Figure S1. Phylogenetic tree constructed with 359 single-copy orthologous genes, which were merged into a supermatrix protein sequences with 127453 sites. The tree was constructed by RaxML under the best-fit model PROTGAMMAIJTTF found by ProtTest. Numbers on the branches are bootstrap values.

Acrostichum aureum (SRR1822234)

Acrostichum aureum (SRR6920722)

Acrostichum aureum (SRR2103733)

Acrostichum speciosum(SRR1822235)

Ceratopteris chingii (SRR4210088)

Ceratopteris chingii (SRR4210089)

Ceratopteris gaudichaudii var. **vulgaris** (SRR2103737)

Ceratopteris thalictroides (SRR1822236)
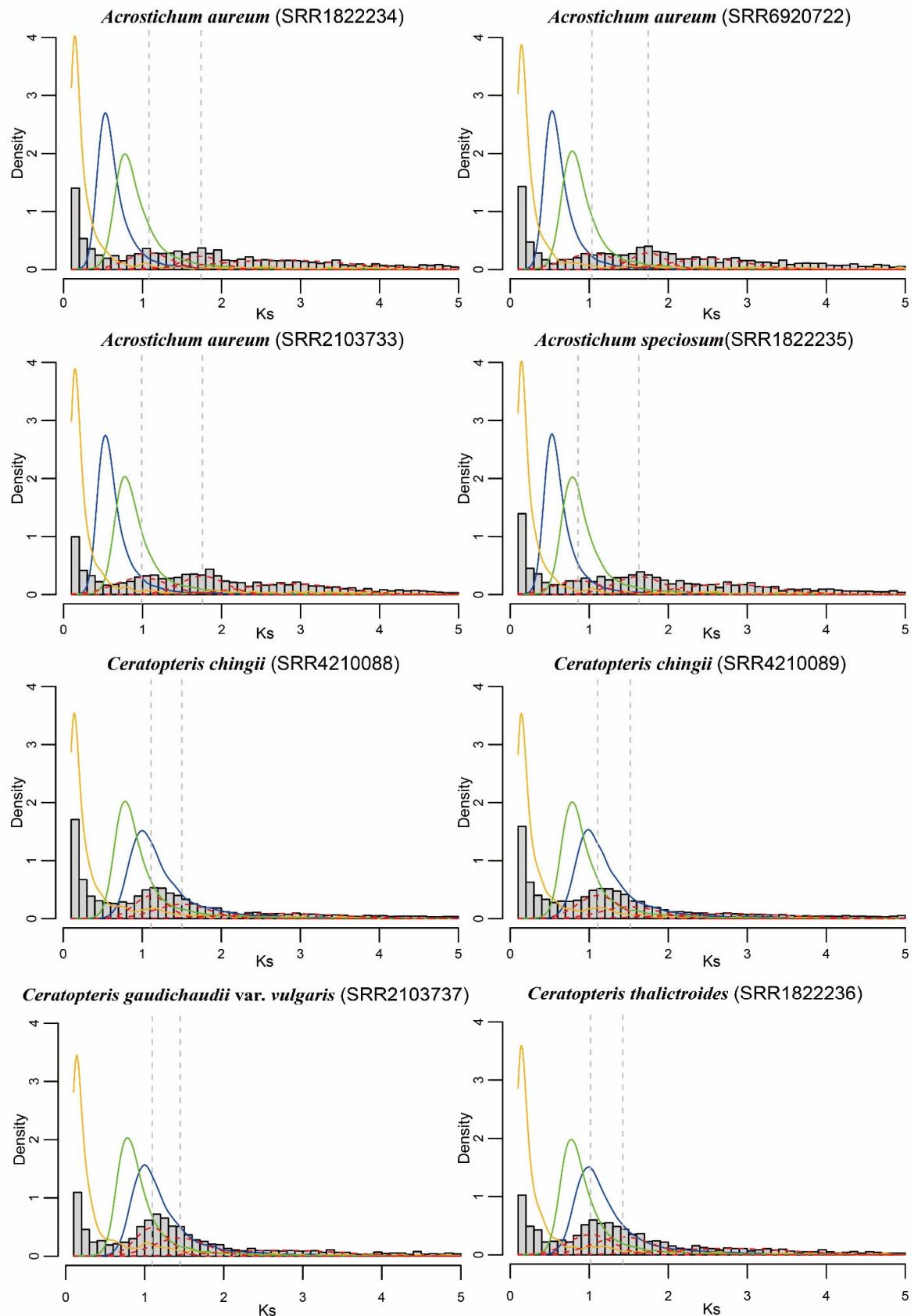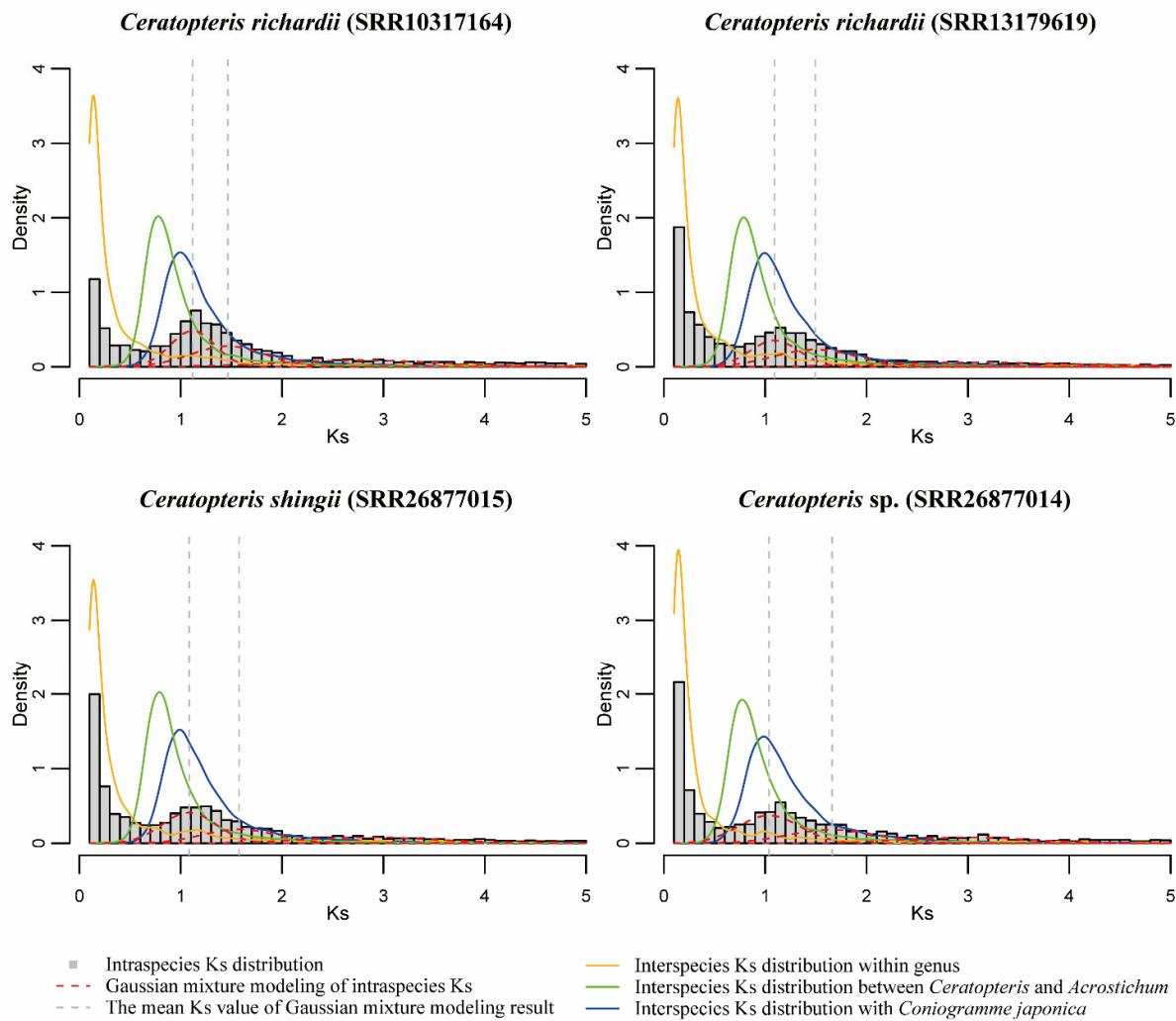
Figure S2. The plots of Ks analysis, including intraspecific and interspecific Ks analysis. The grey histograms presented the Ks distribution of intraspecific paralog pairs with a bin of 0.1 of x-axis, and the Gaussian mixture modeling results were curved in red dashed lines with the peaks marked by vertical grey dashed lines. The interspecific orthologues Ks distribution within genus (between species and *Cer. shingii* within *Ceratopteris*, between species and *Acr. speciosum* within *Acrostichum*), between genera (between the *Acrostichum* species and *Cer. shingii*, the *Ceratopteris* species and *Acr. speciosum*), with *Coniogramme japonica* (between species and *Con. japonica*) were presented by yellow, green, blue solid curves, respectively.
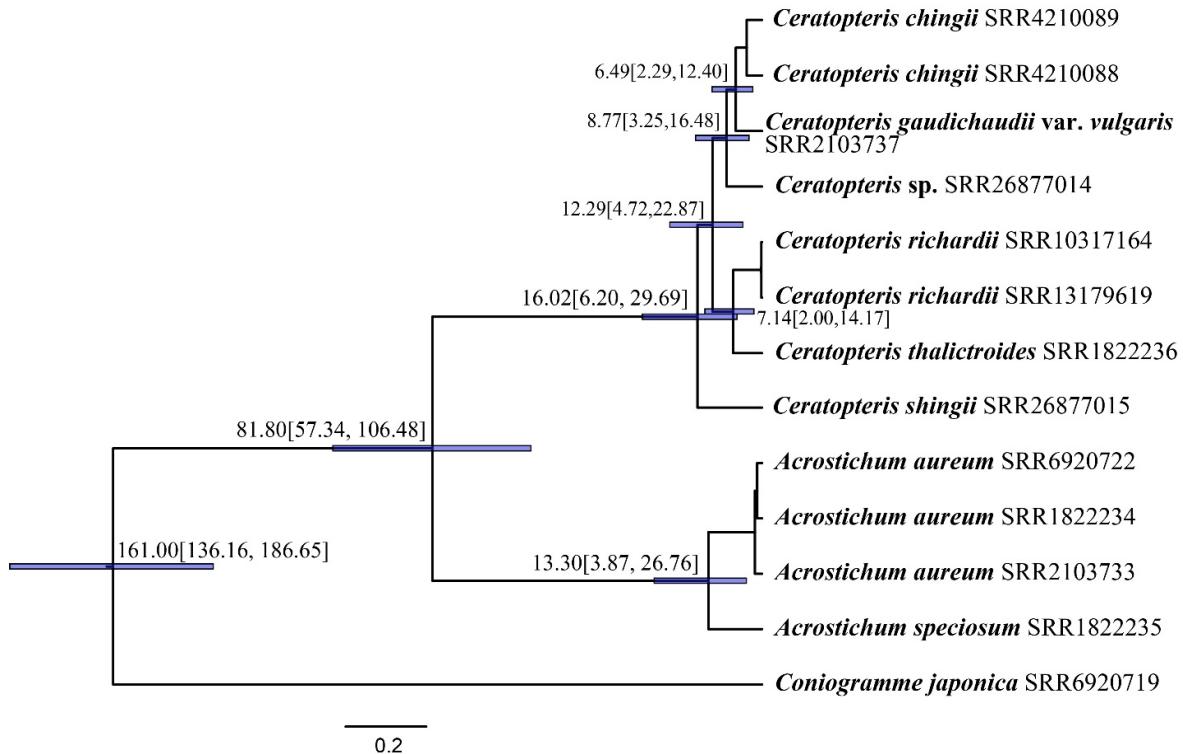
Figure S3. Divergence time estimation using 359 single-copy OGs. The numbers near each node are the corresponding estimated time with a confidence interval of 95%.

