

DMNT对草地贪夜蛾成虫和幼虫行为影响的差异

Effects of DMNT on adult and larval behavior of *Spodoptera frugiperda*

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- 1、研究背景**
- 2、验证序列的准确性**
- 3、蛋白质结构预测**

研究背景

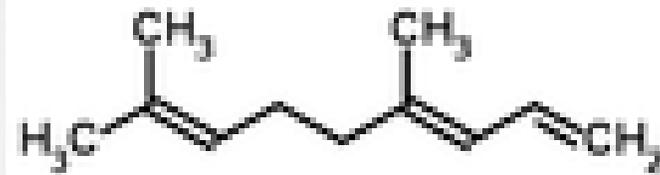
研究对象：草地贪夜蛾 *Spodoptera frugiperda*
DMNT (*E*)-4,8-dimethyl-1,3,7-nonatriene
反式-4,8-二甲基-1,3,7-壬三烯



雄性个体



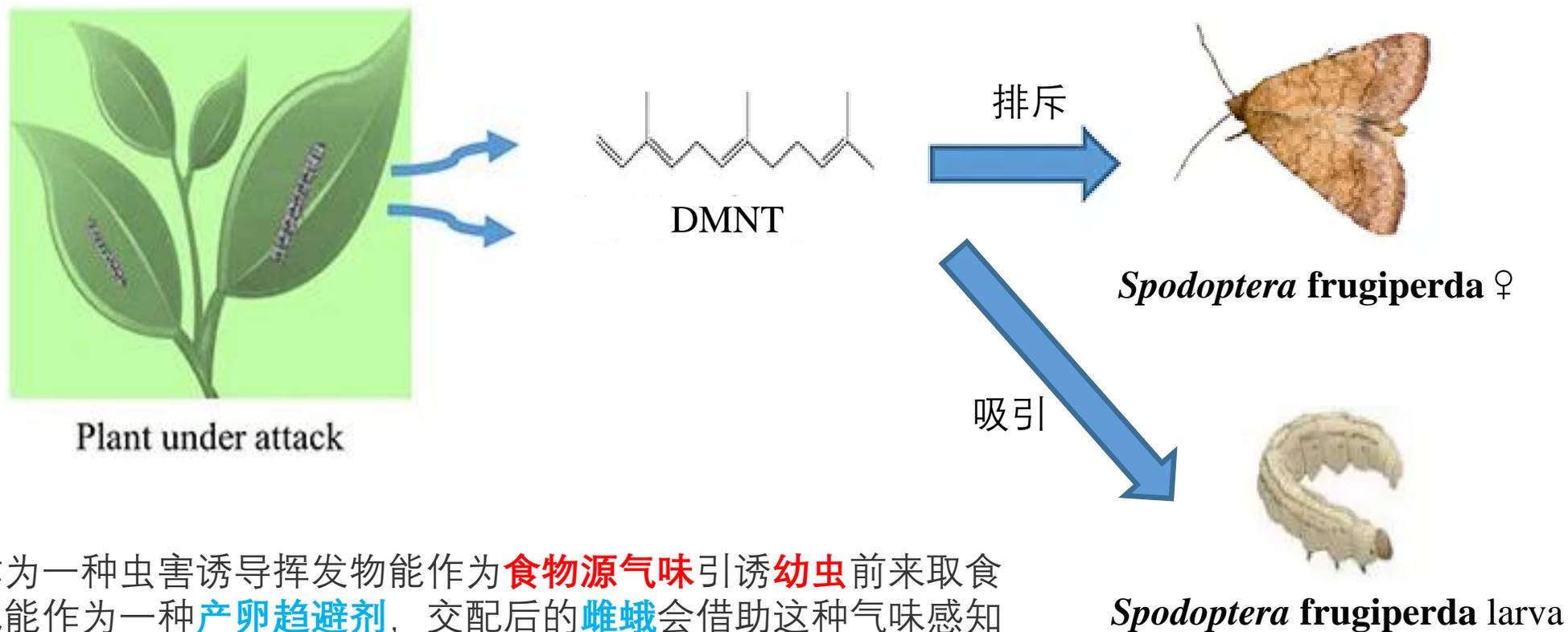
雌性个体



DMNT



文献依据



DMNT作为一种虫害诱导挥发物能作为**食物源气味**引诱**幼虫**前来取食
DMNT也能作为一种**产卵趋避剂**，交配后的**雌蛾**会借助这种气味感知植株被危害的情况，从而选择不产卵。

Yactayo-Chang. *et al.* 2021

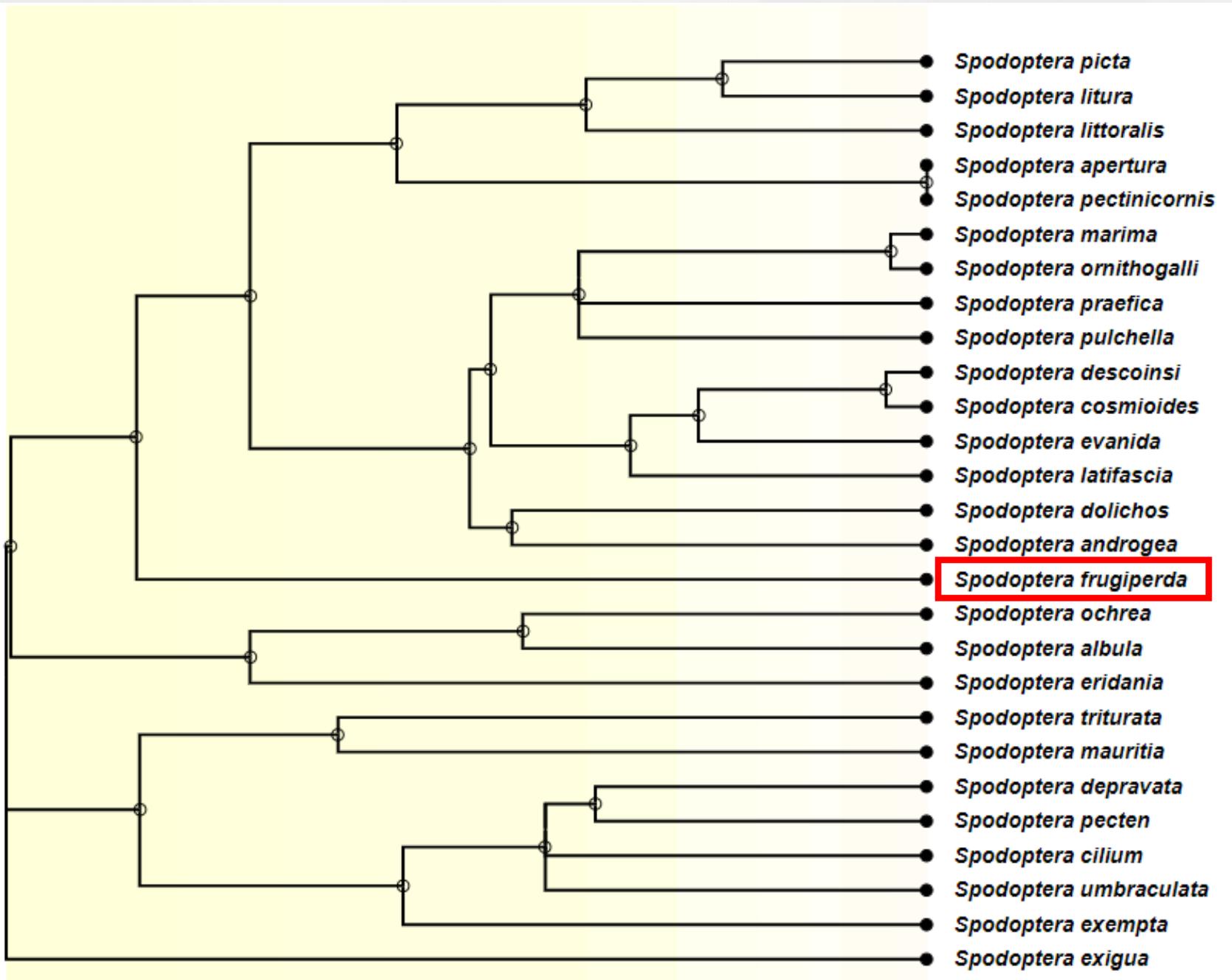
Nascimento. *et al.* 2015

交配后的雌蛾通常不会将卵产在已经有幼虫存在的植株上，
这样会减少其后代的食物来源

夜蛾科noctuidae/灰夜蛾属*Spodoptera*进化时间树



夜蛾科（Noctuidae），昆虫纲，鳞翅目中的1科。全世界已知约2万种，中国已知约1600种。



Spodoptera 灰夜蛾属

草地贪夜蛾

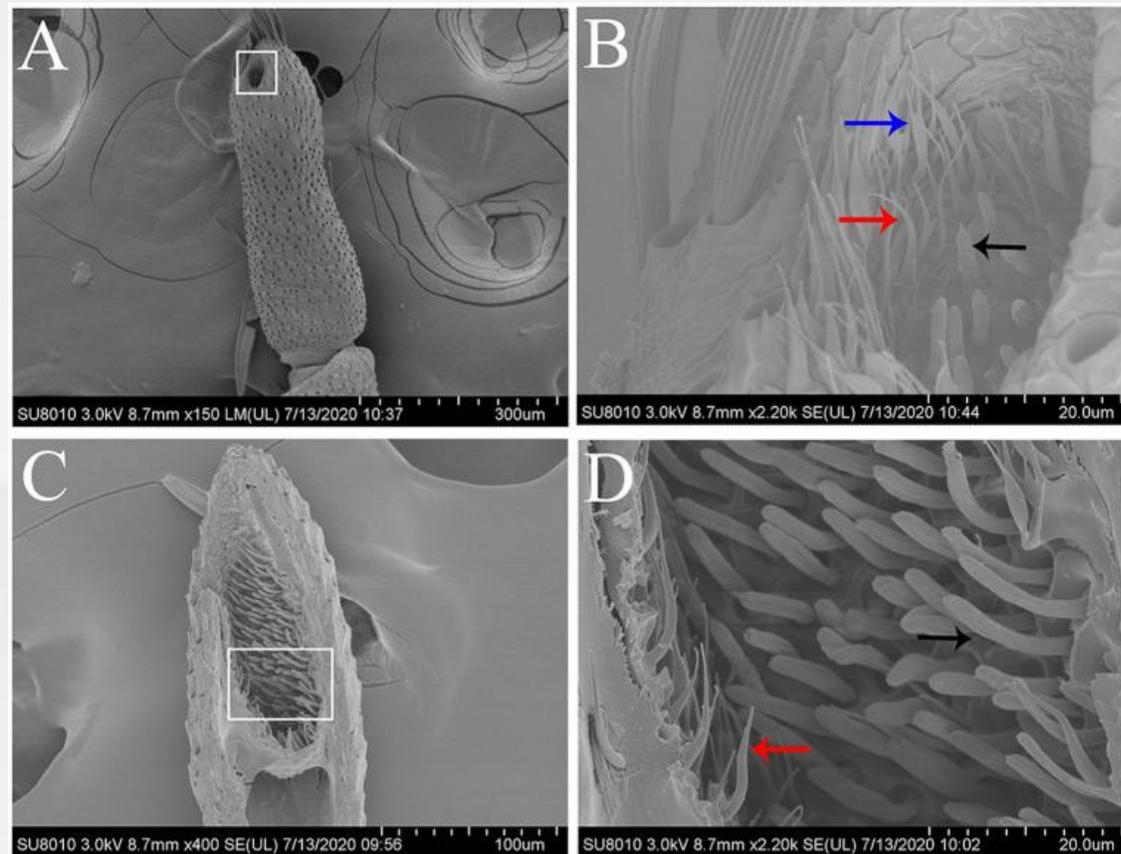
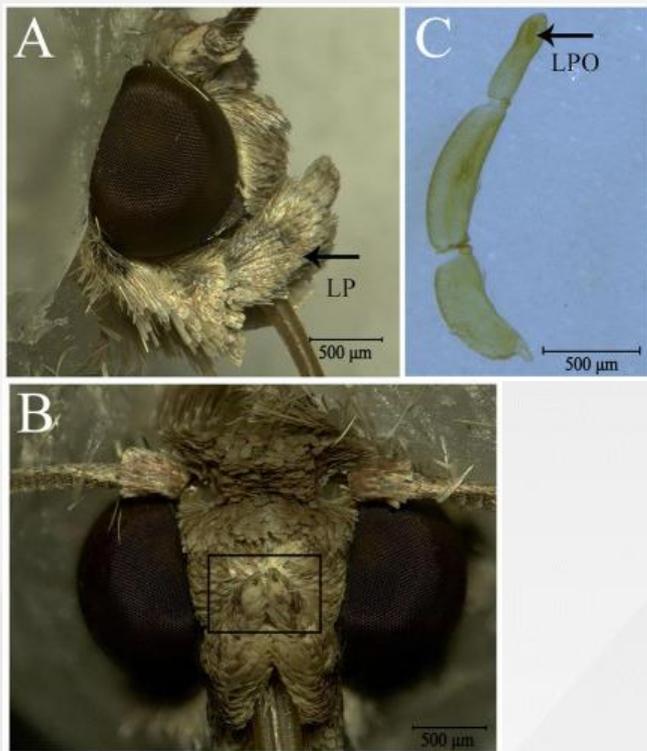
(*Spodoptera frugiperda*)

