

Supplementary figures and tables
for
Genome-wide macroevolutionary signatures of key innovations in
butterflies colonizing new host plants

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Affiliations

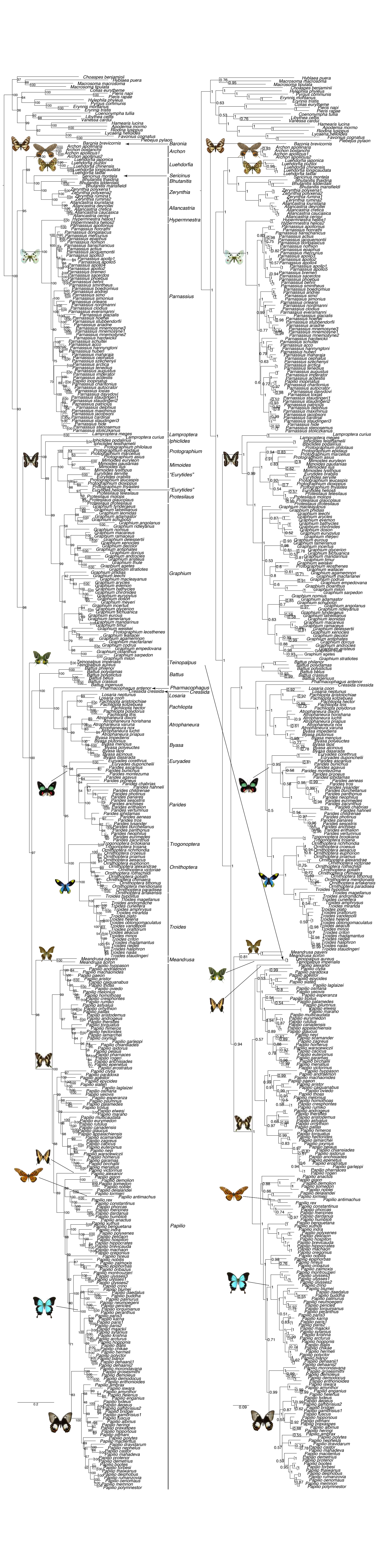
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Correspondence

