

## **Supporting information**

**Figure S1.** Percentage of variable sites and informative sites of 38 mt genes in 107 taxa. The colored lines under the gene names indicate the categories of the genes.

**Figure S2.** The ML tree inferred by RAxML based on concatenated nt sequences of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

**Figure S3.** The ML tree inferred by RAxML based on concatenated aa sequences of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

**Figure S4.** The ML tree inferred by RAxML based on the combined first and second codon positions of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

**Figure S5.** The ML tree inferred by RAxML based on the third codon positions of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

**Figure S6.** The Bayesian tree inferred by MrBayes based on the concatenated nt sequences of 38 mt genes of 107 species. Numbers on branches are posterior probabilities.

**Figure S7.** The Bayesian tree inferred by Phylobayes with the CAT model based on the concatenated amino acid sequences of 38 mt genes of 107 species. Numbers on branches are posterior probabilities.

**Figure S8.** The Bayesian tree inferred by MrBayes based on the combined first and second codon positions of 38 mt genes of 107 species. Numbers on branches are posterior probabilities.

**Figure S9.** The Bayesian tree inferred by MrBayes based on the third codon positions

of 38 mt genes of 107 species. Numbers on branches are posterior probabilities.

**Figure S10.** The MP tree inferred by PAUP based on concatenated nt sequences of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

**Figure S11.** The MP tree inferred by PAUP based on concatenated aa sequences of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

**Figure S12.** The MP tree inferred by PAUP based on the combined first and second codon positions of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

**Figure S13.** The MP tree inferred by PAUP based on the third codon positions of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

**Figure S14.** Comparison of phylogenetic relationships of major angiosperm lineages between mt genomes (based on the nt data) and APG IV (APG IV, 2016).

**Figure S15.** Comparison of eudicots phylogenetic relationships between mt genomes (based on the nt data) and APG IV (APG IV, 2016).

**Figure S16.** Phylogenetic tree with concordance factors annotated. Three numbers beside each node represent bootstrap value, gCF value, and sCF value.

**Table S1.** Eighteen topologies regarding the relationships of the five mesangiosperm lineages.

**Table S2.** List of 107 taxa sampled for the mitochondrial genomic dataset in this study.

**Table S3.** Partition finder results for the concatenated nucleotide dataset.

**Table S4.** Characteristics of 38 mitochondrial genes, including the number of taxa sampled in the data matrix, the number of total aligned characters, the percentage of gaps or missing data, and variable and informative sites.

**Table S5.** Nucleotide GC compositional contents and codon-usage bias of all mt protein-coding genes in 107 taxa.

**Table S6.** Nucleotide GC content and codon-usage bias of 38 mt genes, 79 pt genes, and 59 nuclear genes in 14 taxa.

**Table S7.** Genes with erroneous placings or extremely long branches in single-gene trees, or not being able to align to other taxa.

**Table S8.** Information of assembled mitochondrial contigs.

Table S1 Eighteen topologies of five mesangiosperm lineages recovered by previous studies.

No.	Topology	References (examples)
1	(Mag-Chl)-(Mon-(Eud-Cer))	Jansen et al., 2007; Moore et al., 2007; Moore et al., 2010; Soltis et al., 2011; Ruhfel et al., 2014; Gitzendanner et al., 2018
2	Mon-(Mag-(Eud-(Cer-Chl)))	Moore et al., 2011; Zeng et al., 2014
3	(Cer-Chl)-(Mag-(Mon-Eud))	Qiu et al., 2010
4	(Cer-Chl)-(Eud-(Mag-Mon))	Endress & Doyle, 2009
5	Eud-(Mon-(Mag-(Cer-Chl)))	Zhang et al., 2012
6	Mon-(Cer-(Eud-(Chl-Mag)))	Barkman et al., 2000
7	(Cer-Mon)-(Chl-(Mag-Eud))	Qiu et al., 1999; Zanis et al., 2002
8	(Cer-Eud)-(Mag-(Chl-Mon))	Hilu et al., 2003; Qiu et al., 2005
9	Mon-(Chl-(Mag-(Cer-Eud)))	Qiu et al., 2005
10	Mon-((Eud-Mag)-(Chl-Cer))	Qiu et al., 2005
11	Eud-((Mag-Mon)-(Cer-Chl))	Qiu et al., 2005
12	Chl-(Mag-(Eud-(Cer-Mon)))	Qiu et al., 2005; Moore et al., 2010
13	Chl-(Mon-(Mag-(Eud-Cer)))	Qiu et al., 2006
14	Mag-(Chl-(Mon-(Cer-Eud)))	Moore et al., 2007
15	(Chl-Mag)-(Cer-(Mon-Eud))	Goremykin et al., 2013
16	Chl-(Mag-(Mon-(Eud-Cer)))	Li et al., 2019
		One Thousand Plant
17	Mon-((Mag-Chl)-(Eud-Cer))	Transcriptomes, 2019
18	Mon-(Mag-(Chl-(Eud-(Cer))))	Yang et al., 2020

**Table S2.** List of 107 taxa sampled for the mitochondrial genomic dataset in this study.

Group	Order	Taxon	Voucher / reference	No. of mt genes sampled (38 in total)	GenBank number(s)	accession
Gymnosperms	Cycadales	<i>Cycas taitungensis</i>	(Chaw, et al. 2008)	36	NC_010303	
	Ginkgoales	<i>Ginkgo biloba</i>	(Guo, et al. 2016)	37	NC_027976	
	Gnetales	<i>Welwitschia mirabilis</i>	(Guo, et al. 2016)	13	NC_029130	
ANA grade	Amborellales	<i>Amborella trichopoda</i>	(Rice, et al. 2013)	32	KF754799-KF754803, KF798319-KF798355	
Magnoliids	Nymphaeales	<i>Nymphaea colorata</i>	(Dong, et al. 2018)	38	NC_037468	
	Austrobaileyales	<i>Schisandra sphenanthera</i>	Yu2018_m01	38		
	Magnoliales	<i>Magnolia Grandiflora</i>	Xue2018_m403	38		
		<i>Magnolia sinostellata</i>	Liu2017_m01	38		
		<i>Annona squamosa</i>	Xue2018_m302	38		
		<i>Liriodendron tulipifera</i>	(Richardson, et al. 2013)	38	NC_021152	
		<i>Cinnamomum camphora</i>	Xue2017_m17	38		
	Laurales	<i>Phoebe sheareri</i>	Xue2017_m08	38		
		<i>Machilus thunbergii</i>	Xue2017_FCM13	38		
		<i>Chimonanthus praecox</i>	Xue2017_m07	37		
		<i>Warburgia ugandensis</i>	Xue2018_m402	38		
	Canellales	<i>Asarum splendens</i>	Xue2017_m19	38		
	Piperales	<i>Saururus chinensis</i>	Xue2017_FCM05	37		
		<i>Piper longum</i>	Xue2017_FCM03	38		
		<i>Chloranthus serratus</i>	Xue2017_m22	35		
-	Chloranthales					

		<i>Sarcandra glabra</i>	Xue2018_m401	34	
-	Ceratophyllales	<i>Ceratophyllum demersum</i>	Xue2018_m301	36	
Eudicots	Ranunculales	<i>Clematis terniflora</i>	Xue2017_m15	33	
	Proteales	<i>Nelumbo nucifera</i>	(Gui, et al. 2016)	38	NC_030753
	Rosales	<i>Cannabis sativa</i>	(White, et al. 2016)	37	NC_027223
		<i>Ziziphus jujuba</i>	No	37	NC_029809
	Cucurbitales	<i>Cucurbita pepo</i>	(Alverson, et al. 2010)	38	NC_014050
		<i>Citrullus lanatus</i>	(Alverson, et al. 2010)	38	NC_014043
	Fabales	<i>Vigna radiata</i>	(Alverson, et al. 2011)	32	NC_015121
		<i>Vigna angularis</i>	(Naito, et al. 2013)	32	NC_021092
		<i>Glycine max</i>	(Chang, et al. 2013)	31	NC_020455
		<i>Millettia pinnata</i>	(Kazakoff, et al. 2012)	31	NC_016742
		<i>Lotus japonicus</i>	(Kazakoff, et al. 2012)	31	NC_016743
		<i>Medicago truncatula</i>	(Bi, et al. 2016)	32	NC_029641
	Myrtales	<i>Lagerstroemia indica</i>	No	36	NC_035616
	Malpighiales	<i>Salix purpurea</i>	(Wei, et al. 2016)	33	NC_029693
		<i>Salix suchowensis</i>	(Ye, et al. 2017)	33	NC_029317
		<i>Populus tremula</i>	(Kersten, et al. 2015)	34	NC_028096
		<i>Populus tremula x Populus alba</i>	(Kersten, et al. 2015)	34	NC_028329
		<i>Populus davidiana</i>	(Choi, et al. 2017)	33	NC_035157
	Malvales	<i>Gossypium barbadense</i>	(Tang, et al. 2015)	35	NC_028254
		<i>Gossypium davidsonii</i>	(Chen, et al. 2017)	35	NC_035075
		<i>Gossypium raimondii</i>	(Chen, et al. 2017)	35	NC_029998
		<i>Gossypium harknessii</i>	(Lei, et al. 2013)	35	NC_027407

	<i>Gossypium hirsutum</i>	(Liu, et al. 2013)	35	NC_027406
	<i>Gossypium thurberi</i>	(Chen, et al. 2017)	35	NC_035074
	<i>Gossypium trilobum</i>	(Chen, et al. 2017)	35	NC_035076
	<i>Gossypium arboreum</i>	(Chen, et al. 2017)	35	NC_035073
	<i>Hibiscus cannabinus</i>	(Liao, et al. 2018)	36	NC_035549
Brassicales	<i>Carica papaya</i>	No	38	NC_012116
	<i>Batis maritima</i>	(Grewe, et al. 2014)	38	NC_024429
	<i>Arabidopsis thaliana</i>	(Unseld, et al. 1997)	24	NC_037304
	<i>Brassica napus</i>	(Handa 2003)	33	NC_008285
	<i>Brassica carinata</i>	(Chang, et al. 2011)	33	NC_016120
	<i>Brassica juncea</i>	(Chang, et al. 2011)	34	NC_016123
	<i>Brassica oleracea</i>	(Chang, et al. 2011)	34	NC_016118
	<i>Brassica rapa</i>	(Chang, et al. 2011)	34	NC_016125
	<i>Sinapis arvensis</i>	No	32	NC_031896
	<i>Brassica nigra</i>	(Yamagishi, et al. 2014)	33	NC_029182
	<i>Raphanus sativus</i>	(Tanaka, et al. 2012)	33	NC_018551
Dilleniales	<i>Dillenia indica</i>	Xue2018_m203	38	
Apiales	<i>Daucus carota subsp. sativus</i>	(Iorizzo, et al. 2012)	33	NC_017855
Asterales	<i>Diplostephium hartwegii</i>	(Vargas, et al. 2017)	35	NC_034354
	<i>Helianthus annuus</i>	(Bock, et al. 2014)	32	NC_023337
Ericales	<i>Vaccinium macrocarpon</i>	(Fajardo, et al. 2014)	37	NC_023338
Caryophyllales	<i>Spinacia oleracea</i>	(Cai, et al. 2017)	28	NC_035618
	<i>Beta vulgaris subsp vulgaris</i>	(Darracq, et al. 2011)	30	NC_002511
	<i>Beta vulgaris subsp maritima</i>	(Darracq, et al. 2011)	31	NC_015099