是夜蛾科灰翅夜蛾属的一种蛾，在农业上属于害虫，其幼虫可大量啃食禾本科如水稻、甘蔗和玉米之类细粒禾穀及菊科、十字花科等多种农作物。

实验基础

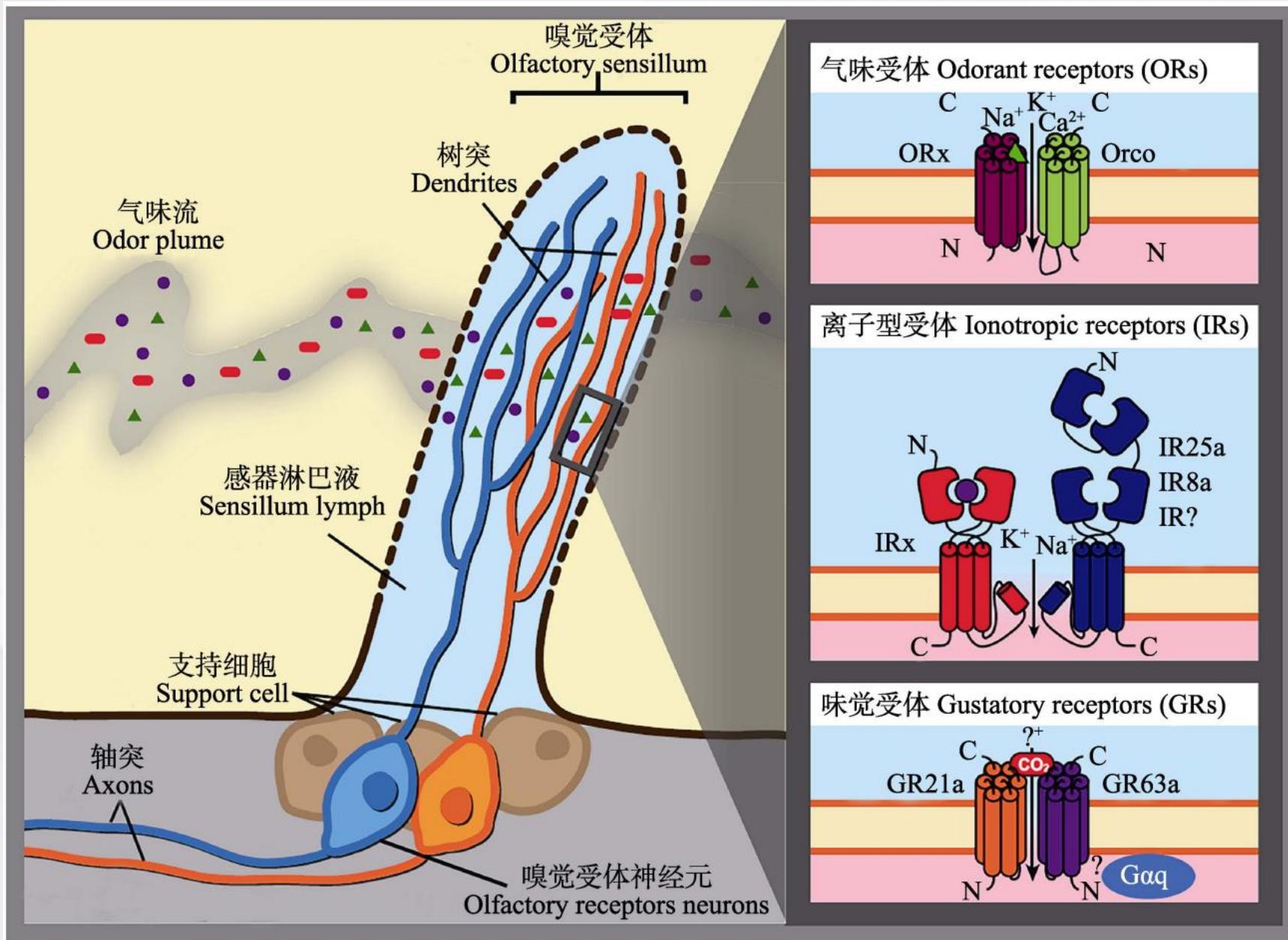
Qiu yan Chen.et al.

Fine Structure and Olfactory Reception of the Labial Palps of *Spodoptera frugiperda*



对其头部和触角进行转录组鉴定并分析，通过爪蟾双电压钳系统进行气味筛选和基因体外功能鉴定

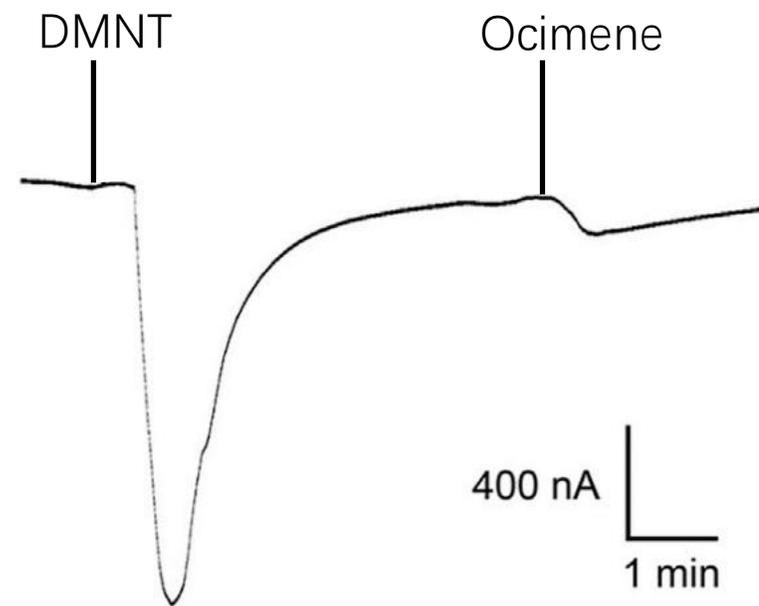
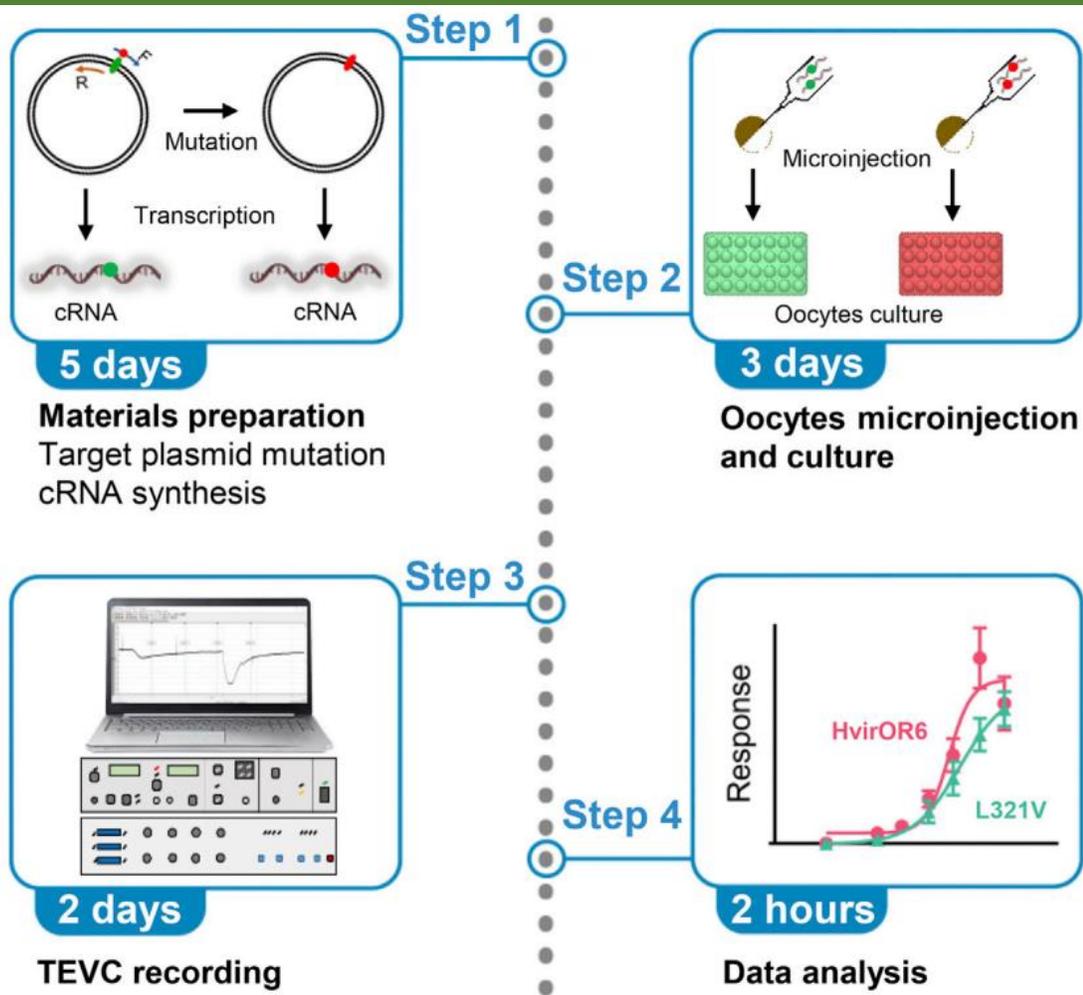
筛选到了SfOR29特异性识别DMNT



Pask and Ray, 2016 绘

每个receptor, 它是由对应的编码的基因来转录翻译得到的

实验基础



将对应的OR基因注射到爪蟾系统里，在体外进行单基因功能的验证

确定基因序列组成以及正确性

通过分离头、触角、胸、腹、足、翅后，进行转录组测序后，
建立cDNA库扩增出来的全长序列
因为**OR基因只在触角**里高表达

```
DNAMAN1
>SfruOR29
ATGAATTCGTTTCTTCAGAGCTTAGAGAATCCAGCGCGACCTTTCCTAGGTCCAAACTACTGGATTCTA
AAGAAAATGGGATTACTTTTACCTAAAAGCAAATTGGGCACAATATTGTACATTTTCTTGCACGAGACT
GTCACATTTTTTGTTCGTTACTCAGTACATGGAGTTGTACGTAATCAGATCAGATTTAGATCTCGTATTG
ACTAACATGAAGATTTCCATGTTAAGCGTGGTTTGCATTTGTTAAAGTGAACACCTTCGTCTTGTGGCAA
AAGCATTGGCGTGAGGTATTGGACTACATTACAGAAGCTGATAATTTTGAACGGCAAAGTGAGGATCCA
GGCAAGATTTCAGATAGTTGAAGCTTACACTAAATACTGCCGGCGGCTCACGTACTTTTACTGGGTTTTG
GTCAGCACAACTTCTTGACAACTACATGTTCACTGATGCGATATTTGTCGTCATCGACTTTTAGA
GAGAACATGCGAAATGGTACAGAACAATTTCCGCACATCTTCAGTTCGTGGATGCCATTTGATAAGTAC
CACTCGCCGGGATGTTGGATCACAGTCCTGTGGCACACAGTACTTTGTGCTTATGGTGCCGCGATTATG
GCGGCCTACGACACTTGTATCGTAGTAACGATGGTATTCTTTGGAGGAAAACCTGGATCTACTTCGTGAG
AGGTGCAAACACATGTTTCGGTTCTTACGGCACTGTAATCACCGACAAGCAGTGCGAGGAGGTAGTACGA
CAGCTGCACGGCATCCATATCATGCTAATAAAGTACTCAAGATTATTTAATTCAGTGTGTCGCCAGTC
ATGTTTTTCTACATGGTCATGTGTTCACTCATGCTTTGTGCGAGCGCCTACCAACTGACTTCCGCTCAG
AATGCCGCGCAGAAGCTTCTGATGGCAGAGTATTTAATTTTTTGAATCGCGCAACTTTTCGTCTTTTGT
TGGCACAGCAACGATGTTTAAATTAATAAATGAGAACATGACGTGAGTCCATTTGAAAGCAACTGGTAC
ACAGCTAACTGTGACAGAAAGAACGTCGCTACTTCTGTGCGGGCAGCTTCGCATCAAGAACATTTTT
ACCGCTGGGCCGTTTCGCCAACCTTACTCTGCCGACCTTCATTAATATACTCAAAGGGGCTTACAGCTAT
TACACATTGCTGAGGAAATAA|
```

Sf OR 29(Spodoptera frugiperda Odorant Receptor 29)

Descriptions

Graphic Summary

Alignments

Taxonomy

Sequences producing significant alignments

Download

Select columns

Show 100



select all 15 sequences selected

[GenBank](#)

[Graphics](#)

[Distance tree of results](#)

[MSA Viewer](#)