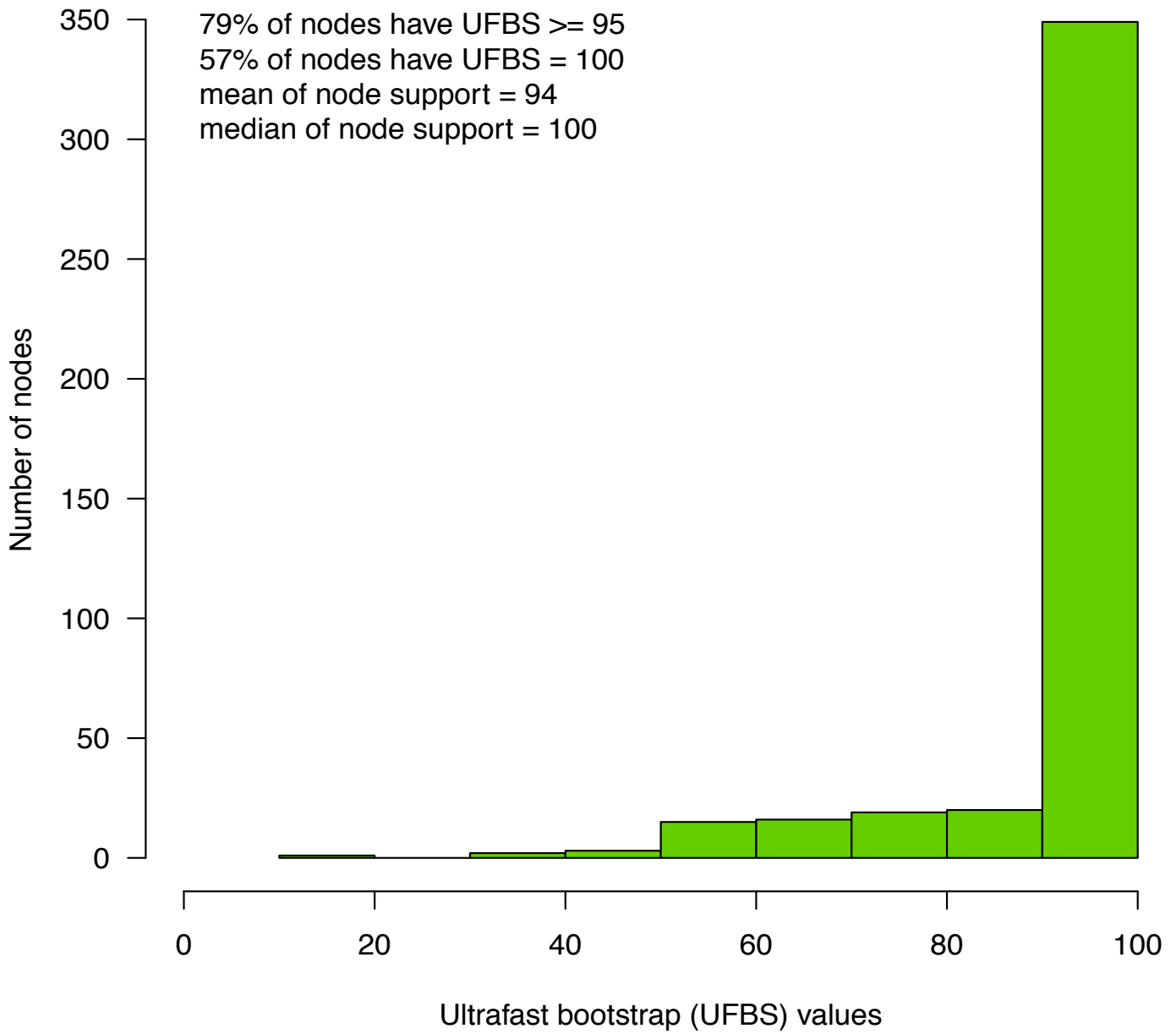
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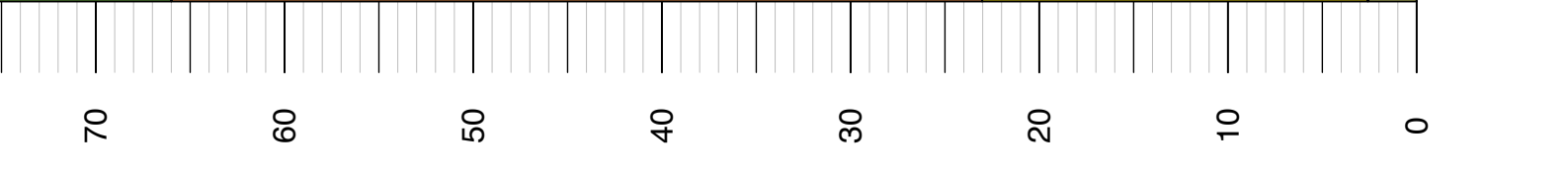
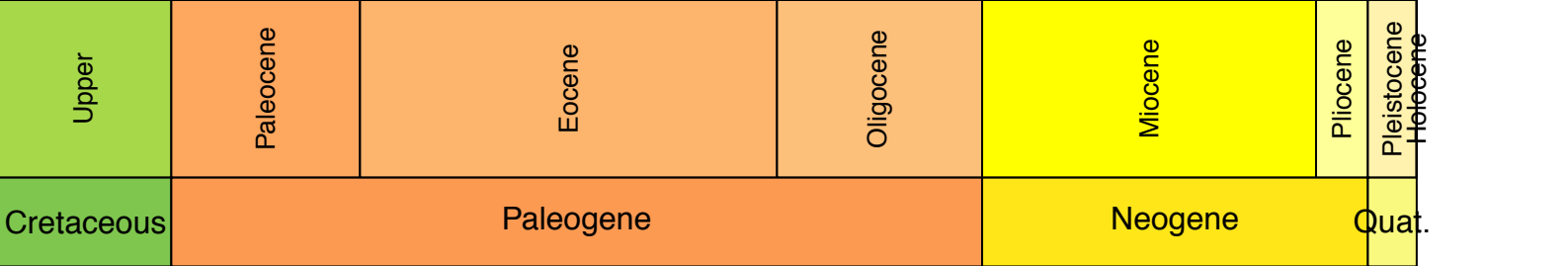
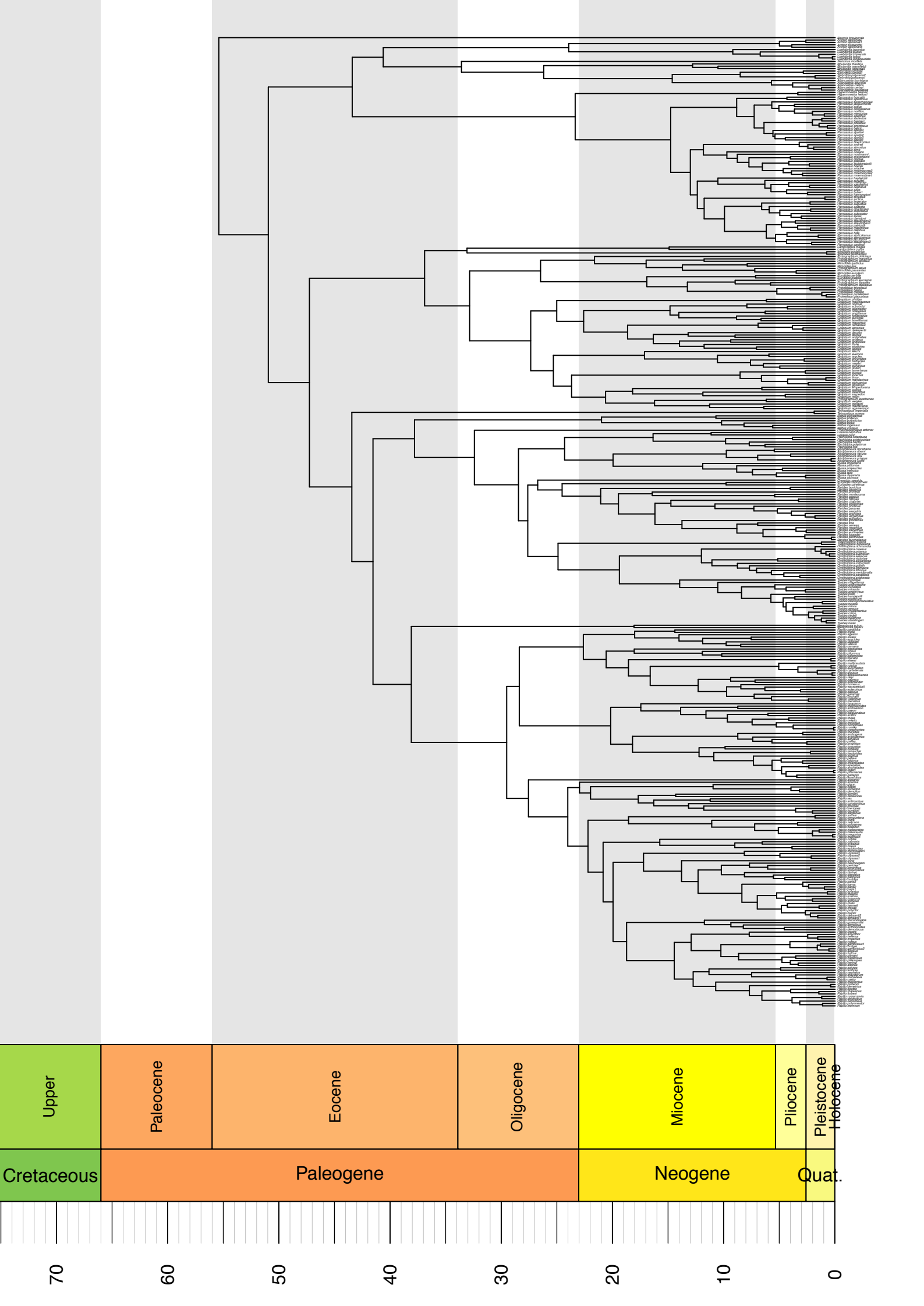
Supplementary figure 1. Phylogenetic relationships of 408 swallowtail butterfly species (Papilionidae). Left phylogeny is inferred with the maximum-likelihood approach implemented with IQ-TREE, and right phylogeny is inferred with the Bayesian approach implemented with MrBayes. Both phylogenies show similar relationships except for the placement of the genus *Teinopalpus*, found as sister to Papilionini + Troidini with IQ-TREE and sister to *Meandrusa* (Papilionini) with MrBayes. Node support is indicated by ultrafast bootstrap and posterior probabilities on the maximum-likelihood and Bayesian phylogenies, respectively, with values of 95% and 0.95 considered as indicative of strong node support. Pictures of butterflies made by Fabien Condamine.

