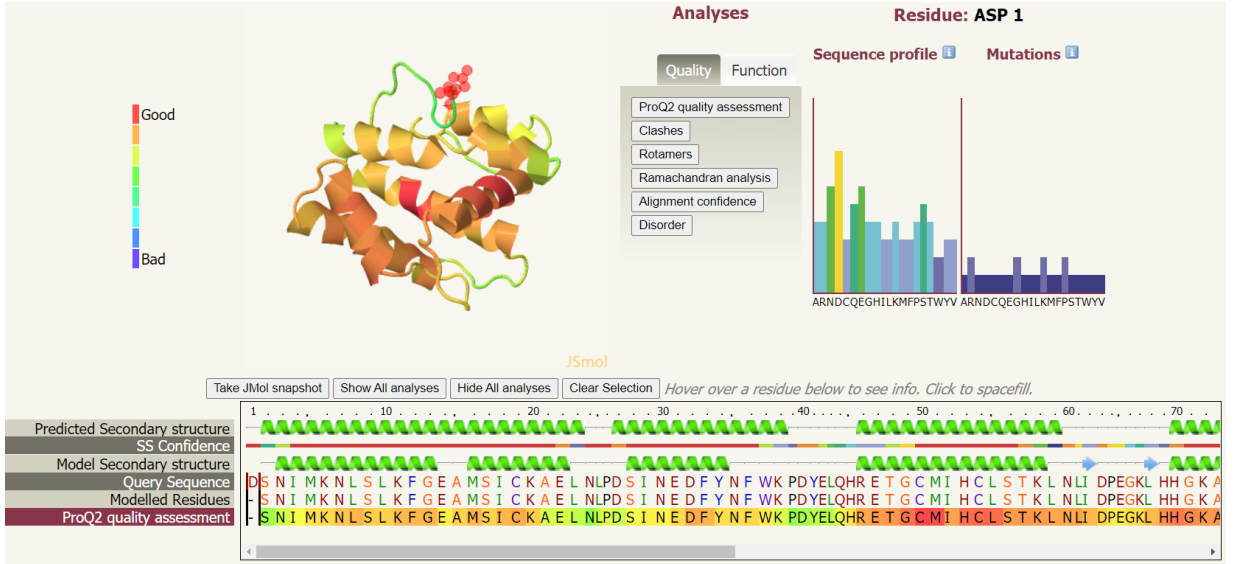
Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

| # | Template | Alignment Coverage | 3D Model | Confidence | % i.d. | Template Information |
|---|---|---|---|---|---|---|
| 1 | c4inwA_ | Alignment |  | 100.0 | 63 | **PDB header:**pheromone-binding protein<br>**Chain:** A: **PDB Molecule:**pheromone-binding protein 1;<br>**PDBTitle:** structure of pheromone-binding protein 1 in complex with (11z,13z)-2 hexadecadienal<br>Run Investigator |
| 2 | c6um9A_ | Alignment |  | 100.0 | 52 | **PDB header:**lipid binding protein<br>**Chain:** A: **PDB Molecule:**pheromone-binding protein 1;<br>**PDBTitle:** gypsy moth pheromone-binding protein 1 (ldispbp1) nmr structure at ph2 4.5<br>Run Investigator |
| 3 | d2jpoa1 | Alignment |  Click to download PDB format model | 100.0 | 65 | **Fold:**EF Hand-like<br>**Superfamily:**Insect pheromone/odorant-binding proteins<br>**Family:**Insect pheromone/odorant-binding proteins<br>Run Investigator |
| 4 | d1dqea_ | Alignment |  | 100.0 | 68 | **Fold:**EF Hand-like<br>**Superfamily:**Insect pheromone/odorant-binding proteins<br>**Family:**Insect pheromone/odorant-binding proteins<br>Run Investigator |


Analyses
Residue: CYS 50
Sequence profile
Mutations
Quality
Function
ProQ2 quality assessment
Clashes
Rotamers
Ramachandran analysis
Alignment confidence
Disorder
Good
Bad
JSmol
Take JMol snapshot
Show All analyses
Hide All analyses
Clear Selection
Hover over a residue below to see info. Click to spacefill.
Predicted Secondary structure
SS Confidence
Model Secondary structure
Query Sequence
Modelled Residues
ProQ2 quality assessment