(a)

Node	GD	GD ratio	(AB)(AB)
0	2,146	28.07%	6.10%
1	107	1.58%	57.01%
2	96	1.35%	75.00%
3	8,587	47.30%	10.97%
4	91	2.14%	20.88%
5	911	3.69%	84.52%
6	**6,348**	**15.71%**	**64.49%**
7	1,288	29.24%	4.66%
8	608	4.23%	56.41%
9	**856**	**4.98%**	**62.97%**
10	1,263	13.09%	32.07%
11	1,963	10.12%	57.67%

(b)

A1
B1
A2
B2

(c)

+ 3884
28960
−3310
Ceratopteris chingii SRR4210088
5628 / 47488

0

+ 950
28386
−2026

+ 411
29462
−2272

1

+ 2103
26322
−4167
Ceratopteris chingii SRR4210089
6 %
4912 / 45003

2146 / 7645

2

107 / 6789
57 %

+ 948
20731
−9679
Ceratopteris gaudichaudii var. *vulgaris* SRR2103737
2023 / 29780

+ 668
31323
−2641

96 / 7128
75 %

+ 4197
23510
−12010
Ceratopteris sp. SRR26877014

+ 4310
33296
−352

5

911 / 24656
85 %

3236 / 27940

+ 918
21476
−6452
Ceratopteris richardii SRR10317164
1032 / 36295

3

+ 656
27010
−3405

8587 / 18153
11 %

+ 4918
29949
−1979
