

*GH3*家族蛋白与抑制剂 *AIEP* 的相互作用研究

Research on the Interaction Between GH3 Protein
Family and AIEP

G01

韩静丹 万俊男 简亚男 曾婷

汇报内容

1. 研究背景



2. 研究目的



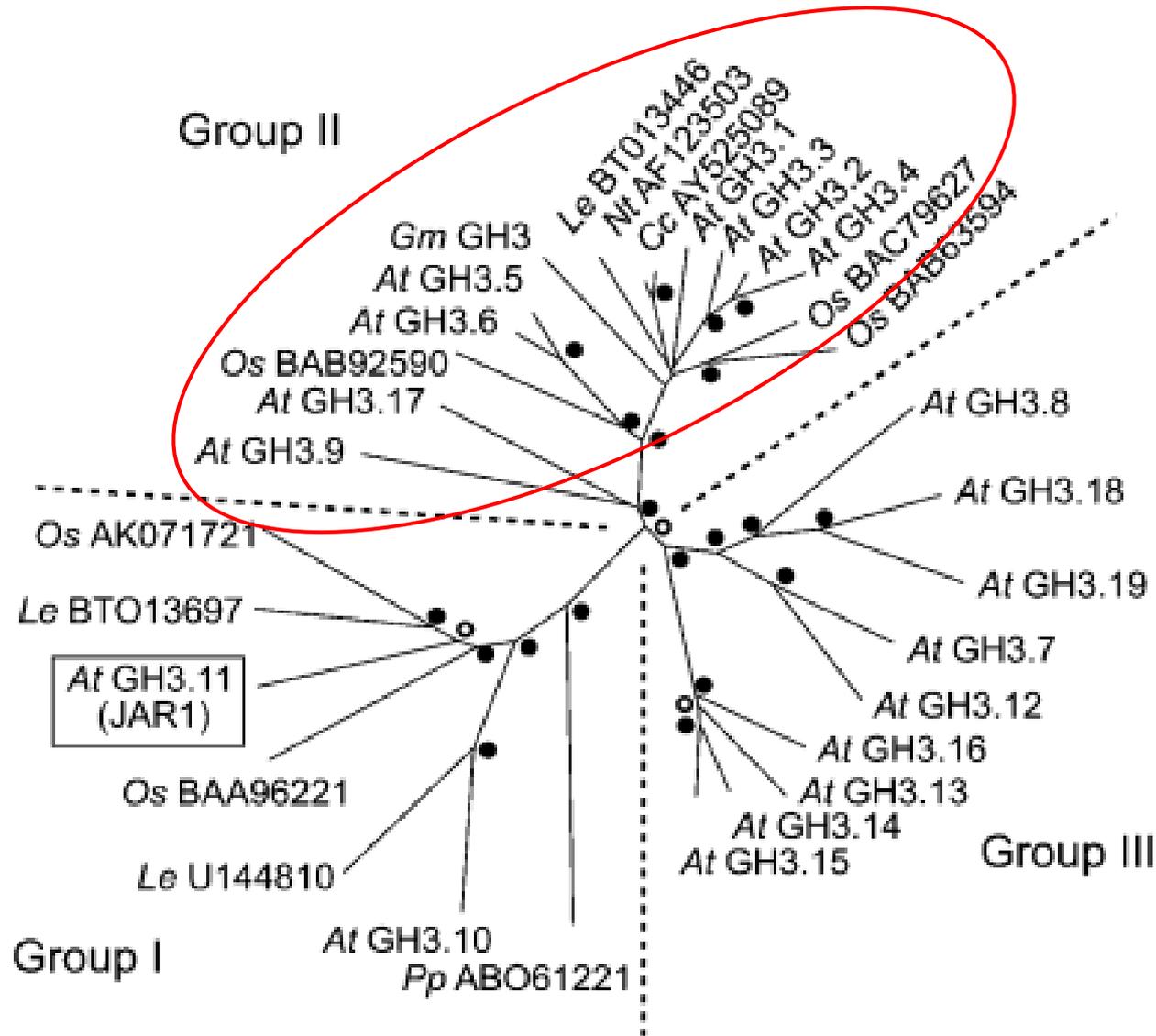
3. 研究流程



4. 研究结果

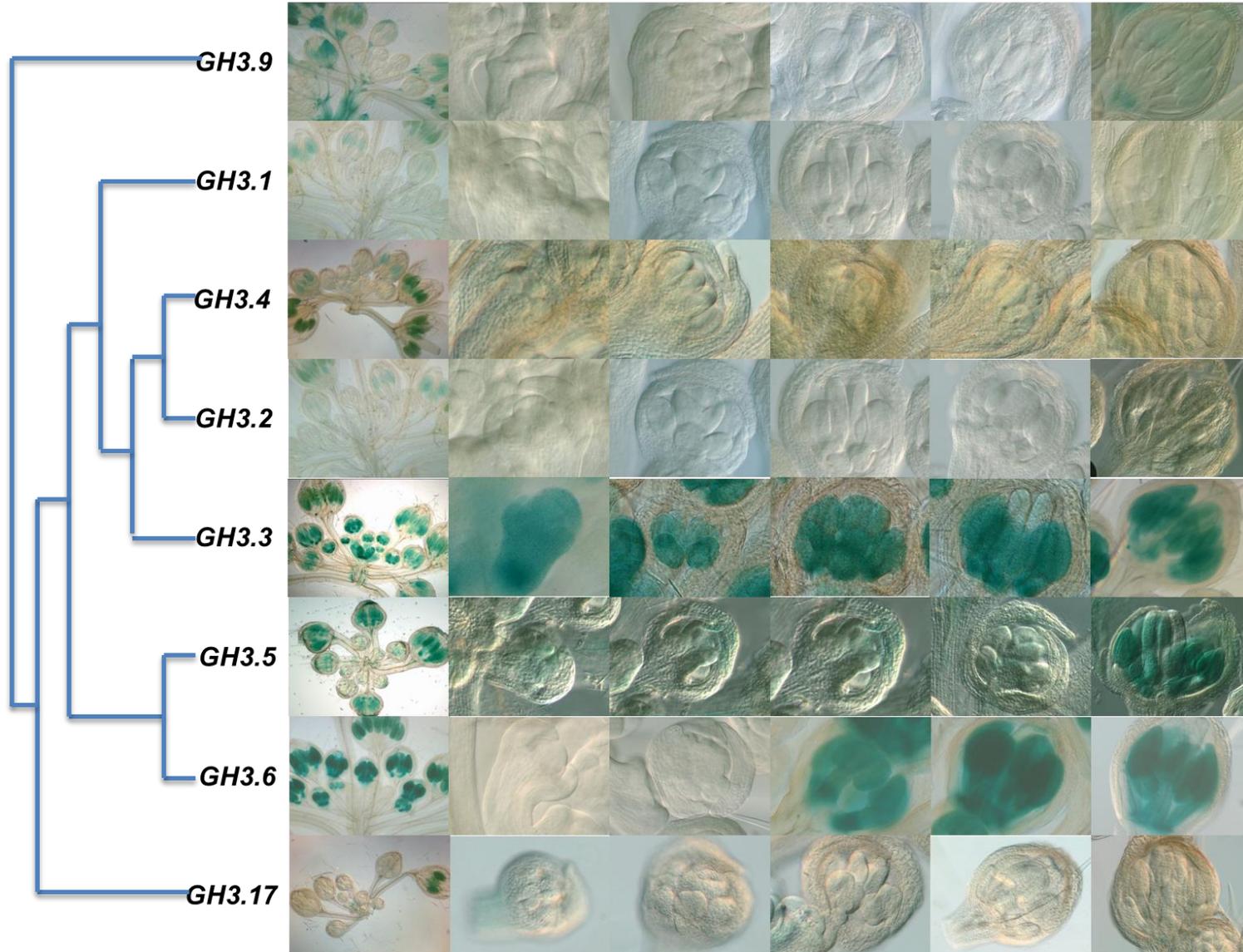


GH3 家族进化关系



GH3 IAA结合亚家族在雄蕊早期表达情况

Stage 1 Stage 2 Stage 3 Stage 4 Stage 5

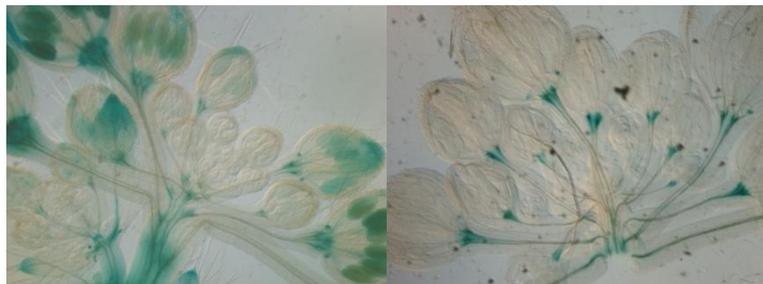


GH3 IAA结合亚家族在*spl*突变体中表达情况

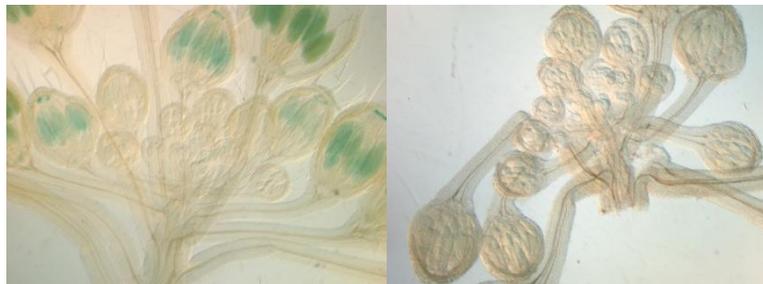
wt

spl^{-/-}