		<i>Beta macrocarpa</i>	(Darracq, et al. 2011)	31	NC_015994
	Gentianales	<i>Asclepias syriaca</i>	(Straub, et al. 2013)	37	NC_022796
		<i>Rhazya stricta</i>	(Park, et al. 2014)	38	NC_024293
	Lamiales	<i>Hesperelaea palmeri</i>	(Van de Paer, et al. 2016)	36	NC_031323
		<i>Boea hygrometrica</i>	(Zhang, et al. 2012)	35	NC_016741
		<i>Utricularia reniformis</i>	(Silva, et al. 2017)	34	NC_034982
		<i>Ajuga reptans</i>	(Zhu, et al. 2014)	26	NC_023103
		<i>Salvia miltiorrhiza</i>	No	33	NC_023209
		<i>Castilleja paramensis</i>	No	34	NC_031806
		<i>Mimulus guttatus</i>	(Mower, et al. 2012)	35	NC_018041
	Solanales	<i>Ipomoea nil</i>	(Hoshino, et al. 2016)	36	NC_031158
			(Sanchez-Puerta et al. 2015)	37	NC_026515
		<i>Hyoscyamus niger</i>			
		<i>Solanum lycopersicum</i>	No	32	NC_035963
		<i>Solanum pennellii</i>	No	36	NC_035964
		<i>Capsicum annuum</i>	No	37	NC_024624
		<i>Nicotiana attenuata</i>	(Xu, et al. 2017)	37	NC_036467
		<i>Nicotiana tabacum</i>	(Sugiyama, et al. 2005)	37	NC_006581
Monocots	Alismatales	<i>Butomus umbellatus</i>	(Cuenca, et al. 2013)	29	NC_021399
		<i>Spirodela polyrhiza</i>	(Wang, et al. 2012)	35	NC_017840
		<i>Zostera marina</i>	(Petersen, et al. 2017)	24	NC_035345
		<i>Stratiotes aloides</i>	(Petersen, et al. 2017)	27	NC_035317
	Asparagales	<i>Asparagus officinalis</i>	Xue2017_m20	34	
		<i>Allium cepa</i>	(Kim, et al. 2016)	25	NC_030100



Arecales	<i>Cocos nucifera</i>	(Aljohi, et al. 2016)	36	NC_031696
	<i>Phoenix dactylifera</i>	(Fang, et al. 2012)	37	NC_016740
Poales	<i>Tripsacum dactyloides</i>	(Allen, et al. 2007)	31	NC_008362
	<i>Zea luxurians</i>	(Allen, et al. 2007)	31	NC_008333
	<i>Zea perennis</i>	(Allen, et al. 2007)	31	NC_008331
	<i>Zea mays subsp parviglumis</i>	(Allen, et al. 2007)	31	NC_008332
	<i>Zea mays</i>	(Clifton, et al. 2004)	30	NC_007982
	<i>Sorghum bicolor</i>	(Allen, et al. 2007)	31	NC_008360
	<i>Saccharum officinarum</i>	(Shearman, et al. 2016)	19	NC_031164
	<i>Oryza sativa Indica cultivar Group</i>	(Tian, et al. 2006)	33	NC_007886
	<i>Oryza sativa Japonica Group</i>	(Notsu, et al. 2002)	34	NC_011033
	<i>Oryza rufipogon</i>	(Fujii, et al. 2010)	35	NC_013816
	<i>Oryza minuta</i>	No	29	NC_029816
	<i>Aegilops speltoides</i>	No	32	NC_022666
	<i>Triticum timopheevii</i>	No	34	NC_022714
	<i>Triticum aestivum cultivar Chinese Yumai</i>	(Cui, et al. 2009)	32	NC_036024
	<i>Triticum aestivum</i>	(Ogihara, et al. 2005)	33	AP008982

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Newly sequenced taxa are highlighted in gray. Voucher information and GenBank accession numbers are listed.

**Table S3.** Partition finder results for the concatenated nucleotide dataset.

Subset	Best Model	Sites	Positions	Partition names
1	GTR+G	505	1-1515\3;	<i>atp1_pos1</i>
2	GTR+G	1032	2-1515\3 20570-21750\3 22295-22692\3;	<i>atp1_pos2, nad7_pos2, rpl10_pos2</i>
3	GTR+I+G	1032	20571-21750\3 3-1515\3 22296-22692\3;	<i>nad7_pos3, atp1_pos3, rpl10_pos3</i>
4	GTR+G	547	22693-23115\3 28474-28914\3 2683-3003\3 1516-1971\3;	<i>rpl16_pos1, rps7_pos1, atp8_pos1, atp4_pos1</i>
5	GTR+G	1717	25441-25785\3 6883-8028\3 1517-1971\3 15870-16221\3 6885-8028\3 19971-20568\3 2684-3003\3 10299-11079\3;	<i>rps13_pos1, cob_pos1, atp4_pos2, nad3_pos3, cob_pos3, nad6_pos3, atp8_pos2, cox3_pos3</i>
6	GTR+G	1311	28476-28914\3 2685-3003\3 1518-1971\3 3226-3819\3 3228-3819\3 21751-22293\3 21752-22293\3 28475-28914\3;	<i>rps7_pos3, atp8_pos3, atp4_pos3, ccmB_pos1, ccmB_pos3, nad9_pos1, nad9_pos2, rps7_pos2</i>
7	GTR+I+G	1332	9592-10296\3 22694-23115\3 3820-4494\3 16222-17703\3 1972-2682\3;	<i>cox2_pos1, rpl16_pos2, ccmC_pos1, nad4_pos1, atp6_pos1</i>
8	GTR+I+G	1786	1973-2682\3 12701-13431\3 16223-17703\3 17705-17997\3 14405-15867\3 3821-4494\3;	<i>atp6_pos2, mttB_pos2, nad4_pos2, nad4L_pos2, nad2_pos2, ccmC_pos2</i>
9	GTR+I+G	2095	18000-19968\3 1974-2682\3 14406-15867\3 3822-4494\3 12700-13431\3 12702-13431\3;	<i>nad5_pos3, atp6_pos3, nad2_pos3, ccmC_pos3, mttB_pos1, mttB_pos3</i>
10	GTR+I+G	896	3004-3225\3 10297-11079\3 19969-20568\3 25072-25440\3 25073-25440\3 25442-25785\3;	<i>atp9_pos1, cox3_pos1, nad6_pos1, rps12_pos1, rps12_pos2, rps13_pos2</i>
11	GTR+I+G	335	3005-3225\3 10298-11079\3;	<i>atp9_pos2, cox3_pos2</i>
12	GTR+I+G	1227	28917-29277\3 23912-24399\3 26082-26307\3 17706-17997\3 25788-26079\3 3006-3225\3 28915-29277\3 24401-24759\3 9593-10296\3 28916-29277\3;	<i>sdh4_pos3, rpl5_pos2, rps19_pos3, nad4L_pos3, rps14_pos3, atp9_pos3, sdh4_pos1, rps1_pos2, cox2_pos2, sdh4_pos2</i>
13	GTR+G	719	3227-3819\3 8030-9591\3;	<i>ccmB_pos2, cox1_pos2</i>
14	GTR+I+G	1601	4495-5553\3 5554-6882\3 11081-12699\3 23118-23910\3;	<i>ccmFC_pos1, ccmFN_pos1, matR_pos2, rpl2_pos3</i>
15	GTR+I+G	1149	4497-5553\3 4496-5553\3 5556-6882\3;	<i>ccmFC_pos3, ccmFC_pos2, ccmFN_pos3</i>
16	GTR+I+G	576	22294-22692\3 5555-6882\3;	<i>rpl10_pos1, ccmFN_pos2</i>
17	GTR+G	500	15868-16221\3 6884-8028\3;	<i>nad3_pos1, cob_pos2</i>

18	GTR	521	8029-9591\3;	<i>cox1_pos1</i>
19	GTR+G	1196	16224-17703\3 8031-9591\3 21753-22293\3;	<i>nad4_pos3, cox1_pos3, nad9_pos3</i>
20	GTR+G	1012	13434-14403\3 22695-23115\3 9594-10296\3 24761-25071\3 24762-25071\3 24760-25071\3;	<i>nad1_pos3, rpl16_pos3, cox2_pos3, rps10_pos2, rps10_pos3, rps10_pos1</i>
21	GTR+I+G	540	11080-12699\3;	<i>matR_pos1</i>
22	GTR+G	540	11082-12699\3;	<i>matR_pos3</i>
23	GTR+G	1177	13432-14403\3 17998-19968\3 25787-26079\3 25786-26079\3;	<i>nad1_pos1, nad5_pos1, rps14_pos2, rps14_pos1</i>
24	GTR+G	981	13433-14403\3 17999-19968\3;	<i>nad1_pos2, nad5_pos2</i>
25	GTR+I+G	586	14404-15867\3 17704-17997\3;	<i>nad2_pos1, nad4L_pos1</i>
26	GTR+G	318	19970-20568\3 15869-16221\3;	<i>nad6_pos2, nad3_pos2</i>
27	GTR+I+G	394	20569-21750\3;	<i>nad7_pos1</i>
28	GTR+I+G	1248	23117-23910\3 26080-26307\3 26081-26307\3 23911-24399\3 23913-24399\3 24402-24759\3 24400-24759\3 23116-23910\3;	<i>rpl2_pos2, rps19_pos1, rps19_pos2, rpl5_pos1, rpl5_pos3, rps1_pos3, rps1_pos1, rpl2_pos1</i>
29	GTR+G	238	25443-25785\3 25074-25440\3;	<i>rps13_pos3, rps12_pos3</i>
30	GTR+I+G	429	26308-27594\3;	<i>rps3_pos1</i>
31	GTR+I+G	858	26309-27594\3 26310-27594\3;	<i>rps3_pos2, rps3_pos3</i>
32	GTR+I+G	879	27595-28473\3 27596-28473\3 27597-28473\3;	<i>rps4_pos1, rps4_pos2, rps4_pos3</i>

**Table S4.** Characteristics of 38 mitochondrial genes, including the number of taxa sampled in the data matrix, the number of total aligned characters, the percentage of gaps or missing data, variable and informative sites.

Gene	No. of taxa (107 in total)	Total aligned characters	Missing (%)	Variable sites	Variable sites (%)	Informative sites	Informative sites (%)
<i>atp1</i>	107	1515	1.3%	734	48.45%	500	33.00%
<i>atp4</i>	105	456	2.1%	259	56.80%	173	37.94%
<i>atp6</i>	105	711	3.1%	333	46.84%	226	31.79%
<i>atp8</i>	106	321	1.1%	218	67.91%	145	45.17%
<i>atp9</i>	99	222	7.5%	103	46.40%	83	37.39%
<i>ccmB</i>	106	594	1.0%	327	55.05%	199	33.50%
<i>ccmC</i>	104	675	3.5%	316	46.81%	208	30.81%
<i>ccmFC</i>	103	1059	5.7%	601	56.75%	350	33.05%
<i>ccmFN</i>	104	1329	3.5%	704	52.97%	458	34.46%
<i>cob</i>	106	1146	1.4%	472	41.19%	252	21.99%
<i>cox1</i>	105	1563	2.3%	475	30.39%	327	20.92%
<i>cox2</i>	103	705	5.9%	295	41.84%	195	27.66%
<i>cox3</i>	106	783	0.9%	311	39.72%	183	23.37%
<i>matR</i>	106	1620	1.9%	884	54.57%	572	35.31%
<i>mttB</i>	101	732	6.2%	404	55.19%	249	34.02%
<i>nad1</i>	102	972	6.4%	281	28.91%	161	16.56%
<i>nad2</i>	104	1464	4.6%	475	32.45%	254	17.35%
<i>nad3</i>	105	354	1.9%	129	36.44%	89	25.14%
<i>nad4</i>	105	1482	2.7%	525	35.43%	318	21.46%
<i>nad4L</i>	104	294	3.3%	113	38.44%	79	26.87%
<i>nad5</i>	103	1971	5.0%	636	32.27%	407	20.65%
<i>nad6</i>	105	600	1.9%	262	43.67%	166	27.67%
<i>nad7</i>	106	1182	1.7%	350	29.61%	188	15.91%
<i>nad9</i>	107	543	0.1%	224	41.25%	135	24.86%
<i>rpl2</i>	68	795	37.8%	410	51.57%	250	31.45%
<i>rpl5</i>	87	489	18.8%	257	52.56%	162	33.13%
<i>rpl10</i>	73	399	36.4%	193	48.37%	111	27.82%
<i>rpl16</i>	96	423	12.3%	229	54.14%	108	25.53%
<i>rps1</i>	71	360	35.2%	188	52.22%	117	32.50%
<i>rps3</i>	101	1287	6.8%	771	59.91%	522	40.56%
<i>rps4</i>	99	879	10.0%	516	58.70%	370	42.09%
<i>rps7</i>	80	441	26.1%	207	46.94%	112	25.40%
<i>rps10</i>	62	312	42.6%	114	36.54%	81	25.96%
<i>rps12</i>	104	369	2.9%	170	46.07%	103	27.91%
<i>rps13</i>	70	345	34.6%	138	40.00%	77	22.32%
<i>rps14</i>	75	294	32.2%	139	47.28%	83	28.23%
<i>rps19</i>	53	228	53.2%	140	61.40%	83	36.40%
<i>sdh4</i>	72	363	33.9%	197	54.27%	118	32.51%

