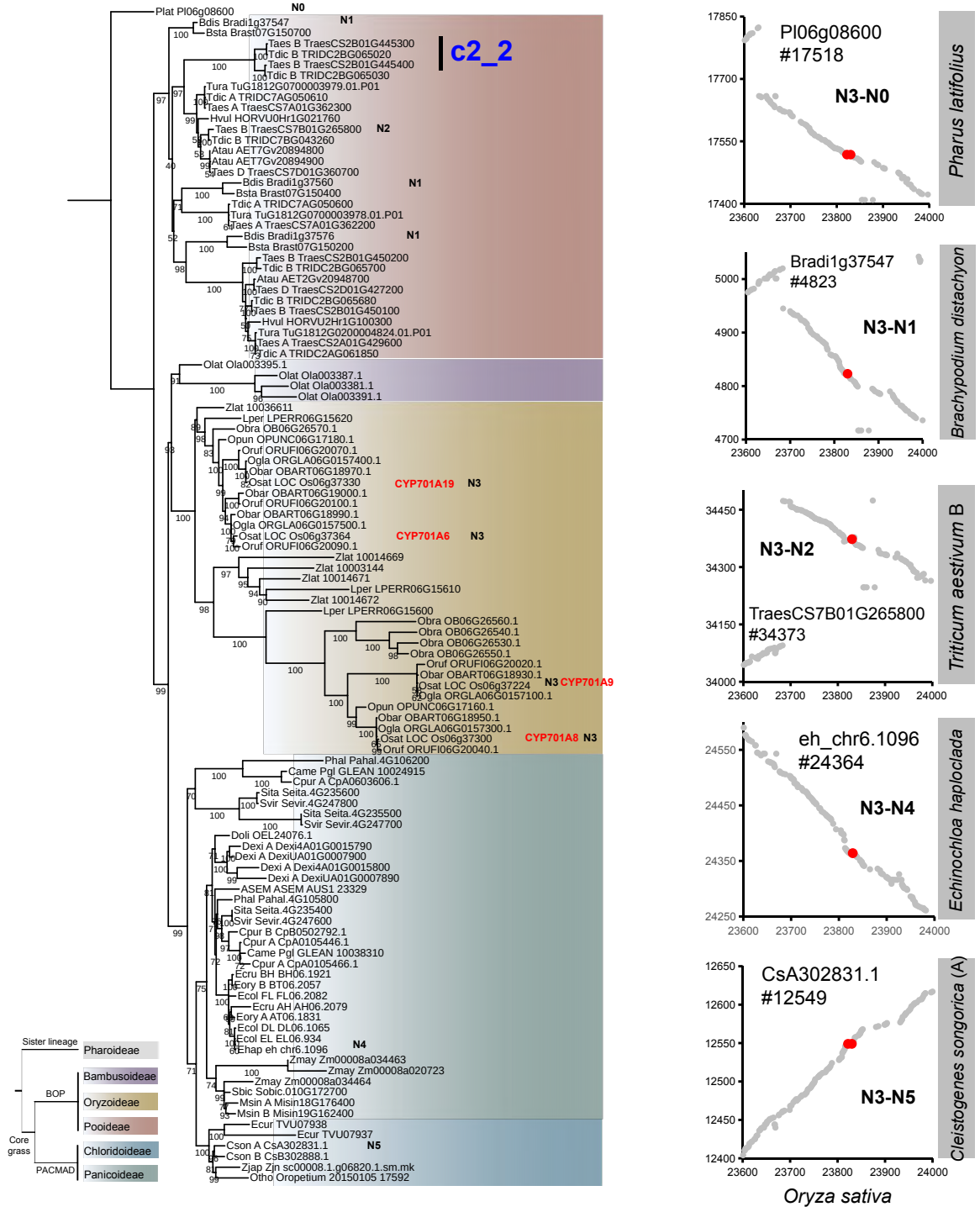


Figure S1. Phylogeny and genomic synteny of *CYP701A8* homologs in grass. Genes in different subfamilies are marked in different color backgrounds. Genes used in synteny analysis are marked in the phylogenetic tree from N0 to N3. Homologs in Triticeae subgenomes B and four *CYP701A8* homologs in *O. sativa* are highlighted. The red syntenic dots represent pairs of native homologs between genomes.