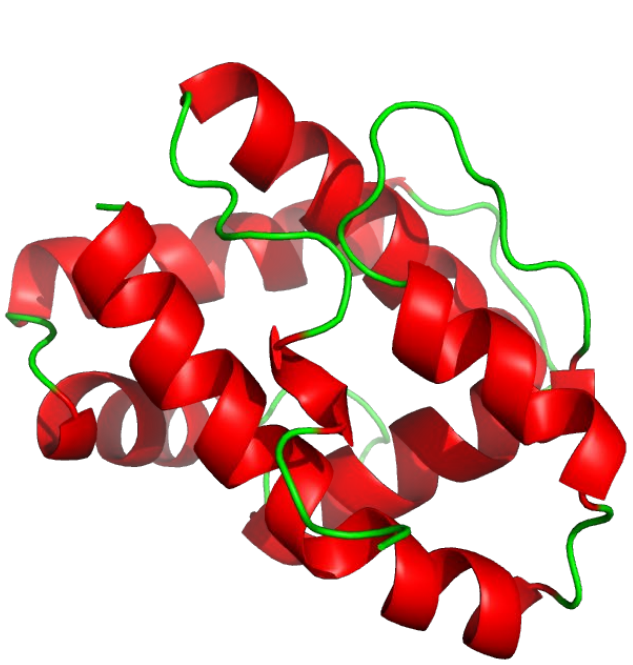

Analyses
Residue: ASN 30
Sequence profile
Mutations
Quality
Function
ProQ2 quality assessment
Clashes
Rotamers
Ramachandran analysis
Alignment confidence
Disorder
Good
Bad
JSmol
Take JMol snapshot
Show All analyses
Hide All analyses
Clear Selection
Hover over a residue below to see info. Click to spacefill.
Predicted Secondary structure
SS Confidence
Model Secondary structure
Query Sequence
Modelled Residues
ProQ2 quality assessment

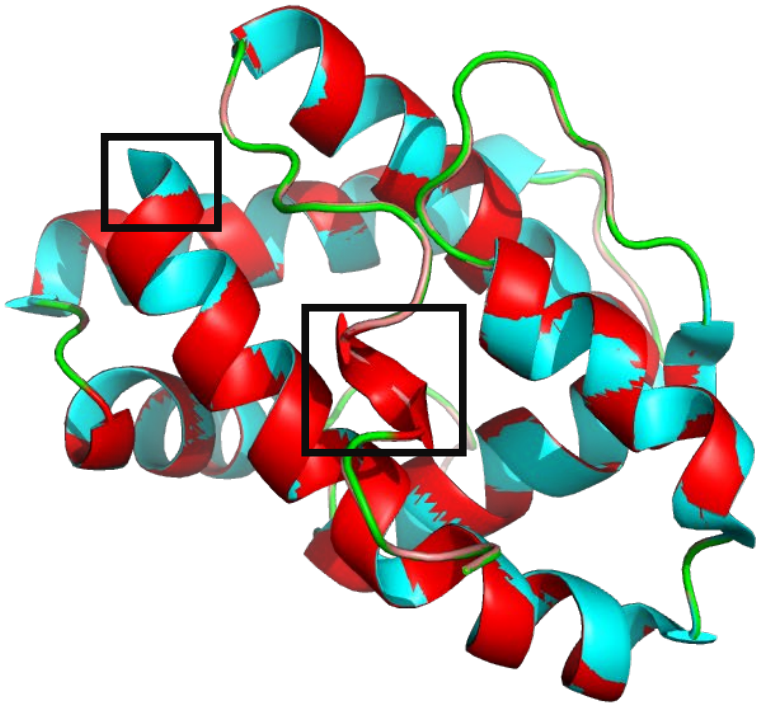

Analyses
Residue: ASP 1
Sequence profile
Mutations
Quality
Function
ProQ2 quality assessment
Clashes
Rotamers
Ramachandran analysis
Alignment confidence
Disorder
Good
Bad
JSmol
Take JMol snapshot
Show All analyses
Hide All analyses
Clear Selection
Hover over a residue below to see info. Click to spacefill.
Predicted Secondary structure
SS Confidence
Model Secondary structure
Query Sequence
Modelled Residues
ProQ2 quality assessment