**Table S5.** Nucleotide GC compositional contents and codon-usage bias of all mt protein-coding genes in 107 taxa.

Group	Taxon	GC	GC1s	GC2s	GC3s	SCUO
Gymnosperm	<i>Cycas taitungensis</i>	0.4470	0.4950	0.4702	0.3758	0.0540
	<i>Ginkgo biloba</i>	0.4571	0.5037	0.4790	0.3887	0.0449
	<i>Welwitschia mirabilis</i>	0.4359	0.5041	0.4205	0.3832	0.0563
Amborellales	<i>Amborella trichopoda</i>	0.4418	0.4932	0.4490	0.3832	0.0485
Nymphaeales	<i>Nymphaea colorata</i>	0.4437	0.4960	0.4462	0.3888	0.0493
Austrobaileyales	<i>Schisandra sphenanthera</i>	0.4437	0.4953	0.4514	0.3845	0.0506
Magnoliids	<i>Annona squamosa</i>	0.4410	0.4921	0.4468	0.3843	0.0500
	<i>Asarum splendens</i>	0.4364	0.4857	0.4432	0.3802	0.0531
	<i>Chimonanthus praecox</i>	0.4364	0.4869	0.4403	0.3820	0.0526
	<i>Cinnamomum camphora</i>	0.4415	0.4915	0.4498	0.3833	0.0504
	<i>Liriodendron tulipifera</i>	0.4426	0.4919	0.4507	0.3851	0.0498
	<i>Magnolia Grandiflora</i>	0.4419	0.4918	0.4506	0.3833	0.0508
	<i>Magnolia sinostellata</i>	0.4420	0.4922	0.4505	0.3833	0.0507
	<i>Machilus thunbergii</i>	0.4414	0.4912	0.4495	0.3834	0.0510
	<i>Phoebe sheareri</i>	0.4409	0.4909	0.4484	0.3833	0.0505
	<i>Piper longum</i>	0.4330	0.4814	0.4394	0.3780	0.0521
	<i>Saururus chinensis</i>	0.4307	0.4822	0.4383	0.3716	0.0561
	<i>Warburgia ugandensis</i>	0.4395	0.4904	0.4465	0.3815	0.0505
	Chloranthales	<i>Chloranthus serratus</i>	0.4414	0.4910	0.4510	0.3821
<i>Sarcandra glabra</i>		0.4413	0.4927	0.4497	0.3815	0.0524
Ceratophyllales	<i>Ceratophyllum demersum</i>	0.4412	0.4913	0.4440	0.3882	0.0497
Monocots	<i>Aegilops speltoides</i>	0.4256	0.4810	0.4245	0.3713	0.0573
	<i>Allium cepa</i>	0.4341	0.4905	0.4368	0.3750	0.0544
	<i>Asparagus officinalis</i>	0.4327	0.4863	0.4378	0.3739	0.0543
	<i>Butomus umbellatus</i>	0.4430	0.4913	0.4439	0.3939	0.0496
	<i>Cocos nucifera</i>	0.4388	0.4903	0.4457	0.3805	0.0505
	<i>Oryza minuta</i>	0.4304	0.4845	0.4248	0.3819	0.0482
	<i>Oryza rufipogon</i>	0.4268	0.4805	0.4250	0.3749	0.0537
	<i>Oryza sativa Indica cultivar Group</i>	0.4272	0.4846	0.4248	0.3721	0.0556
	<i>Oryza sativa Japonica Group</i>	0.4258	0.4804	0.4248	0.3722	0.0560
	<i>Phoenix dactylifera</i>	0.4362	0.4865	0.4423	0.3798	0.0515
	<i>Saccharum officinarum</i>	0.4320	0.4922	0.4239	0.3799	0.0518
	<i>Sorghum bicolor</i>	0.4252	0.4803	0.4266	0.3688	0.0578
	<i>Spirodela polyrhiza</i>	0.4314	0.4854	0.4376	0.3713	0.0538
	<i>Stratiotes aloides</i>	0.4398	0.4924	0.4382	0.3888	0.0510
	<i>Tripsacum dactyloides</i>	0.4258	0.4800	0.4274	0.3699	0.0564
	<i>Triticum aestivum</i>	0.4257	0.4808	0.4243	0.3721	0.0571
	<i>Triticum aestivum cultivar Chinese Yumai</i>	0.4255	0.4800	0.4242	0.3724	0.0566
	<i>Triticum timopheevii</i>	0.4258	0.4811	0.4251	0.3713	0.0572

	<i>Zea luxurians</i>	0.4256	0.4795	0.4267	0.3705	0.0565
	<i>Zea mays</i>	0.4254	0.4809	0.4267	0.3686	0.0580
	<i>Zea mays</i> subsp <i>parviglumis</i>	0.4258	0.4799	0.4272	0.3703	0.0564
	<i>Zea perennis</i>	0.4257	0.4798	0.4271	0.3702	0.0566
	<i>Zostera marina</i>	0.4372	0.4939	0.4339	0.3837	0.0523
Eudicots	<i>Ajuga reptans</i>	0.4371	0.4884	0.4255	0.3976	0.0434
	<i>Arabidopsis thaliana</i>	0.4215	0.4821	0.4194	0.3630	0.0634
	<i>Asclepias syriaca</i>	0.4231	0.4754	0.4252	0.3687	0.0568
	<i>Batis maritima</i>	0.4262	0.4794	0.4264	0.3726	0.0553
	<i>Beta macrocarpa</i>	0.4150	0.4739	0.4087	0.3624	0.0623
	<i>Beta vulgaris</i> subsp <i>maritima</i>	0.4147	0.4740	0.4083	0.3618	0.0624
	<i>Beta vulgaris</i> subsp <i>vulgaris</i>	0.4140	0.4739	0.4082	0.3599	0.0642
	<i>Boea hygrometrica</i>	0.4189	0.4698	0.4229	0.3641	0.0602
	<i>Brassica carinata</i>	0.4241	0.4784	0.4242	0.3697	0.0571
	<i>Brassica juncea</i>	0.4234	0.4775	0.4230	0.3698	0.0574
	<i>Brassica napus</i>	0.4237	0.4781	0.4243	0.3688	0.0577
	<i>Brassica nigra</i>	0.4245	0.4777	0.4206	0.3753	0.0518
	<i>Brassica oleracea</i>	0.4235	0.4775	0.4230	0.3699	0.0574
	<i>Brassica rapa</i>	0.4235	0.4780	0.4230	0.3695	0.0578
	<i>Cannabis sativa</i>	0.4243	0.4781	0.4230	0.3718	0.0567
	<i>Capsicum annuum</i>	0.4258	0.4775	0.4295	0.3704	0.0561
	<i>Carica papaya</i>	0.4286	0.4821	0.4301	0.3736	0.0548
	<i>Castilleja paramensis</i>	0.4208	0.4750	0.4227	0.3648	0.0619
	<i>Citrullus lanatus</i>	0.4296	0.4819	0.4310	0.3760	0.0551
	<i>Clematis terniflora</i>	0.4385	0.4892	0.4466	0.3796	0.0507
	<i>Cucurbita pepo</i>	0.4303	0.4814	0.4298	0.3796	0.0527
	<i>Daucus carota</i>	0.4315	0.4845	0.4327	0.3771	0.0516
	<i>Dillenia indica</i>	0.4255	0.4773	0.4309	0.3682	0.0571
	<i>Diplostephium hartwegii</i>	0.4259	0.4785	0.4278	0.3713	0.0575
	<i>Glycine max</i>	0.4277	0.4814	0.4294	0.3723	0.0553
	<i>Gossypium arboreum</i>	0.4247	0.4752	0.4251	0.3738	0.0549
	<i>Gossypium barbadense</i>	0.4247	0.4753	0.4251	0.3737	0.0550
	<i>Gossypium davidsonii</i>	0.4247	0.4752	0.4251	0.3738	0.0549
	<i>Gossypium harknessii</i>	0.4247	0.4755	0.4249	0.3737	0.0548
	<i>Gossypium hirsutum</i>	0.4247	0.4751	0.4251	0.3738	0.0549
	<i>Gossypium raimondii</i>	0.4245	0.4750	0.4250	0.3734	0.0550
	<i>Gossypium thurberi</i>	0.4245	0.4750	0.4251	0.3735	0.0549
	<i>Gossypium trilobum</i>	0.4245	0.4750	0.4251	0.3734	0.0550
	<i>Helianthus annuus</i>	0.4268	0.4797	0.4293	0.3714	0.0554
	<i>Hesperelaea palmeri</i>	0.4240	0.4767	0.4272	0.3680	0.0574
	<i>Hibiscus cannabinus</i>	0.4250	0.4747	0.4246	0.3757	0.0531
	<i>Hyoscyamus niger</i>	0.4250	0.4771	0.4291	0.3689	0.0575
	<i>Ipomoea nil</i>	0.4221	0.4746	0.4262	0.3656	0.0585
	<i>Lagerstroemia indica</i>	0.4239	0.4754	0.4263	0.3701	0.0585

<i>Lotus japonicus</i>	0.4271	0.4791	0.4306	0.3716	0.0545
<i>Medicago truncatula</i>	0.4263	0.4813	0.4279	0.3699	0.0550
<i>Millettia pinnata</i>	0.4280	0.4808	0.4296	0.3735	0.0547
<i>Mimulus guttatus</i>	0.4219	0.4738	0.4258	0.3661	0.0599
<i>Nelumbo nucifera</i>	0.4380	0.4893	0.4457	0.3789	0.0517
<i>Nicotiana attenuata</i>	0.4245	0.4773	0.4290	0.3672	0.0582
<i>Nicotiana tabacum</i>	0.4247	0.4767	0.4289	0.3685	0.0574
<i>Populus davidian</i>	0.4195	0.4715	0.4160	0.3711	0.0597
<i>Populus tremula</i>	0.4198	0.4718	0.4182	0.3694	0.0606
<i>Populus tremula</i> x <i>Populus alba</i>	0.4198	0.4718	0.4182	0.3695	0.0605
<i>Raphanus sativus</i>	0.4234	0.4780	0.4217	0.3703	0.0575
<i>Rhazya stricta</i>	0.4242	0.4774	0.4274	0.3678	0.0580
<i>Salix purpurea</i>	0.4196	0.4715	0.4177	0.3696	0.0610
<i>Salix suchowensis</i>	0.4197	0.4716	0.4177	0.3696	0.0607
<i>Salvia miltiorrhiza</i>	0.4211	0.4752	0.4235	0.3646	0.0606
<i>Sinapis arvensis</i>	0.4239	0.4790	0.4243	0.3684	0.0583
<i>Solanum lycopersicum</i>	0.4303	0.4822	0.4293	0.3795	0.0498
<i>Solanum pennellii</i>	0.4262	0.4790	0.4289	0.3708	0.0561
<i>Spinacia oleracea</i>	0.4148	0.4733	0.4087	0.3624	0.0607
<i>Utricularia reniformis</i>	0.4237	0.4736	0.4287	0.3688	0.0584
<i>Vaccinium macrocarpon</i>	0.4222	0.4764	0.4204	0.3697	0.0581
<i>Vigna angularis</i>	0.4276	0.4783	0.4289	0.3756	0.0544
<i>Vigna radiata</i>	0.4279	0.4785	0.4293	0.3760	0.0543
<i>Ziziphus jujuba</i>	0.4297	0.4829	0.4335	0.3726	0.0562

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GC, CG1, GC2 and GC3 indicate GC compositional contents of all codon positions and 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> codon positions, respectively. SCUO indicates the degree of codon-usage bias.