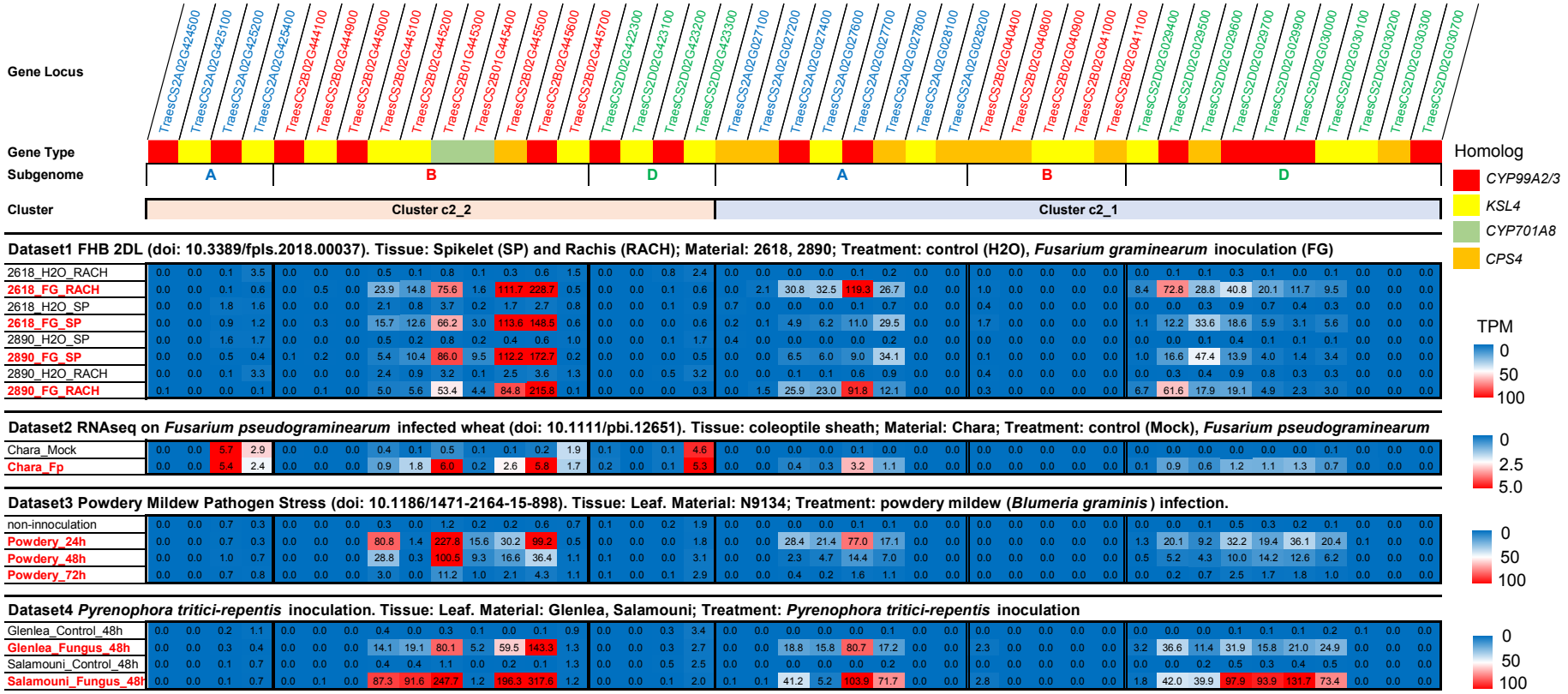
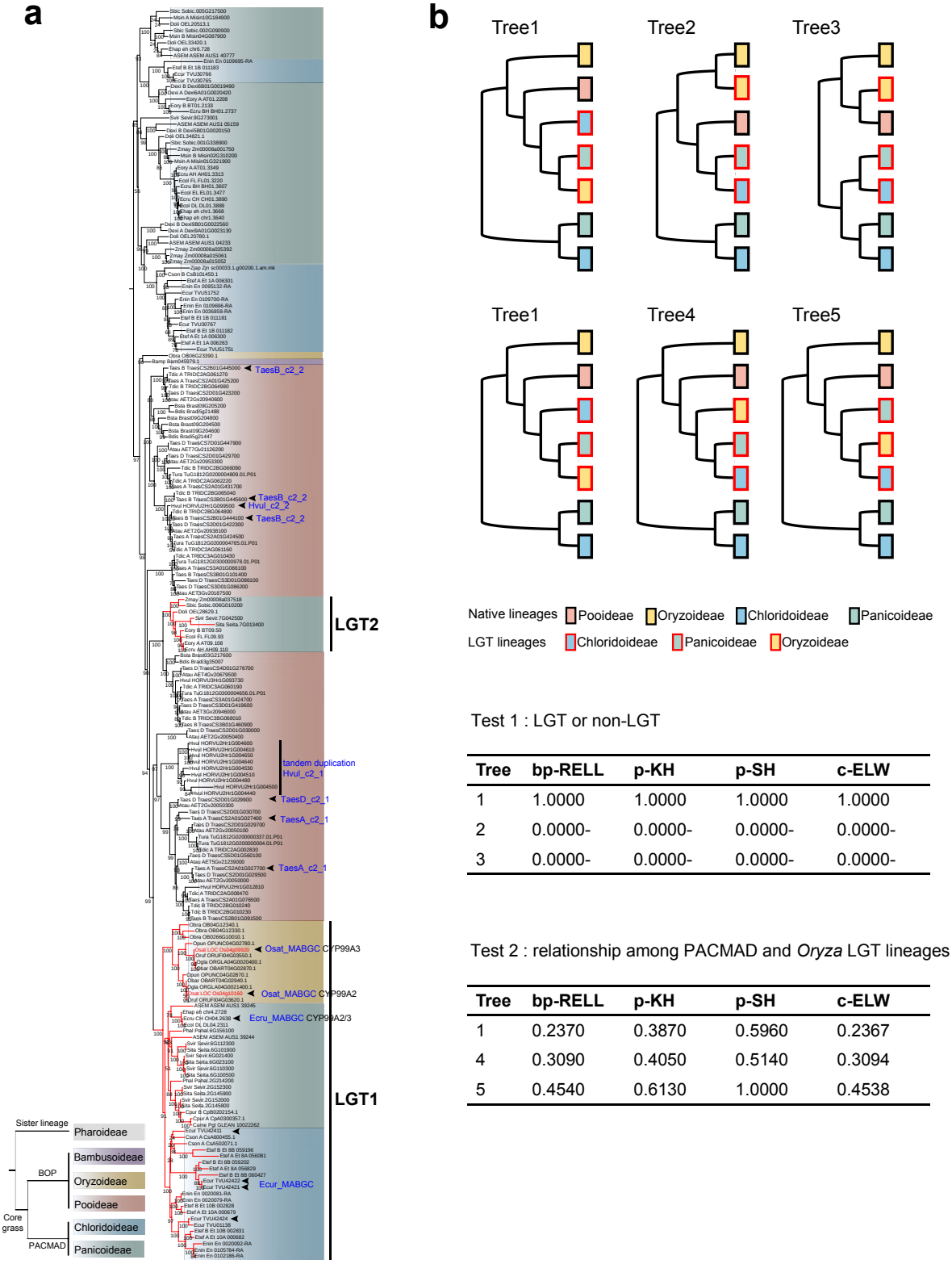