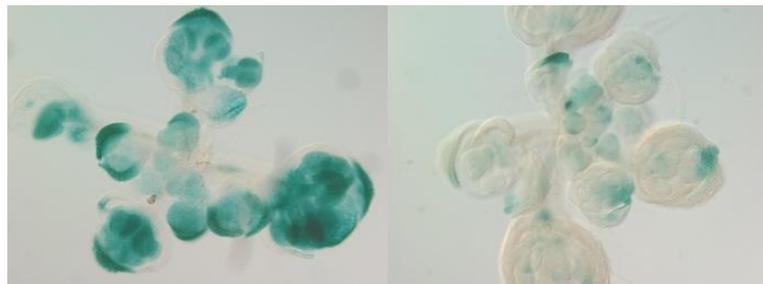
GH3.9



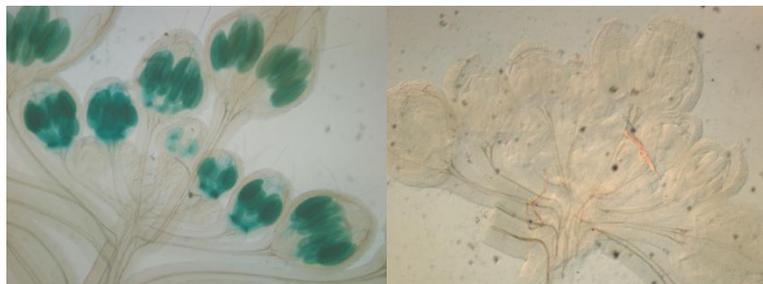
GH3.1



GH3.5



GH3.6



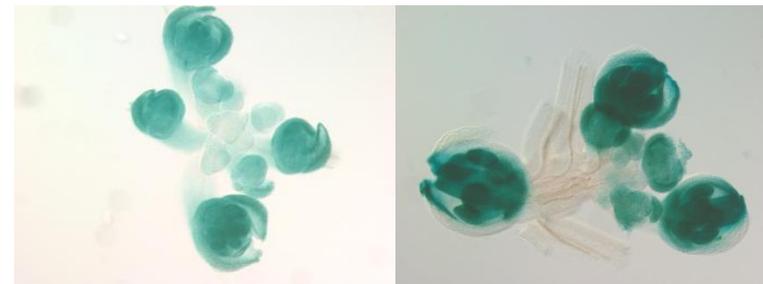
wt

spl^{-/-}

GH3.2



GH3.3



郑亚风 未发表数据

研究目的

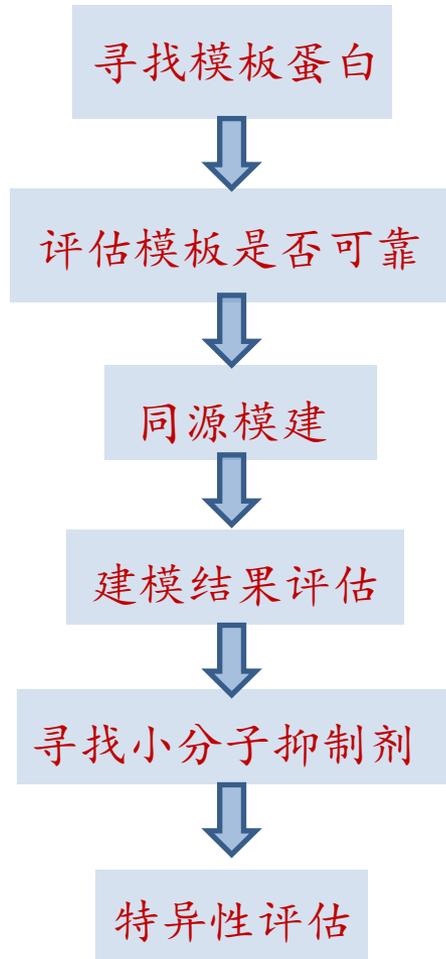
模拟GH3.3/5/6蛋白结构

找到特异小分子抑制剂

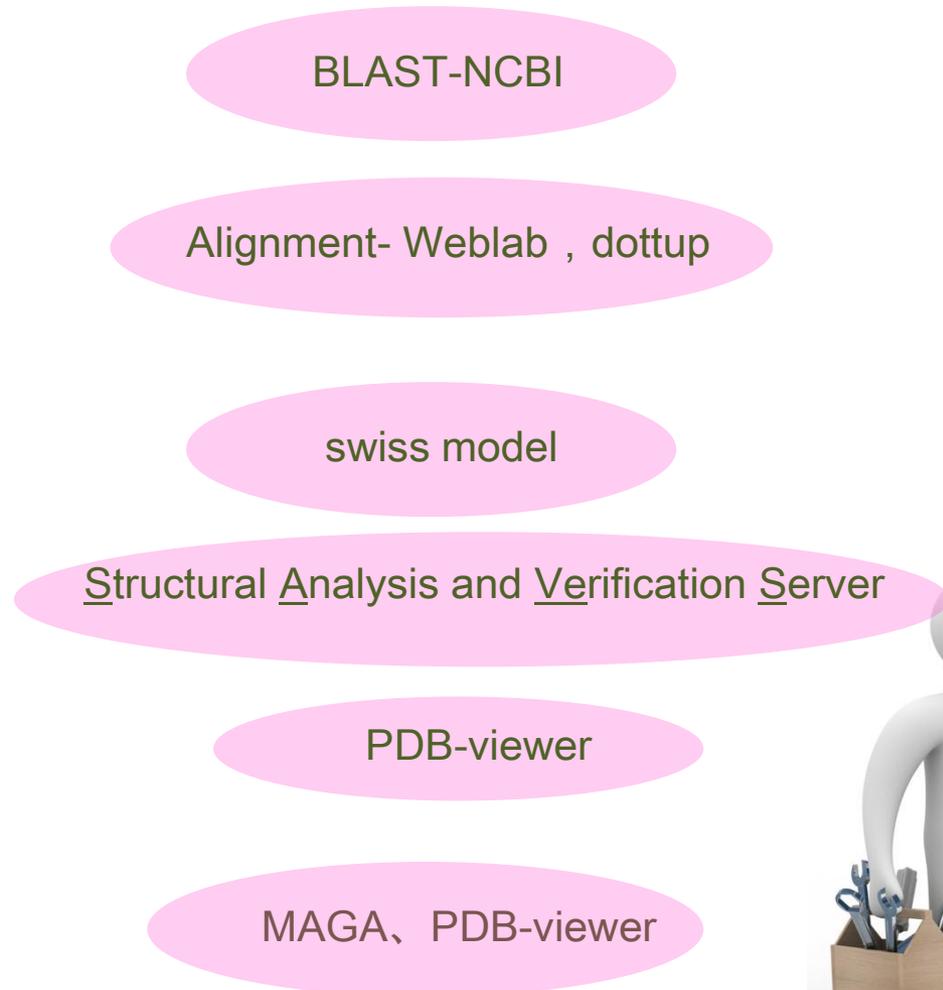


实验设计

流程

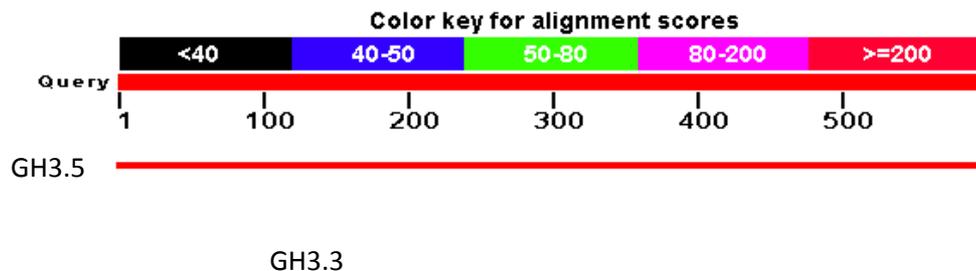


工具

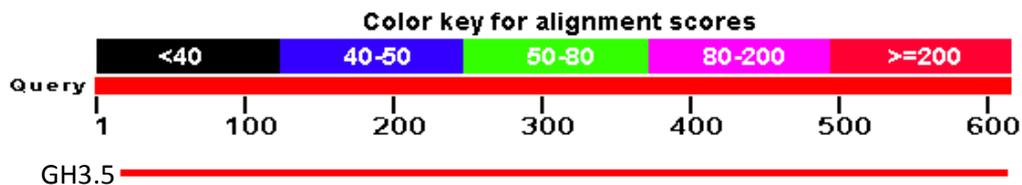


1. 寻找模板蛋白