**Table S6.** Nucleotide GC content and codon-usage bias of 38 mt genes, 79 cp genes and 59 nuclear genes in 14 taxa.

species	SCUO			GC			GC1			GC2			GC3		
	pt	mt	nu	pt	mt	nu	pt	mt	nu	pt	mt	nu	pt	mt	nu
<i>Amborella trichopoda</i>	0.1044	0.0485	0.0556	0.3937	0.4418	0.4353	0.4713	0.4932	0.5338	0.3956	0.4490	0.3597	0.3141	0.3832	0.4122
<i>Arabidopsis thaliana</i>	0.1381	0.0634	0.0479	0.3741	0.4215	0.4386	0.4587	0.4821	0.5254	0.3832	0.4194	0.3882	0.2806	0.3630	0.4021
<i>Asparagus officinalis</i>	0.1186	0.0543	0.0404	0.3897	0.4327	0.4559	0.4745	0.4863	0.5367	0.3976	0.4378	0.3964	0.2970	0.3739	0.4346
<i>Ceratophyllum demersum</i>	0.1149	0.0497	0.0815	0.3872	0.4412	0.4141	0.4693	0.4913	0.5122	0.3909	0.4440	0.3810	0.3015	0.3882	0.3490
<i>Chimonanthus praecox</i>	0.1034	0.0526	0.0507	0.3948	0.4364	0.4446	0.4740	0.4869	0.5317	0.3948	0.4403	0.3912	0.3156	0.3820	0.4108
<i>Cinnamomum camphora</i>	0.0997	0.0504	0.0453	0.3950	0.4415	0.4528	0.4719	0.4915	0.5387	0.3939	0.4498	0.3932	0.3193	0.3833	0.4266
<i>Ginkgo biloba</i>	0.1212	0.0449	0.0711	0.3954	0.4571	0.4364	0.4842	0.5037	0.5391	0.4020	0.4790	0.3959	0.2999	0.3887	0.3742
<i>Glycine max</i>	0.1546	0.0553	0.0491	0.3646	0.4277	0.4458	0.4509	0.4814	0.5321	0.3761	0.4294	0.3878	0.2667	0.3723	0.4176
<i>Gossypium raimondii</i>	0.1149	0.0550	0.0539	0.3862	0.4245	0.4357	0.4670	0.4750	0.5272	0.3873	0.4250	0.3834	0.3043	0.3734	0.3966
<i>Liriodendron tulipifera</i>	0.1037	0.0498	0.0550	0.3944	0.4426	0.4373	0.4731	0.4919	0.3744	0.3955	0.4507	0.4175	0.3146	0.3851	0.5200
<i>Medicago truncatula</i>	0.1488	0.0550	0.0726	0.3686	0.4263	0.4237	0.4570	0.4813	0.5207	0.3778	0.4279	0.3903	0.2710	0.3699	0.3600
<i>Solanum lycopersicum</i>	0.1173	0.0498	0.0666	0.3858	0.4303	0.4308	0.4672	0.4822	0.5276	0.3900	0.4293	0.3864	0.3002	0.3795	0.3785
<i>Sorghum bicolor</i>	0.1151	0.0578	0.0243	0.3936	0.4252	0.4923	0.4795	0.4803	0.5615	0.3984	0.4266	0.4018	0.3029	0.3688	0.5136
<i>Zea mays</i>	0.1152	0.0580	0.0231	0.3930	0.4254	0.4968	0.4793	0.4809	0.5615	0.3978	0.4267	0.4060	0.3019	0.3686	0.5230
average	0.1193	0.0532	0.0526	0.3869	0.4339	0.4457	0.4699	0.4863	0.5230	0.3915	0.4382	0.3913	0.2993	0.3771	0.4228
standard deviation	0.0168	0.0047	0.0169	0.0103	0.0100	0.0233	0.0092	0.0074	0.0449	0.0078	0.0156	0.0132	0.0161	0.0082	0.0575

GC, GC1, GC2 and GC3 indicate GC content of all codon positions and 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> codon position, respectively. SCUO indicates the degree of codon-usage bias. Pt, plastid; mt, mitochondrial; nu, nuclear.



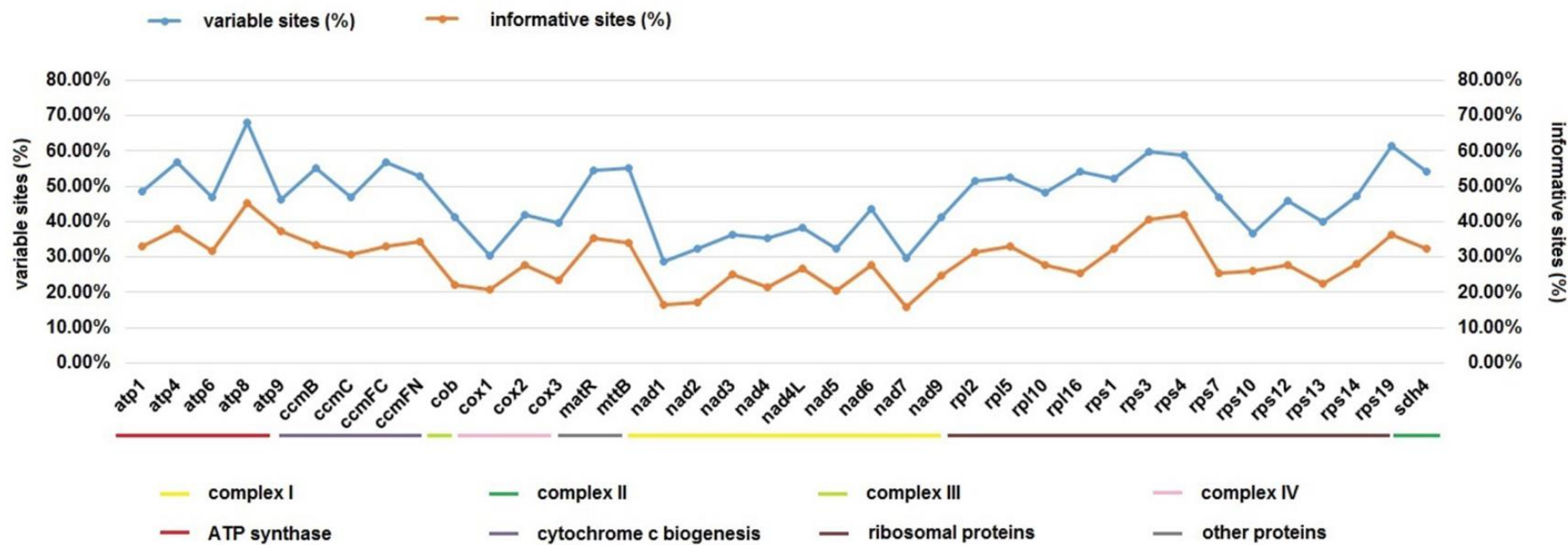
**Table S7.** Genes with erroneous placings or extremely long branches in single-gene trees, or not being able to align to other taxa.

Gene	Species						
atp1	<i>Viscum album</i>						
atp4	<i>Acorus gramineus</i>						
atp6	<i>Welwitschia mirabilis</i>	<i>Acorus gramineus</i>	<i>Viscum album</i>				
atp9	<i>Bupleurum falcatum</i>	<i>Glycine max</i>	<i>Lotus japonicus</i>	<i>Medicago truncatula</i>	<i>Millettia pinnata</i>	<i>Vigna angularis</i>	<i>Vigna radiata</i>
ccmFC	<i>Acorus gramineus</i>	<i>Vitis vinifera</i>					
ccmB	<i>Geranium maderense</i>						
ccmC	<i>Viscum album</i>						
ccmFC	<i>Acorus gramineus</i>	<i>Welwitschia mirabilis</i>	<i>Vitis vinifera</i>				
ccmFN	<i>Acorus gramineus</i>	<i>Welwitschia mirabilis</i>	<i>Vitis vinifera</i>				
cox1	<i>Vitis vinifera</i>	<i>Geranium maderense</i>	<i>Viscum album</i>	<i>Acorus gramineus</i>			
cox2	<i>Vitis vinifera</i>	<i>Acorus gramineus</i>	<i>Viscum album</i>				
cox3	<i>Viscum album</i>						
matR	<i>Acorus gramineus</i>	<i>Vitis vinifera</i>					
mttB	<i>Oryza sativa indica</i>	<i>Oryza sativa japonica</i>	<i>Acorus gramineus</i>				
nad1	<i>Welwitschia mirabilis</i>	<i>Acorus gramineus</i>	<i>Vitis vinifera</i>				
nad2	<i>Welwitschia mirabilis</i>	<i>Vitis vinifera</i>					
nad3	<i>Welwitschia mirabilis</i>	<i>Acorus gramineus</i>					
nad4	<i>Welwitschia mirabilis</i>	<i>Vitis vinifera</i>					
nad4L	<i>Welwitschia mirabilis</i>	<i>Acorus gramineus</i>					
nad5	<i>Welwitschia mirabilis</i>	<i>Vitis vinifera</i>					
nad6	<i>Vitis vinifera</i>						
nad7	<i>Vitis vinifera</i>						
nad9	<i>Vitis vinifera</i>	<i>Acorus gramineus</i>					

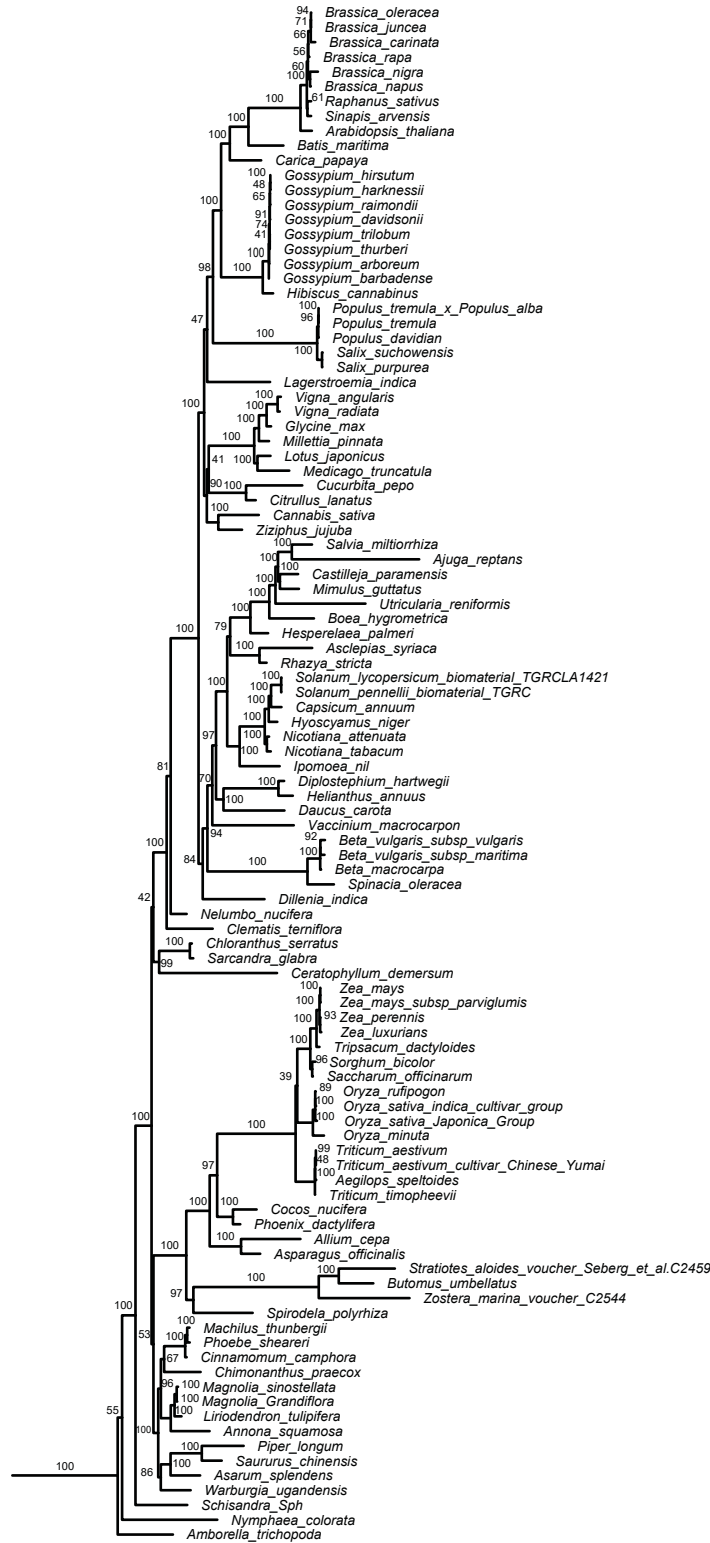
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rpl5	<i>Acorus gramineus</i>	<i>Sarcandra glabra</i>	<i>Acorus gramineus</i>	<i>Vitis vinifera</i>
rpl10	<i>Acorus gramineus</i>	<i>Welwitschia mirabilis</i>		
rpl16	<i>Welwitschia mirabilis</i>	<i>Butomus umbellatus</i>		
rps1	<i>Acorus gramineus</i>	<i>Clematis terniflora</i>		
rps3	<i>Acorus gramineus</i>	<i>Geranium maderense</i>		
rps4	<i>Acorus gramineus</i>	<i>Ajuga reptans</i>	<i>Welwitschia mirabilis</i>	
rps7	<i>Butomus umbellatus</i>	<i>Zostera marina</i>	<i>Acorus gramineus</i>	
rps10	<i>Acorus gramineus</i>			
rps12	<i>Viscum album</i>			
rps13	<i>Acorus gramineus</i>			
rps19	<i>Ceratophyllum demersum</i>			