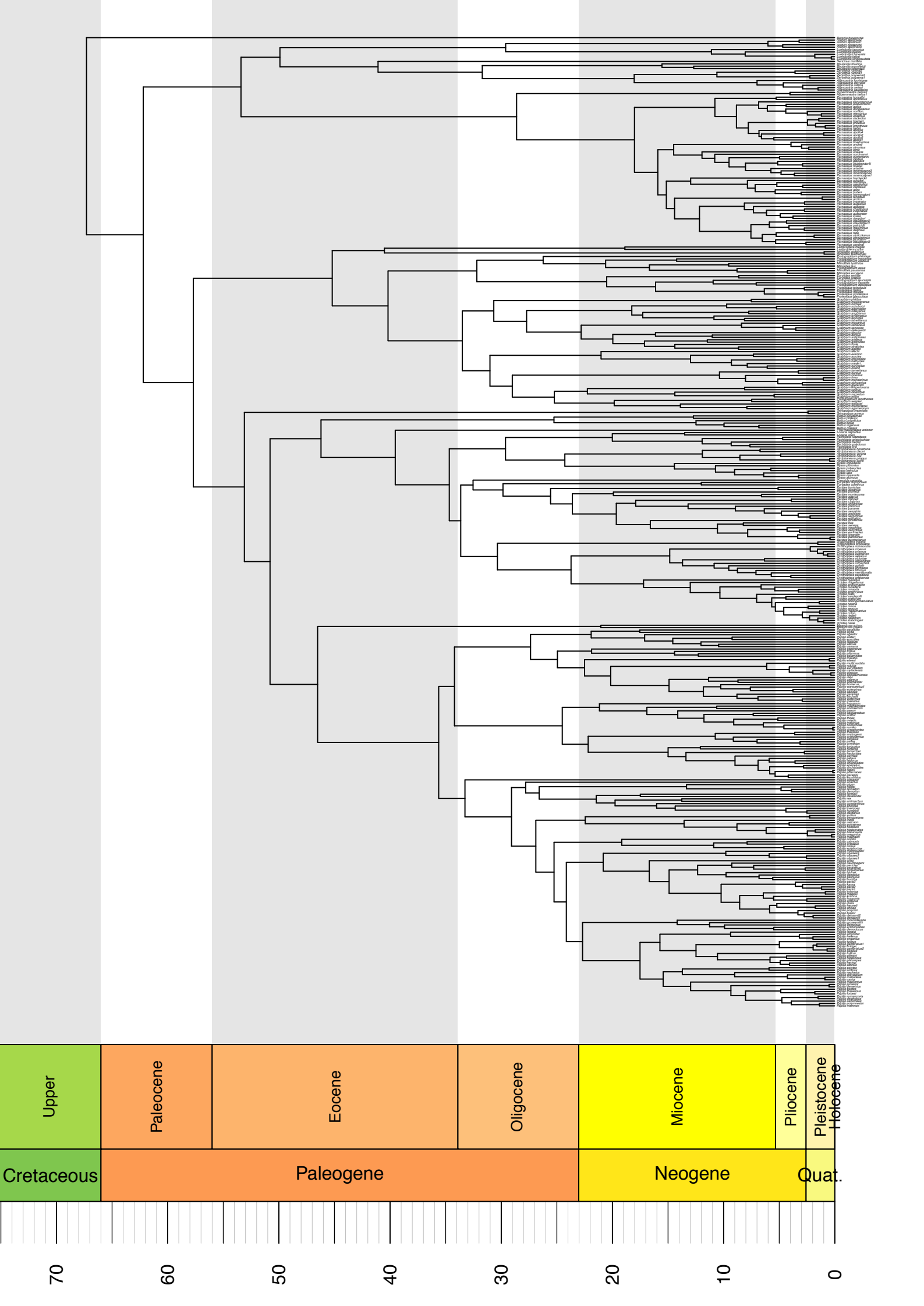


Supplementary figure 2. Node support (ultrafast bootstrap) of the maximum-likelihood phylogeny. The histogram shows the distribution of node support for all Papilionidae, and indicates a high overall tree resolution with ~80% of nodes having ultrafast bootstrap values $\geq 95\%$.



Supplementary figure 3. Bayesian estimates of divergence times for swallowtail butterflies. The first inference was performed with exponential priors on fossil calibrations, while the second inference was carried out with uniform priors. The analysis based on exponential priors estimated a crown age for the family at 55.4 Ma (95% CI: 47.8-71.0 Ma), while the analysis based on uniform priors estimated the origin at 67.2 Ma (95% CI: 47.8-112 Ma).





Supplementary figure 4. Estimation of ancestral host-plant preferences for the two molecular dated trees with the Dispersal-Extinction-Cladogenesis (DEC) model. The results show that the family Aristolochiaceae is recovered as the ancestral feeding habit of the Papilionidae. K = Cretaceous, Pl = Pliocene, P = Pleistocene. Pictures of butterflies made by Fabien Condamine.