Analyses
Residue: ASP 1
Sequence profile
Mutations
Quality
Function
ProQ2 quality assessment
Clashes
Rotamers
Ramachandran analysis
Alignment confidence
Disorder
Good
Bad
JSmol
Take JMol snapshot
Show All analyses
Hide All analyses
Clear Selection
Hover over a residue below to see info. Click to spacefill.
Predicted Secondary structure
SS Confidence
Model Secondary structure
Query Sequence
Modelled Residues
ProQ2 quality assessment

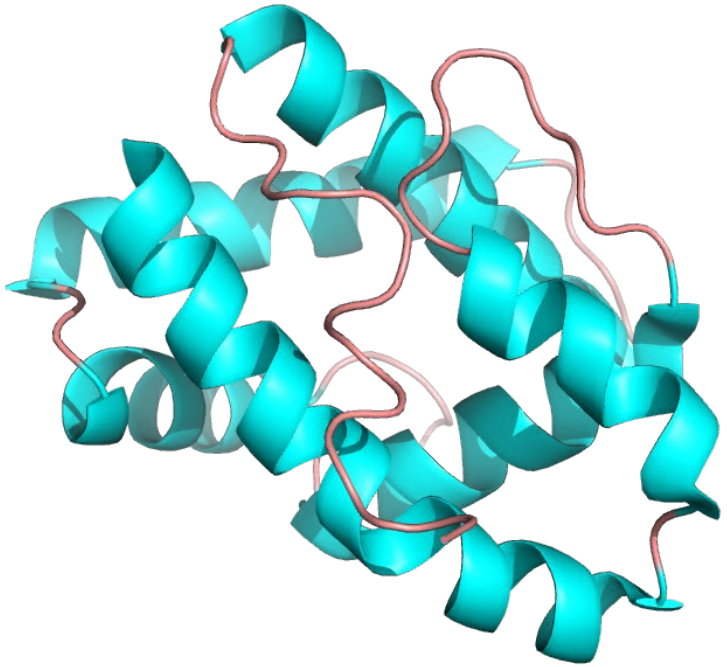
# Model Compare

EbolPBP4





4INW



# Follow-up

- 设计实验验证是否茶尺蠖信息素结合蛋白4位于触角上的毛形感受器上
- 用荧光竞争结合实验探明茶尺蠖信息素结合蛋白4是否有亲和性很高的信息素分子
- 如果有亲和性很高的信息素分子，用软件预测结合分子生物学技术分析它们之间的结合机制，为开发高效杀虫剂提供一个分子基础。

# Thanks for listening !

# Welcome to criticize and correct

# 参考文献


1. Fleischer, J., Pregitzer, P., Breer, H. & Krieger, J. Access to the odor world: olfactory receptors and their role for signal transduction in insects. Cellular and molecular life sciences : CMLS 75, 485–508; 10.1007/s00018-017-2627-5 (2018).
2. Conchou, L. et al. Insect Odorscapes: From Plant Volatiles to Natural Olfactory Scenes. Frontiers in physiology 10, 972; 10.3389/fphys.2019.00972 (2019).
3. Schmidt, H. R. & Benton, R. Molecular mechanisms of olfactory detection in insects: beyond receptors. Open biology 10, 200252; 10.1098/rsob.200252 (2020).
4. Leal, W. S. Odorant reception in insects: roles of receptors, binding proteins, and degrading enzymes. Annual review of entomology 58, 373–391; 10.1146/annurev-ento-120811-153635 (2013).
5. Xu, H. & Turlings, T. C. J. Plant Volatiles as Mate-Finding Cues for Insects. Trends in plant science 23, 100–111; 10.1016/j.tplants.2017.11.004 (2018).