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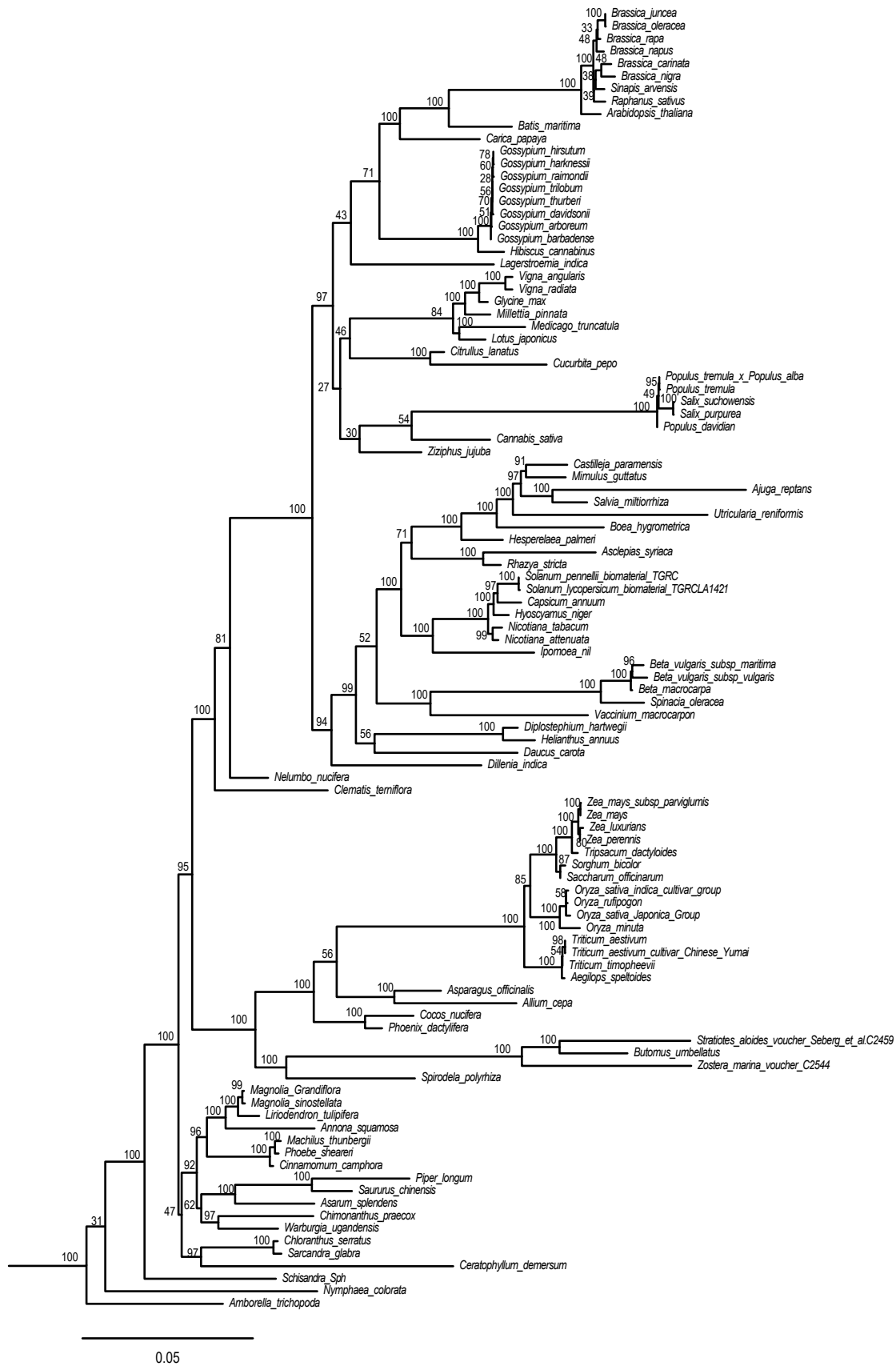


**Figure S1.** Percentage of variable sites and informative sites of 38 mt genes in 107 taxa. The colored lines under the gene names indicate the categories the genes.

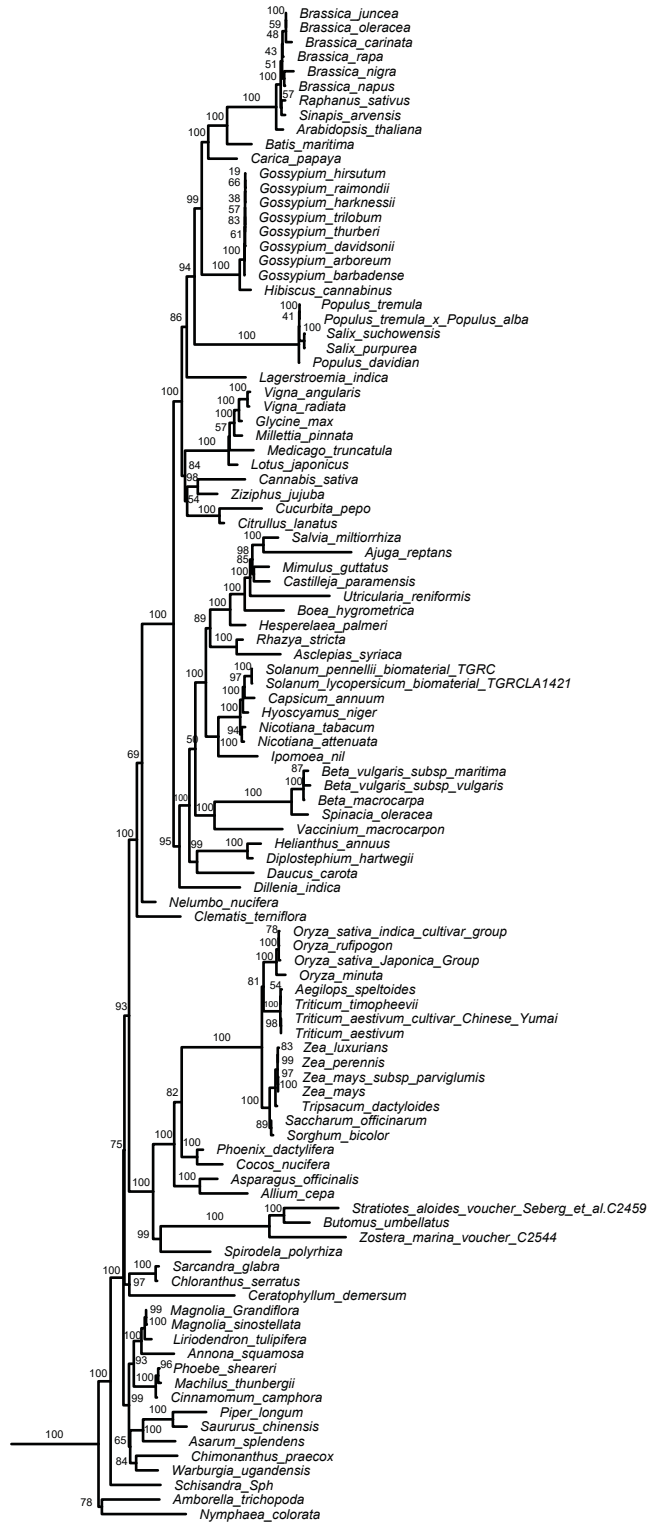


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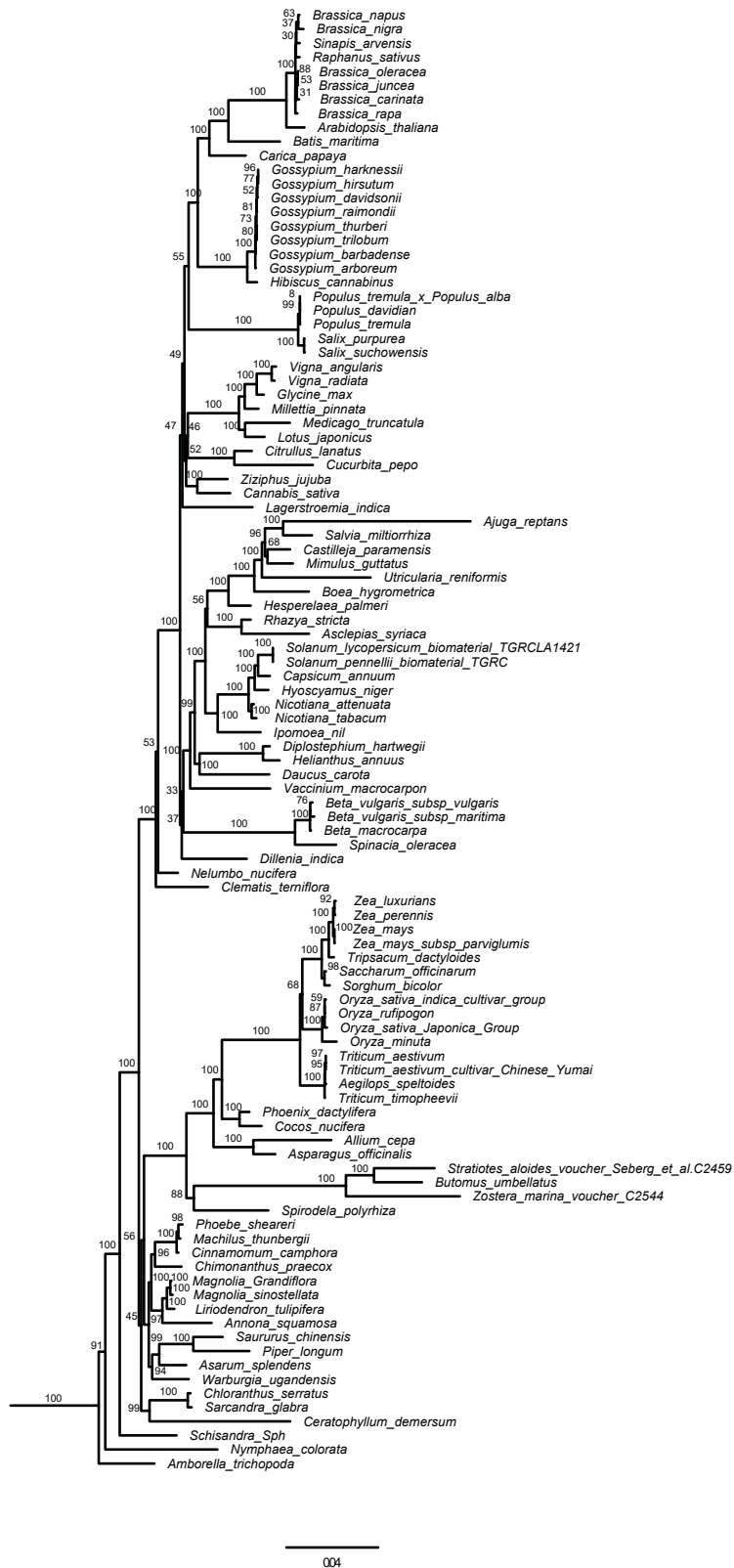
**Figure S2.** The ML tree inferred by RAxML based on concatenated nt sequences of 38 mt genes of 107 species. Numbers on branches are bootstrap values.



**Figure S3.** The ML tree inferred by RAXML based on concatenated aa sequences of 38 mt genes of 107 species. Numbers on branches are bootstrap values.