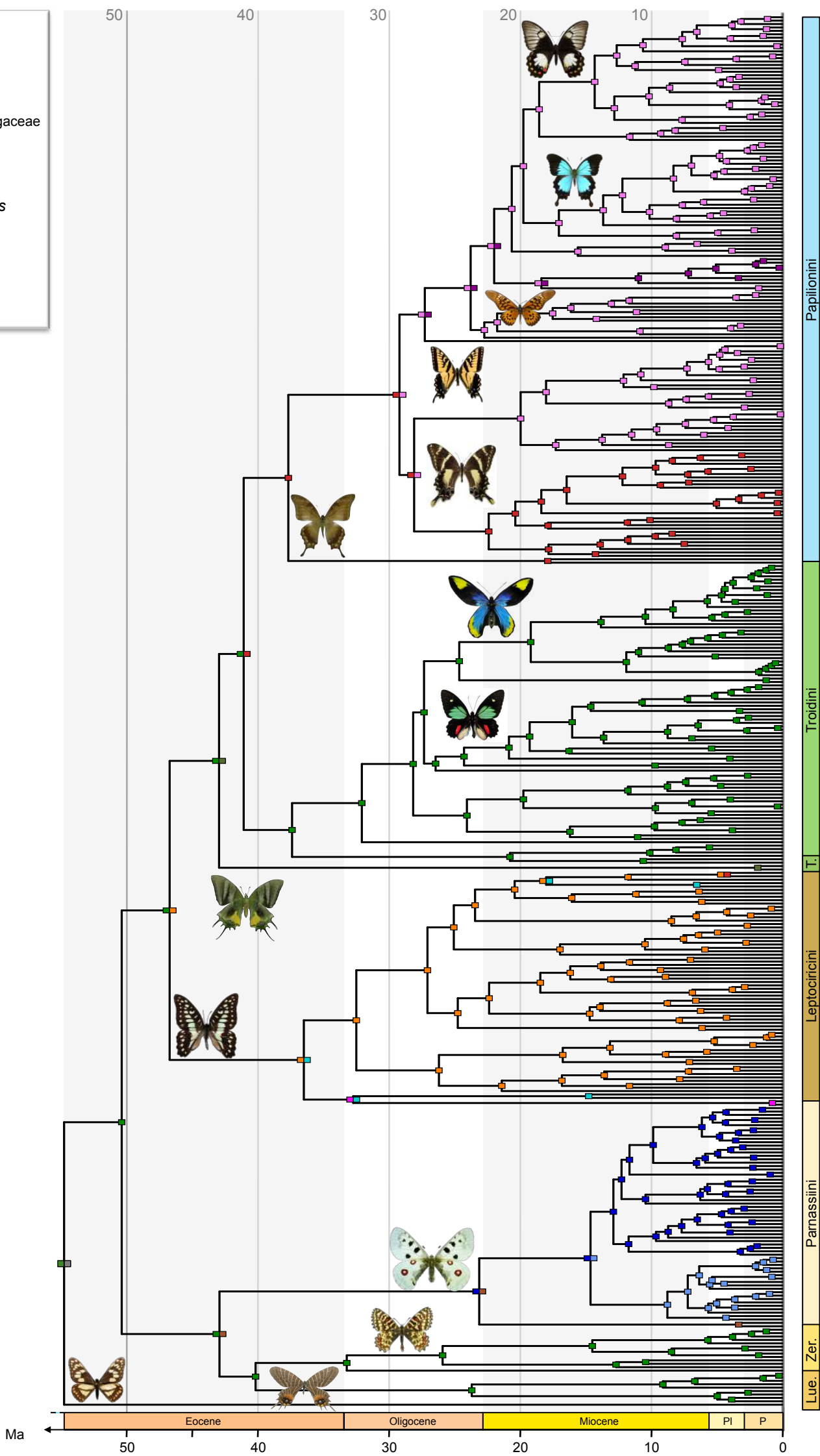
Legend

Main host plants

- Aristolochiaceae
- Rutaceae
- Annonaceae
- Crassulaceae + Saxifragaceae
- Apiaceae
- Lauraceae
- Papaveraceae

Secondary host plants

- Fabaceae (*Acacia*)
- Zygophyllaceae
- Hernandiaceae
- Rosaceae
- Magnoliaceae



Ma

50

40

30

20

10

Papilionini

Trodini

T.

Leptocircini

Parnassiini

Lue. Zer.

Eocene

Oligocene

Miocene

PI

P

Supplementary figure 5. Estimation of ancestral host-plant preferences with the maximum-likelihood model of Markov 1-parameter (Mk) and the Bayesian approach of BayesTraits. The results are represented by pie charts indicating the relative probability for each state inferred at a given node. The results consistently show that (1) the family Aristolochiaceae is recovered as the ancestral feeding habit of the Papilionidae, and (2) the host-plant shifts are recovered at the same nodes, except at the root of Papilionini and at the root of *Iphiclides* + *Lamproptera* (due to the fact the the Mk model can include only 10 states).

Aristolochiaceae
 Hernandiaceae
 Rosaceae
 Zygophyllaceae
 Apiaceae
 Rutaceae

Lauraceae
 Magnoliaceae
 Annonaceae
 Crassulaceae + Saxifrag
 Papaveraceae
 Fabaceae (Acacia)

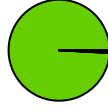
Markov 1-parameter

BayesTraits

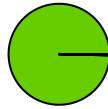
root of Papilionidae



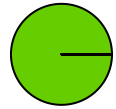
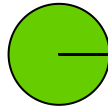
root of Parnassiinae + Papilioninae



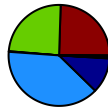
root of Parnassiinae



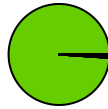
root of Zerynthiini + Luehdorfiini



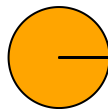
root of Parnassiini



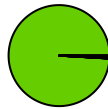
root of Papilioninae



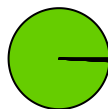
root of Leptocircini



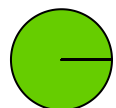
root of Papilionini + Troidini + Teinopal



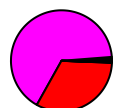
root of Papilionini + Troidini



root of Troidini



root of Papilionini



Aristolochiaceae
 Hernandiaceae
 Rosaceae
 Zygophyllaceae
 Apiaceae
 Rutaceae

Lauraceae
 Magnoliaceae
 Annonaceae
 Crassulaceae + Saxifrag
 Papaveraceae
 Fabaceae (Acacia)

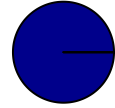
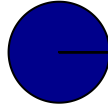
Markov 1-parameter

BayesTraits

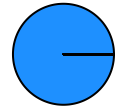
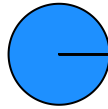
root of Parnassius



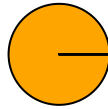
root of Parnassius subgenus Parnass



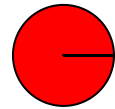
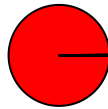
root of Parnassius other subgenera



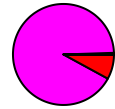
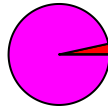
root of Iphiclides + Lamproptera



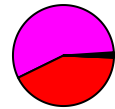
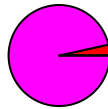
root of Meandrusa



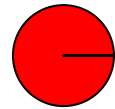
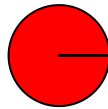
root of Papilio



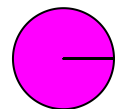
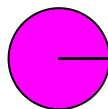
root of New World Papilio



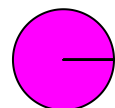
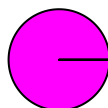
root of Papilio subgenera Pterourus and Chik



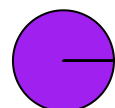
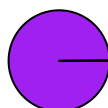
root of Papilio subgenus Heraclides



root of Old World Papilio



root of Papilio subgenus Papilio



Supplementary figure 6. Estimation of ancestral host-plant preferences for the Aristolochiaceae feeders with the Dispersal-Extinction-Cladogenesis (DEC) model. The results show that the genus *Aristolochia* is the primary Aristolochiaceae host plant while being also recovered as the ancestral feeding habit of the Papilionidae. Pictures of butterflies made by Fabien Condamine.

Supplementary figure 7. Phylogenetic relationships within the Aristolochiaceae (perianth-bearing Piperales) for 247 species. The phylogeny is inferred with the Bayesian approach of MrBayes. Node support is indicated by posterior probabilities, with values ≥ 0.95 considered as strong node support. Pictures of plants made by Fabien Condamine.