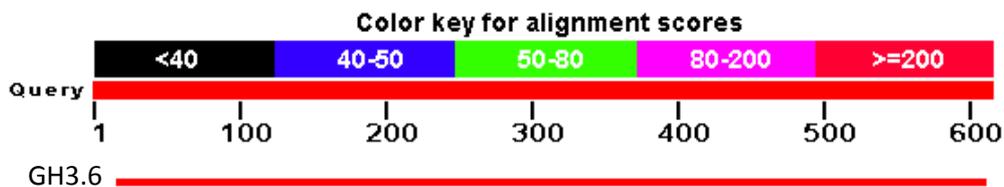
GH3.3/5/6 BLAST 结果



Max score	Max score	Total score	Query cover	E value	Max ident	Accession
961	961	961	100%	0.0	77%	4B2G_A
587	587	587	93%	0.0	50%	4EWW_A
564	564	564	93%	0.0	48%	4EQ4_A



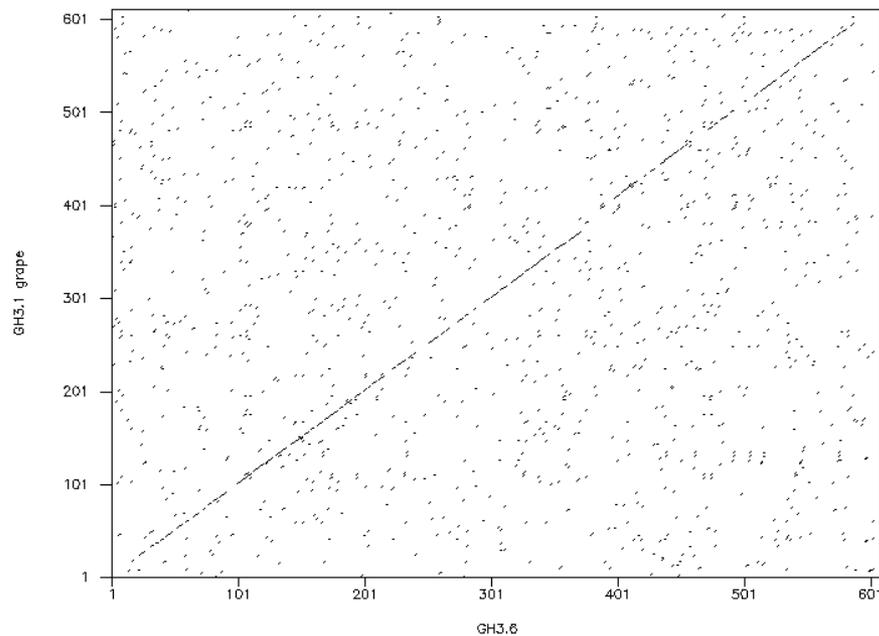
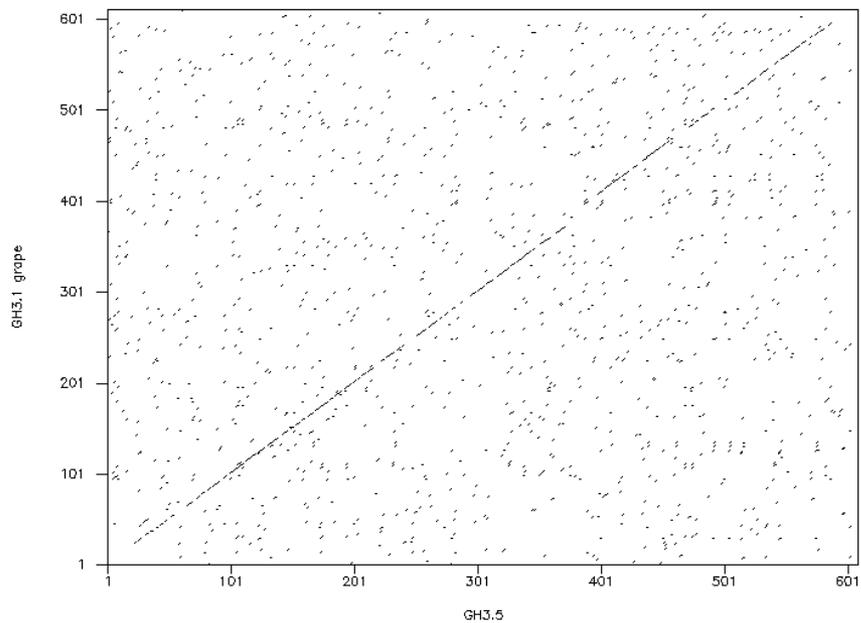
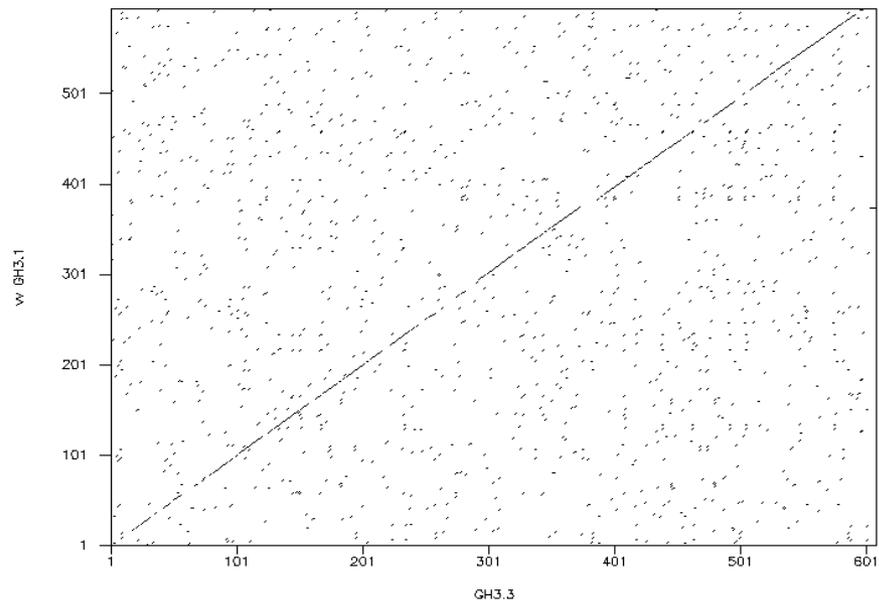
Max score	Total score	Query cover	E value	Max ident	Accession
835	835	96%	0.0	67%	4B2G_A
568	568	92%	0.0	49%	4EWW_A