	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
<input checked="" type="checkbox"/>	PREDICTED: Spodoptera frugiperda uncharacterized LOC118282435 (LOC118282435), m...	Spodoptera frugiperda	2012	2012	99%	0.0	97.22%	5700	XM_035603511.1
<input checked="" type="checkbox"/>	PREDICTED: Spodoptera frugiperda uncharacterized LOC118282434 (LOC118282434), m...	Spodoptera frugiperda	1962	1962	99%	0.0	96.46%	5674	XM_035603510.1
<input checked="" type="checkbox"/>	PREDICTED: Spodoptera litura uncharacterized LOC111349337 (LOC111349337), mRNA	Spodoptera litura	1714	1714	99%	0.0	92.62%	2938	XM_022960430.1
<input checked="" type="checkbox"/>	Mythimna separata olfactory receptor 51 mRNA, complete cds	Mythimna separata	819	819	99%	0.0	79.16%	1194	MN171159.1
<input checked="" type="checkbox"/>	PREDICTED: Trichoplusia ni uncharacterized LOC113495192 (LOC113495192), mRNA	Trichoplusia ni	577	577	97%	1e-159	75.64%	5983	XM_026873800.1
<input checked="" type="checkbox"/>	Sesamia inferens clone SinfOR32 putative odorant receptor mRNA, partial cds	Sesamia inferens	536	536	95%	2e-147	75.30%	1208	KC960479.1
<input checked="" type="checkbox"/>	Agrochola circellaris genome assembly, chromosome: 6	Agrochola circellaris	531	531	64%	1e-145	79.02%	20906342	OU611845.1
<input checked="" type="checkbox"/>	Noctua pronuba genome assembly, chromosome: 4	Noctua pronuba	470	470	59%	3e-127	78.70%	19064865	LR999896.1
<input checked="" type="checkbox"/>	Diarsia rubi genome assembly, chromosome: 7	Diarsia rubi	468	561	75%	9e-127	77.81%	22522638	OW026418.1
<input checked="" type="checkbox"/>	Griposia aprilina genome assembly, chromosome: 13	Griposia aprilina	457	457	65%	2e-123	77.35%	24562086	OU744296.1
<input checked="" type="checkbox"/>	Eilema depressum genome assembly, chromosome: 6	Eilema depressum	265	265	54%	1e-65	74.28%	23371365	OU612018.1
<input checked="" type="checkbox"/>	Atethmia centrigo genome assembly, chromosome: 8	Atethmia centrigo	156	229	16%	8e-33	84.62%	33210846	HG995374.1
<input checked="" type="checkbox"/>	Acronicta aceris genome assembly, chromosome: 6	Acronicta aceris	73.1	73.1	3%	8e-08	95.56%	17505600	OU342763.1
<input checked="" type="checkbox"/>	Hypena proboscidalis genome assembly, chromosome: 3	Hypena proboscidalis	67.6	67.6	3%	4e-06	97.44%	24208453	LR990129.1
<input checked="" type="checkbox"/>	Protodeltote pygarga genome assembly, chromosome: 3	Protodeltote pygarga	62.1	62.1	3%	2e-04	94.87%	16884165	OW388251.1

LOC118282435

LOC118282434

对SfOR29进行blast, Database选择Nucleotide collection(nr/nt)

Nucleotide Advanced Help

GenBank

Send to

PREDICTED: *Spodoptera frugiperda* uncharacterized LOC118282435 (LOC118282435) mRNA

- Complete Record
- Coding Sequences
- Gene Features

Download features.

Format

NCBI Reference Sequence: XM_035603511.1
[FASTA](#) [Graphics](#)

Go to

LOCUS XM_035603511 5700 bp mRNA linear INV 24-JUL-2020
DEFINITION PREDICTED: *Spodoptera frugiperda* uncharacterized LOC118282435 (LOC118282435), mRNA.
ACCESSION XM_035603511
VERSION XM_035603511.1
DELINK BioProject: [PRJNA647344](#)
KEYWORDS RefSeq; includes ab initio.
SOURCE *Spodoptera frugiperda* (fall armyworm)
ORGANISM [Spodoptera frugiperda](#)
Eukaryota; Metazoa; Ecdysozoa; Arthropoda; Hexapoda; Insecta; Pterygota; Neoptera; Endopterygota; Lepidoptera; Glossata; Ditrysia; Noctuoidea; Noctuidae; Amphipyrinae; Spodoptera.
COMMENT MODEL [REFSEQ](#): This record is predicted by automated computational analysis. This record is derived from a genomic sequence ([NC_049712.1](#)) annotated using gene prediction method: Gnomon.
Also see:
[Documentation](#) of NCBI's Annotation Process

##Genome-Annotation-Data-START##
Annotation Provider :: NCBI

Reference sequence information

RefSeq protein product
See the reference protein sequence for uncharacterized protein LOC118282435 (XP_035459404.1).

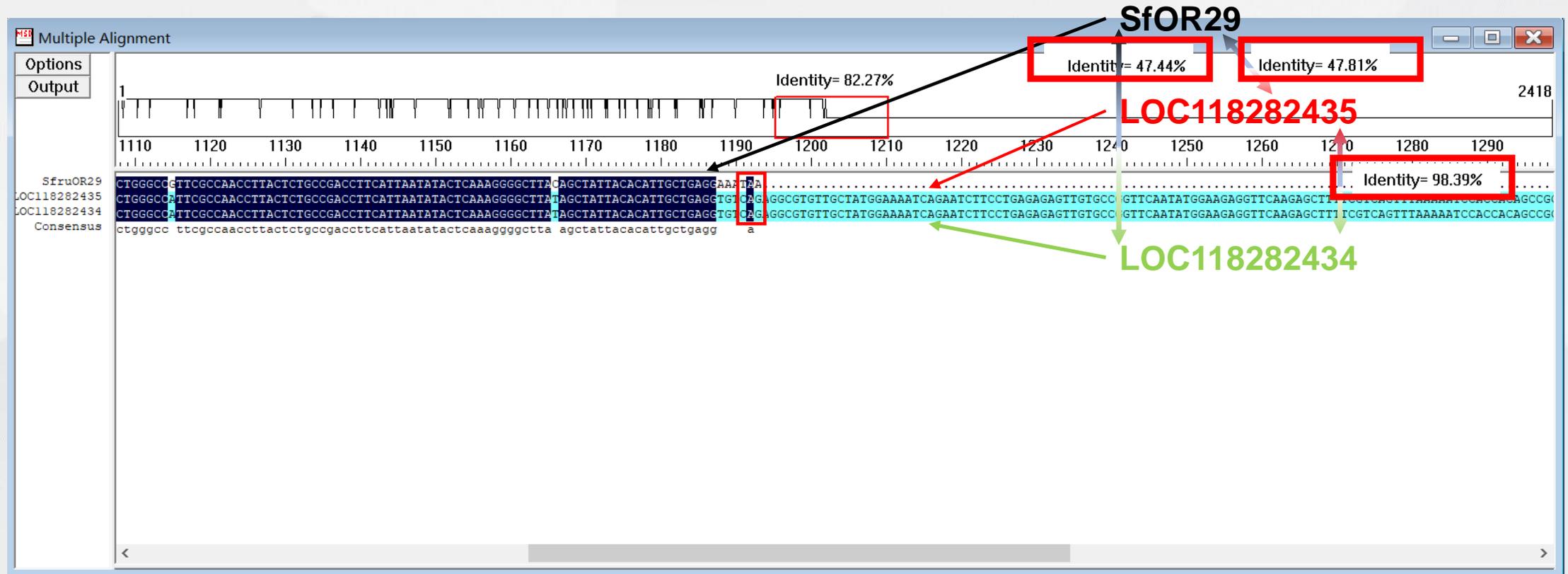
More about the gene LOC118282435

LOC118282435 gene

Related information

BioProject

SfOR29是通过测转录组后用cDNA扩增出的，
NCBI里的是根据基因组测序后预测的，
且根据之前实验室里鳞翅目夜蛾科的转录组测序结果，
编码嗅觉受体序列的长度一般都是**1200bp**左右



蛋白质成分分析

用Expasy内翻译软件对SfruOR29的cDNA进行翻译，选择最合适的氨基酸序列

工具：Expasy-translate

Translate is a tool which allows the translation of a nucleotide (DNA/RNA) sequence to a protein sequence.

DNA or RNA sequence

```
acagaagctgataatTTTgaacggcaagtgaggatccaggcaagattcagatagttgaagcttacactaaactgcccggcgtcacgtactttactgg  
gTTTTggtcagcacaaccttcttgacaactacatgttcaccactgatcogataTTTgctcatcogactTTtagagagaacatgcgaaatgggtacagaaca  
ttccgcacatcttcagttcgtggatgccatttgataagtaaccactcggcgggatggtgacagctcctgtggcacacagctactttgtgcttatgggtcc  
gcatattggcggcctacgacactgtatcgttagtaacgatggtattctttggagaaaactggatcactcgtgagaggtgcaaacacatgttcggttct  
tacggcactgtaatcaccgacaagcagtcgaggaggtagtagcacagctgcacggcattccatcatgctaataaagtactcaagattatttaattcactg  
ctgtcgcagtcactgTTTTctacatgggtcattgttcaactcatgctttgtgcagcgcctaccaactgacttccgctcagaatgccgcgcagaagcttctg  
atggcagagtatttaattttggaatcgcgcaacttttctcttttggcagcagcaacgatgtttaattaaaaatgagaacatgacgtcaggtcattt  
gaaagcaactggtacacagctaacgtgcacagaagaagacgtgctacttctgtcggggcagcttcgatcaagaacattttaccgctgggocgttcgcc  
aaccttactctgccaccttcattaatatactcaaggggcttacagctattacacattgctgaggaaata
```

Output format

- Verbose: Met, Stop, spaces between residues
- Compact: M, -, no spaces
- Includes nucleotide sequence
- Includes nucleotide sequence, no spaces

DNA strands

- forward
- reverse

Genetic codes - See NCBI's genetic codes

Standard

reset

TRANSLATE!

Results of translation

- Open reading frames are highlighted in red
- Select your initiator on one of the following frames to retrieve your amino acid sequence

Download all the translated frames

5'3' Frame 1

```
MNSFLQSLNPARPFLGPNYWILKKMGLLLPKSKLGTILYIFLHETVTFVVTQYMELYVIRSDLDLVLTNMKISMLSVVCIVKVNTFVLWQKHWREVLVDYITEADNFERQSEDPGKIQIVEAYTKYCRRLTYF  
YWVLVSTTFLTTTCSPLMRYLSSSTFRENMRNGTEQFPHFSSWMPFDKYHSPGCWITVLWHTVLCAYGAAI MAAYDTCIVVTMVFFGGKLDLLRERCKHMFGSYGTVITDKQCEEVVRQLHGIHIMLIKYSRL  
FNSLLSPVMFFYMVMCSLMLCASAYQLTSAQNAAQKLLMAEYLIFGIAQLFVFCWHSNDVLIKNNENMTSGPFESNWTANCQRQKDVLLLSGQLRIKNIFTAGPFANLTLPTFINILKGAYSYYTLLRK-
```

>SfruOR29

```
MNSFLQSLNPARPFLGPNYWILKKMGLLLPKSKLGTILYIFLHETVTFVVTQYMELYVIRSDLDLVLTNMKISMLSVVCIVKVNTFVLWQKHWREVLVDYITEADNFERQSEDPGKIQI  
VEAYTKYCRRLTYFYWVLVSTTFLTTTCSPLMRYLSSSTFRENMRNGTEQFPHFSSWMPFDKYHSPGCWITVLWHTVLCAYGAAI MAAYDTCIVVTMVFFGGKLDLLRERCKHMFG  
SYGTVITDKQCEEVVRQLHGIHIMLIKYSRLFNSLLSPVMFFYMVMCSLMLCASAYQLTSAQNAAQKLLMAEYLIFGIAQLFVFCWHSNDVLIKNNENMTSGPFESNWTANCQRQKDV  
VLLLSGQLRIKNIFTAGPFANLTLPTFINILKGAYSYYTLLRK-
```

蛋白质成分分析

UniProt

[BLAST](#) [Align](#) [Retrieve/ID mapping](#) [Peptide search](#) [SPARQL](#)

We are aiming to switch to the new UniProt website on Monday, May 9. Please explore and share your feedback. [Take me to the new website.](#)

UniParc 2022_01 results

UniParc is a comprehensive and non-redundant database that contains most of the publicly available protein **sequences** in the world. Proteins may exist in different source databases and in multiple copies in the same database. UniParc avoids such redundancy by storing each unique sequence only once and giving it a stable and unique identifier (UPI).

A UPI is never removed, changed or reassigned. UniParc contains only protein **sequences**. All other information about the protein must be retrieved from the source databases using the database cross-references.

[Help](#) [UniParc help video](#) [Other tutorials and videos](#) [Downloads](#)

[BLAST](#) [Align](#) [Download](#) [Add to basket](#) [Columns](#) [Share](#)

1 to 1 of 1 Show 100

<input type="checkbox"/>	Entry	Organisms	UniProtKB	First seen	Last seen	Length	<input type="button" value="edit"/>
<input type="checkbox"/>	UPI0015DEDA1	Spodoptera frugiperda (Fall armyworm)		2020-07-25	2021-11-05	805	

1 to 1 of 1 Show 100

UniParc - UPI0015DEDAD1

[BLAST](#) [Format](#) [Add to basket](#) [Columns](#)

- Databases
- Sequence
- InterPro

Filter by:

Active (2)

Organisms

SPOFR (2) ✕

uncharacterized protein LOC118282434 [Spodoptera frugiperda]
NCBI Reference Sequence: XP_035459403.1
[Identical Proteins](#) [FASTA](#) [Graphics](#)

Database	Identifier	Version	Organism	First seen	Last seen	Active
RefSeq	XP_035459403	1	Spodoptera frugiperda (Fall armyworm)	2020-07-25	2021-11-05	Yes
RefSeq	XP_035459404	1	Spodoptera frugiperda (Fall armyworm)	2020-07-25	2021-11-05	Yes

Sequence

uncharacterized protein LOC118282435 [Spodoptera frugiperda]
NCBI Reference Sequence: XP_035459404.1
[Identical Proteins](#) [FASTA](#) [Graphics](#)