0.94
 Gymnotheca chinensis
 Gymnotheca involucriata
 Anemopsis californica
 Saururus cernuus
 Saururus chinensis

Saururaceae



Saruma

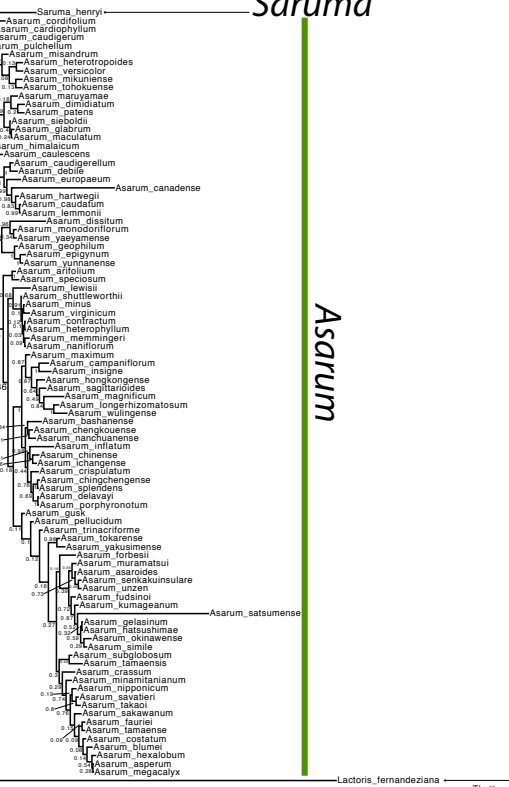


Asarum



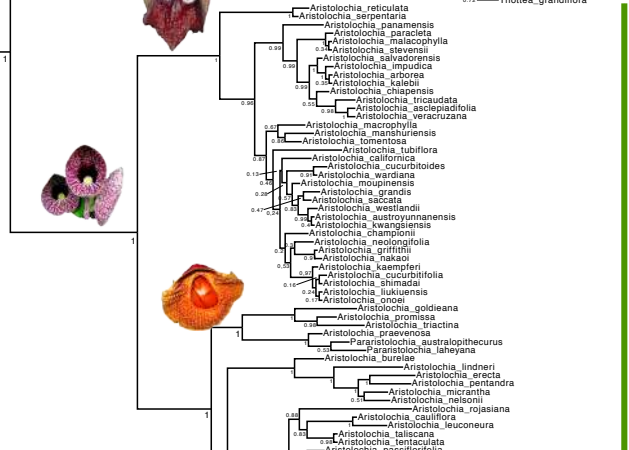
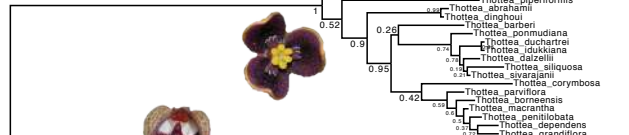
Perianth-bearing Piperales