Max score	Total score	Query cover	E value	Max ident	Accession
852	852	96%	0.0	68%	4B2G_A
573	573	92%	0.0	49%	4EWW_A
552	552	92%	0.0	48%	4EQ4_A

2. 模板蛋白评估

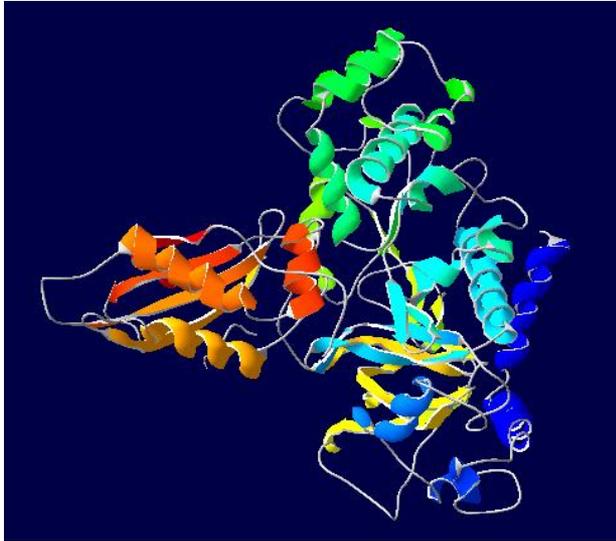
序列比对结果



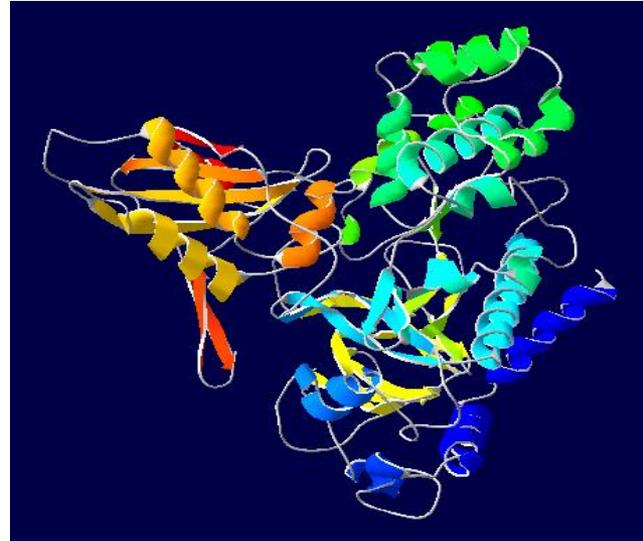
3. 同源模建

同源模建结果

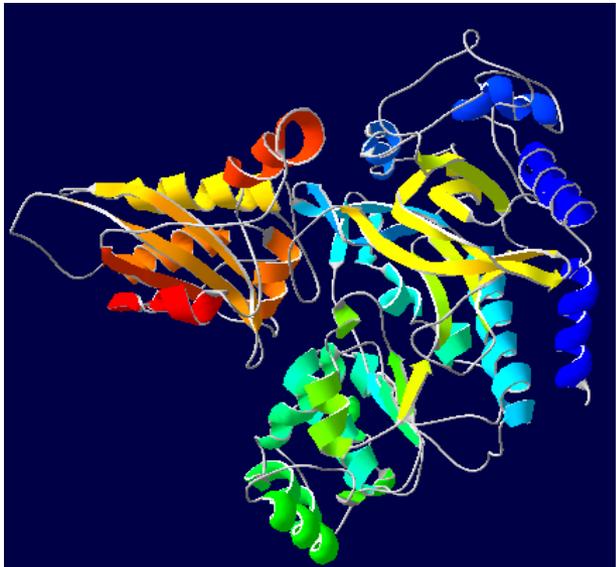
wv GH3.1



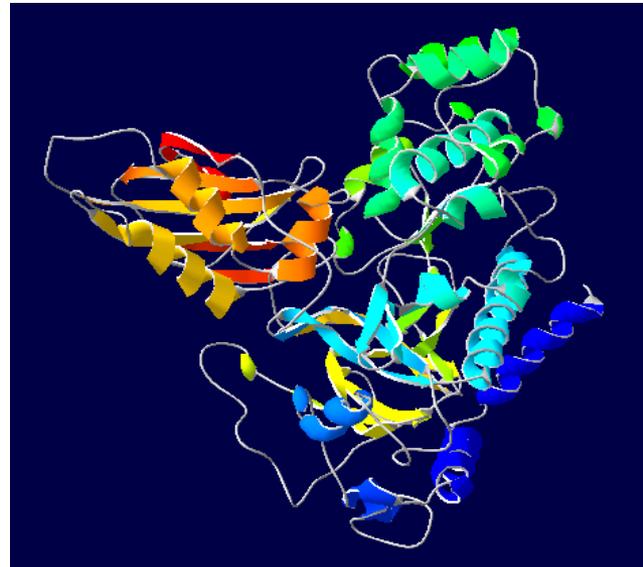
wv GH3.3



wv GH3.5



wv GH3.6



4. 建模结果评估

建模结果评估

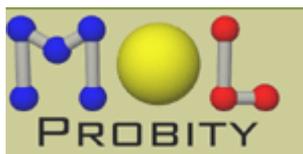


People • Seminars
Lectures • Webmail
Links • Facilities
Software • Home



评价建模结果的合理性
全面、简单

<http://nihserver.mbi.ucla.edu/SAVES/>



评价、优化建模结果
逐步分析，能够得到每一个原子的
具体信息，并在线改动不合理
结构
专业、可信度高

<http://molprobity.biochem.duke.edu/index.php>



各种有用的帖子，在线请教

<http://www.mdbbs.org/viewthread.php?tid=26753>

4. 建模结果评估

SAVES results for GH3.1grape.pdb

PASS

Procheck

Summary

1	Warning	+ Ramachandran plot: 91.9% core 7.5% allow 0.6% gener 0.0% disall [PostScript] • [PDF] • [JPG]
2	Warning	+ All Ramachandrans: 7 labelled residues (out of 558) [PostScript] • [PDF] Images: 1 2 3
3	Warning	+ Chi1-chi2 plots: 4 labelled residues (out of 328) [PostScript] • [PDF] Images: 1 2
4	Note	Main-chain params: 6 better 0 inside 0 worse [PostScript] • [PDF] • [JPG]
5	Note	Side-chain params: 5 better 0 inside 0 worse [PostScript] • [PDF] • [JPG]
6	Warning	+ Residue properties: Max.deviation: 5.5 Bad contacts: 5 Bond len/angle: 3.0 Morris et al class: 1 2 2 + 2 cis-peptides G-factors Dihedrals: -0.11 Covalent: 0.53 Overall: 0.14 [PostScript] • [PDF] Images: 1 2 3 4 5 6
7	Note	G-factors Dihedrals: -0.11 Covalent: 0.53 Overall: 0.14 [PostScript] • [PDF] • [JPG]
8	Note	M/c bond lengths: 100.0% within limits 0.0% highlighted [PostScript] • [PDF] Images: 1 2
9	Note	M/c bond angles: 99.5% within limits 0.5% highlighted [PostScript] • [PDF] • [JPG]
10	Note	Planar groups: 100.0% within limits 0.0% highlighted [PostScript] • [PDF] • [JPG]

View the interactive [Ramachandran Plot](#)

What_check

All Text		TeX file	
1	2	3	4
10	11	12	13
14	15	16	17
18	19	20	21
22	23	24	25
26	27	28	29
30	31	32	33
34	35	36	37
38	39	40	41
42	43	44	45
46	47	48	49
50	51	52	53
54	55	56	57
58	59	60	

Verify_3D

97.88% of the residues had an averaged 3D-1D score > 0.2

Pass

[View Plot](#)
[Averaged Data](#)
[Raw Data](#)
[View the 3D-1D table](#)