Figure S2. Transcriptomic profiling of wheat genes in MABGC-like clusters under pathogen infections. Genes in different colors are from different subgenomes (blue, subgenome A; red, subgenome B; green, subgenome D). Homolog information is shown by red (*CYP99A2/3*), yellow (*KSL4*), green (*CYP701A8*) and orange (*CPS4*). Dataset1, the spikelet (SP) and rachis (RACH) from two wheat accessions 2618 and 2890 were infected by *Fusarium* head blight (*Fusarium graminearum*) (FG) and water (control). Dataset2, coleoptile sheaths of wheat accession Chara were infected by crown rot (*Fusarium pseudograminearum*) (Fp). Dataset3, leaves from accession N9134 were inoculated by powdery mildew (*Blumeria graminis*). Dataset4, leaves from Glenlea and Salamouni were infected by tan splot (*Pyrenophora tritici-repentis*). All the quantified gene expression (TPM) values were obtained from WheatOmics 1.0 (Ma et al., 2021).



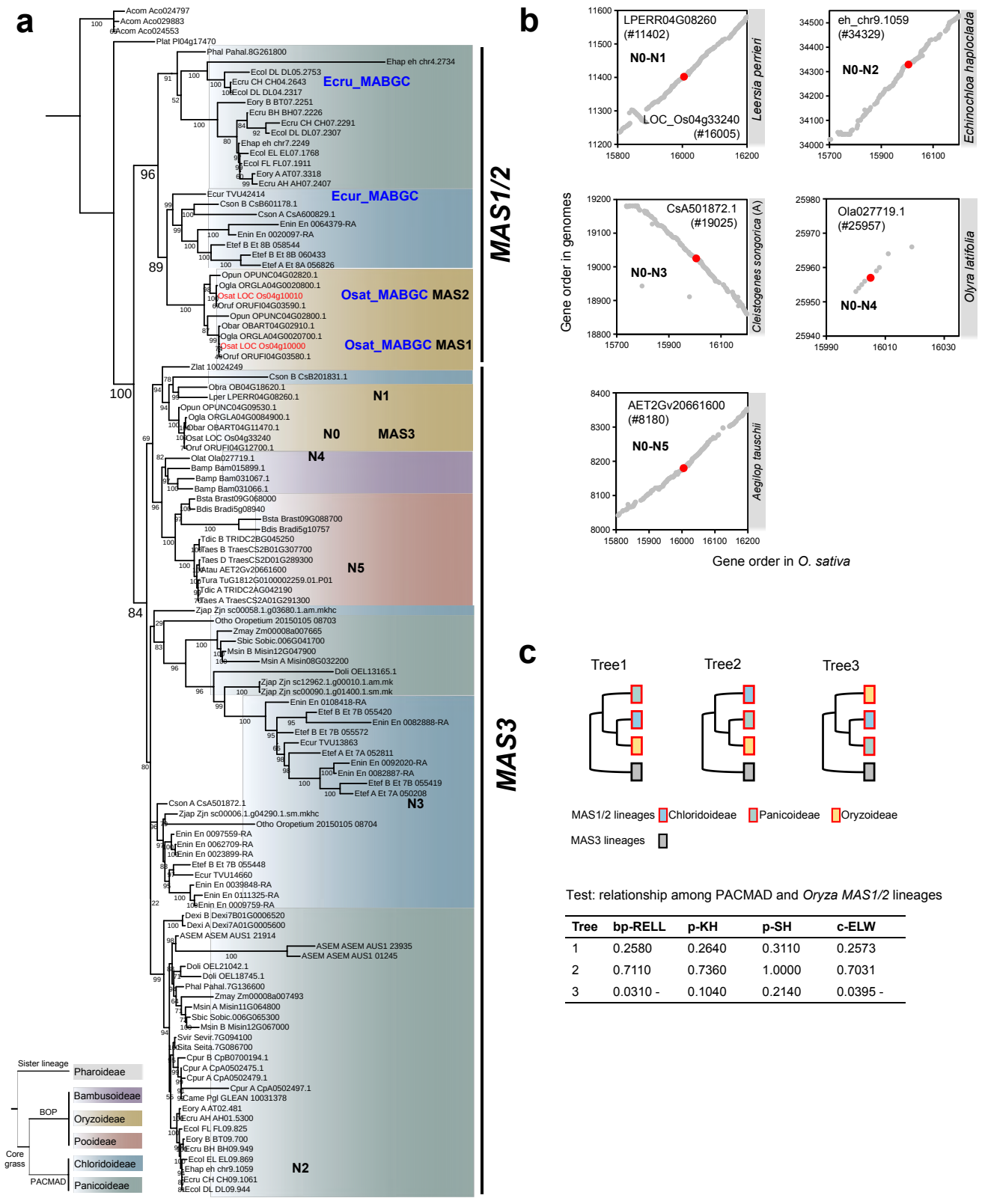
Test 1 : LGT or non-LGT

Tree	bp-RELL	p-KH	p-SH	c-ELW
1	1.0000	1.0000	1.0000	1.0000
2	0.0000-	0.0000-	0.0000-	0.0000-
3	0.0000-	0.0000-	0.0000-	0.0000-

Test 2 : relationship among PACMAD and *Oryza* LGT lineages

Tree	bp-RELL	p-KH	p-SH	c-ELW
1	0.2370	0.3870	0.5960	0.2367
4	0.3090	0.4050	0.5140	0.3094
5	0.4540	0.6130	1.0000	0.4538

Figure S3. Phylogeny of *CYP99A2/3* homologs in grass and topology tests. (a) Homolog phylogeny of *CYP99A2/3* homologs. Genes in different subfamilies are marked in different color backgrounds. Cluster information of some homologs in Triticeae and MABGCs are suggested. **(b)** Topology tests. Three (Tree 1, 2, 3) and three (Tree 1, 4, 5) constrained trees were set for Test 1 and Test 2, respectively. Minus signs "-" represent that the corresponding topology could be rejected significantly (p-value < 0.05).