Ceratopteris richardii SRR13179619
6504 / 58559

+ 5671
29338
−1668

6

6348 / 40413
64 %

+ 278
29759
−3815

4

91 / 4247
21 %

+ 1608
21901
−9466
Ceratopteris thalictroides SRR1822236
3036 / 28677

+ 2967
25886
−6419
Ceratopteris shingii SRR26877015

12203 / 43739

+ 1973
21482
−3697
Acrostichum aureum SRR1822234
1347 / 24790

7

+ 458
23206
−1509

1288 / 4405

+ 1774
20504
−4476
Acrostichum aureum SRR6920722
5 %
2122 / 25953

+ 5968
25335
0

10

1263 / 9652
32 %

+ 1059
24257
−1152

8

608 / 14376
56 %

+ 1257
18888
−6626
Acrostichum aureum SRR2103733
705 / 21194

+ 19367
19367
0

11

1963 / 19401
58 %

+ 1605
24350
−2590

9

856 / 17188
63 %

+ 2169
19787
−6732
Acrostichum speciosum SRR1822235
4113 / 21704

+ 6066
25433
0
Coniogramme japonica SRR6920719
8375 / 21885

Figure S4. Two WGD events inferred by the phylogenetic method. (a) The top-left table contains the number of duplicated gene families (GD), the ratio of GD to gene families (GD ratio), and the proportion of (AB)(AB) type GD of each node. The nodes that may experience WGD events are in bold. (b) A schematic tree of (AB)(AB) type GD. (c) In the tree file, the GD/gene families (yellow box) and the proportion of (AB)(AB) type GD (green box) are also marked below each node. The upper, along and below branch numbers, with green, blue and red colors, indicate the expansion and contraction of gene families. The putative WGD events are marked with grey arrows.
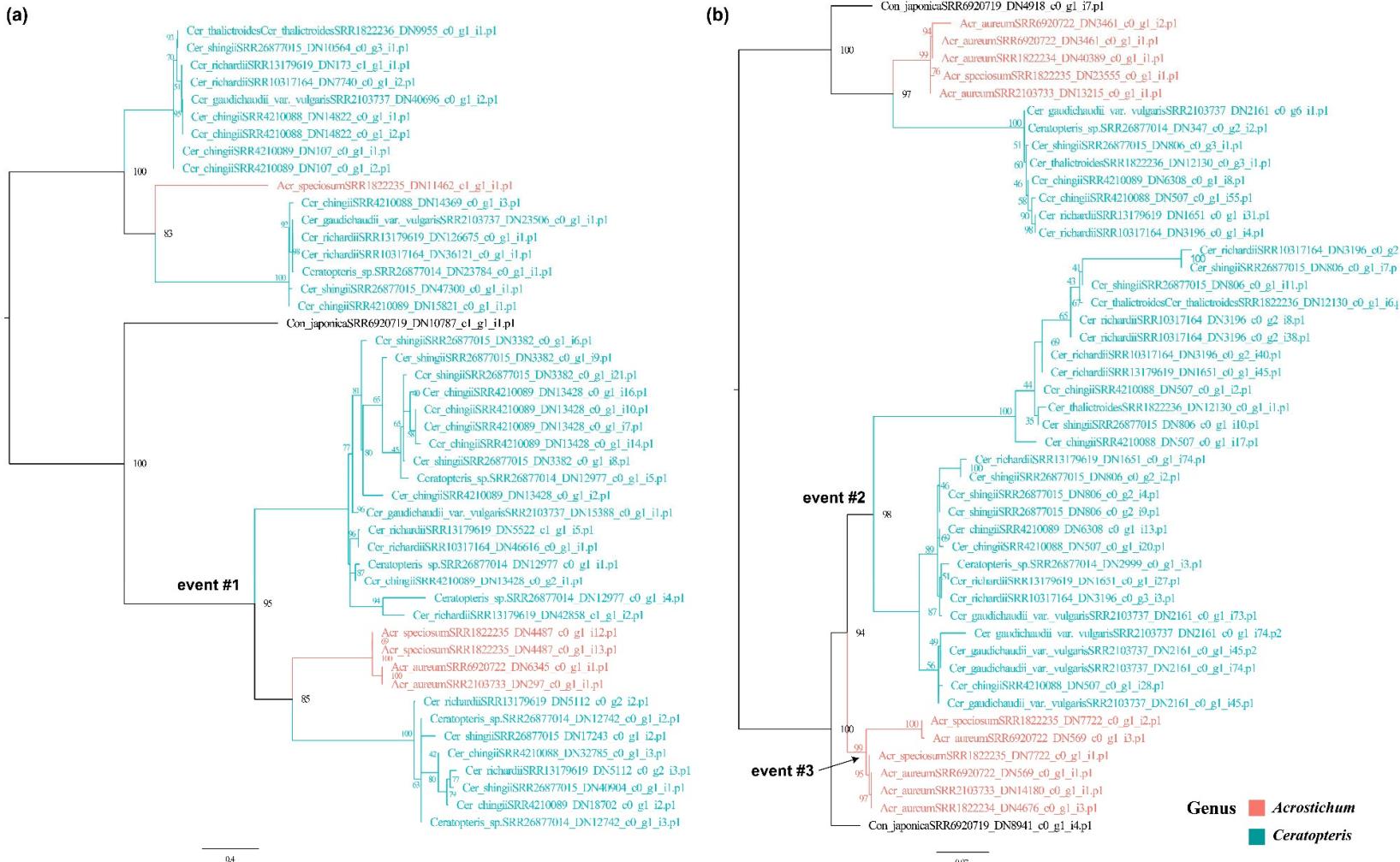
Figure S5. Phylogenetic gene trees of cluster 1109 (a) and cluster 1004 (b) constructed in Tree2GD. The two trees were selected randomly and could find the signals of three putative WGD events. The cluster 1109 and cluster 1004 contained 47 sequences of 12 samples, and 48 sequences of 13 samples, respectively. The