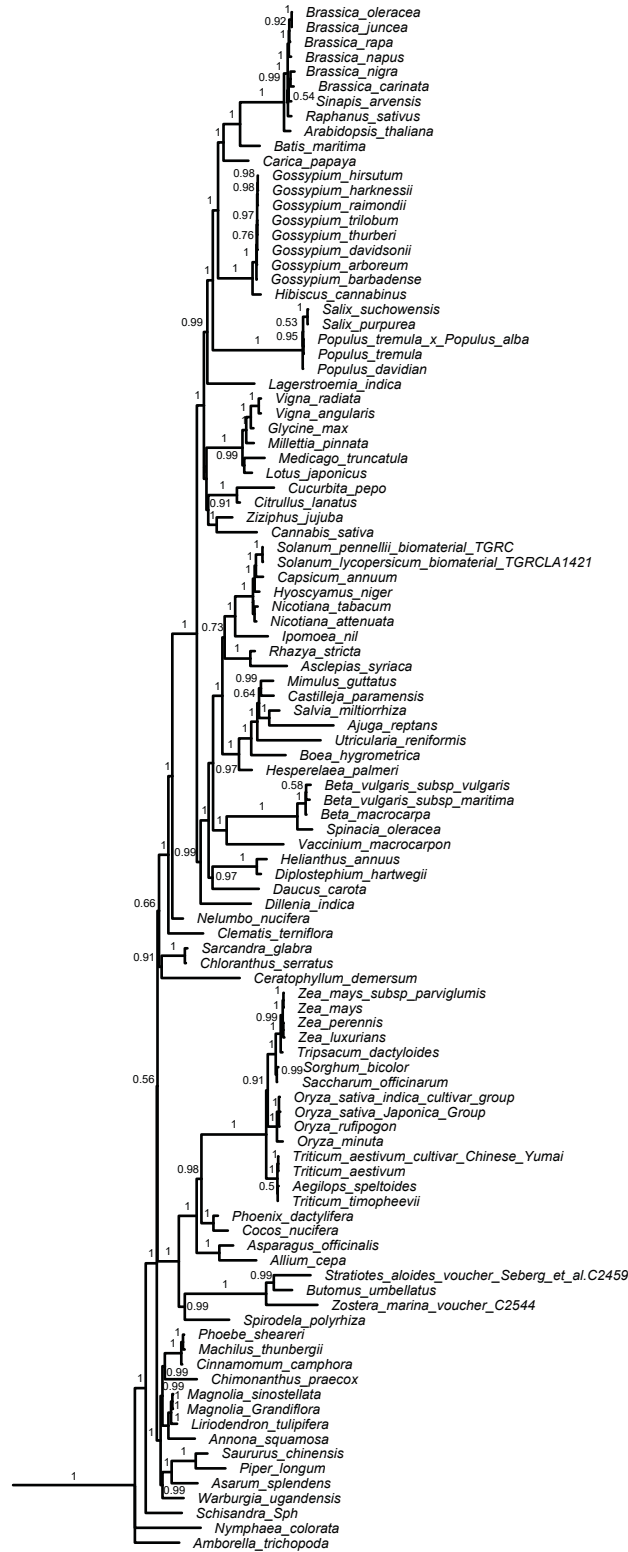
**Figure S4.** The ML tree inferred by RAxML based on the 1<sup>st</sup>+2<sup>nd</sup> codon positions of 38 mt genes of 107 species. Numbers on branches are bootstrap values.



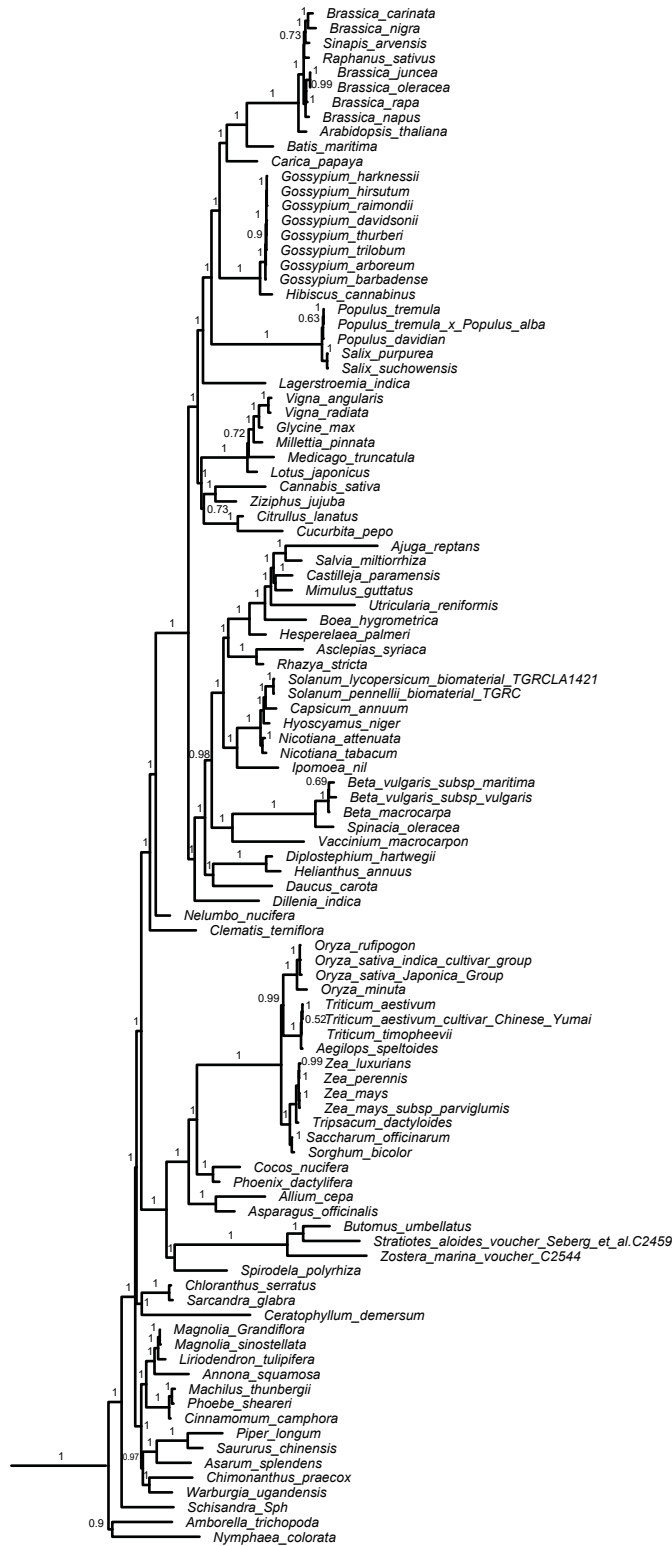
**Figure S5.** The ML tree inferred by RAxML based on the 3<sup>rd</sup> codons positions of 38 mt genes of 107 species. Numbers on branches are bootstrap values.



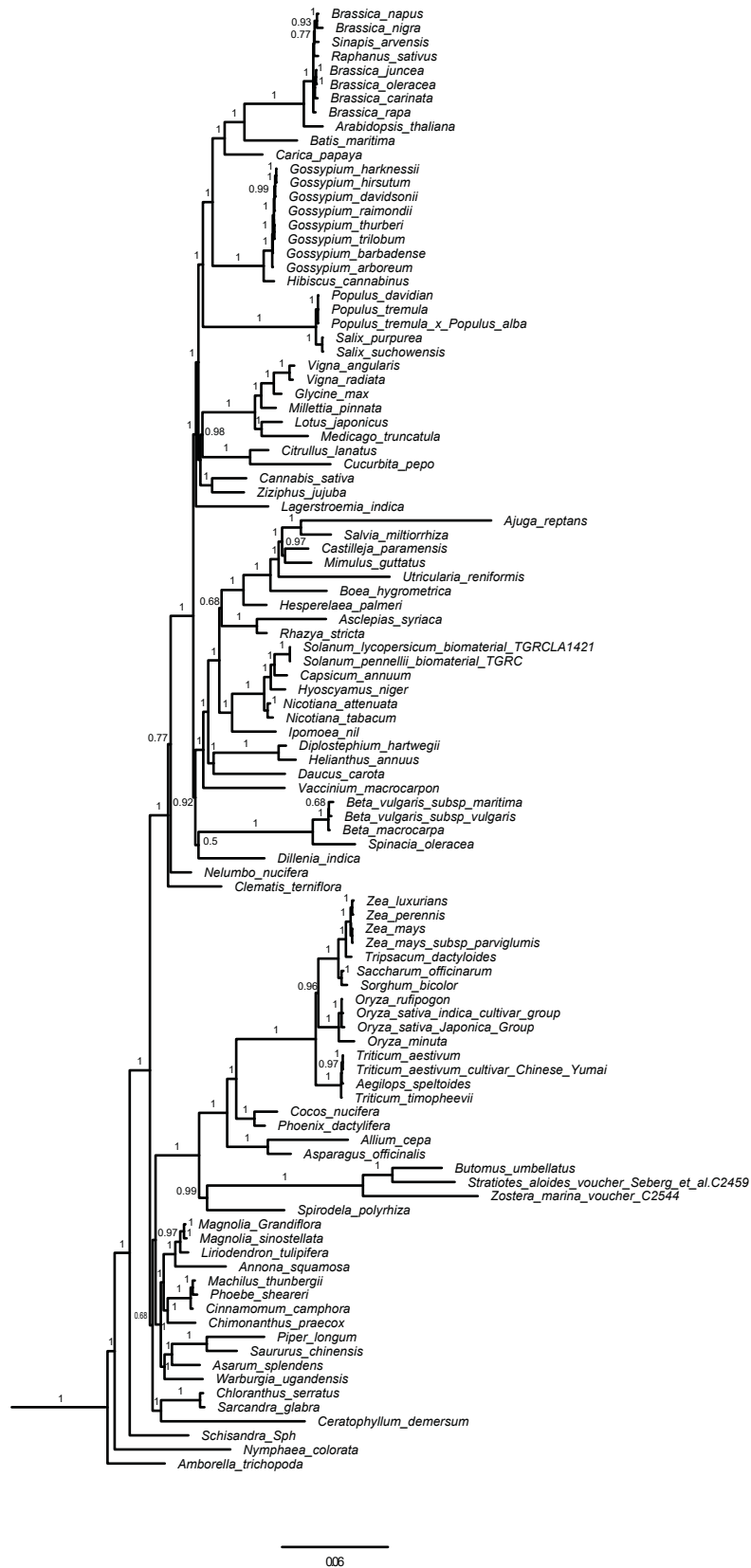




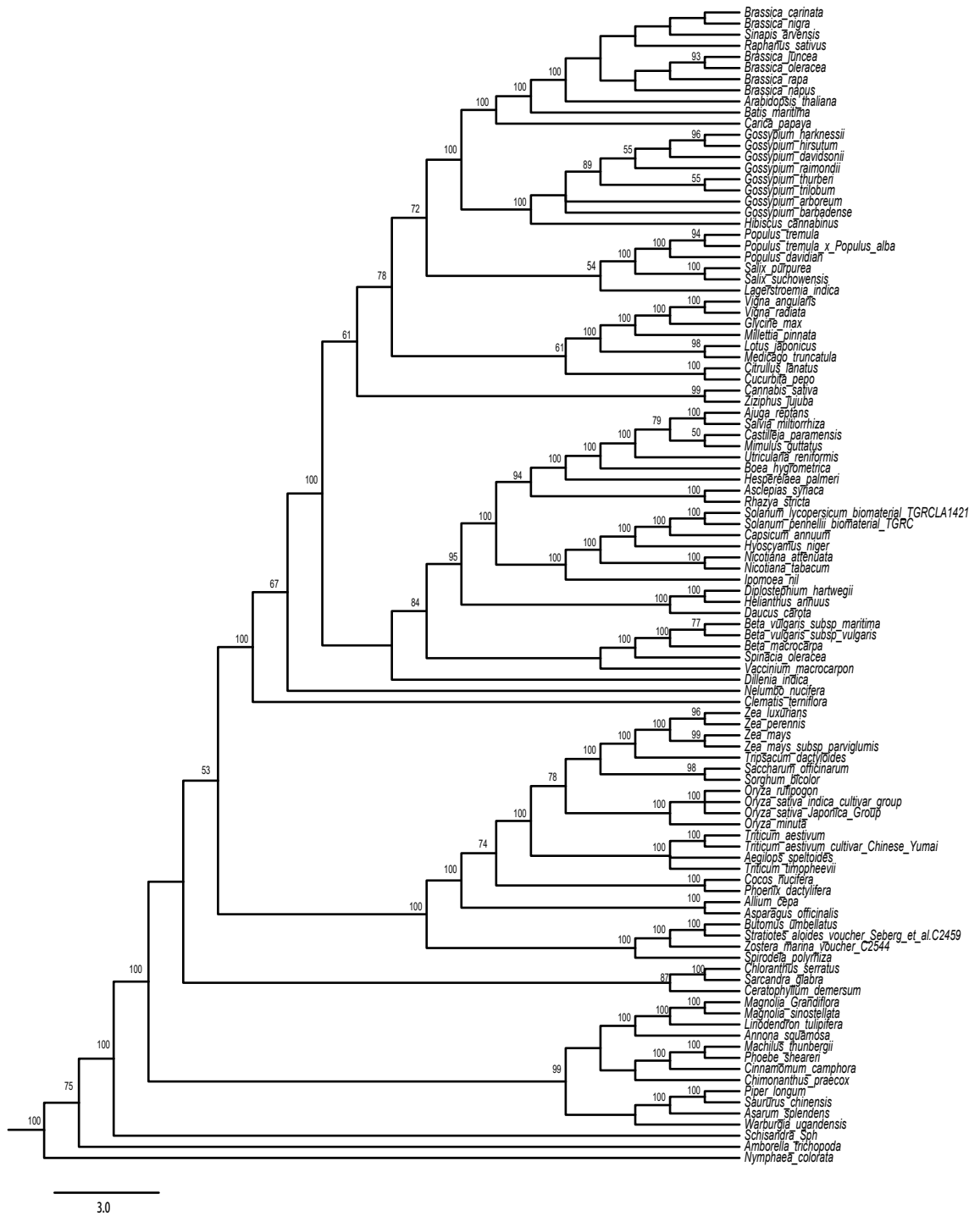
**Figure S7.** The Bayesian tree inferred by Phylobayes with CAT model based on the concatenated amino acid sequences of 38 mt genes of 107 species. Numbers on branches are posterior probabilities.