Errat

Overall quality factor
92.986
[\[PostScript\]](#) • [\[PDF\]](#)
JPGs: [[1](#)]
[\[Output Log\]](#)

Prove

- [PROVE output](#)
- [PostScript](#)
- [PDF](#)

JPGs:

- [Image1](#)
- [Image2](#)
- [Image3](#)
- [Image4](#)
- [Image5](#)

4. 建模结果评估

SAVES results for GH3.3.pdb



Procheck

1	Error	* Ramachandran plot: 89.7% core 9.1% allow 1.0% gener 0.2% dlsall [PostScript] • [PDF] • [JPG]
2	Warning	+ All Ramachandrans: 13 labelled residues (out of 577) [PostScript] • [PDF] Images: 1 2 3
3	Warning	+ Chi1-chi2 plots: 3 labelled residues (out of 351) [PostScript] • [PDF] Images: 1 2
4	Note	Main-chain params: 6 better 0 inside 0 worse [PostScript] • [PDF] • [JPG]
5	Note	Side-chain params: 5 better 0 inside 0 worse [PostScript] • [PDF] • [JPG]
6	Error	* Residue properties: Max. deviation: 5.5 Bad contacts: 5 * Bond len/angle: 8.2 Morris et al class: 1 1 2 * 5 cis-peptides G-factors Dihedrals: -0.03 Covalent: 0.31 Overall: 0.11 [PostScript] • [PDF] Images: 1 2 3 4 5 6
7	Note	G-factors Dihedrals: -0.03 Covalent: 0.31 Overall: 0.11 [PostScript] • [PDF] • [JPG]
8	Error	* M/c bond lengths: 99.6% within limits 0.4% highlighted 1 off graph [PostScript] • [PDF] Images: 1 2
9	Error	* M/c bond angles: 98.3% within limits 1.7% highlighted 1 off graph [PostScript] • [PDF] • [JPG]
10	Error	* Planar groups: 87.8% within limits 12.2% highlighted 4 off graph [PostScript] • [PDF] Images: 1 2

View the interactive
[Ramachandran Plot](#)

What_check

All Text		TeX file	
1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16
17	18	19	20
21	22	23	24
25	26	27	28
29	30	31	32
33	34	35	36
37	38	39	40
41	42	43	44
45	46	47	48
49	50	51	52
53	54		

Verify_3D

92.93% of the
residues had an
averaged 3D-1D
score > 0.2

Pass

[View Plot](#)
[Averaged Data](#)
[Raw Data](#)
[View the 3D-1D table](#)

Errat

Overall quality factor
92.389
[PostScript] •
[PDF]
JPGs: [1]
[Output Log]

Prove

- PROVE
output
- PostScript
- PDF
- JPGs:
- image1
- image2
- image3
- image4
- image5

4. 建模结果评估

SAVES results for GH3.5.pdb



Procheck

Summary

1	Error	* Ramachandran plot: 88.5% core 10.2% allow 1.0% gener 0.4% disall [PostScript] • [PDF] • [JPG]
2	Error	* All Ramachandrans: 19 labelled residues (out of 587) [PostScript] • [PDF] Images: 1 2 3
3	Warning	+ Chi1-chi2 plots: 3 labelled residues (out of 351) [PostScript] • [PDF] Images: 1 2
4	Note	Main-chain params: 6 better 0 inside 0 worse [PostScript] • [PDF] • [JPG]
5	Note	Side-chain params: 5 better 0 inside 0 worse [PostScript] • [PDF] • [JPG]
6	Error	* Residue properties: Max. deviation: 19.6 Bad contacts: 27 * Bond len/angle: 17.7 Morris et al class: 1 1 2 * 3 cis-peptides 1 D amino acids G-factors Dihedrals: -0.02 Covalent: 0.07 Overall: 0.03 [PostScript] • [PDF] Images: 1 2 3 4 5 6
7	Note	G-factors Dihedrals: -0.02 Covalent: 0.07 Overall: 0.03 [PostScript] • [PDF] • [JPG]
8	Error	* M/c bond lengths: 98.8% within limits 1.2% highlighted 6 off graph [PostScript] • [PDF] Images: 1 2
9	Error	* M/c bond angles: 97.3% within limits 2.7% highlighted 16 off graph [PostScript] • [PDF] • [JPG]
10	Warning	+ Planar groups: 90.4% within limits 9.6% highlighted 3 off graph [PostScript] • [PDF] Images: 1 2 3

View the Interactive
[Ramachandran Plot](#)

What_check

All Text		TeX file	
1	2	3	4
10	11	12	13
14	15	16	17
18	19	20	21
22	23	24	25
26	27	28	29
30	31	32	33
34	35	36	37
38	39	40	41
42	43	44	45
46	47	48	49
50	51	52	53
54	55	56	57

Verify_3D

88.31% of the
residues had an
averaged 3D-1D
score > 0.2

Pass

[View Plot](#)

[Averaged Data](#)

[Raw Data](#)

[View the 3D-1D table](#)

Errat

Overall quality factor
83.536
[\[PostScript\]](#) •
[\[PDF\]](#)
 JPGs: [1]
[\[Output Log\]](#)

Prove

- PROVE output
- PostScript
- PDF
- JPGs:
- Image1
- Image2
- Image3
- Image4
- Image5

4. 建模结果评估 SAVES results for GH3.6.pdb



Procheck

Summary

1	Error	* Ramachandran plot: 88.1% core 10.6% allow 1.2% gener 0.2% disall [PostScript] • [PDF] • [JPG]
2	Warning	+ All Ramachandrans: 17 labelled residues (out of 588) [PostScript] • [PDF] Images: 1 2 3
3	Warning	+ Chi1-chi2 plots: 3 labelled residues (out of 346) [PostScript] • [PDF] Images: 1 2
4	Note	Main-chain params: 6 better 0 Inside 0 worse [PostScript] • [PDF] • [JPG]
5	Note	Side-chain params: 5 better 0 Inside 0 worse [PostScript] • [PDF] • [JPG]
6	Error	* Residue properties: Max. deviation: 14.1 Bad contacts: 3 * Bond len/angle: 11.2 Morris et al class: 1 1 2 + 3 cis-peptides G-factors Dihedrals: -0.02 Covalent: 0.27 Overall: 0.10 [PostScript] • [PDF] Images: 1 2 3 4 5 6
7	Note	G-factors Dihedrals: -0.02 Covalent: 0.27 Overall: 0.10 [PostScript] • [PDF] • [JPG]
8	Error	* M/c bond lengths: 99.6% within limits 0.4% highlighted 2 off graph [PostScript] • [PDF] Images: 1 2
9	Error	* M/c bond angles: 98.0% within limits 2.0% highlighted 5 off graph [PostScript] • [PDF] • [JPG]
10	Error	* Planar groups: 86.2% within limits 13.8% highlighted 2 off graph [PostScript] • [PDF] Images: 1 2

View the Interactive

What_check

All Text		TeX file	
1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16
17	18	19	20
21	22	23	24
25	26	27	28
29	30	31	32
33	34	35	36
37	38	39	40
41	42	43	44
45	46	47	48
49	50	51	52

Verify_3D

91.20% of the residues had an averaged 3D-1D score > 0.2

Pass

[View Plot](#)
[Averaged Data](#)
[Raw Data](#)
[View the 3D-1D table](#)

Errat

Overall quality factor 85.889
[\[PostScript\]](#) • [\[PDF\]](#)
 JPGs: [1]
[\[Output Log\]](#)

Prove

- [PROVE output](#)
- [PostScript](#)
- [PDF](#)
- JPGs:
 - [Image1](#)
 - [Image2](#)
 - [Image3](#)
 - [Image4](#)
 - [Image5](#)

小分子抑制剂寻找

Crystal Structure of an Indole-3-Acetic Acid Amido Synthetase from Grapevine Involved in Auxin Homeostasis^W

Thomas S. Peat,^a Christine Böttcher,^b Janet Newman,^a Del Lucent,^a Nathan Cowieson,^c and Christopher Davies^{b,1}