Sequence
UPI0015DEDAD1
Checksum¹: 028D2DF63A53A6B3

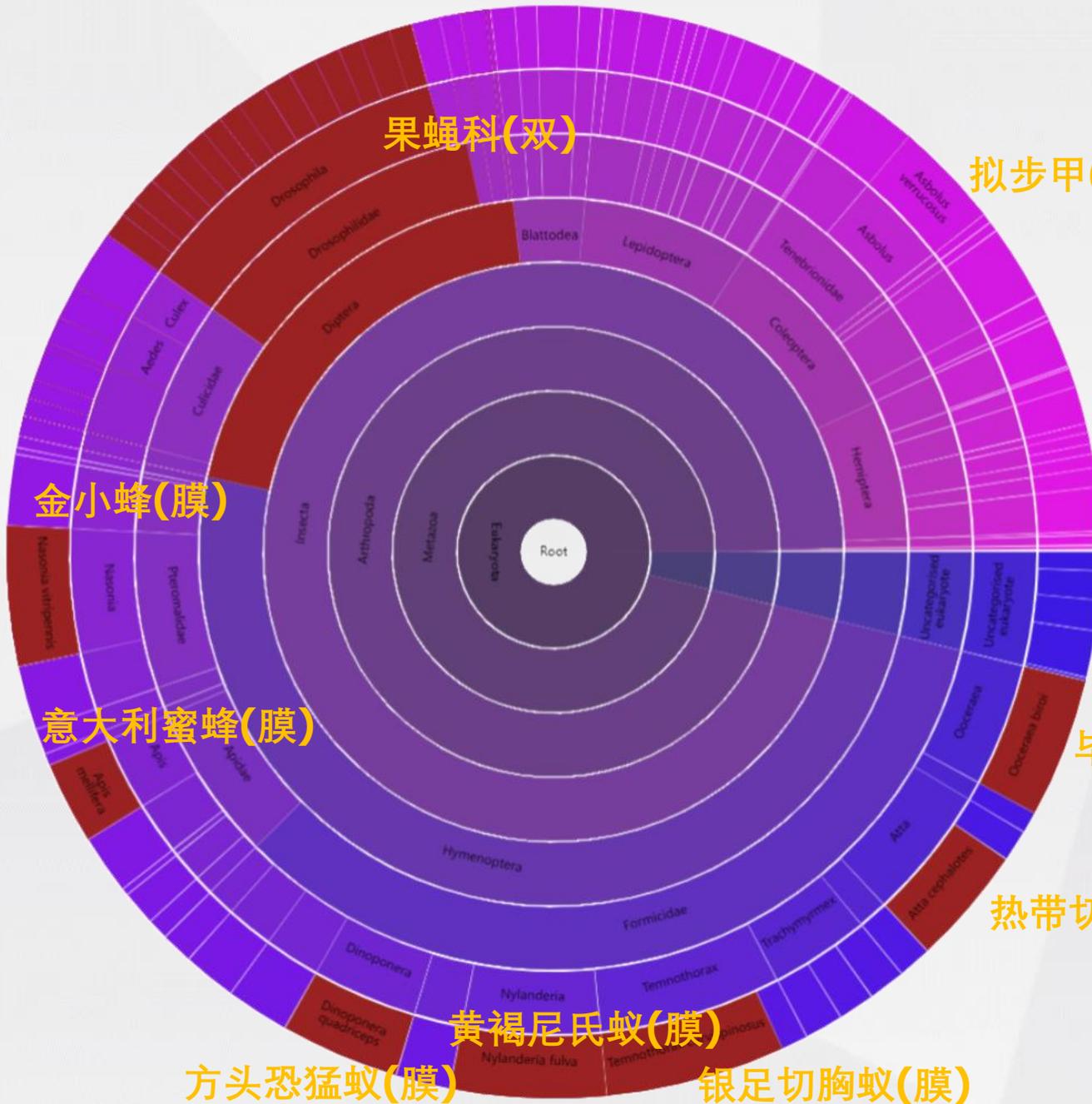
InterPro

InterPro group name	Database Identifier	Graphical view
<u>Olfactory receptor, insect</u>	Pfam PF02949	
	PANTHER PTHR21137	

0 125 250 375 500 625 750

```
AYGAAIMAAY DTCIVVTMVF FGGKLDLLRE RCKHMFSGSYG TVITDKQCEE
    260    270    280    290    300
VVRQLHGIHI MLIKYSRLFN SLLSPVMFFY MVMCSMLCA SAYQLTSAQN
    310    320    330    340    350
AAQKLLMAEY LIFGIAQLFV FCWHSNDVLI KENNTSGPF ESNWYTANCR
    360    370    380    390    400
```

工具: <https://pfam.xfam.org> (EMBL.EBI)



目前昆虫内嗅觉跨膜受体的研究主要集中在模式生物**果蝇**和**膜翅目**以及一些**鞘翅目**昆虫中，*Spodoptera frugiperda*(**鳞**)的还尚未被研究

Search

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PANTHER FAMILY INFORMATION ?

Family: **ODORANT RECEPTOR (PTHR21137)**

Subfamilies: [10](#)

PANTHER Links:



[Tree](#) [MSA](#)

PANTHER GO-slim Molecular Function:

[olfactory receptor activity](#)

PANTHER GO-slim Biological Process:

[response to chemical detection of stimulus](#)
[sensory perception of chemical stimulus](#)

PANTHER GO-slim Cellular Component:

[integral component of membrane](#)
[plasma membrane](#)

PANTHER protein class: **G-protein coupled receptor**

Pathway Categories: No pathway information available

Genes: [359](#)

HMM Length: 379

Downloads: [HMM](#) (HMMER format)

GENES ASSIGNED TO THIS FAMILY

Species	Count
Anopheles gambiae	83
Drosophila melanogaster	60
Tribolium castaneum	216

冈比亚按蚊 双翅目
黑腹果蝇 双翅目
赤拟谷盗 鞘翅目

工具: <http://www.pantherdb.org/panther/>

PTHR21137家族

G-蛋白偶联受体

Family: 7tm_6 (PF02949)

118 architectures

10148 sequences

0 interactions

103 species

4 structures

Summary

Domain organisation

Clan

Alignments

HMM logo

Trees

Curation & model

Species

Structures

AlphaFold Structures

trRosetta Structure

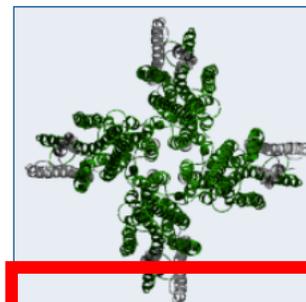
Jump to...  **Summary: 7tm Odorant receptor**

Pfam includes annotations and additional family information from a range of different sources. These sources can be accessed via the tabs below.

This tab holds the annotation information that is stored in the Pfam database. As we move to using Wikipedia as our main source of annotation, the contents of this tab will be gradually replaced by the Wikipedia tab.

7tm Odorant receptor

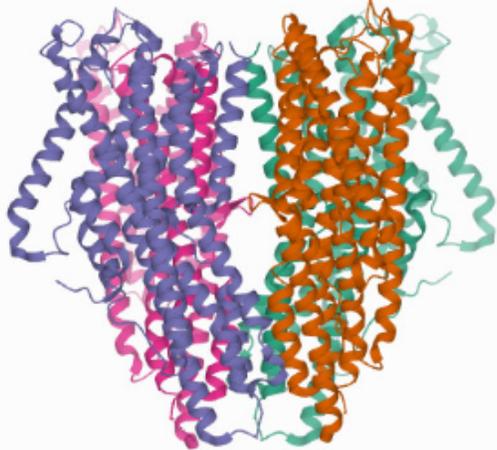
This family is composed of 7 transmembrane receptors, that are probably drosophila odorant receptors.

Internal database linksSCOOP: [7tm_7 Trehalose_recip](#)Similarity to PfamA
using HHSearch: [7tm_7](#)

PDB entry 6C70: Cryo-EM structure of Orco

7 transmembrane=7tm

Biological Assembly 1 ?



3D View: [Structure](#) | [1D-3D View](#) | [Electron Density](#) | [Validation Report](#) | [Predict Membrane](#) ⓘ

Global Symmetry: Cyclic - C4 ⓘ ([3D View](#))
Global Stoichiometry: Homo 4-mer - A4 ⓘ

[Find Similar Assemblies](#)

6C70

Cryo-EM structure of Orco

PDB DOI: [10.2210/pdb6C70/pdb](https://doi.org/10.2210/pdb6C70/pdb) EM Map [EMD-7352:EMDBEMDataResource](#)

Classification: **MEMBRANE PROTEIN**

Organism(s): **Apocrypta bakeri** 榕小蜂(膜翅目)

Expression System: *Homo sapiens*

Mutation(s): No ⓘ

Membrane Protein: Yes ⓘ [OPM](#) [PDBTM](#) [MemProtMD](#) [mpstruc](#)

Deposited: 2018-01-19 Released: 2018-08-22

Deposition Author(s): [Butterwick, J.A.](#), [Kim, K.H.](#), [Walz, T.](#), [Ruta, V.](#)

Funding Organization(s): National Institutes of Health/National Institute Of Allergy and Infectious Diseases (NIH/NIAID)

Experimental Data Snapshot

Method: ELECTRON MICROSCOPY

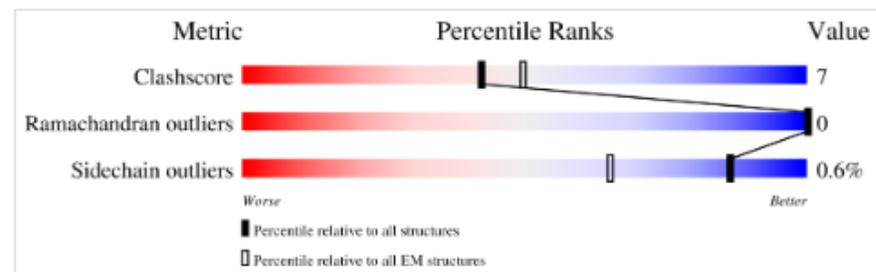
Resolution: 3.50 Å

Aggregation State: PARTICLE

Reconstruction Method: SINGLE PARTICLE

wwPDB Validation ⓘ

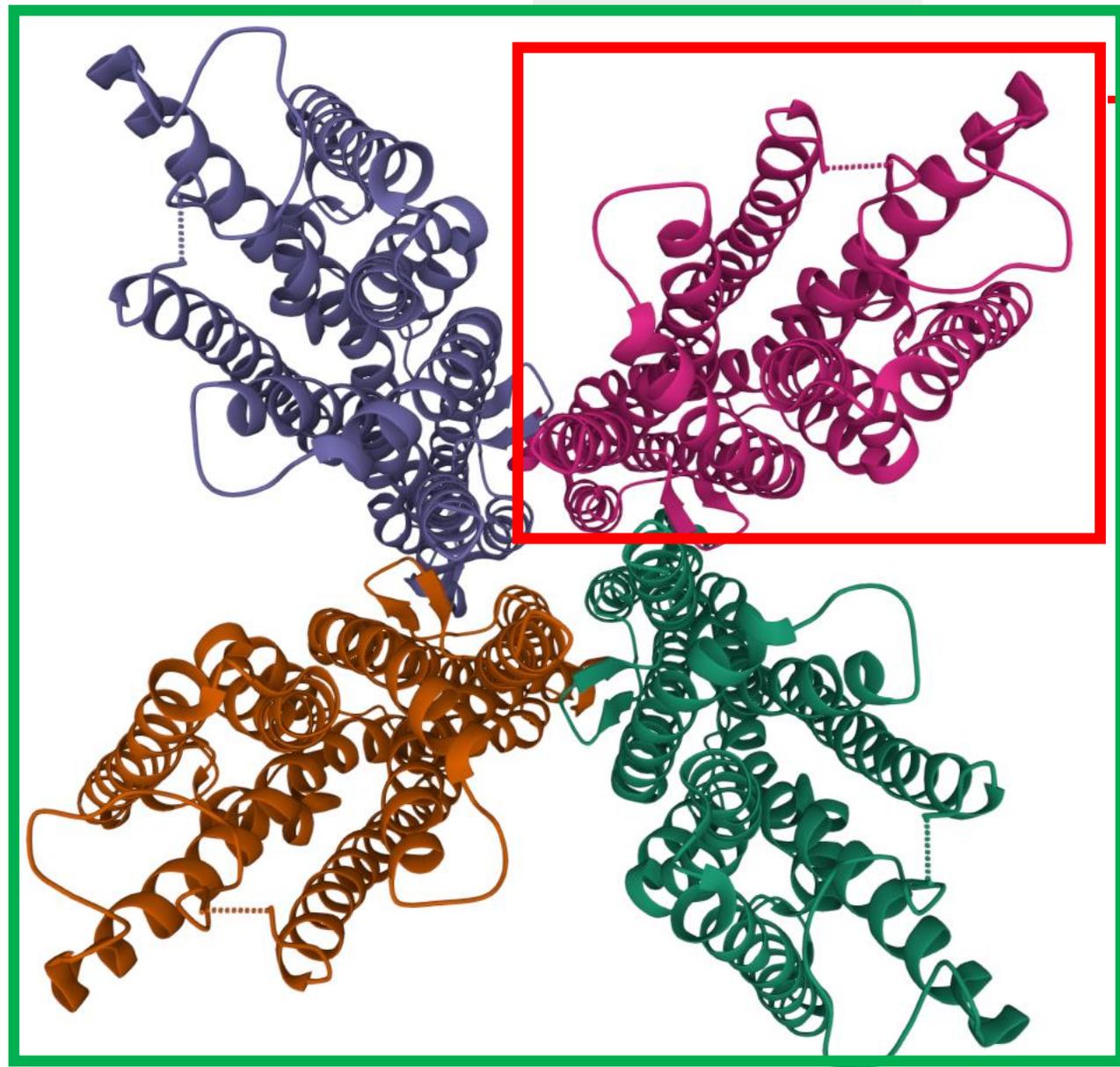
[3D Report](#) [Full Report](#)