Test: relationship among PACMAD and *Oryza MAS1/2* lineages

Tree	bp-RELL	p-KH	p-SH	c-ELW
1	0.2580	0.2640	0.3110	0.2573
2	0.7110	0.7360	1.0000	0.7031
3	0.0310 -	0.1040	0.2140	0.0395 -

Figure S4. Phylogeny and genomic synteny of *MAS1/2* homologs in grass. (a) A maximum-likelihood tree of *MAS1/2* and homologs across the grass family. The homolog in *A. comosus* is set as an outgroup. Different background colors represent different subfamilies. **(b)** Genomic synteny among the native *MAS3* homologs. Red dots represent that the two *MAS3* homologs from two genomes are in good synteny. **(c)** Topology tests on three constrained trees. The top panel shows the topologies of constrained trees used in tests. The bottom panels show the results of the test on the LGT event of *MAS1/2* from PACMAD to *Oryza*. Minus signs "-" represent that the corresponding topology could be rejected significantly (*p*-value < 0.05).

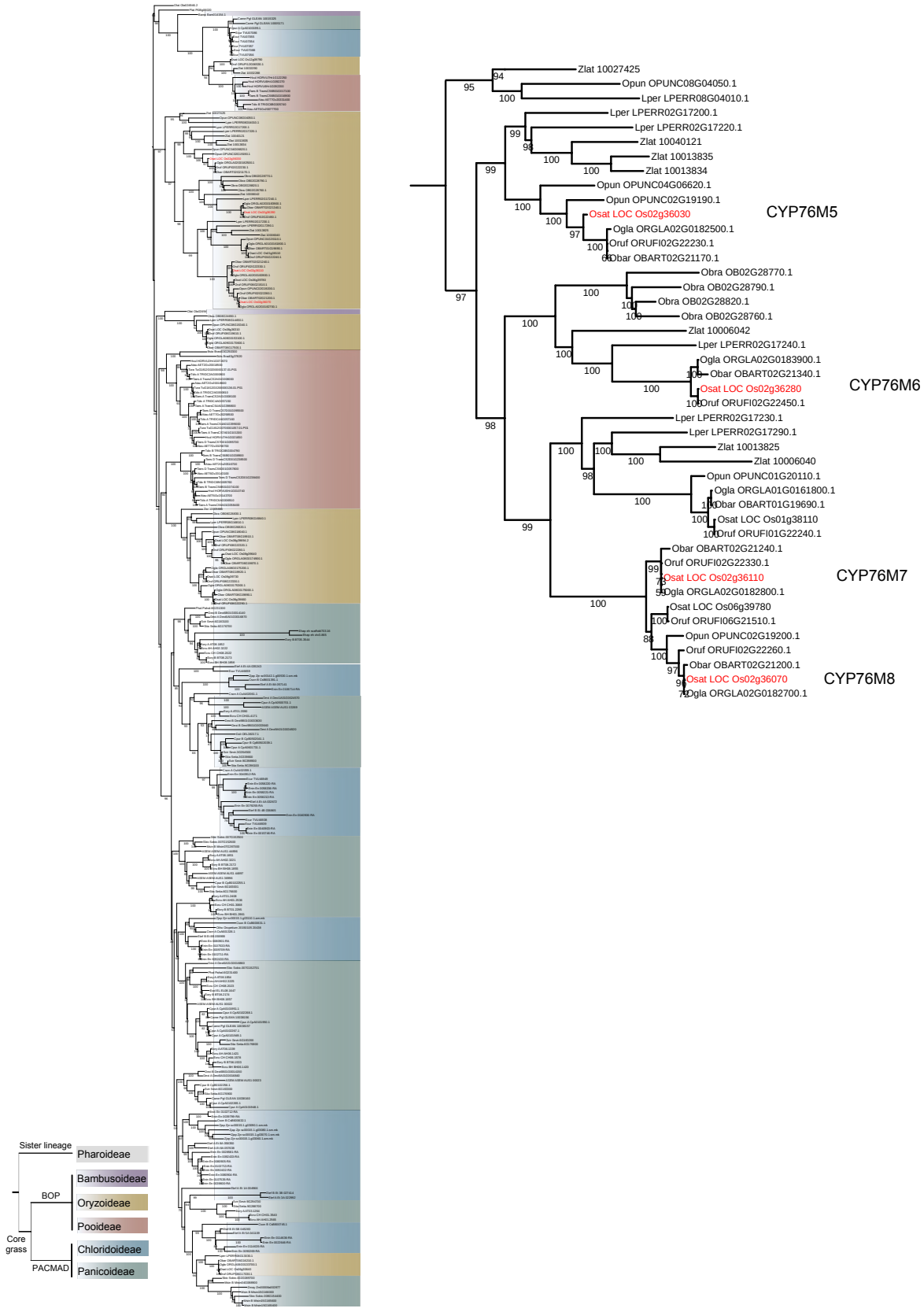


Figure S5. A maximum-likelihood phylogenetic tree of *CYP76M5/6/7/8* homologs in grass. Different background colors represent different subfamilies. The branch containing *CYP76M5/6/7/8* from *O. sativa* is zoomed in.