^aThe Commonwealth Scientific and Industrial Research Organization (CSIRO) Materials, Science and Engineering, Parkville, Victoria 3052, Australia

^bCSIRO Plant Industry, Glen Osmond, South Australia 5064, Australia

^cAustralian Synchrotron, Clayton, Victoria 3168, Australia

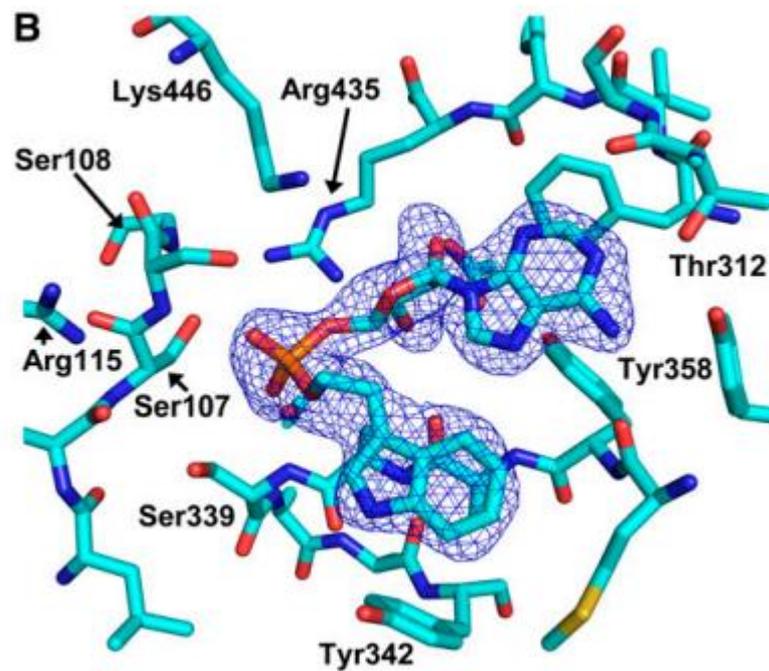
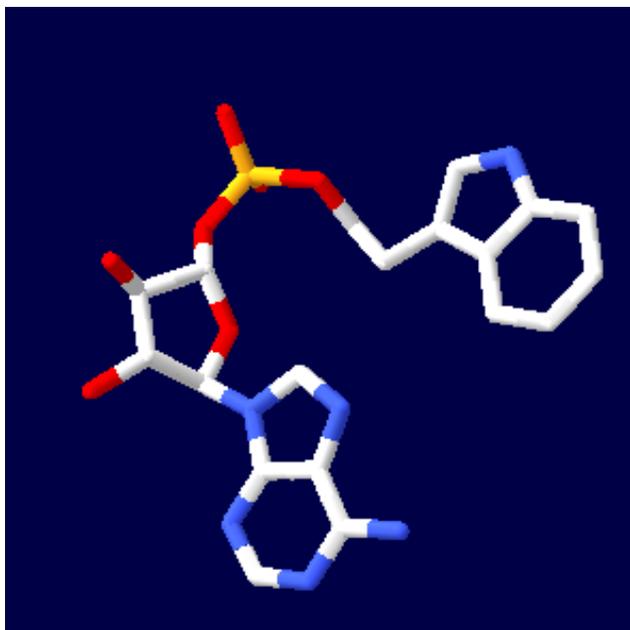
A Novel Tool for Studying Auxin-Metabolism: The Inhibition of Grapevine Indole-3-Acetic Acid-Amido Synthetases by a Reaction Intermediate Analogue

Christine Böttcher^{1*}, Eric G. Dennis¹, Grant W. Booker², Steven W. Polyak², Paul K. Boss¹,
Christopher Davies¹

¹CSIRO Plant Industry, Glen Osmond, South Australia, Australia, ²The School of Molecular and Biomedical Science, University of Adelaide, Adelaide, South Australia, Australia