This is version 1.3 of the entry. See [complete history](#).

```
Sequence of 6C70 | Cryo-EM structure of Orco | Chain 1: Odorant rec... | A
7 17 27 37 47 57 67 77 87 97 107 117 127 137 147 177 187
GPGRKFKHQ GLVADLLPNI RVMQGVGHFM FNYSEGGKF PHRIYCVITL LLLLQYGM AVNLMESDD VDDLTANTIT MLFFLHPVVK MIYFFVRSKI FYKTLAIWNN PSHPLFAES NARFHALAIT KMRRLLFCVA GATIFSVISW IGITFIEDSV KRITDPEINE TTIIPIPRLM IRTIFYPFNAM SGAGHVFAI
197 207 217 227 237
YQFYVLVISM AVSNSLDLVLF CSWLLFACEQ LQHLKAIMKP LMELSAITLDT VVPSNGELFK AGSADHLRES QGVQPSGNGD NVLDVDLRLGI YSNRQDFTAT FRPTAGTTFN GVGNGNLTG KQEMLVRSAL KYWVERHKHV VRLVIAVGDA YGVALLHML TTIITLTLA YQATKNGVN VYARTVIGYL LYTLGQVFLF
397 407 417 427 437 447 457 467
CIFGNRLIEE SSSVMEAAYS CHWYDGSEEA KTFVQIVCQQ CQKAMSISGA KFFTSLDLF ASVLGAVVY FMLVQLK
```

按 F11 即可退出全屏模式



由七股 α 螺旋组成的受体

由四个同源受体组成的聚合物

Structure

6C70 | Cryo-EM structure of Orco

Type	Assembly
Asm Id	1: Author And Software ...
Dynamic Bonds	× Off
Nothing Focused	

Measurements

Structure Motif Search

Components 6C70

Preset + Add

Polymer Cartoon

Density

Quality Assessment

Assembly Symmetry

Export Models

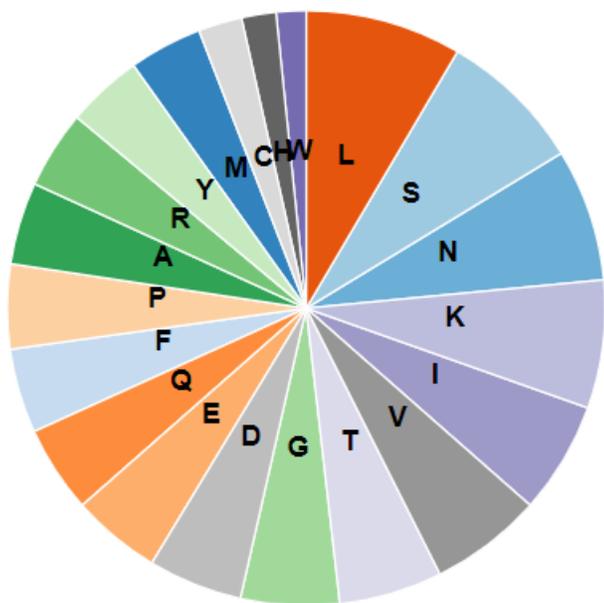
Export Animation

Export Geometry

蛋白理化性质分析——利用Expasy下ProtParam工具

蛋白质氨基酸组成：

Amino Acid composition



Ala (A)	36	4.5%
Arg (R)	34	4.2%
Asn (N)	58	7.2%
Asp (D)	41	5.1%
Cys (C)	19	2.4%
Gln (Q)	38	4.7%
Glu (E)	39	4.8%
Gly (G)	43	5.3%
His (H)	15	1.9%
Ile (I)	49	6.1%
Leu (L)	68	8.4%
Lys (K)	56	7.0%
Met (M)	32	4.0%
Phe (F)	37	4.6%
Pro (P)	37	4.6%
Ser (S)	63	7.8%
Thr (T)	45	5.6%
Trp (W)	13	1.6%
Tyr (Y)	33	4.1%
Val (V)	49	6.1%
Pyl (O)	0	0.0%
Sec (U)	0	0.0%
(B)	0	0.0%
(Z)	0	0.0%
(X)	0	0.0%

(氨基酸数量) Number of amino acids: 805

(分子质量) Molecular weight: 91951.48

(分子式) Formula: $C_{4096}H_{6386}N_{1102}O_{1203}S_{51}$

氨基酸数量前三位：

(亮氨酸) Leu 8.4%

(丝氨酸) Ser 7.8%

(天冬酰胺) Asn 7.2%

(理论等电点) Theoretical pI: 8.61

(不稳定指数) Instability index: 40.24

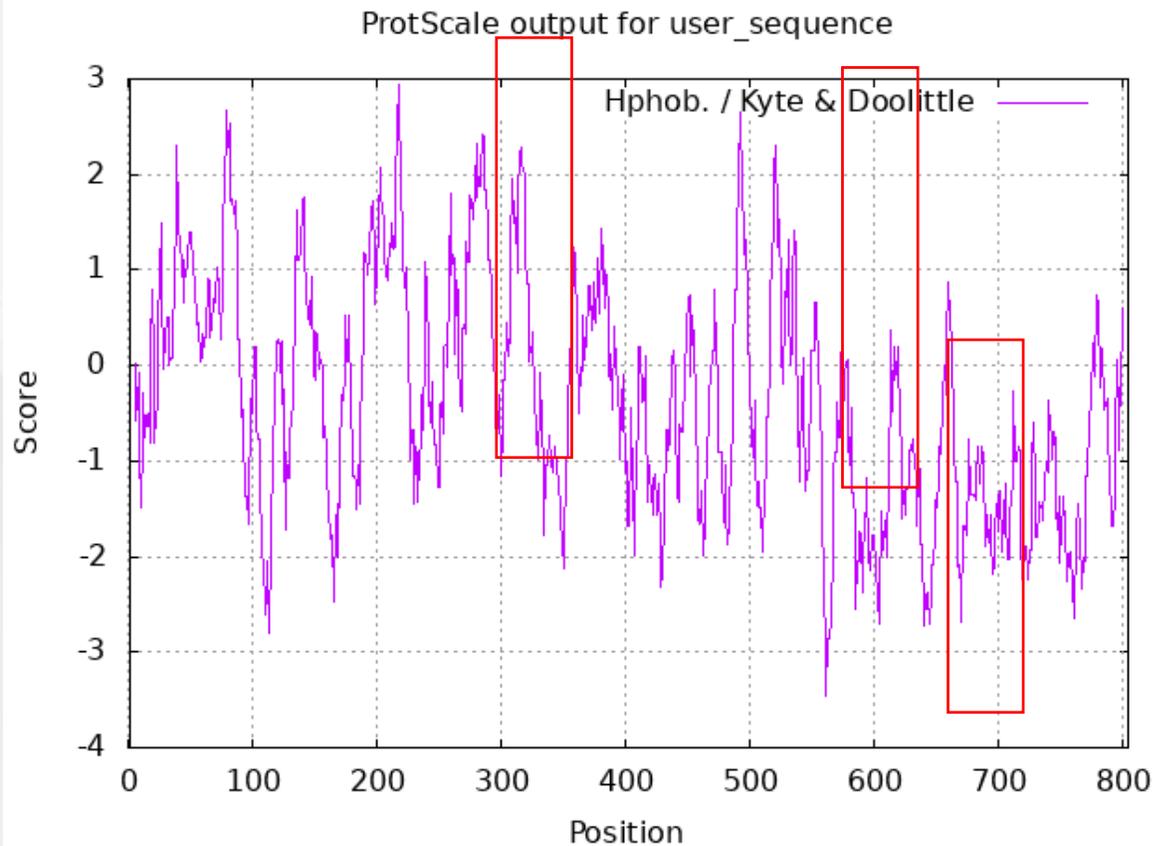
大于40显示蛋白质可能不稳定

(总平均亲水性) GRAVY: -0.356

预测蛋白亲疏水性质——利用Expasy下ProtScale工具

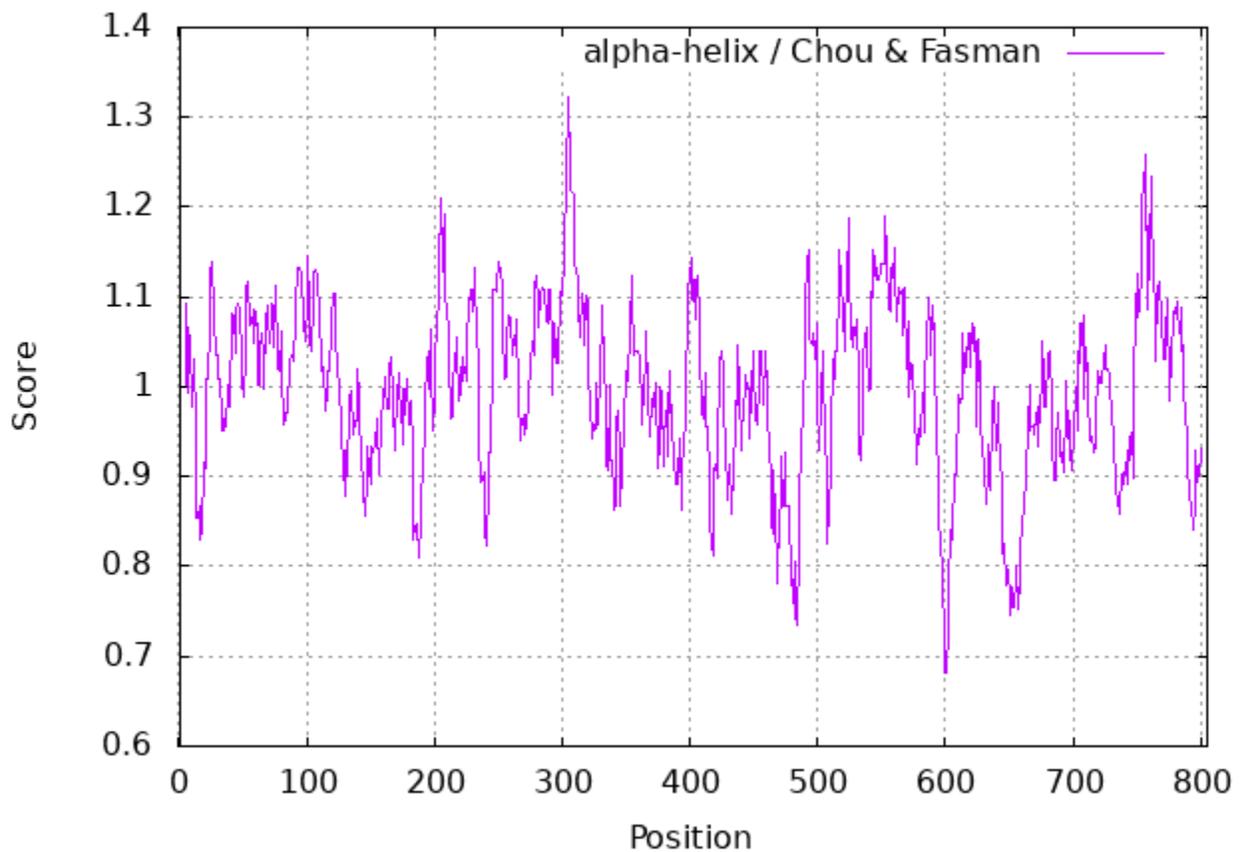
Using the scale **Hphob. / Kyte & Doolittle**, the individual values for the 20 amino acids are:

Ala: 1.800	Arg: -4.500	Asn: -3.500	Asp: -3.500	Cys: 2.500	Gln: -3.500
Glu: -3.500	Gly: -0.400	His: -3.200	Ile: 4.500	Leu: 3.800	Lys: -3.900
Met: 1.900	Phe: 2.800	Pro: -1.600	Ser: -0.800	Thr: -0.700	Trp: -0.900
Tyr: -1.300	Val: 4.200	: -3.500	: -3.500	: -0.490	