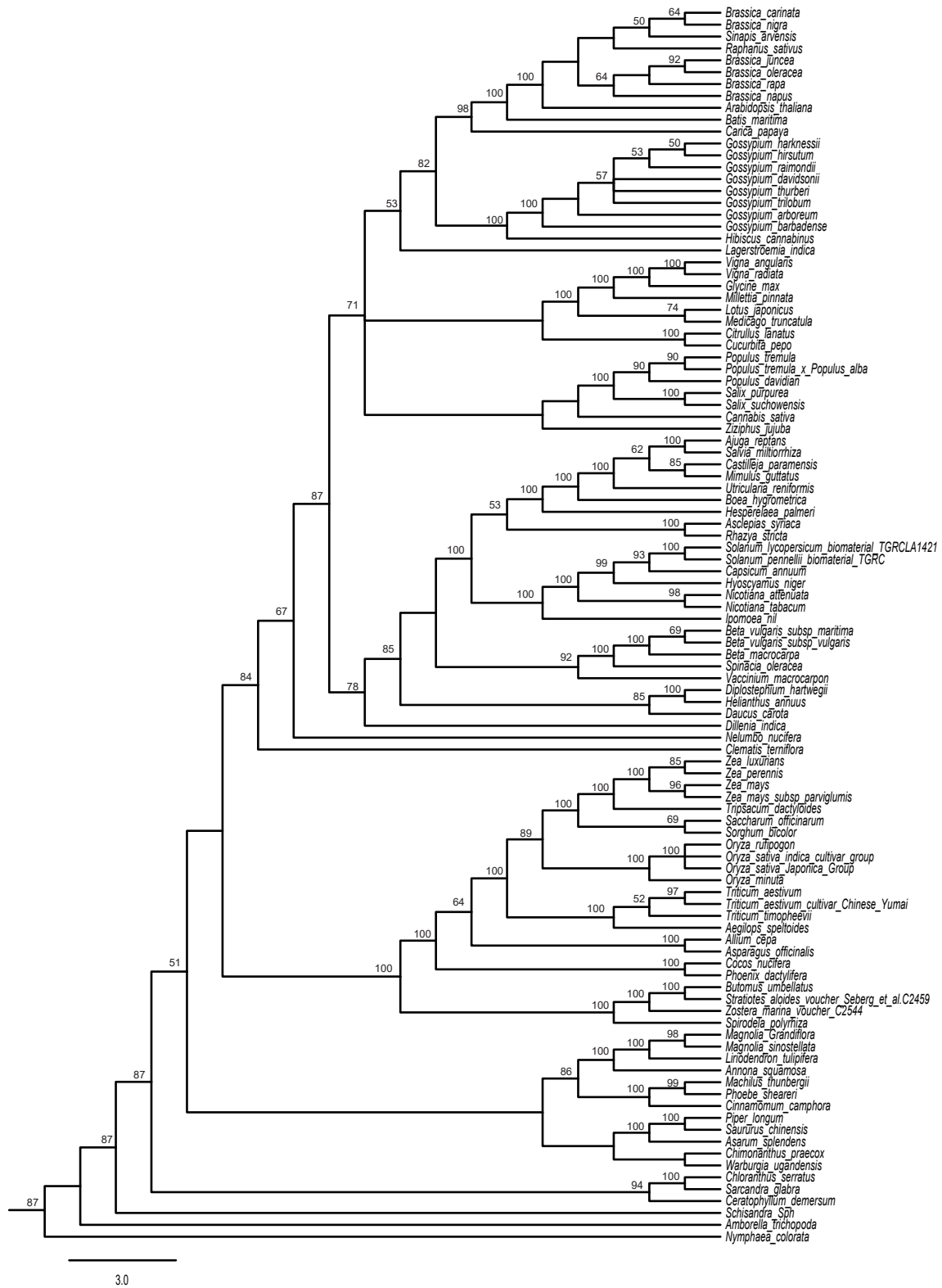
**Figure S8.** The Bayesian tree inferred by MrBayes based on the 1<sup>st</sup>+2<sup>nd</sup> codon positions of 38 mt genes of 107 species. Numbers on branches are posterior probabilities.



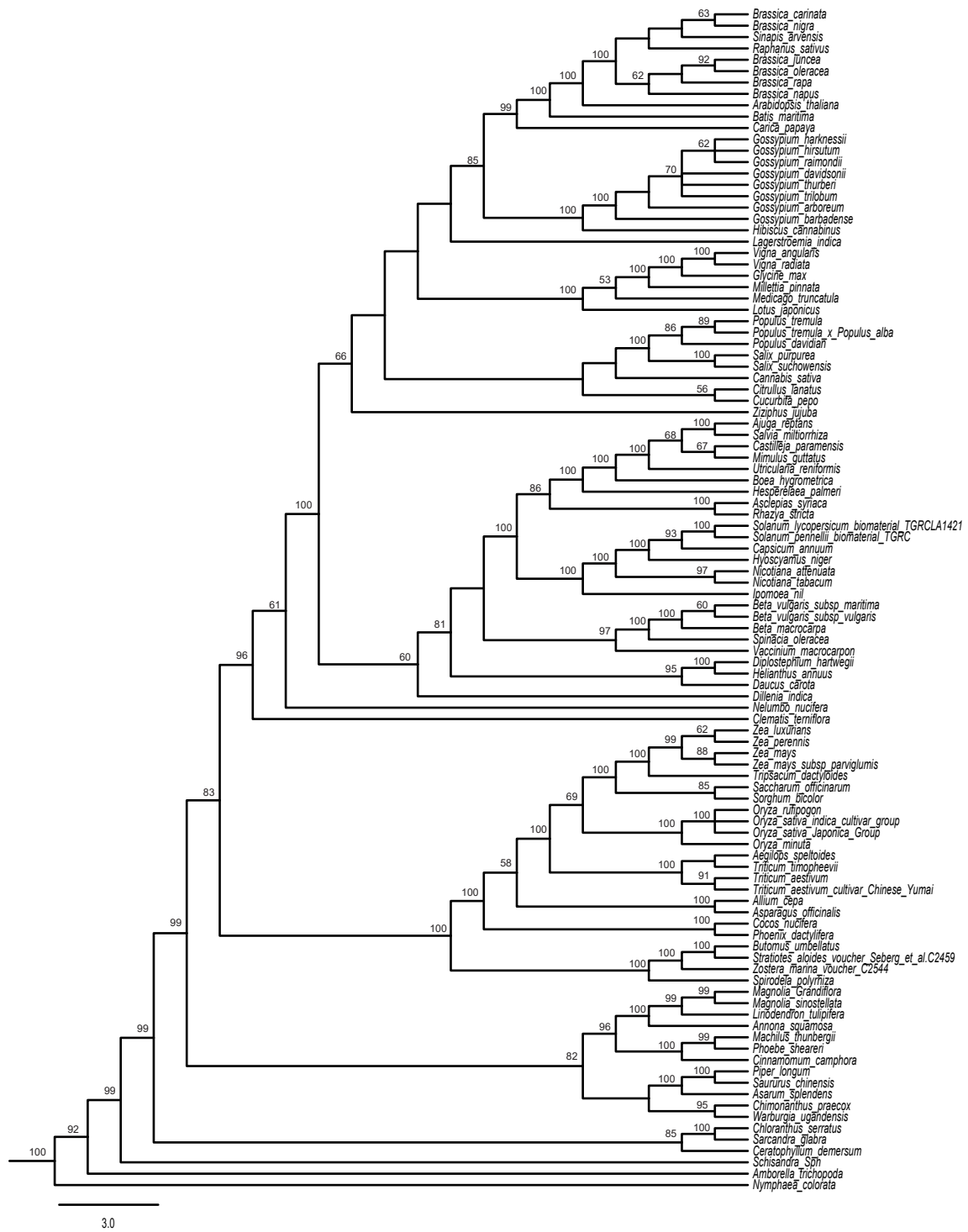
**Figure S9.** The Bayesian tree inferred by MrBayes based on the 3<sup>rd</sup> codon positions of 38 mt genes of 107 species. Numbers on branches are posterior probabilities.



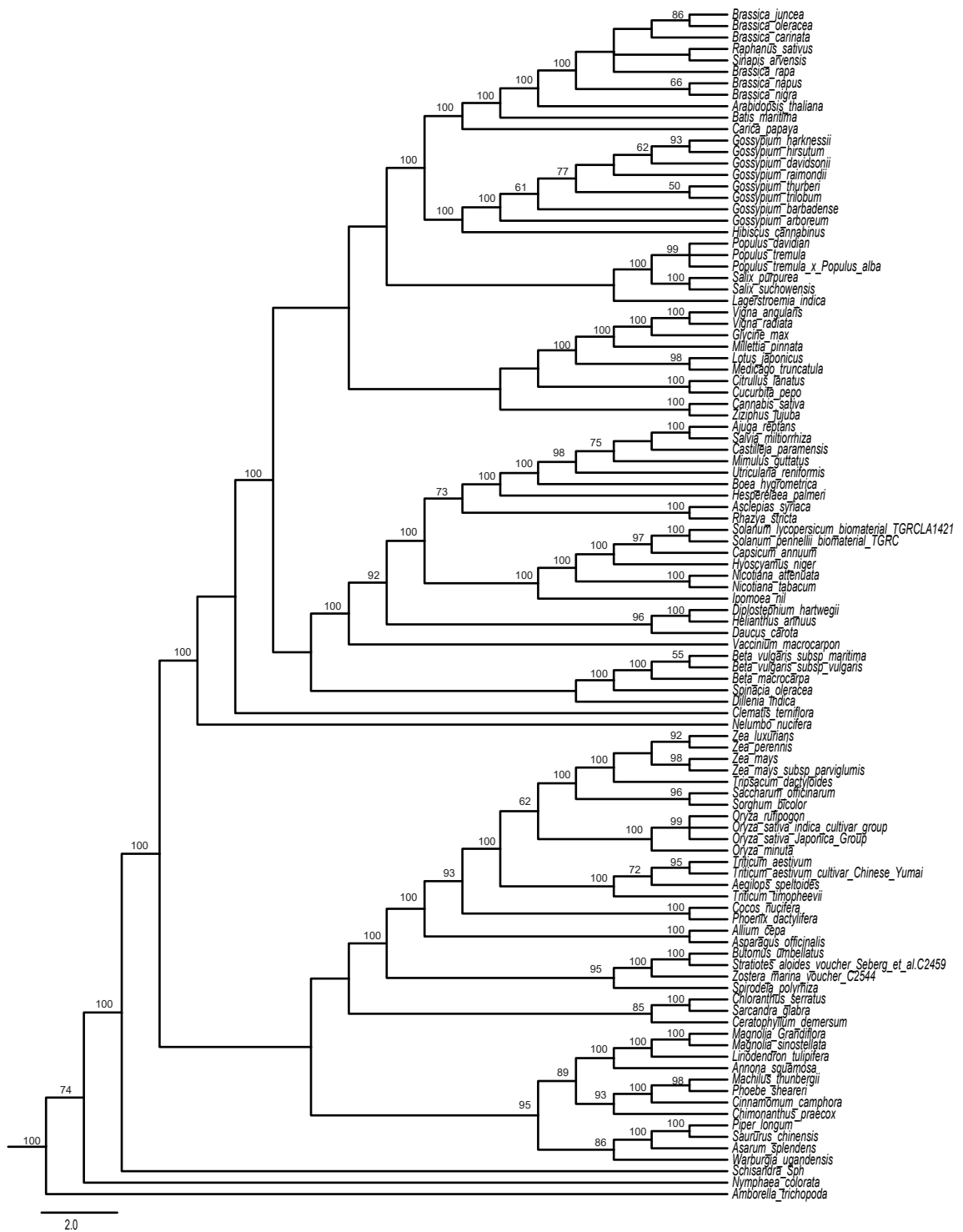
**Figure S10.** The MP tree inferred by PAUP based on concatenated nt sequences of 38 mt genes of 107 species. Numbers on branches are bootstrap values.