1

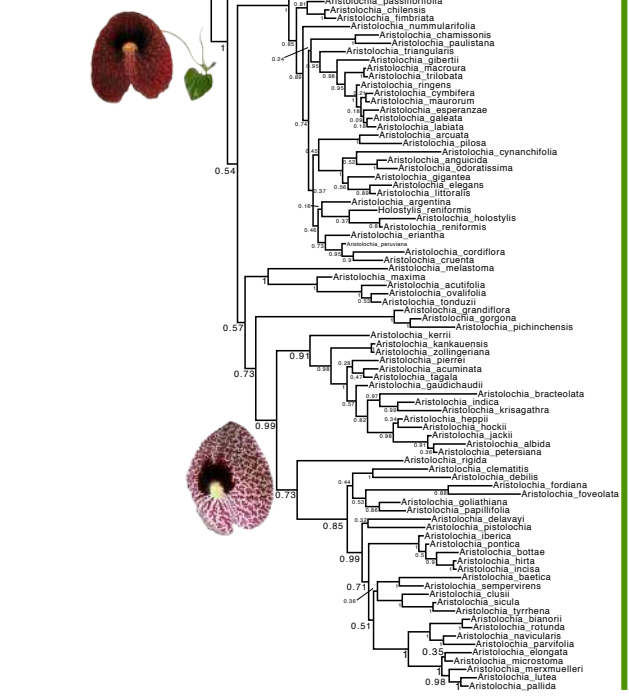


Lactoris

Thottea

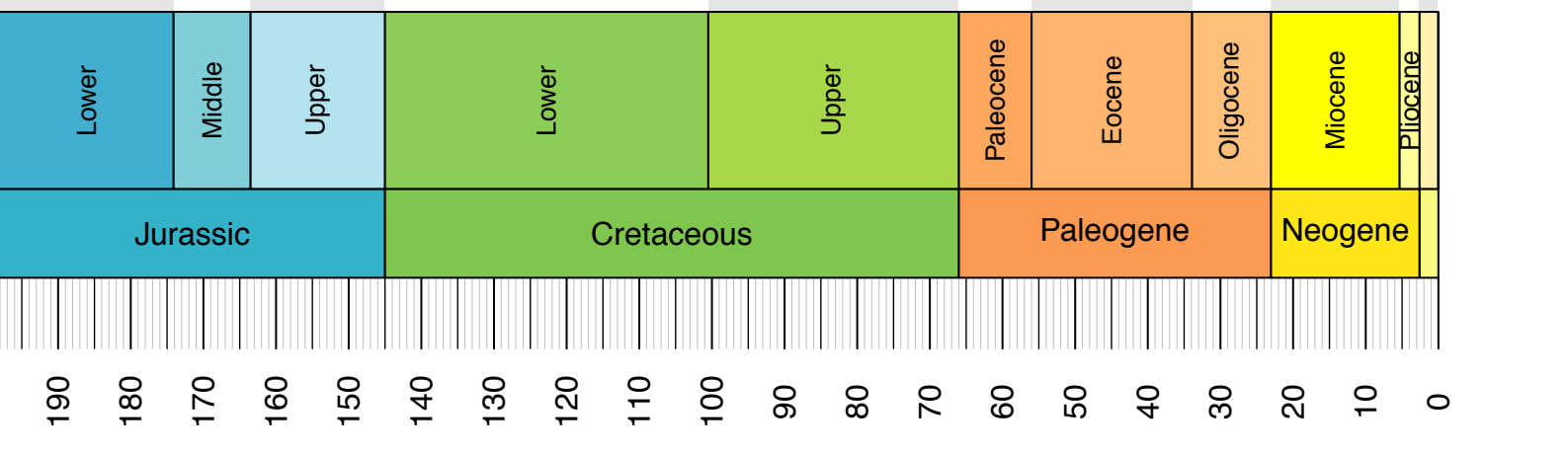
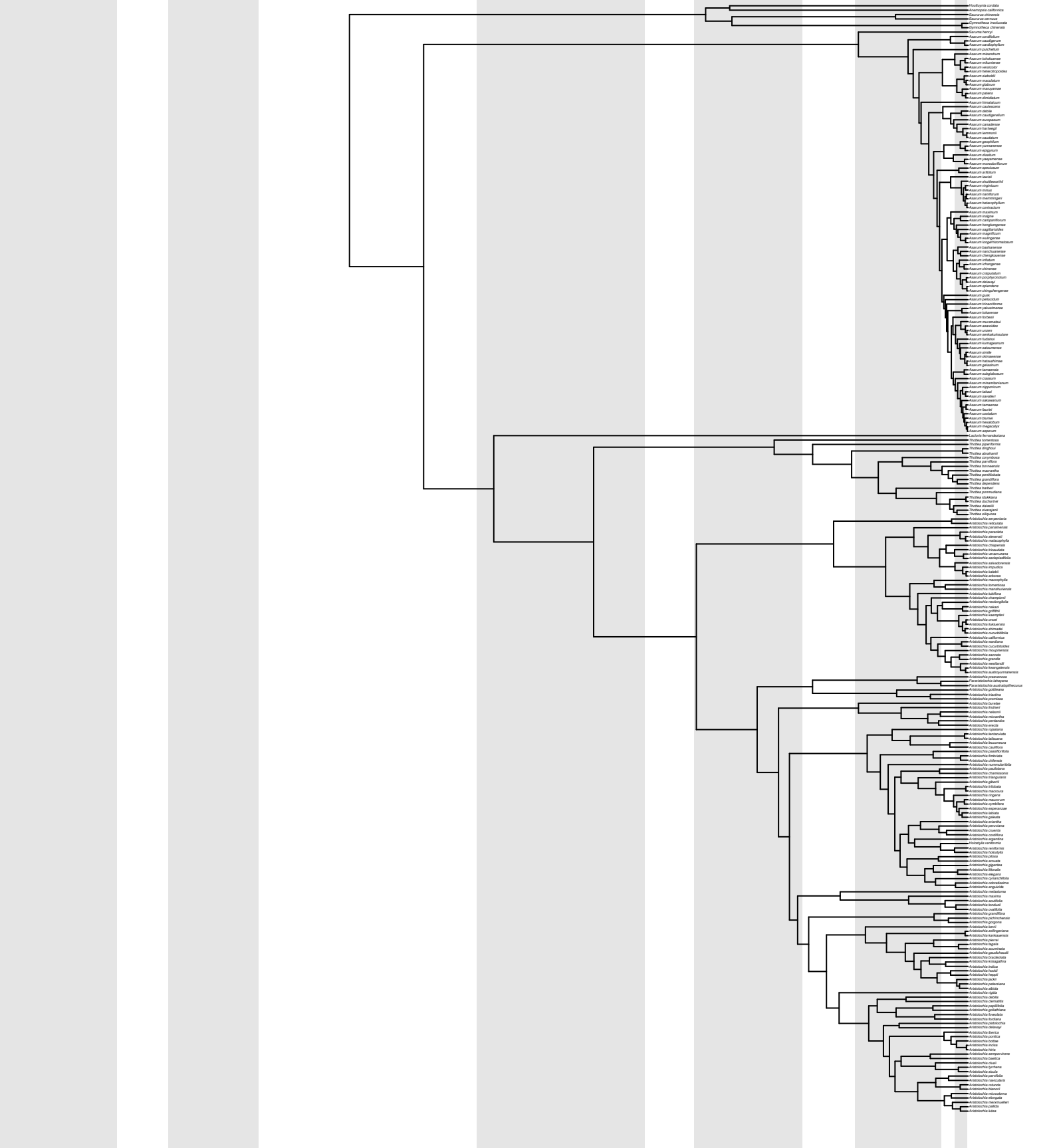
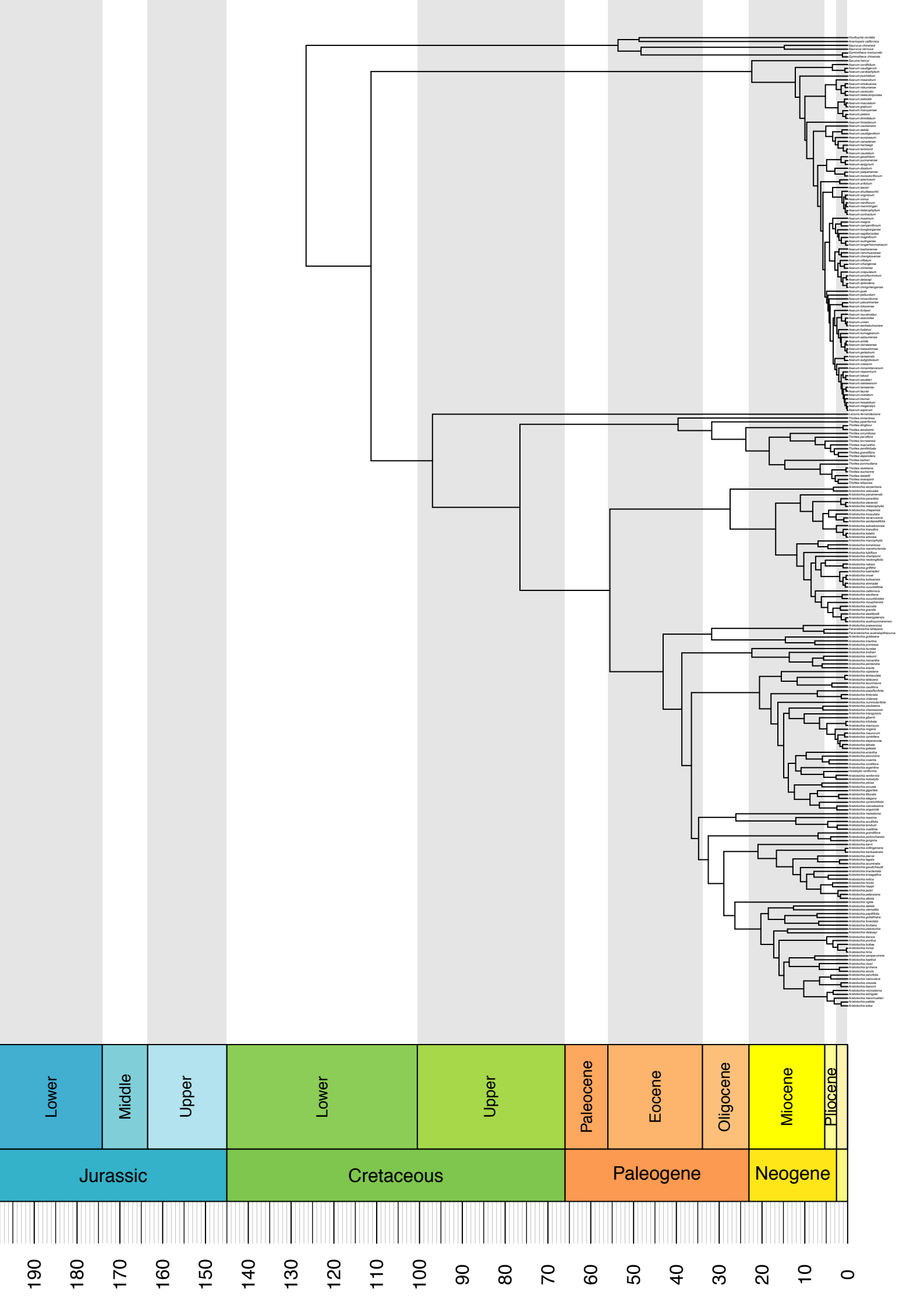