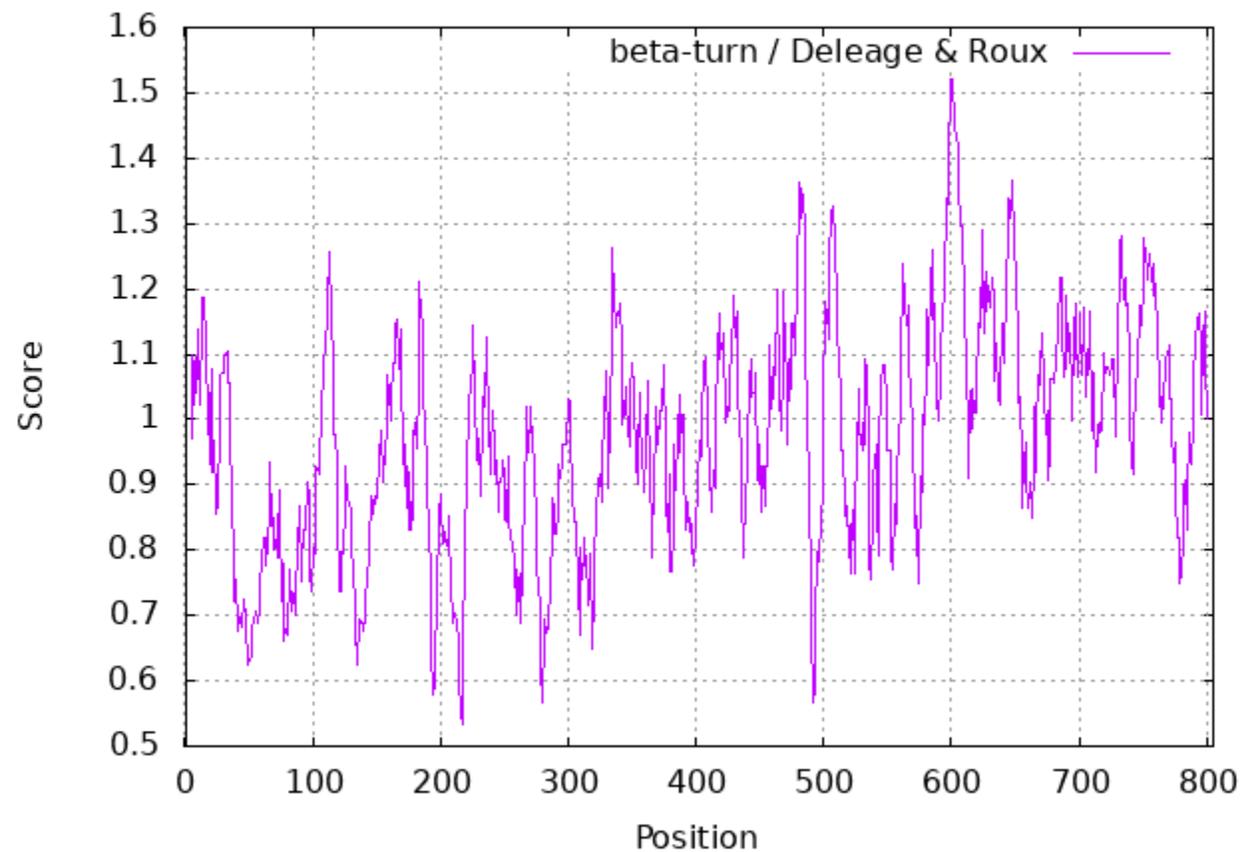


正值表示疏水
负值表示亲水

ProtScale output for user_sequence



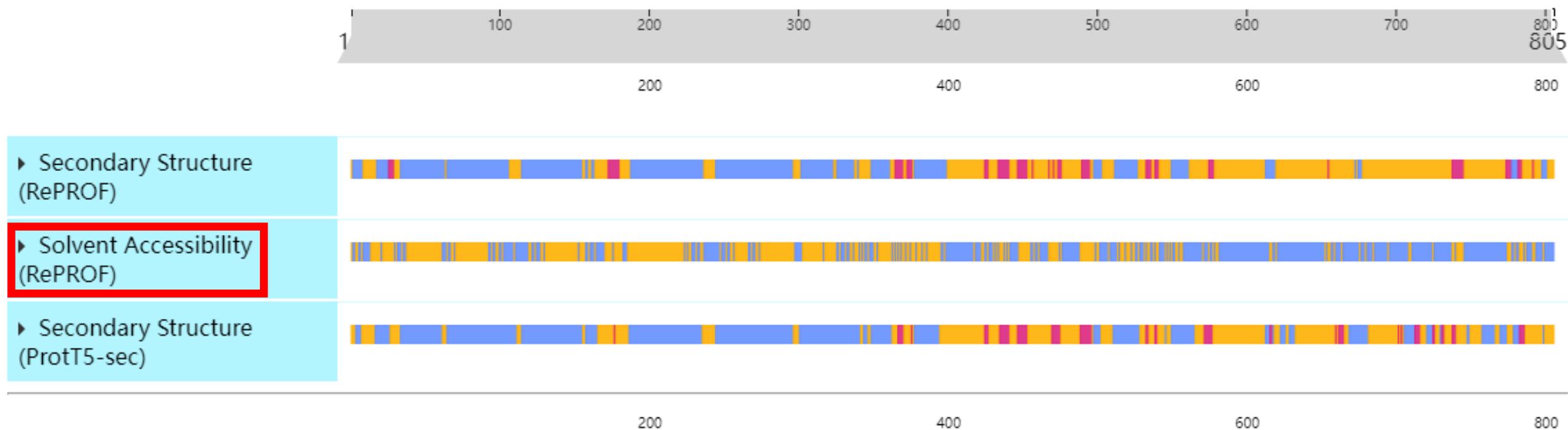
ProtScale output for user_sequence



预测蛋白结构, α 螺旋和 β 折叠

预测蛋白二级结构——工具：PredictProtein

Secondary Structure and Solvent Accessibility Prediction



蛋白质点突变分析



Domains:

Archaea

Bacteria

Eukarya

预测蛋白二级结构——工具: PredictProtein



Predicted localization for the Eukarya domain: Plasma Membrane (GO term ID: [GO:0005886](#)) Prediction confidence 1

蛋白质位点预测显示，他是在质膜上表达功能的，这符合我们预测蛋白质的主要功能

蛋白质结构预测

工具: <https://swissmodel.expasy.org/>



Oligo-State Ligands
Monomer None

GMQE QMEANDisCo Global
0.09 **0.53** ± 0.08

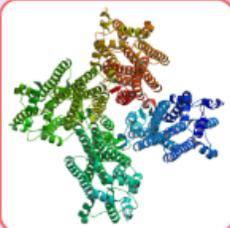
QMEANDisCo Local | QMEAN Z-Scores

Template	Seq Identity	Coverage	Description
4cse.1.A	21.93%	<div style="width: 20%;"></div>	PIH1 DOMAIN-CONTAINING PROTEIN 1 PIH N-terminal domain

Model 02 ▾

Structure Assessment

Model-Template Alignment



Oligo-State Ligands
Homo-tetramer (matching prediction) None

GMQE QMEANDisCo Global
0.26 **0.54** ± 0.05

QMEANDisCo Local | QMEAN Z-Scores

Membrane annotation has been transferred from template.
 Show / Hide

Template	Seq Identity	Coverage	Description
7lid.1.A	15.14%	<div style="width: 15%;"></div>	MhOR5 The structure of the insect olfactory receptor OR5 from <i>Machilis hrabei</i> in complex with eugenol

Model 01 ▾

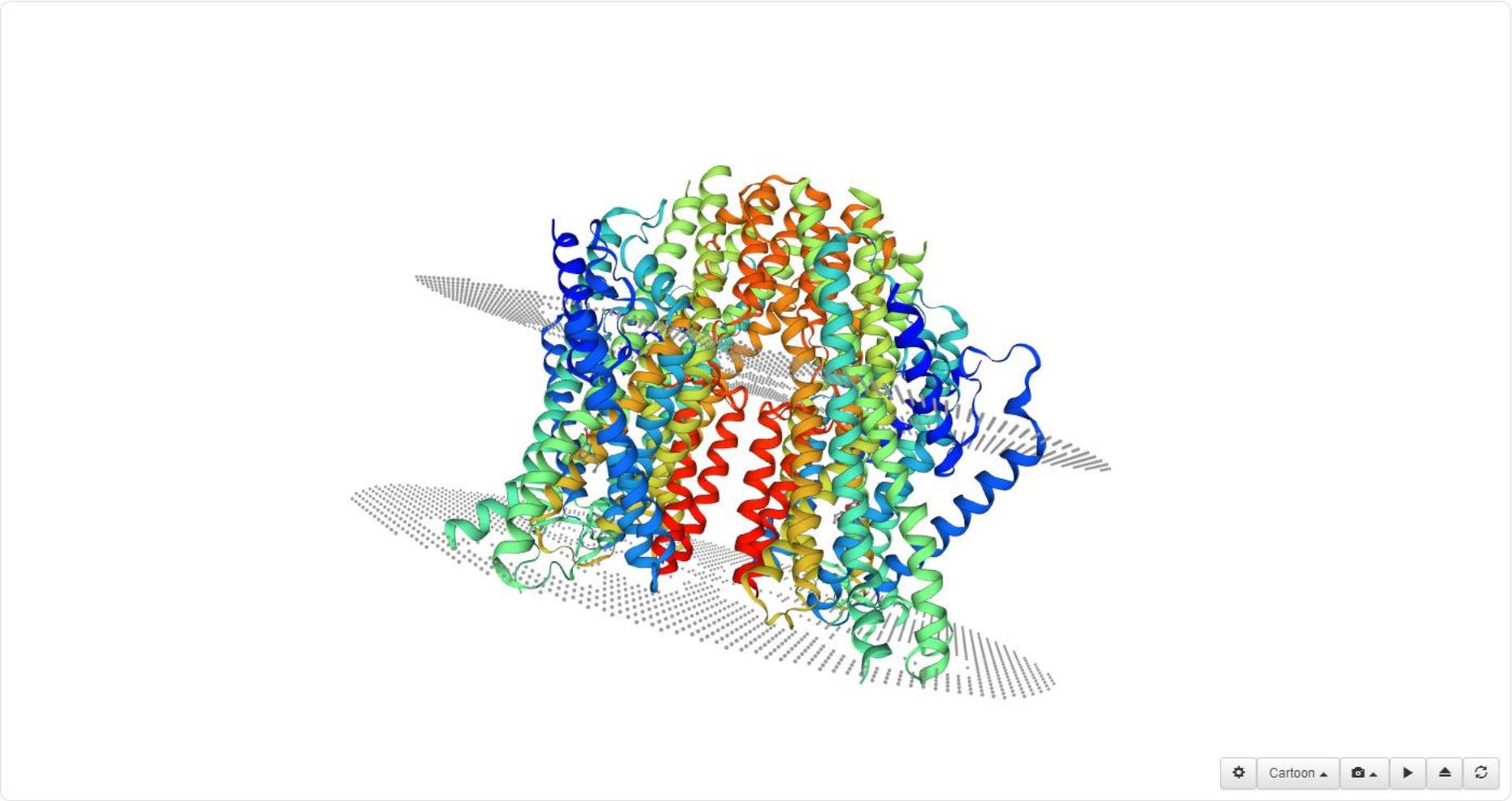
Structure Assessment

Machilis hrabei 石蛎

SMTL ID : 7lid.1

The structure of the insect olfactory receptor OR5 from *Machilis hrabei* in complex with eugenol

Coordinates	PDB Format
Method	ELECTRON MICROSCOPY
Oligo State	homo-tetramer
Ligands	4 x EOL: 2-methoxy-4-(prop-2-en-1-yl)phenol (Non-covalent)
Links	RCSB PDB PDBE-KB PDB PDBsum CATH PLIP
Citation	Del Marmol, J. et al., The structural basis of odorant recognition in insect olfactory receptors. Nature (2021) doi
Release Date	2021-08-11
Peptides	MhOR5: A B C D
SMTL:PDB	SMTL Chain Id: A B C D PDB Chain Id: A B C D
Membrane	We predict this structure to be a membrane protein. <input checked="" type="checkbox"/> Show / Hide



Cartoon | Camera | Play | Home | Refresh

MhOR5

Toggle Identical (ABCD)

Seqes	SFGRAKIDVDSVDHIDDYIHLRKKWKRI	30
7lid.1. (ABCD)	SDYIHLRKKWKRI	30
Seqes	ILRISGHWPFLPHEKRNQHKSKFRQVYSC	60
7lid.1. (ABCD)	ILRISGHWPFLPHEKRNQHKSKFRQVYSC	60
Seqes	LVITLGFITCSCYICGLCLSESIQAALNNI	90
7lid.1. (ABCD)	LVITLGFITCSCYICGLCLSESIQAALNNI	90

Machilis hrabei (3)

TAXONOMY

 Eukaryota (3)

EXPERIMENTAL METHOD

 ELECTRON MICROSCOPY (3)

POLYMER ENTITY TYPE

 Protein (3)

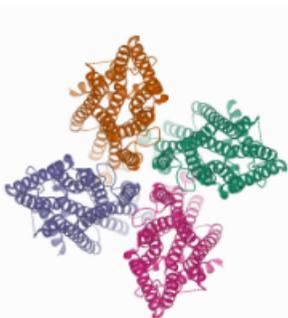
REFINEMENT RESOLUTION (Å)

 2.5 - 3.0 (2) 3.0 - 3.5 (1)

RELEASE DATE

 2020 - 2024 (3)

SYMMETRY TYPE

 Cyclic (3)

3D View

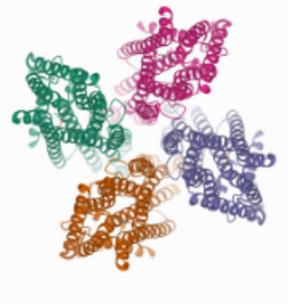
7LIC

The structure of the insect olfactory receptor **OR5 from Machilis hrabei**

del Marmol, J., Ruta, V.

(2021) Nature **597**: 126-131

Released 2021-08-11
Method ELECTRON MICROSCOPY 3.3 Å
Organisms Machilis hrabei
Macromolecule MhOR5 (protein)

[Download File](#) [View File](#) 

3D View

7LID

The structure of the insect olfactory receptor **OR5 from Machilis hrabei** in complex with eugenol **丁香子酚**

del Marmol, J., Ruta, V.