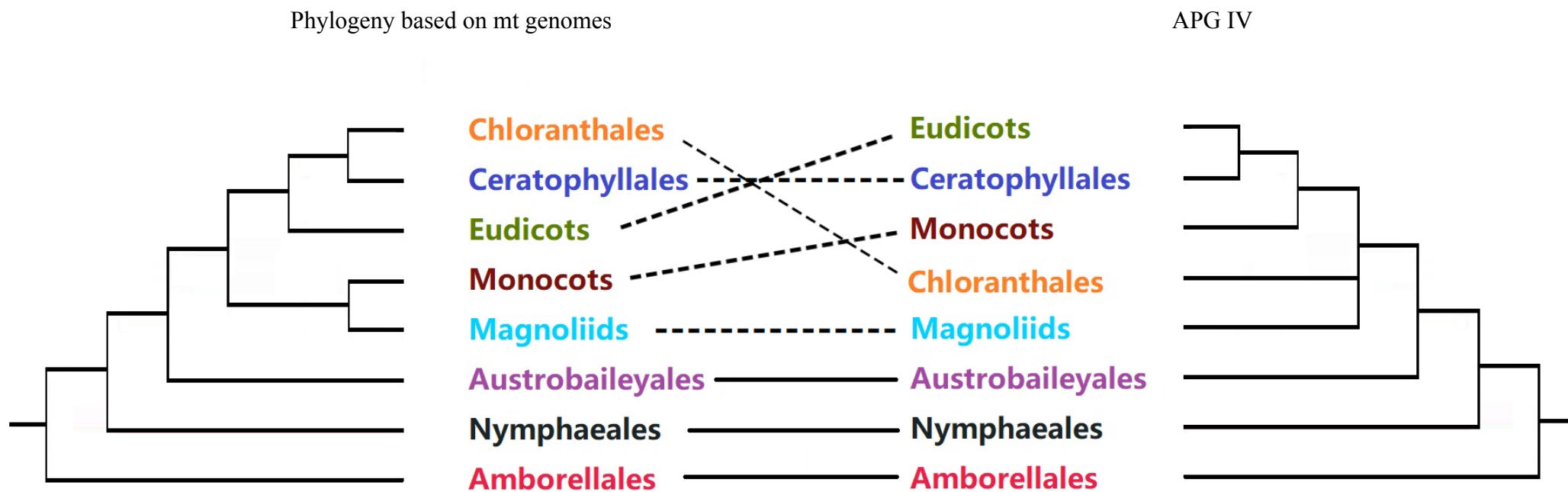
**Figure S11.** The MP tree inferred by PAUP based on concatenated aa sequences of 38 mt genes of 107 species. Numbers on branches are bootstrap values.



**Figure S12.** The MP tree inferred by PAUP based on the 1st+2nd codon positions of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

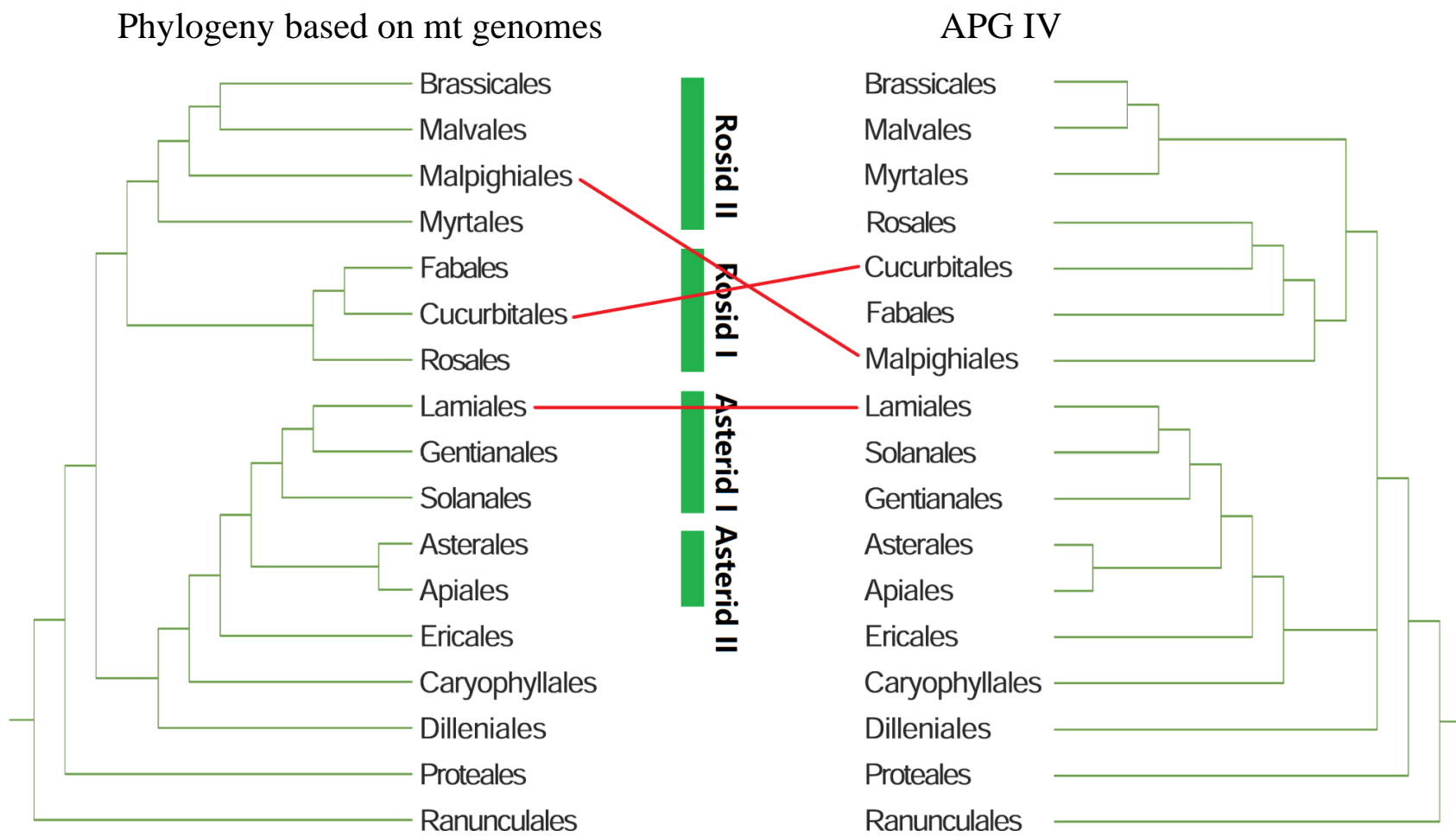


**Figure S13.** The MP tree inferred by PAUP based on the 3rd codon positions of 38 mt genes of 107 species. Numbers on branches are bootstrap values.

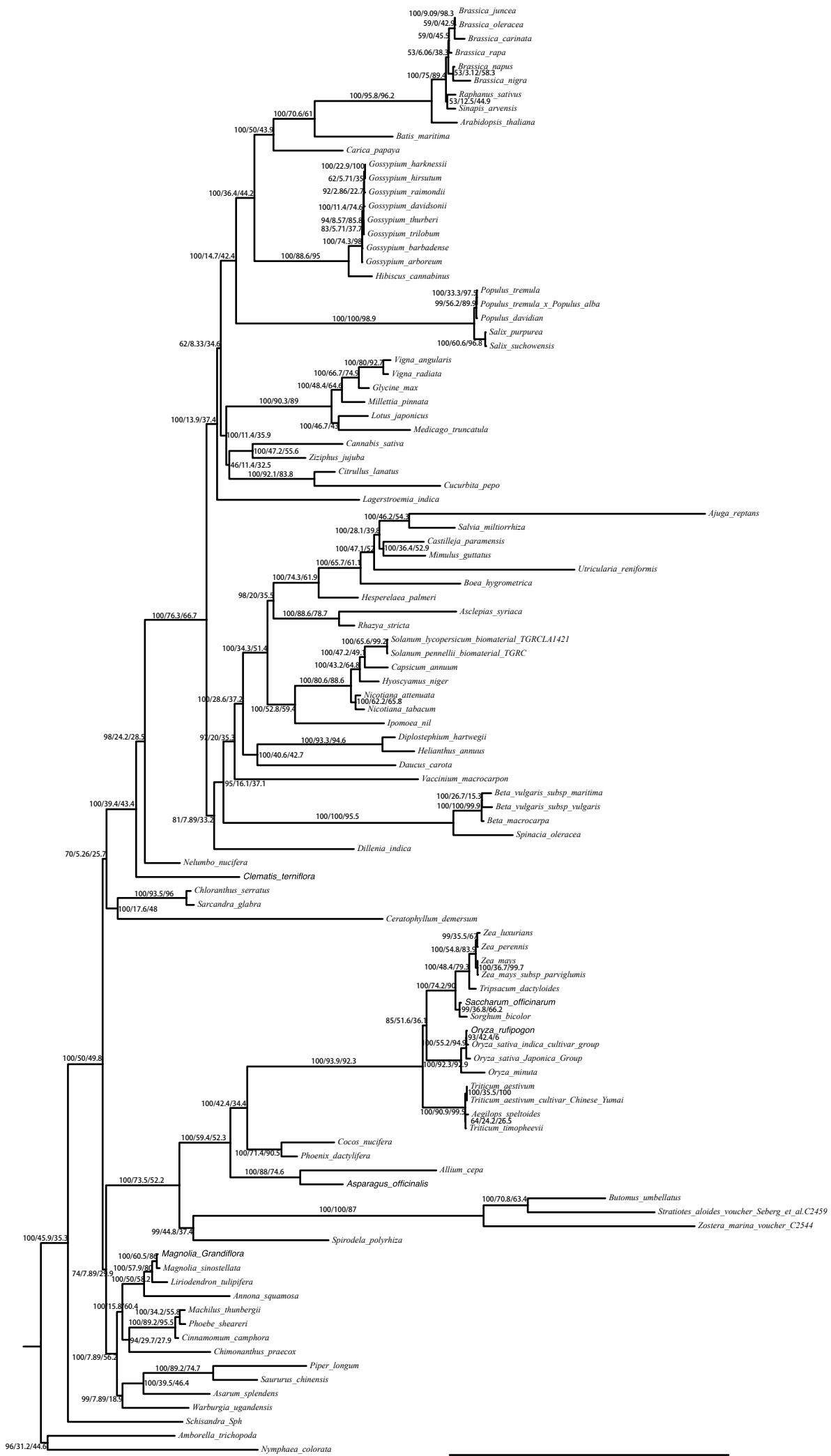


**Figure S14.** Comparison of phylogenetic relationships of major angiosperm lineages between mt genomes (based on the nt data) and APG IV (Byng et al., 2016).





**Figure S15.** Comparison of eudicots phylogenetic relationships between mt genomes (based on the nt data) and APG IV (Byng et al., 2016).



0.04

**Figure S16.** Phylogenetic tree with concordance factors annotated. Three numbers beside each node represent bootstrap value, gCF value, and sCF value.

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