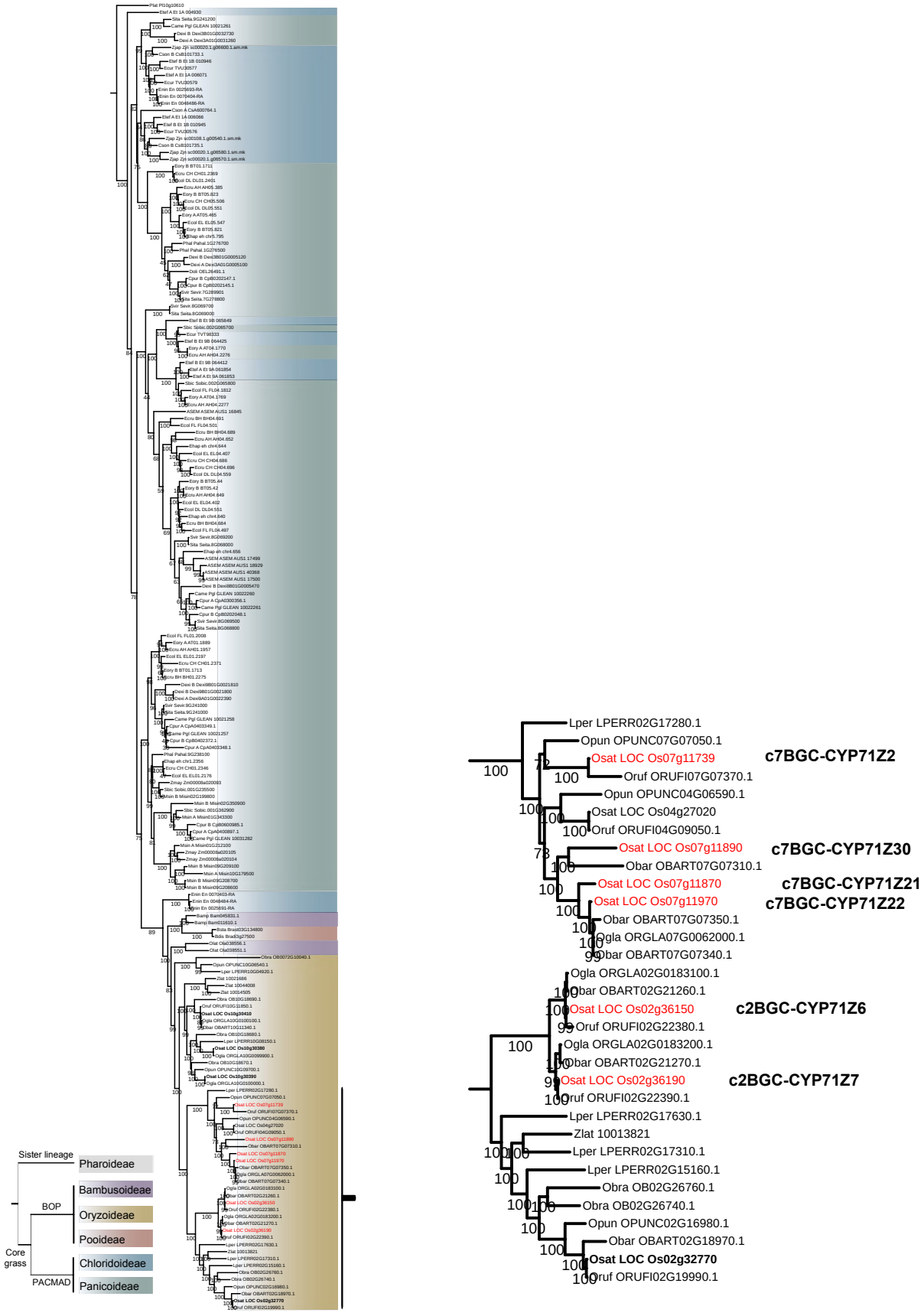


Figure S6. A maximum-likelihood phylogeny of *CYP71Z6/7* homologs in grass. Different background colors represent different subfamilies. The branch containing CYP71Z genes from *O. sativa* is zoomed in and their cluster information (c2BGC and c7BGC) is shown.