gene trees were constructed by IQ-TREE with the JTT+G4 model and 1000 times ultrafast bootstrap. The detailed procedures can be find in the section of Materials and Methods. When inferred a duplicated gene (GD) candidate, the last common ancestor (LCA) of the two sub-branches should have depths with a difference of zero i.e. with topology as ((A,B), (A,B)) or a difference of one, i.e. with topology as ((A,B), B). The depth is calculated by the number of steps it takes to travel from the current node to the root on the species tree.
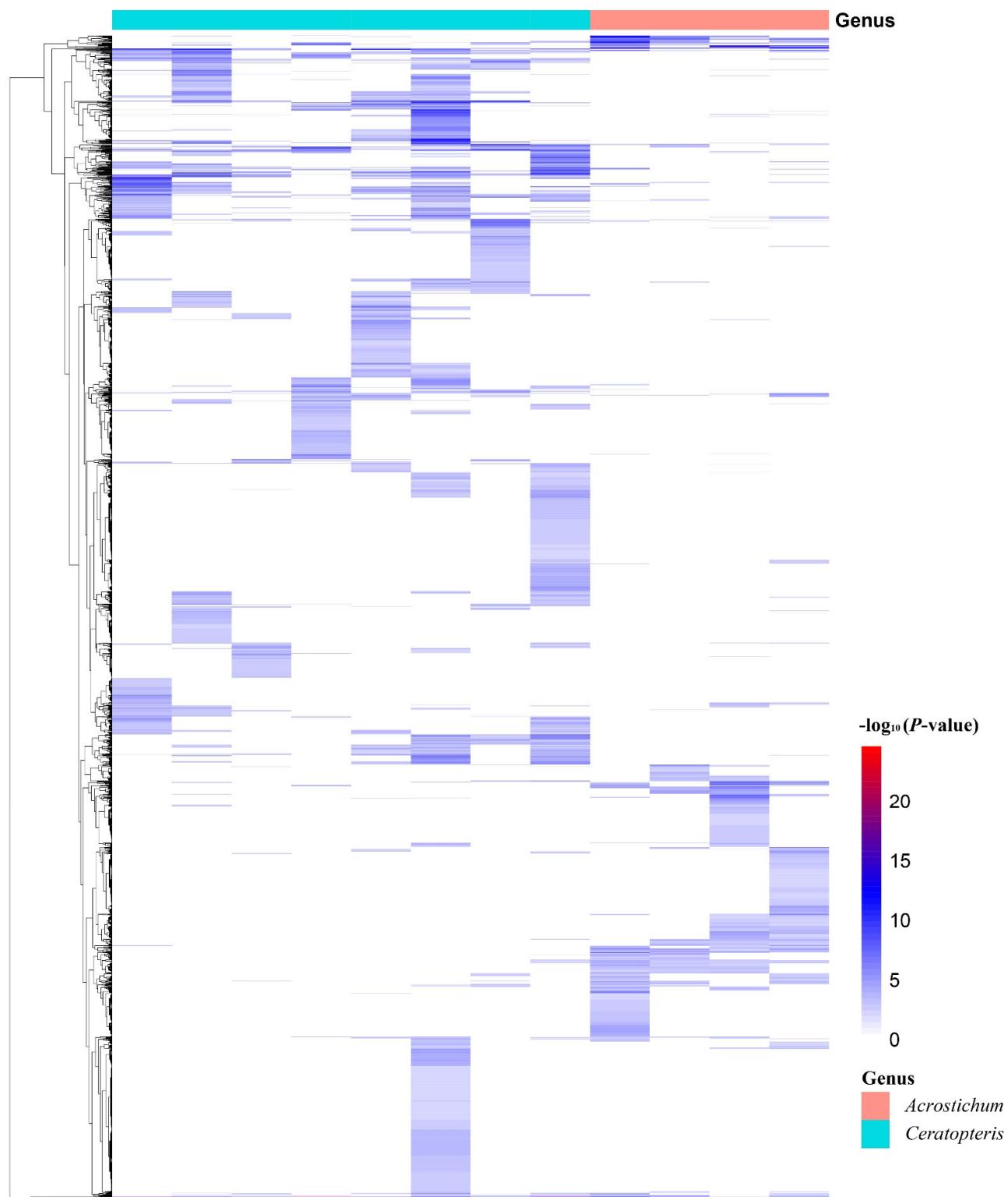
Figure S6. Functional enrichment heatmap of duplicated genes retained from two putative WGD events. The duplicated genes of each putative WGD event were functional enrichment analyzed, respectively, resulting in different patterns of functional terms.
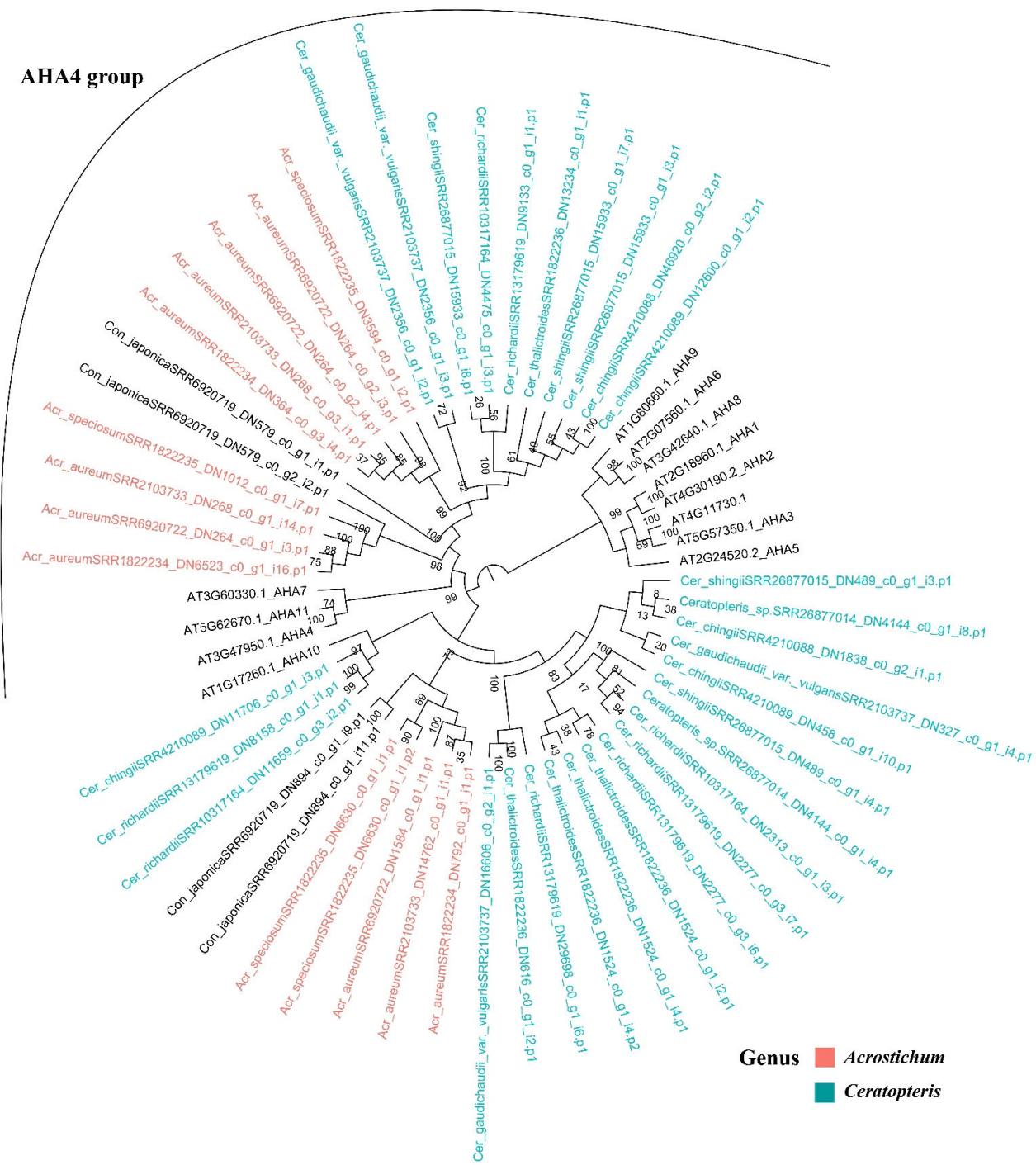