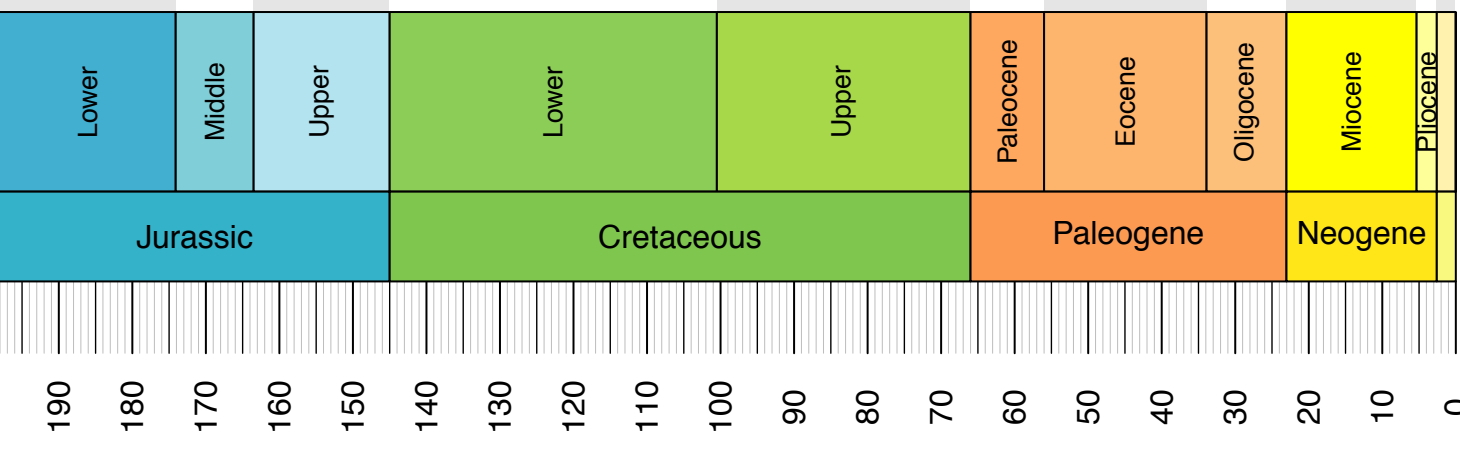
Aristolochia



0.03

Supplementary figure 8. Bayesian estimates of divergence times for Aristolochiaceae. The first inference was performed with exponential priors on fossil calibrations and 150 Ma as maximum age. The second inference was performed with exponential priors on fossil calibrations and 221 Ma as maximum age. The third inference was performed with uniform priors on fossil calibrations and 150 Ma as maximum age. The fourth inference was performed with uniform priors on fossil calibrations and 221 Ma as maximum age. The origin of the genus *Aristolochia* is estimated at 55.5 Ma (95% CI: 39.2-72.8 Ma) in the first analysis, at 58.8 Ma (95% CI: 42.5-76.2 Ma) in the second analysis, at 60.7 Ma (95% CI: 43.9-80.5 Ma) in the third analysis, and at 64.8 Ma (95% CI: 47.3-83.1 Ma) in the fourth analysis.





Supplementary figure 9. Median node ages and 95% credibility intervals (CI) for the two dating analyses of Papilionidae and the four dating analyses of Aristolochiaceae. The 95% CI overlap substantially between the two groups regardless of the dating analysis. J = Jurassic, Pl = Pliocene, P = Pleistocene. Pictures of the plant and butterfly made by Fabien Condamine.

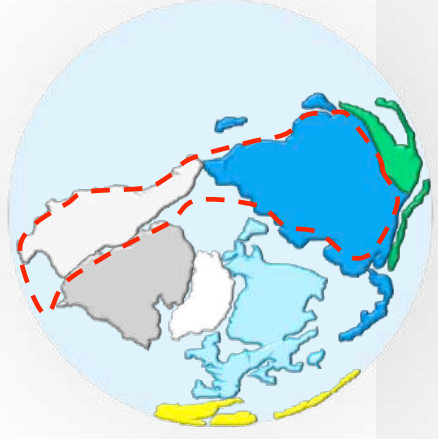
Supplementary figure 10. Estimation of the historical biogeography for the two molecular dated trees of Papilionidae with the Dispersal-Extinction-Cladogenesis (DEC) model. For each tree, two DEC analyses were performed: one with time-stratified palaeogeographic constraints, and one without such constraints. The swallowtail butterflies originated in a northern region centred around the Bering land bridge. K = Cretaceous, Pl = Pliocene, P = Pleistocene. Pictures of the butterflies and the world maps made by Fabien Condamine.

a) Dating with exponential priors (max. 150 Ma) and biogeographic inference with adjacency matrix

Global paleogeography 25 Ma



Papilionidae appeared **55.4 Ma**
(95% CI: 47.8-70.9 Ma)