5. 寻找小分子抑制剂

AIEP及其结合位点



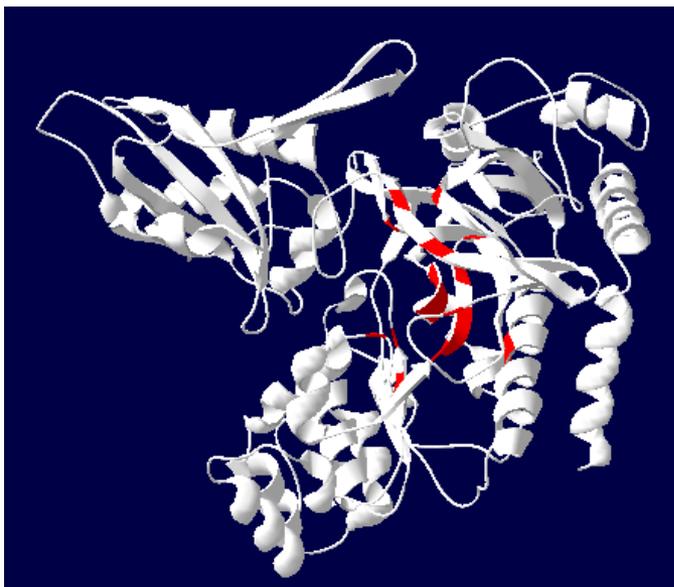
5. 寻找小分子抑制剂

活性位点展示

wv GH3.1



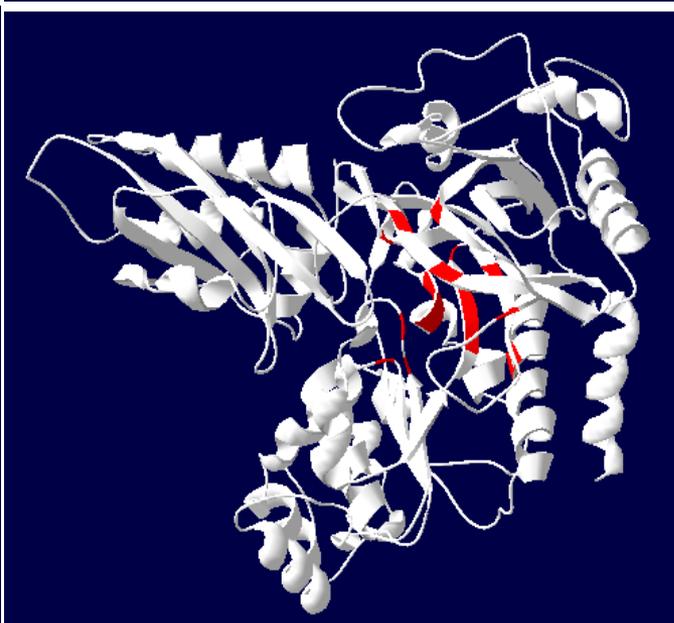
wv GH3.3



wv GH3.5



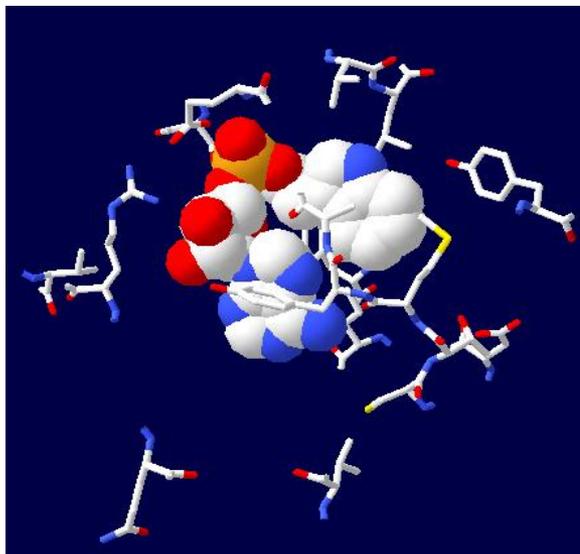
wv GH3.6



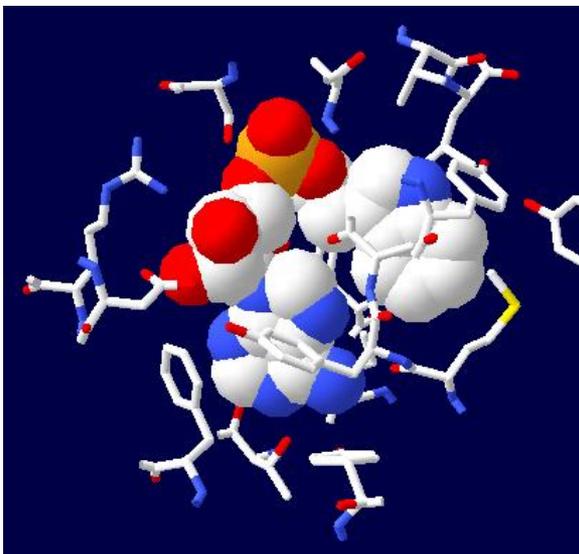
5. 寻找小分子抑制剂

小分子结合情况

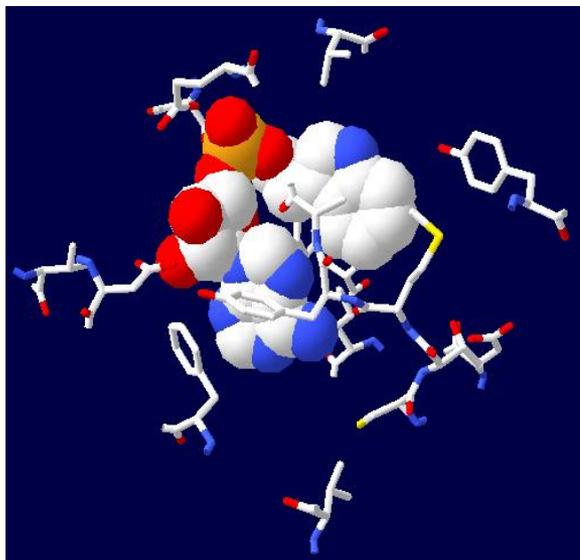
wv GH3.1



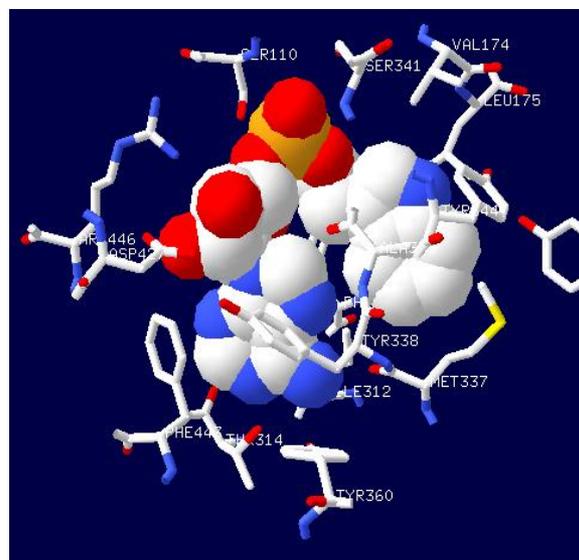
wv GH3.3



wv GH3.5

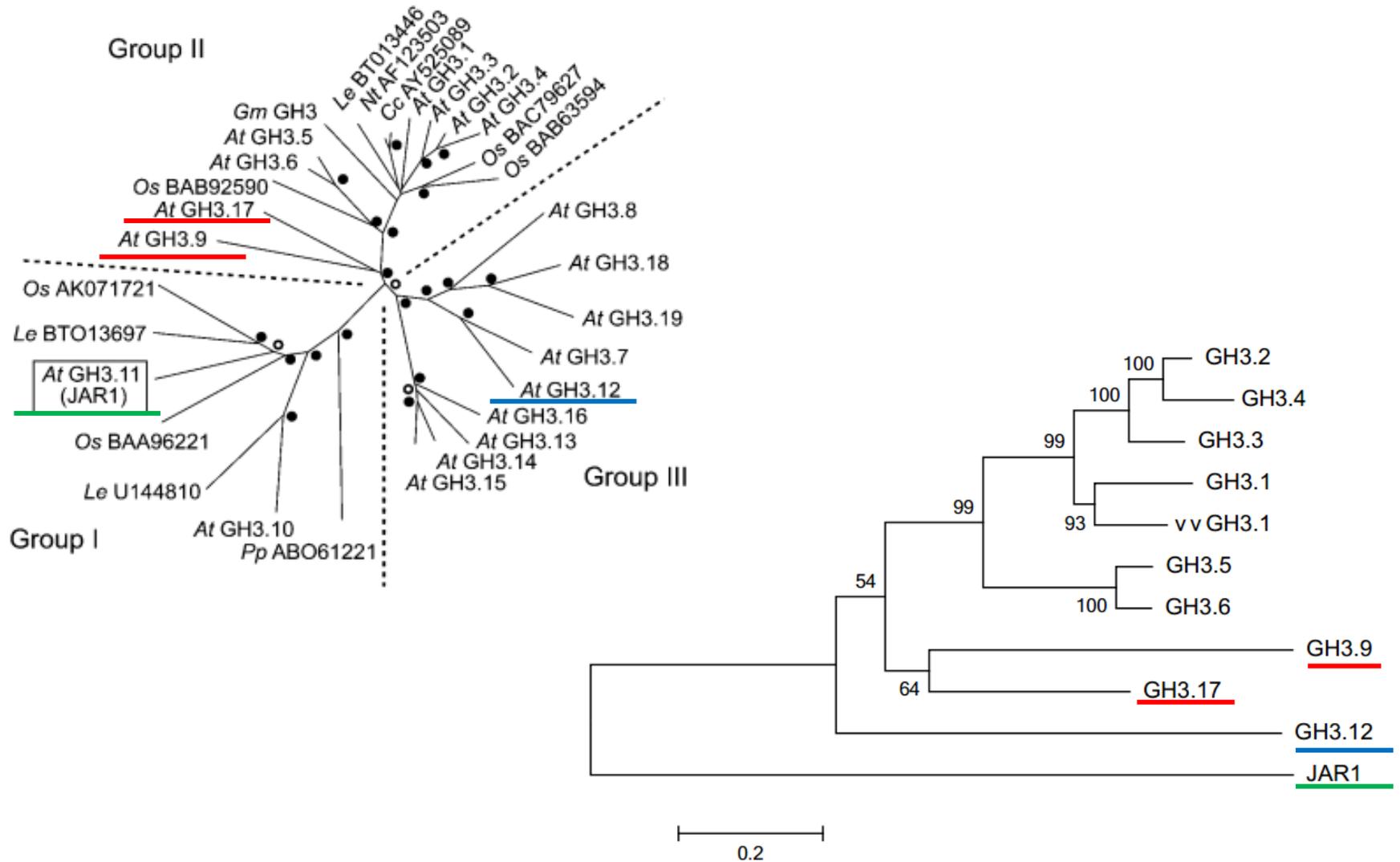


wv GH3.6



6. 特异性评估

GH3家族其他成员与AIEP结合情况



Family: GH3 (PF03321)

6 architectures 647 sequences 0 interactions 276 species 0 structures

Summary

Summary: GH3 auxin-responsive promoter

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

[No Wikipedia article](#) [Pfam](#) [Interpro](#)

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.

GH3 auxin-responsive promoter [Add annotation](#)

No Pfam abstract.

Literature references

1. Walker L, Estelle M; , Curr Opin Plant Biol 1998;1:434-439.: Molecular mechanisms of auxin action. [PUBMED:10066623](#)

Clan

This family is a member of clan [ANL](#) (CL0378), which has a total of [3 members](#).