(2021) Nature **597**: 126-131

Released 2021-08-11
Method ELECTRON MICROSCOPY 2.9 Å
Organisms Machilis hrabei
Macromolecule MhOR5 (protein)
Unique Ligands EOL

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3D View

7LIG

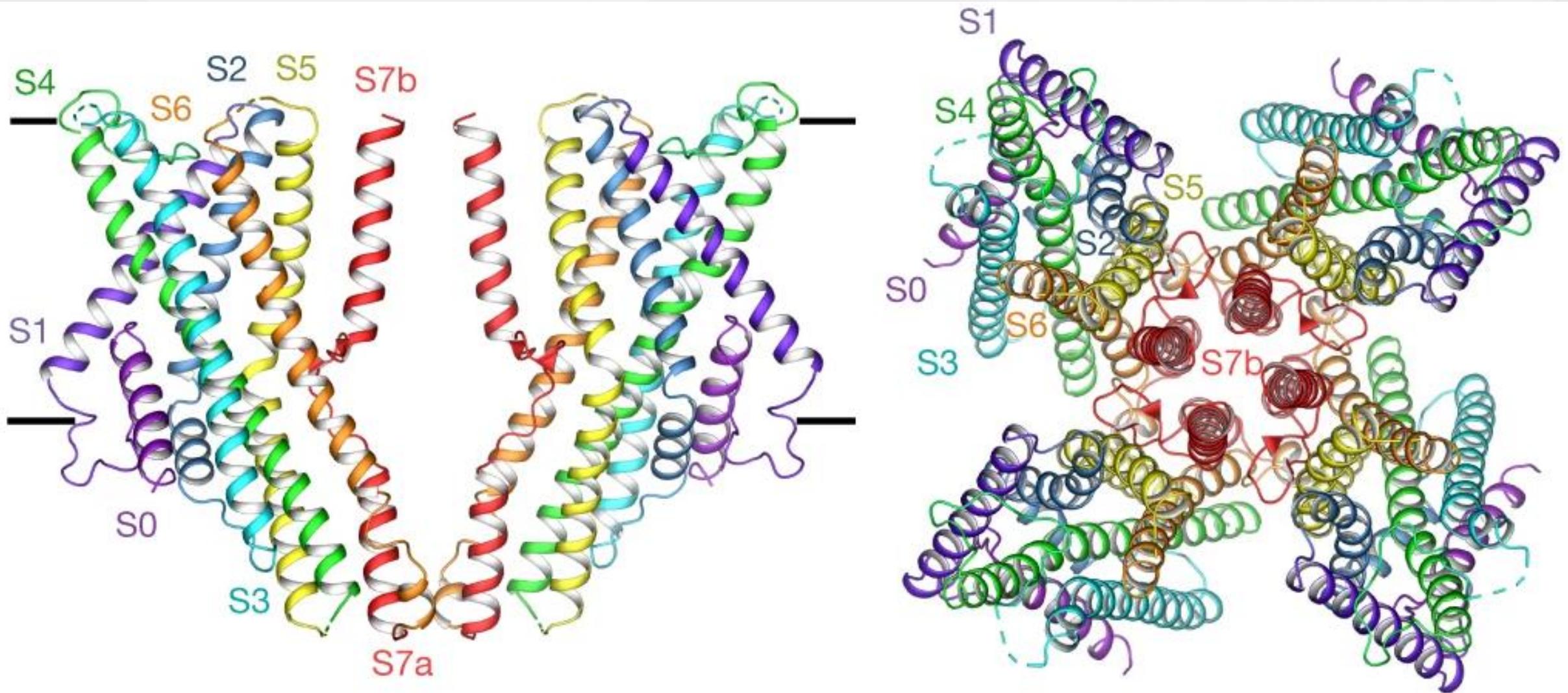
The structure of the insect olfactory receptor **OR5 from Machilis hrabei** in complex with DEET **避蚊胺**

del Marmol, J., Ruta, V.

(2021) Nature **597**: 126-131

Released 2021-08-11
Method ELECTRON MICROSCOPY 2.9 Å
Organisms Machilis hrabei
Macromolecule MhOR5 (protein)
Unique Ligands DE3

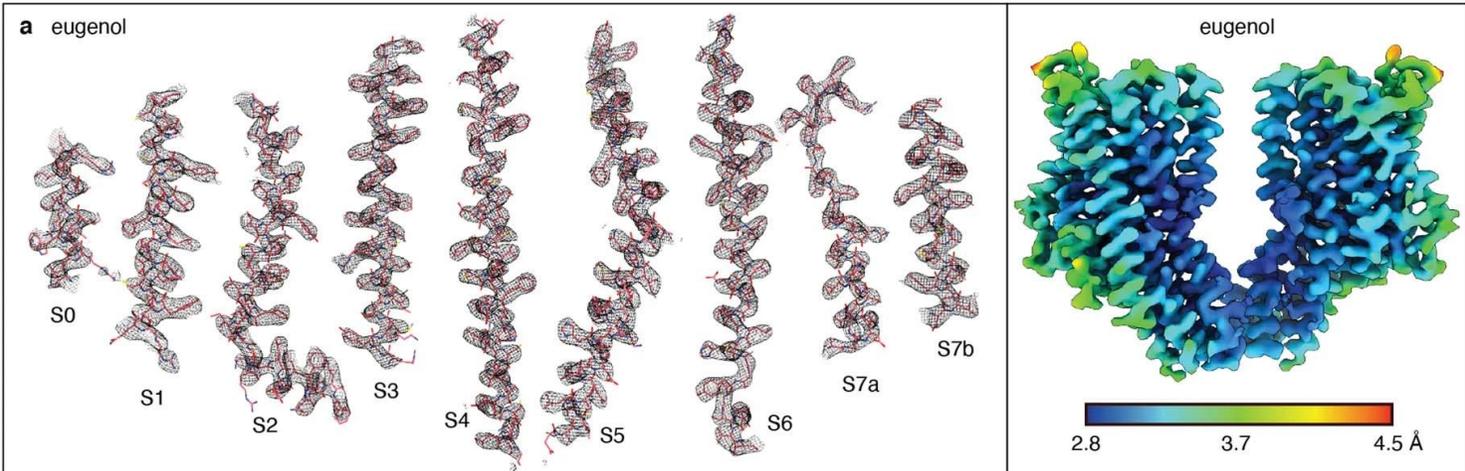
[Download File](#) [View File](#)



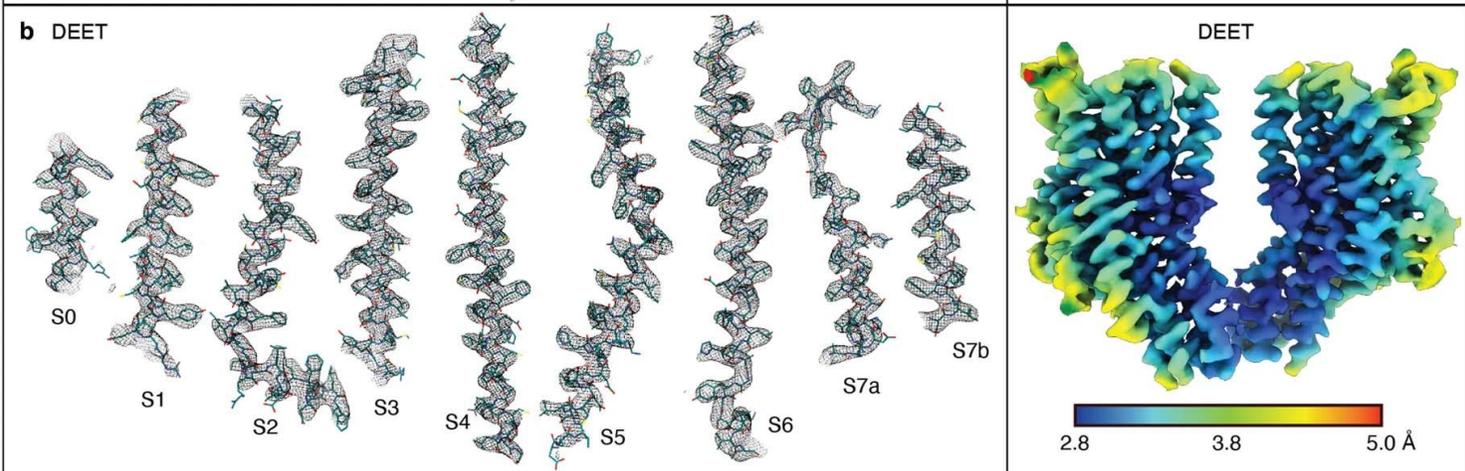
S0-S6是固定结构，S7由a和b组成，S7b为可活动臂，整个聚合体靠**四个可活动的S7b**来结合气味分子

Josefina Del Marmol . *et al.*

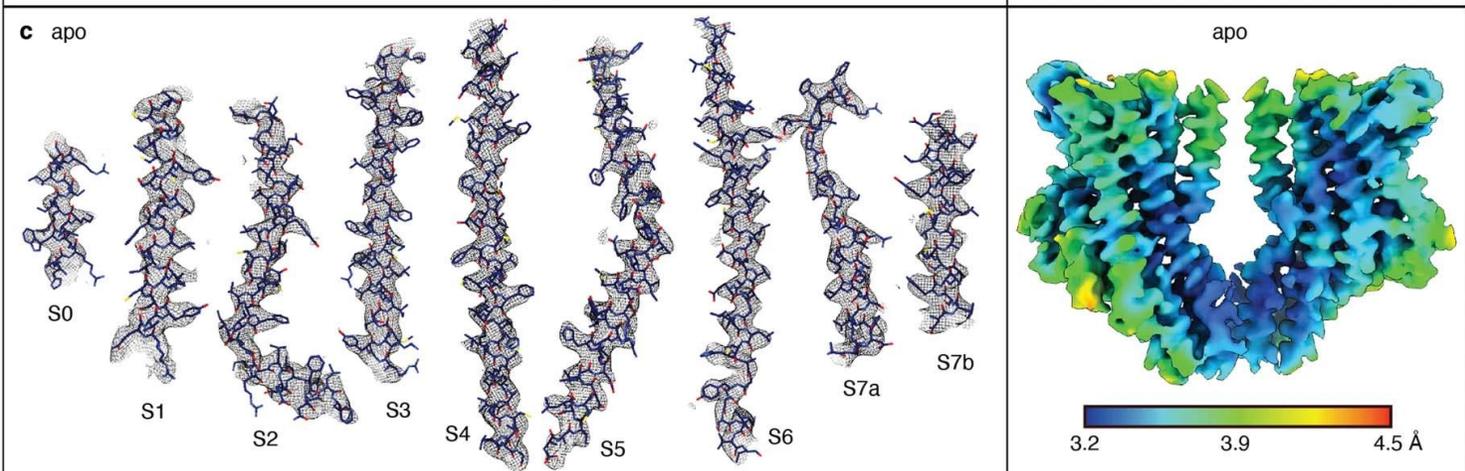
The structural basis of odorant recognition in insect olfactory receptors