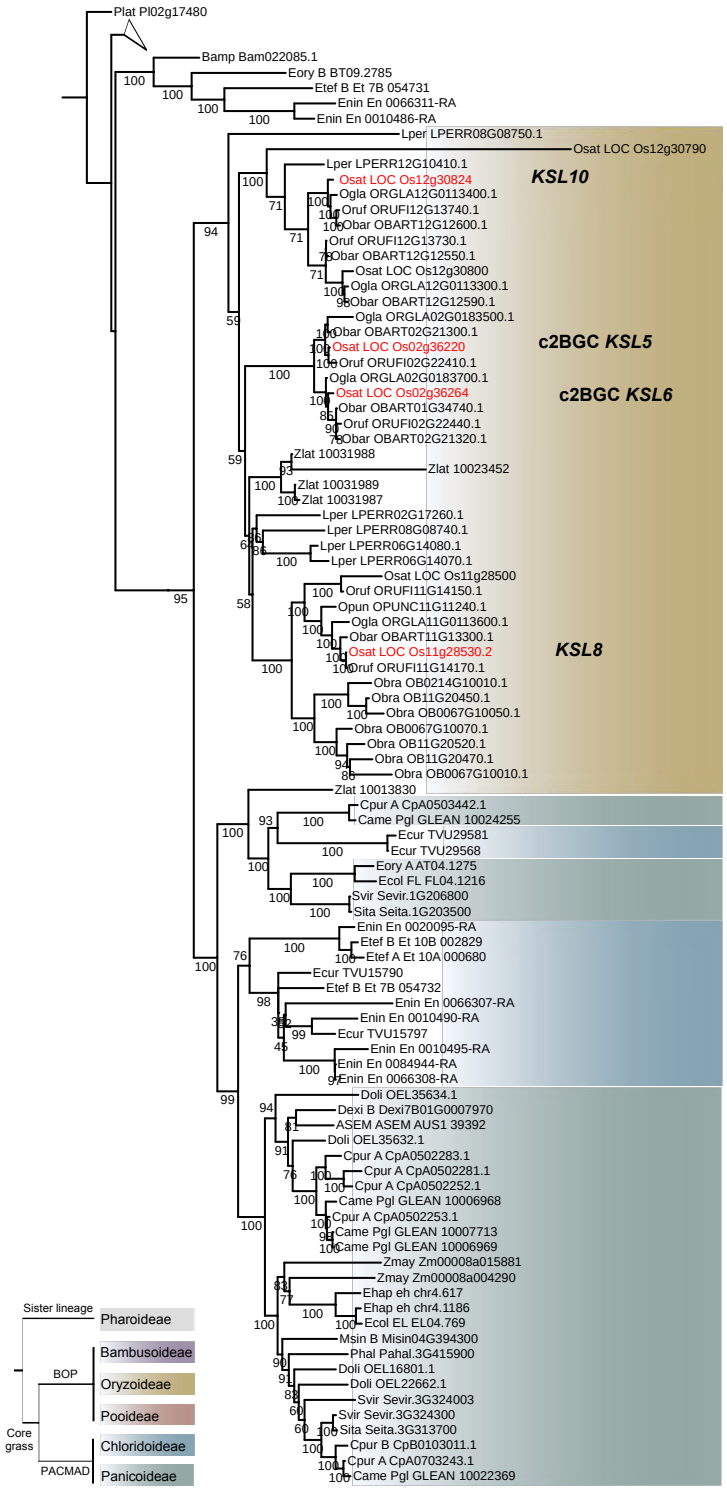
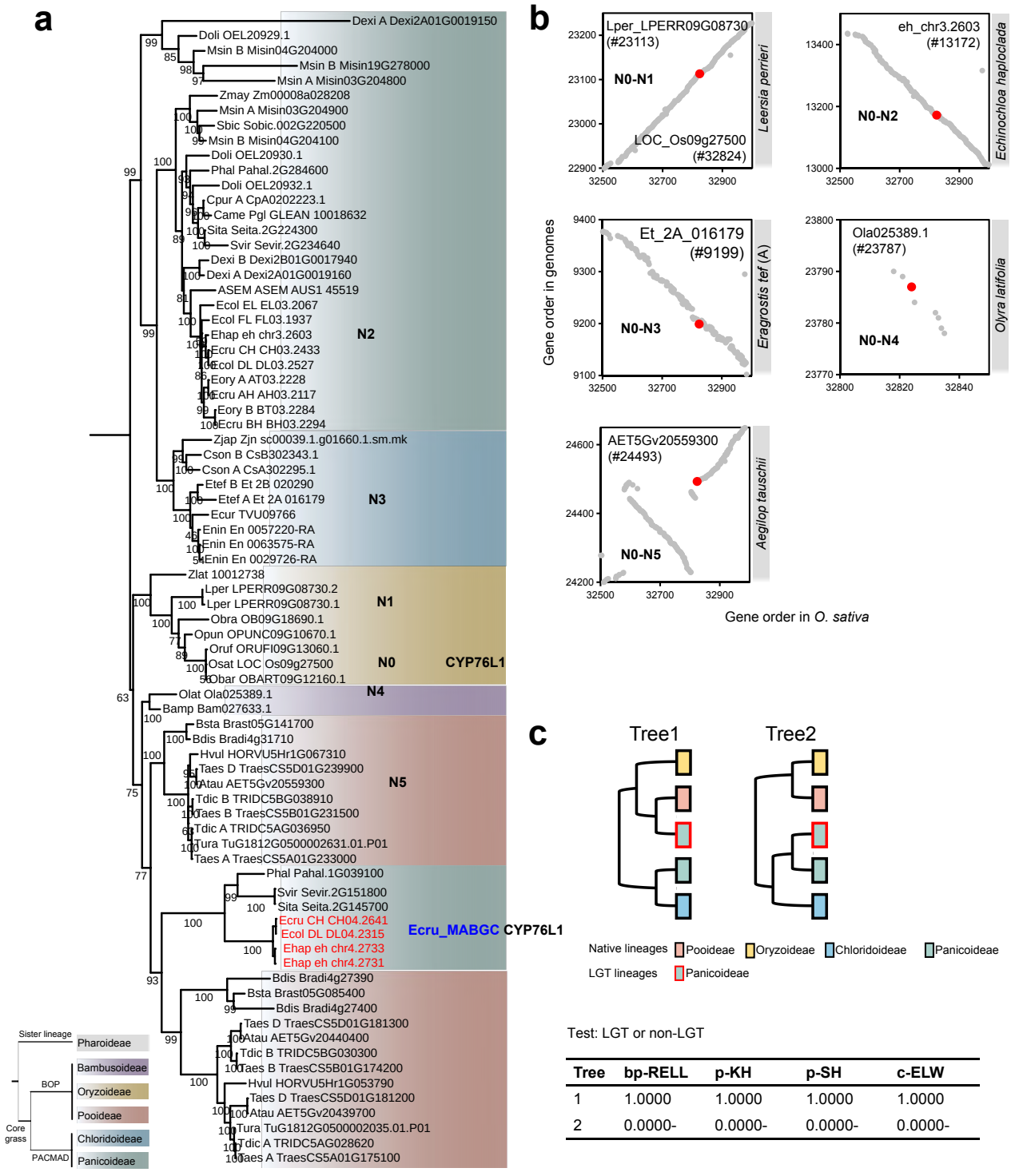


Figure S7. A maximum-likelihood phylogeny of *KSL5/6* homologs in grass. Different background colors represent different subfamilies.