Internal database links

SCOOP:	AMP-binding
Similarity to PfamA using HHSearch:	AMP-binding

External database links

PANDIT:	PF03321
Pseudofam:	PF03321
SYSTEMS:	GH3

- Domain organisation
- Clan
- Alignments
- HMM logo
- Trees
- Curation & model
- Species
- Interactions
- Structures

Jump to...

enter ID/acc [Go](#)

推荐分析基因家族的网站



Species > Tools > Info > Help > Contact Us

phytozome

Composite Arabidopsis thaliana columbia family (20 families, 20 members)

Ath 20

Classification ? Find related families Align family members Get Data Display options

Composite family

Genes in this family ? Functional Annotation Multiple Sequence Alignment Family History

	ORG	DBXREF	SYMBOL	DEFINITION	DOMAINS	SYNTENY	EXONS	
F	G	B	Ath	AT1G23160.1	Auxin-responsive GH3 family pr...			579
F	G	B	Ath	AT1G28130.1	GH3.17 Auxin-responsive GH3 family pr...			610
F	G	B	Ath	AT1G48660.1	Auxin-responsive GH3 family pr...			574
F	G	B	Ath	AT1G48670.1	auxin-responsive GH3 family pr...			526
F	G	B	Ath	AT1G48690.1	Auxin-responsive GH3 family pr...			191
F	G	B	Ath	AT1G59500.1	GH3.4 Auxin-responsive GH3 family pr...			598
F	G	B	Ath	AT2G14960.1	GH3.1 Auxin-responsive GH3 family pr...			591
F	G	B	Ath	AT2G23170.1	GH3.3 Auxin-responsive GH3 family pr...			596
F	G	B	Ath	AT2G46370.4	JAR1 Auxin-responsive GH3 family pr...			587
F	G	B	Ath	AT2G47750.1	GH3.9 putative indole-3-acetic acid-...			586
F	G	B	Ath	AT4G03400.1	DFL2 Auxin-responsive GH3 family pr...			592
F	G	B	Ath	AT4G27260.1	WES1 Auxin-responsive GH3 family pr...			613
F	G	B	Ath	AT4G37390.1	AUR3 Auxin-responsive GH3 family pr...			604
F	G	B	Ath	AT5G13320.1	PBS3 Auxin-responsive GH3 family pr...			576
F	G	B	Ath	AT5G13350.1	Auxin-responsive GH3 family pr...			588
F	G	B	Ath	AT5G13360.3	Auxin-responsive GH3 family pr...			673
F	G	B	Ath	AT5G13370.1	Auxin-responsive GH3 family pr...			596
F	G	B	Ath	AT5G13380.1	Auxin-responsive GH3 family pr...			625
F	G	B	Ath	AT5G51470.1	Auxin-responsive GH3 family pr...			582
F	G	B	Ath	AT5G54510.1	PF03321: GH3 auxin-responsive promoter (24 - 583)			613

Center for Integrative Genomics

JGI Joint Genome Institute ©2011 University of California

6. 特异性评估

亚家族代表BLAST

Max score	Total score	Query cover	E value	Max ident	Accession
849	849	98%	0.0	76%	4B2G_A
530	530	93%	0.0	49%	4EWV_A
511	511	93%	2e-175	48%	4EQ4_A

GH 3.2

Max score	Total score	Query cover	E value	Max ident	Accession
693	693	98%	0.0	55%	4B2G_A
637	637	97%	0.0	52%	4EWV_A
616	616	97%	0.0	51%	4EQ4_A

GH 3.17

Max score	Total score	Query cover	E value	Max ident	Accession
624	624	98%	0.0	52%	4B2G_A
565	565	97%	0.0	48%	4EWV_A
547	547	97%	0.0	48%	4EQ4_A

GH 3.9

Max score	Total score	Query cover	E value	Max ident	Accession
1198	1198	100%	0.0	100%	4EPL_A
414	414	98%	2e-136	38%	4B2G_A

JAR1

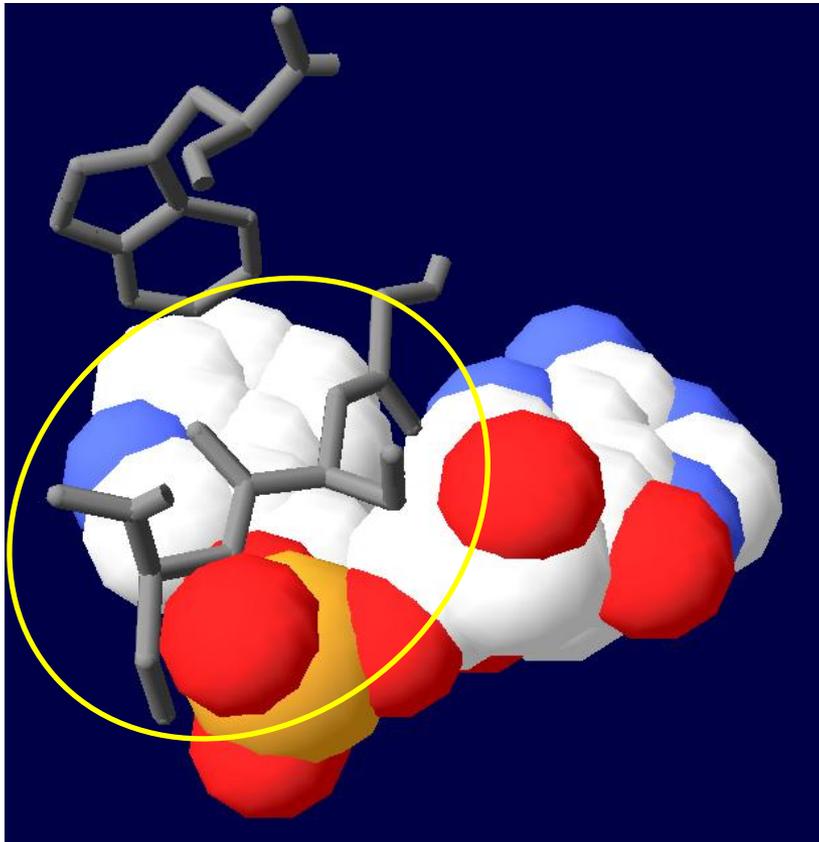
Max score	Total score	Query cover	E value	Max ident	Accession
1189	1189	100%	0.0	100%	4EWV_A

GH 3.12

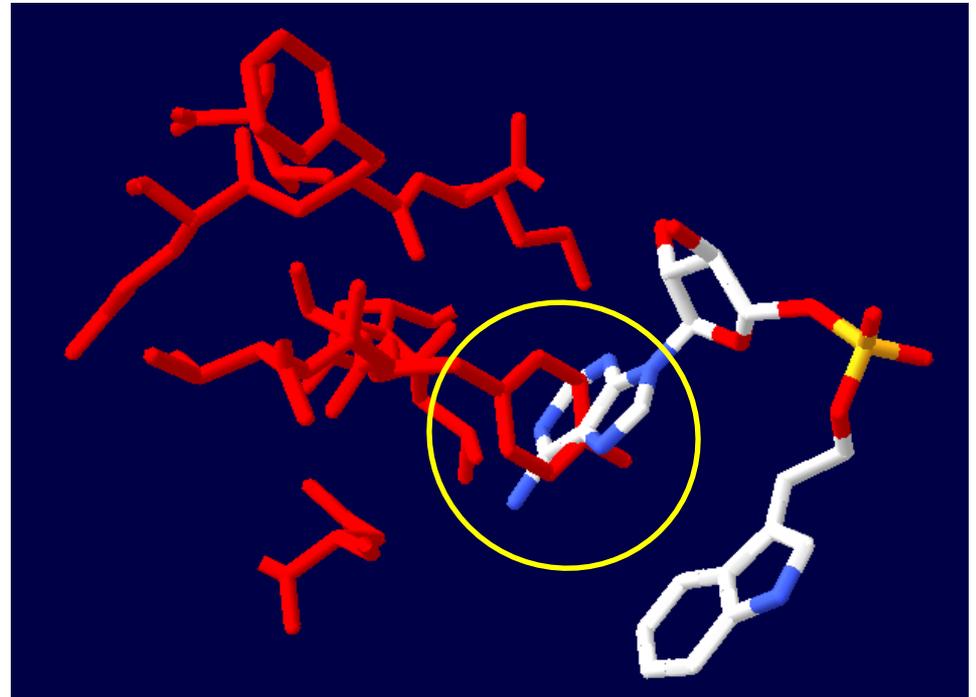
6. 特异性评估

JAR1 活性位点与 AIEP 结合情况

JAR1



GH 3.12



结论



AIEP能够抑制GH3. 3/5/6结合活性



AIEP可能对GH3结合IAA亚家族都具有抑制效应



AIEP对其他亚家族没有抑制效应



THANKS!



简亚男

曾婷

G01

韩静丹

万俊男