Figure S7. Phylogenetic tree of *AHA* genes. The alignment of *AHA* genes contained 59 protein sequences and 1077 sites. The tree was constructed by maximum likelihood method with the automatically determined substitution model (-m MFP) and 1000 bootstrapping repeats (-b 1000).
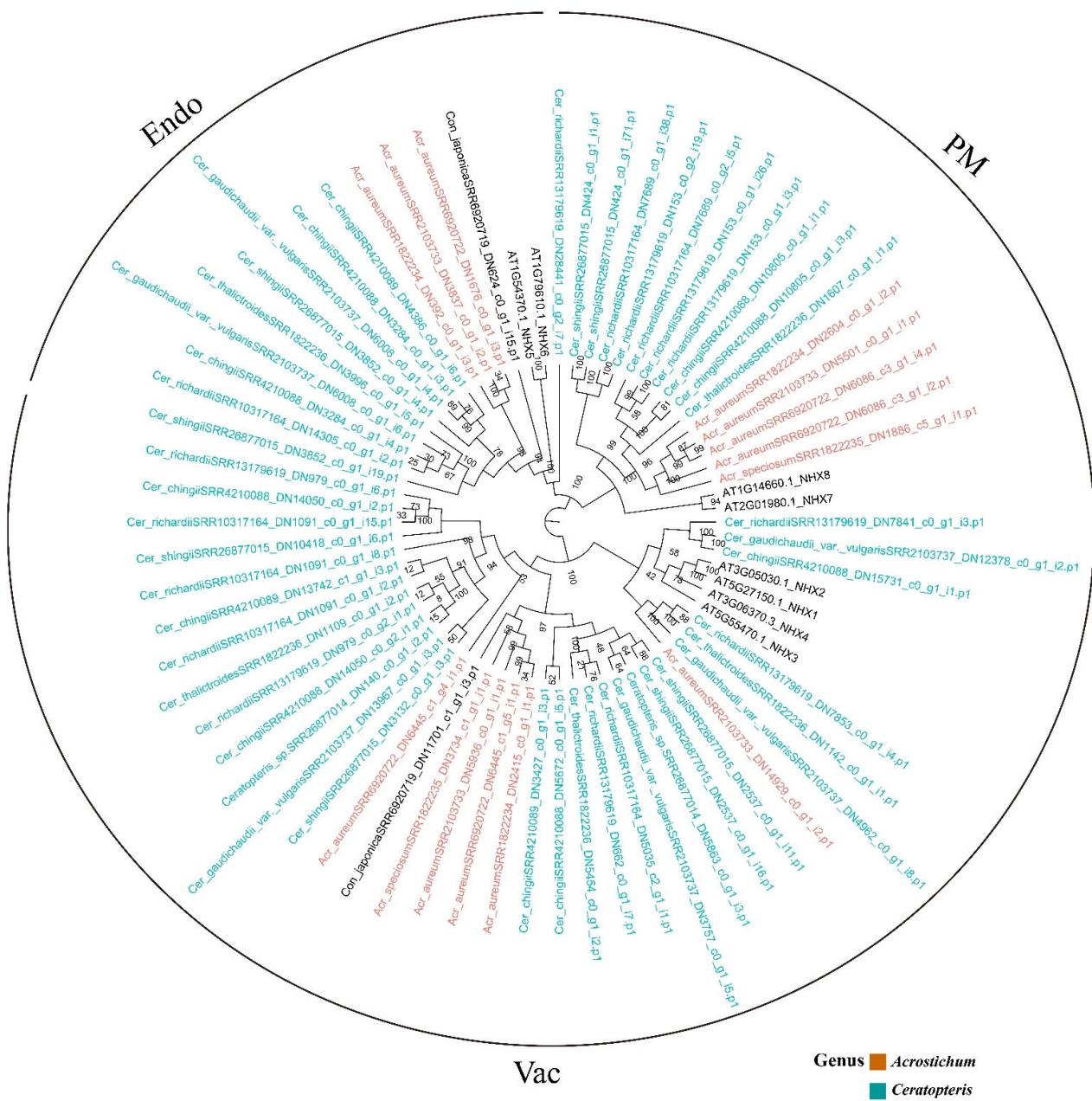
Figure S8. Phylogenetic tree of *NHX* genes. The alignment of *NHX* genes contained 72 protein sequences and 1313 sites. The tree was constructed by maximum likelihood method with the automatically determined substitution model (-m MFP) and 1000 bootstrapping repeats (-b 1000).
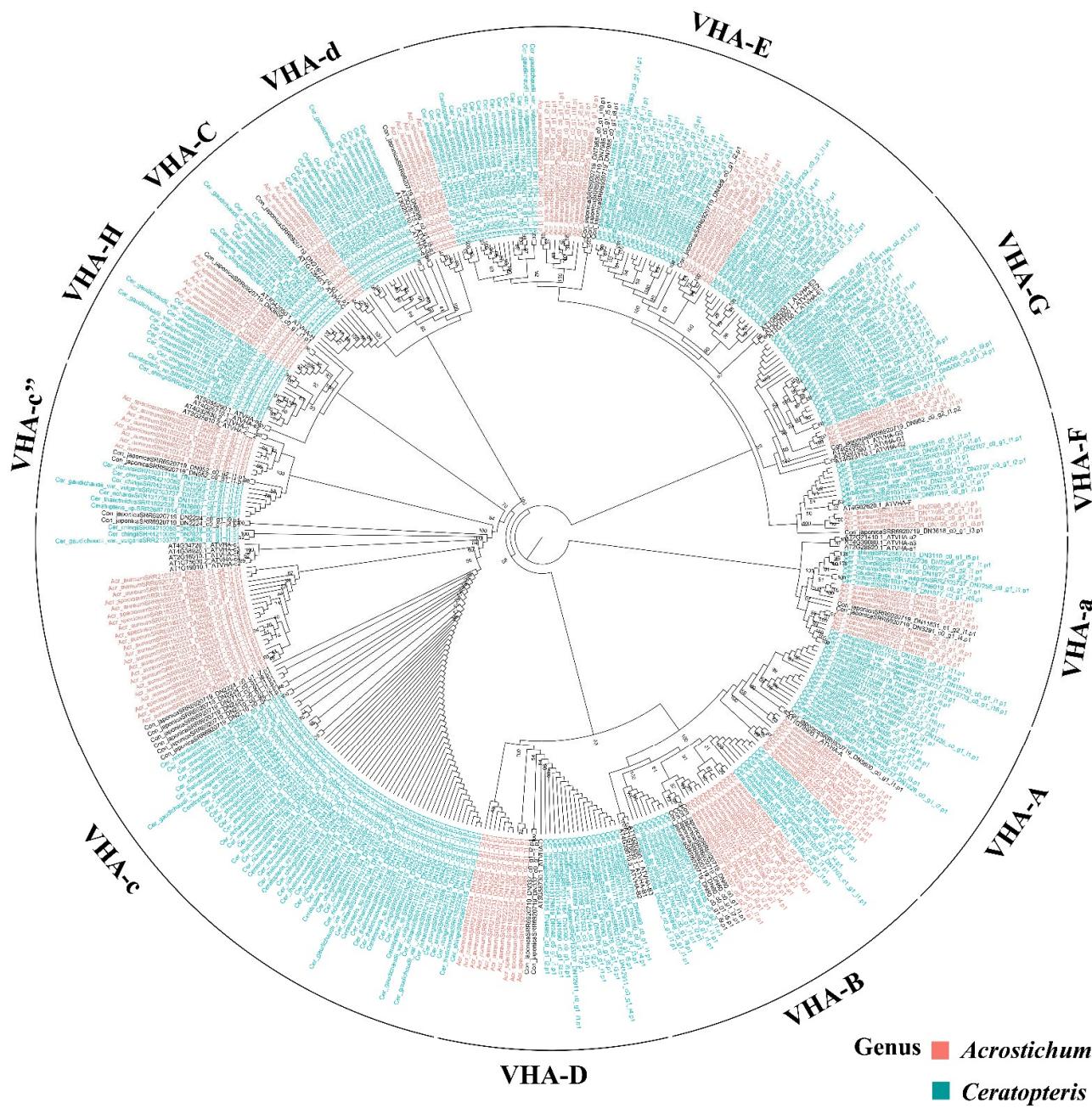
Figure S9. Phylogenetic tree of *VHA* genes. The alignment of *VHA* genes contained 399 protein sequences and 1239 sites. The tree was constructed by maximum likelihood method with the automatically determined substitution model (-m MFP) and 1000 bootstrapping repeats (-bb 1000).