Tree	bp-RELL	p-KH	p-SH	c-ELW
1	1.0000	1.0000	1.0000	1.0000
2	0.0000-	0.0000-	0.0000-	0.0000-

Figure S8. Phylogeny and genomic synteny of *CYP76L1* homologs in grass and topology tests. (a) A maximum-likelihood tree of *CYP76L1* and its homologs across the grass family. Different background colors represent different subfamilies. Genes used in synteny analysis are marked in the phylogenetic tree from N0 to N5. **(b)** Genomic synteny among the native *CYP76L1* homologs. Red dots represent that the two homologs from two genomes are in good synteny. **(c)** Topology tests on two constrained trees. The top panel shows the topologies of constrained trees under tests. The bottom panels show the test results on the LGT of *CYP76L1* from Pooideae to Panicoideae.Minus signs "-" represent that the corresponding topology could be rejected significantly (*p*-value < 0.05).

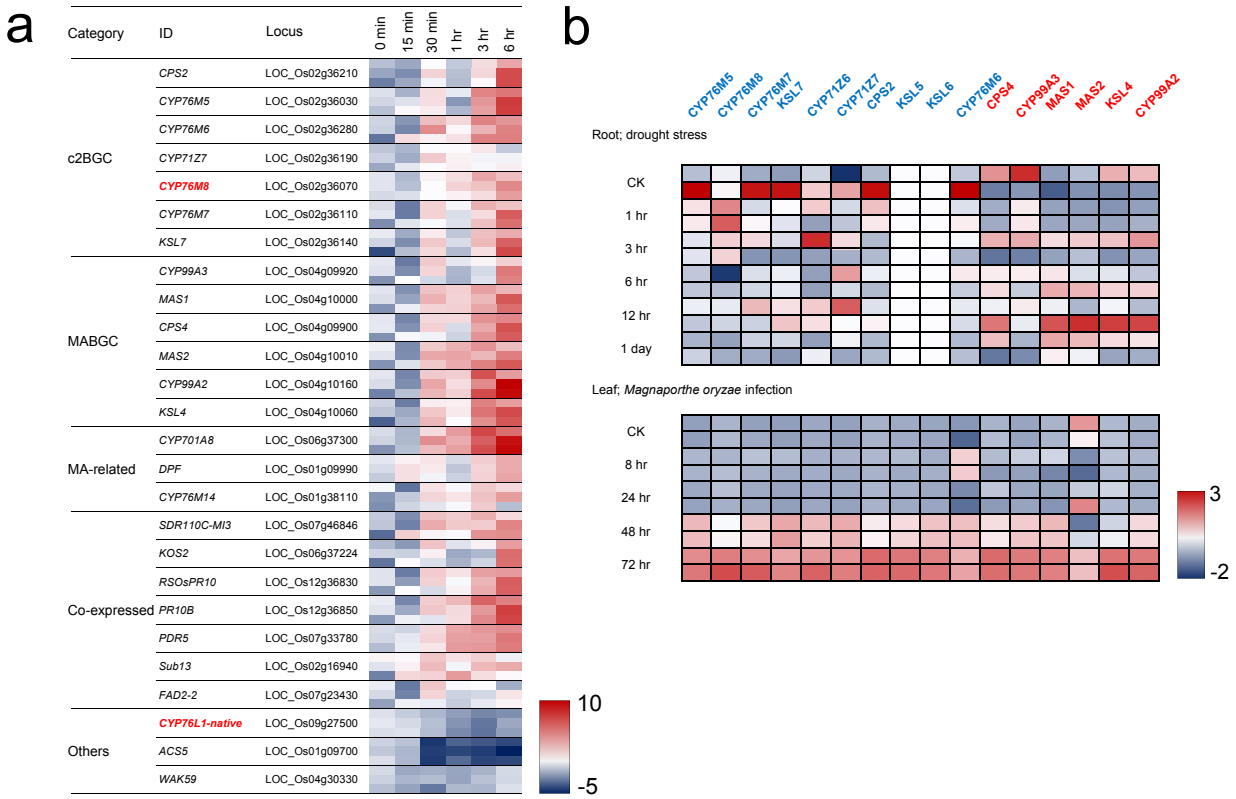


Figure S9. Expression of MABGC, c2BGC and related genes in rice under JA treatment (a), drought and rice blast fungus *M. oryzae* infection (b).