常规状态

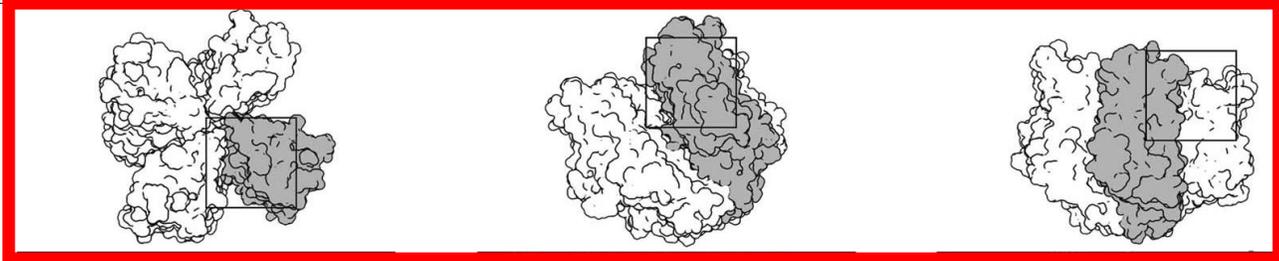


识别丁香子酚时



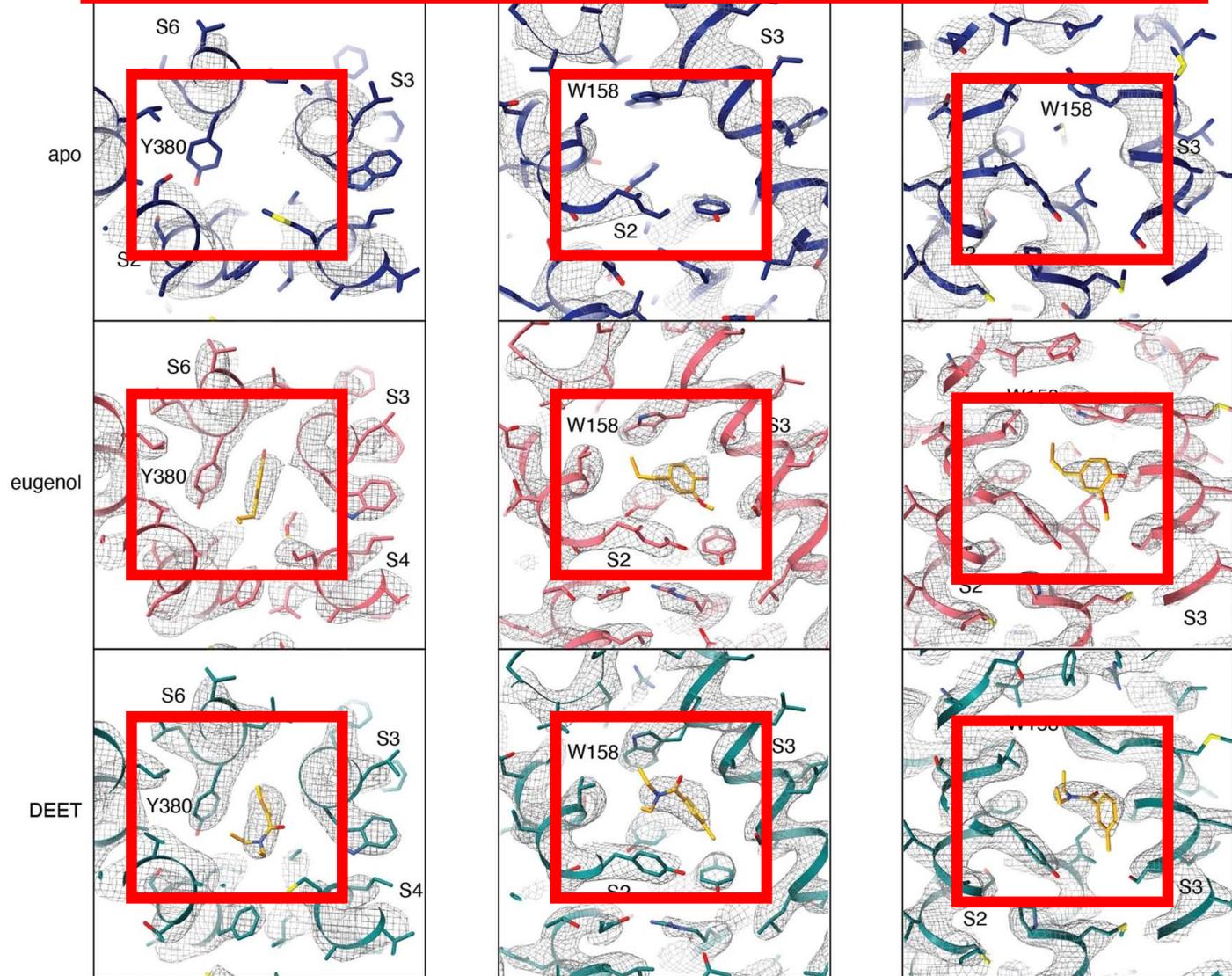
识别避蚊胺时

b



扫描位置

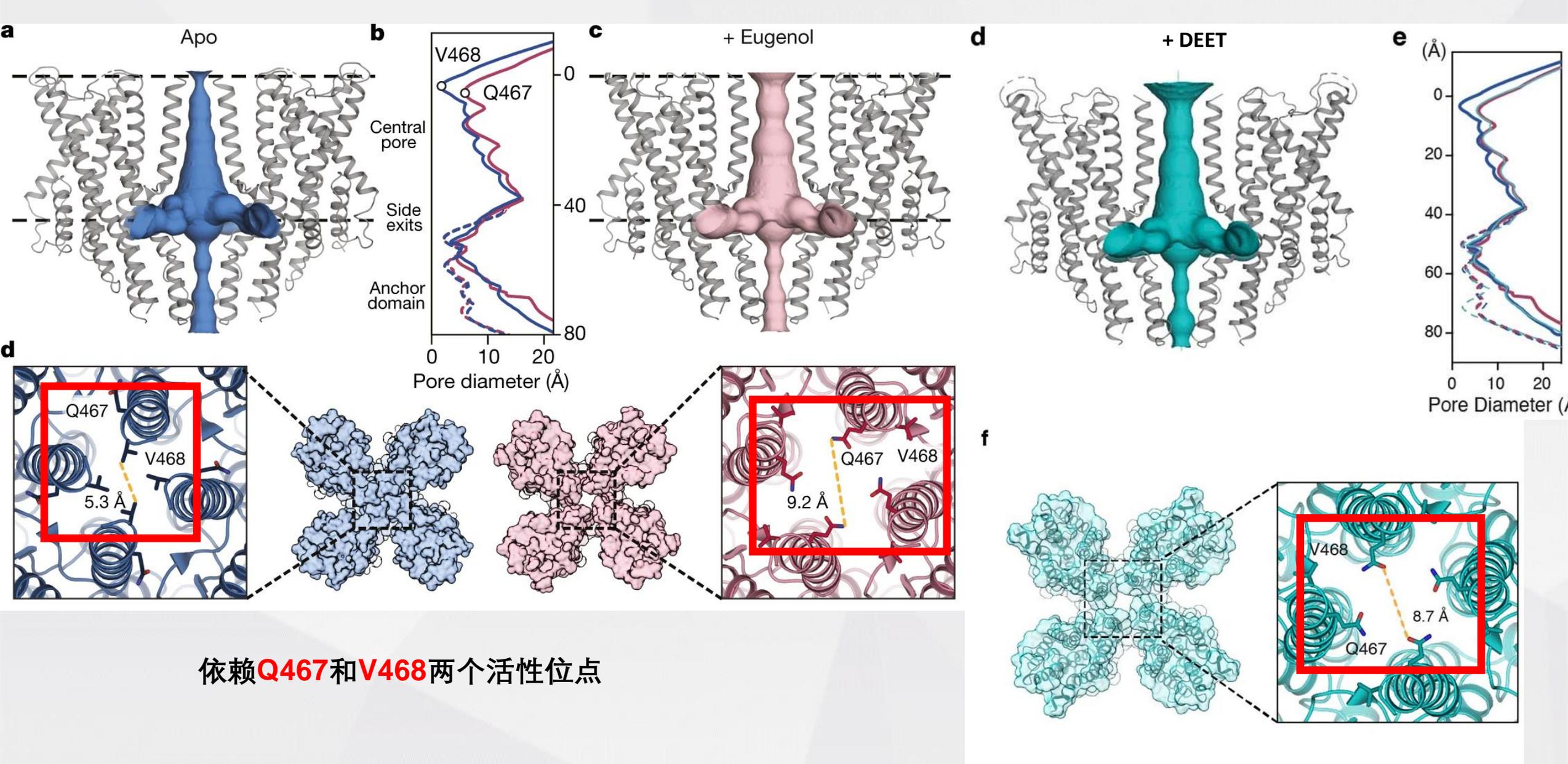
顶部, 侧部, 底部



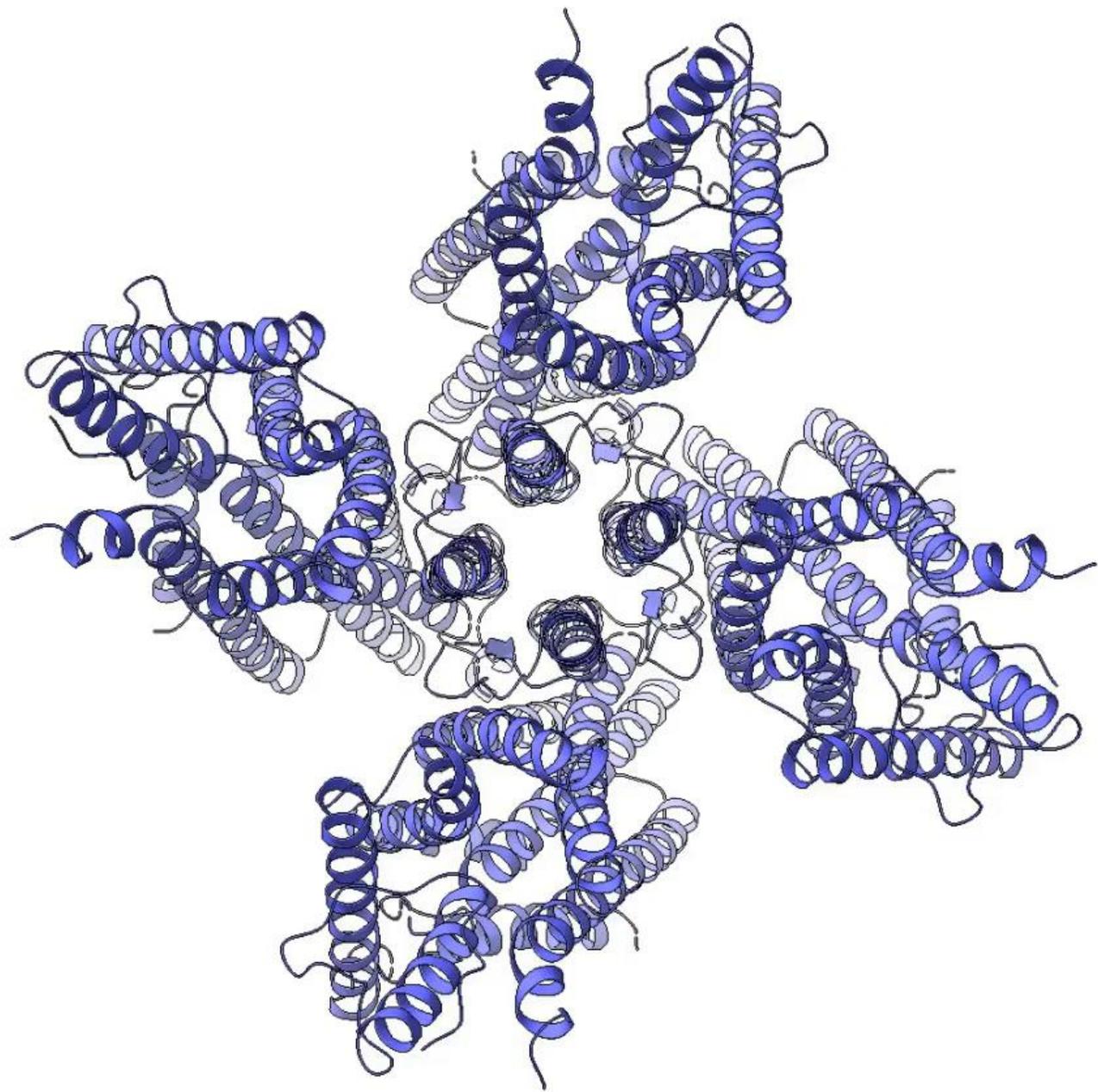
常规状态

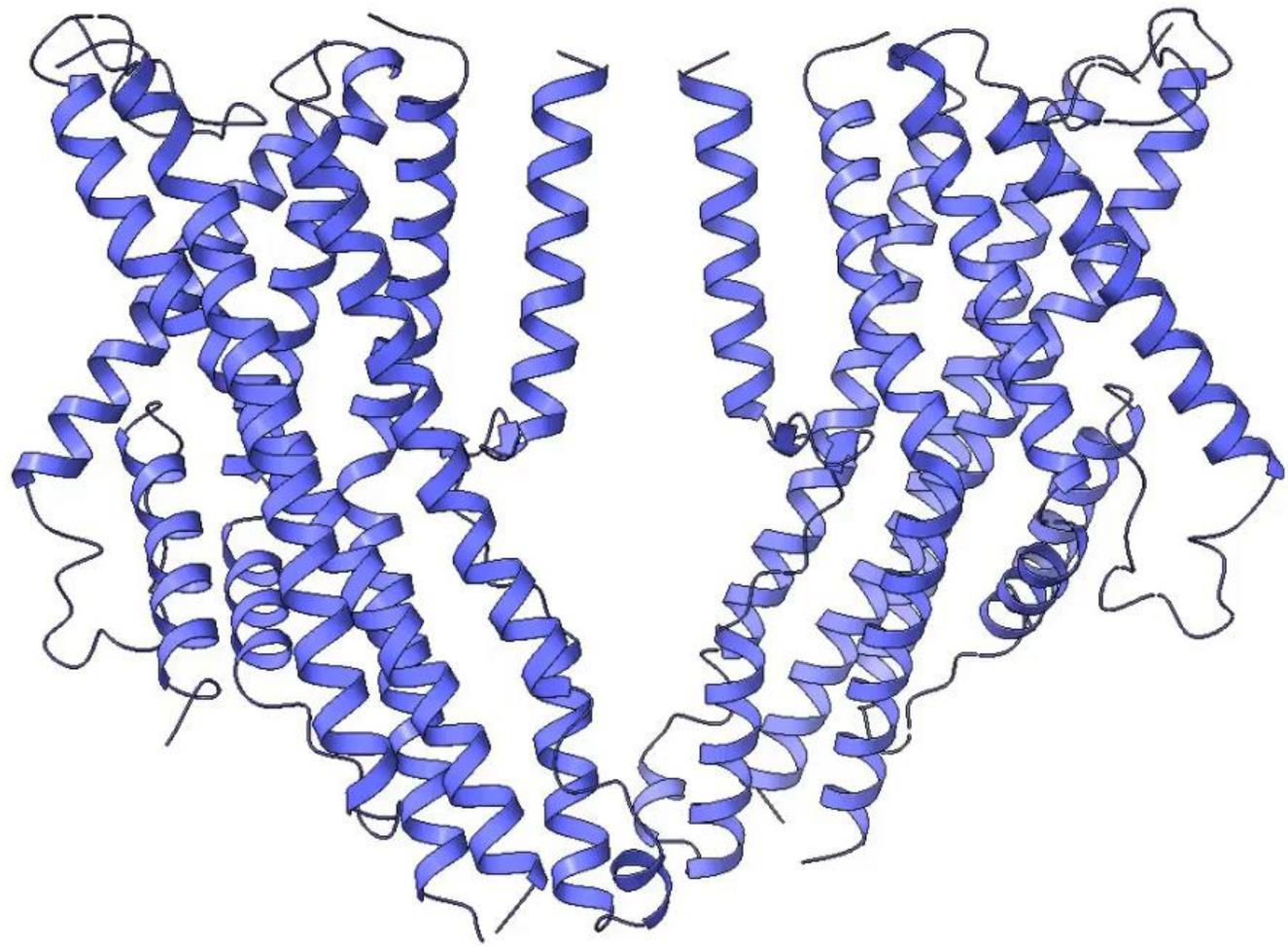
识别丁香子酚时

识别避蚊胺时



依赖**Q467**和**V468**两个活性位点





总结

- 1、通过将所获的cDNA序列与NCBI和Uniprot的同源性较高的序列进行比对，侧面验证了序列的准确性
- 2、结合文献和模型构建，预测Sf OR29的三级结构应为由四个七股 α 螺旋组成的同源四聚体复合物，明确了其结合原理
- 3、Sf OR29应该是PTHR21137家族的一个跨膜蛋白，为G蛋白偶联受体

展望

1. 确定并验证Sf OR29体外的功能

— 爪蟾电压钳系统

2. 对比突变体和野生型的行为实验

— Crispr定向敲除
— 触角电生理实验

3. 探究DMNT识别的神经通路

— 钙离子脑部成像技术

4. 夜蛾科家族食物源信息素的探究

— 基因比对找同源性基因

谢谢！

欢迎大家批评指正！