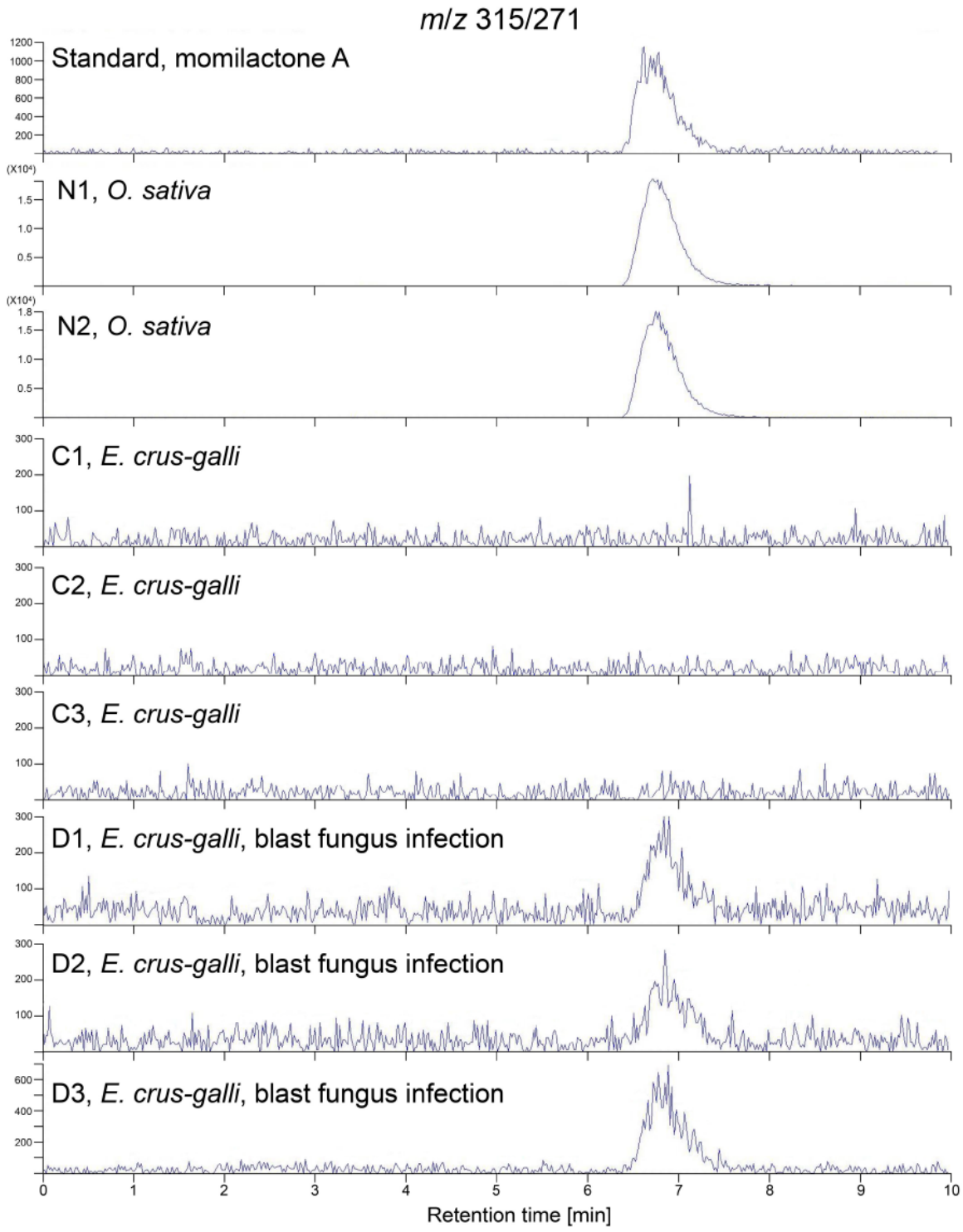


Figure S10. Liquid chromatography-tandem mass spectrometry (LC-MS/MS) analyses of momilactone A in rice and barnyardgrass leaves. Extracts from fresh leaves of rice (*O. sativa*) Nipponbare and barnyardgrass (*E. crus-galli*) STB08 under mock and blast fungus infection treatment were analyzed. Momilactone A was detected with the selected reaction monitoring (*m*/*z* 315/271).

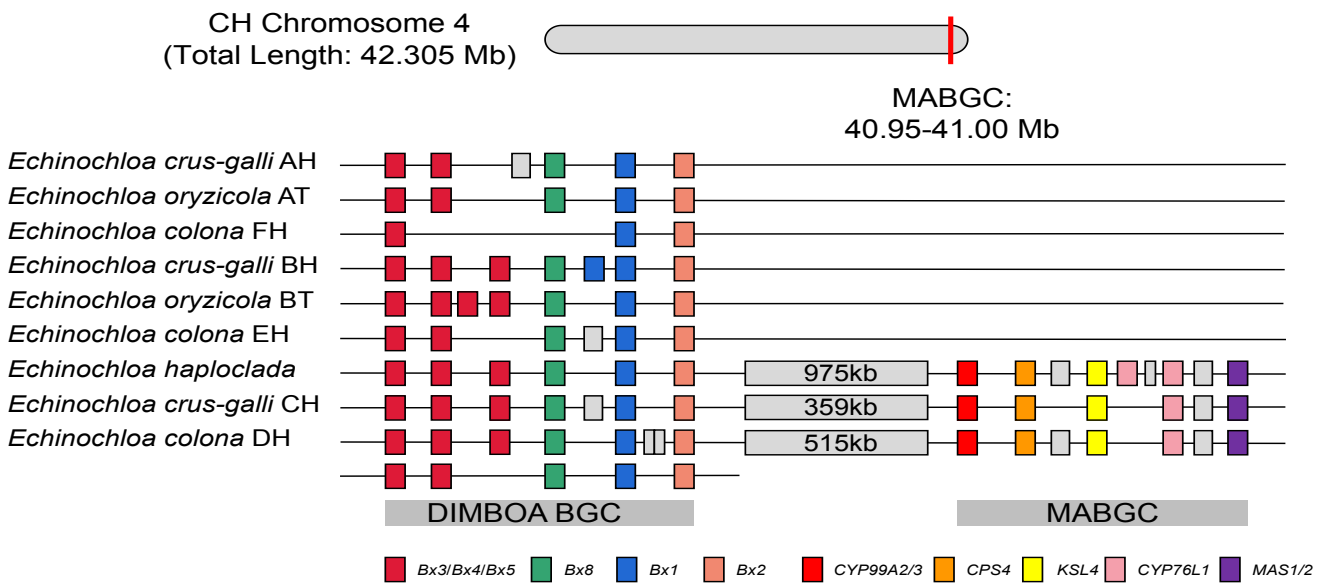


Figure S11. The structures of MABGCs and DIMBOA Bx clusters on chromosomes 4 in nine *Echinochloa* subgenomes.