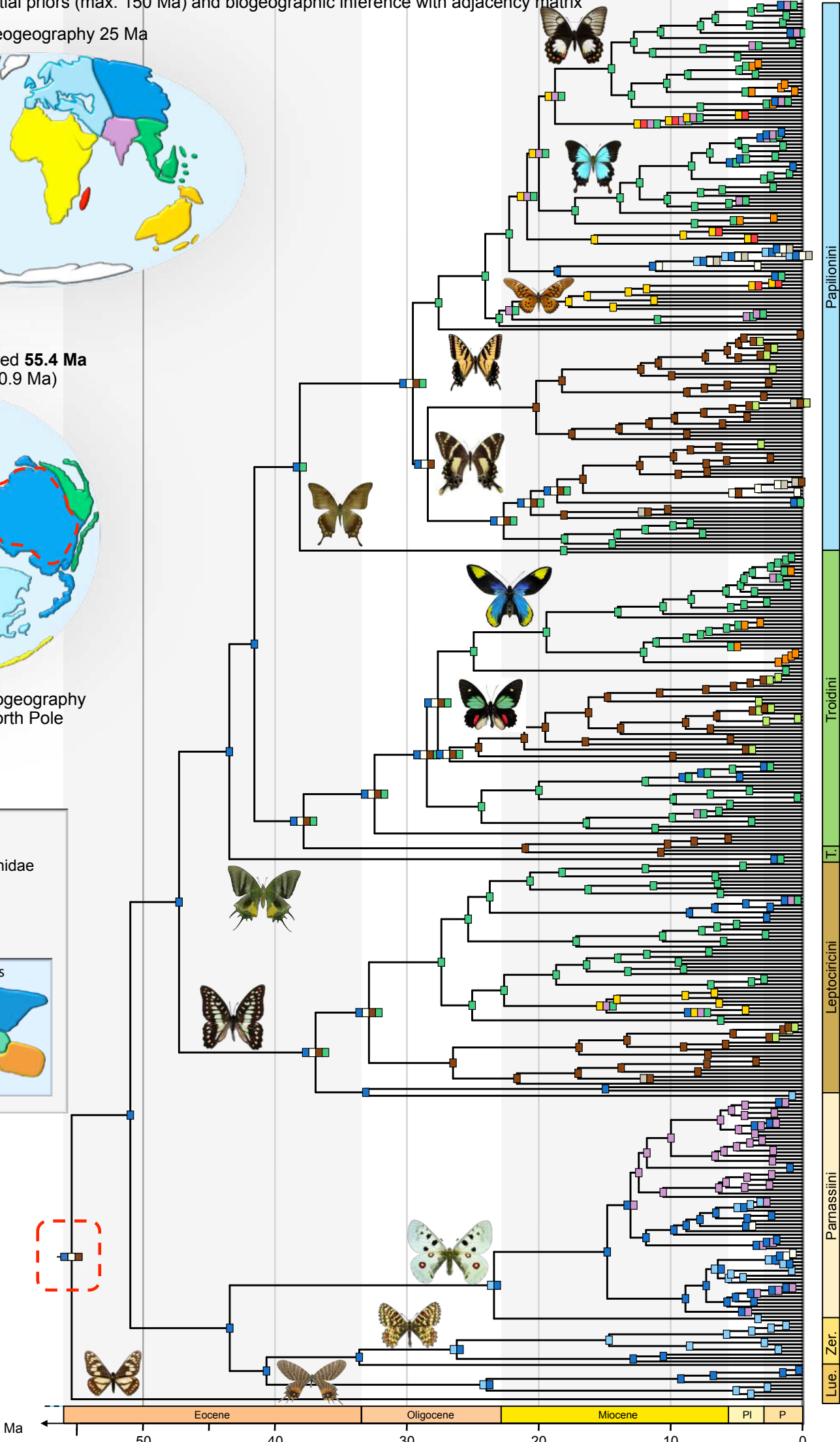


Early Eocene paleogeography
Viewed from North Pole

Legend

- Origin of Papilionidae
- Ancestral area

Color code for areas



b) Dating with exponential priors (max. 150 Ma) and biogeographic inference with unconstrained matrix

Global paleogeography 25 Ma

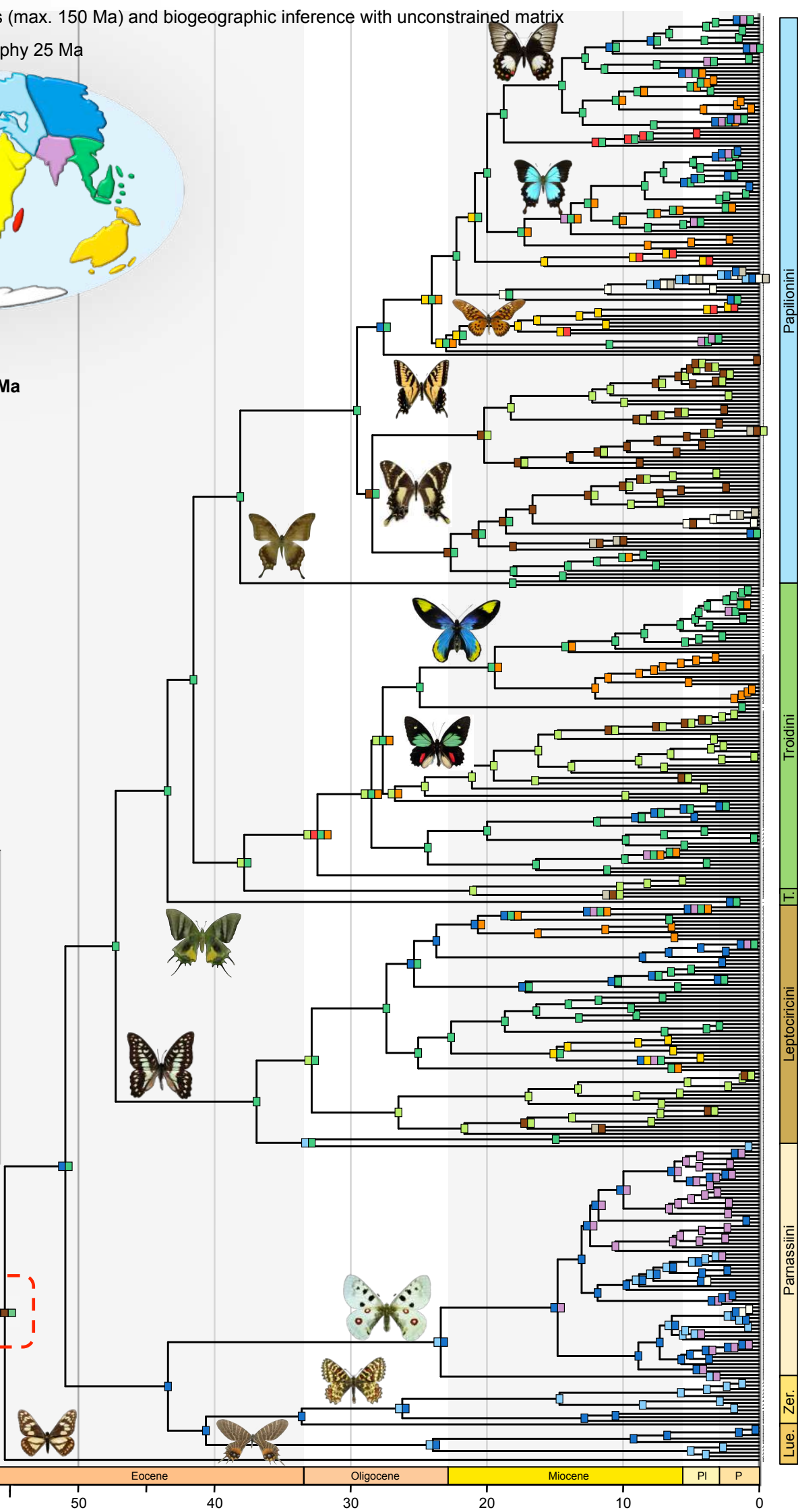


Papilionidae appeared **55.4 Ma**
(95% CI: 47.8-70.9 Ma)

Legend

- Origin of Papilionidae
- Ancestral area

Color code for areas



Ma

Eocene

Oligocene

Miocene

PI

P

Parnassiini

Leptocircini

Trodini

Papilionini

T.

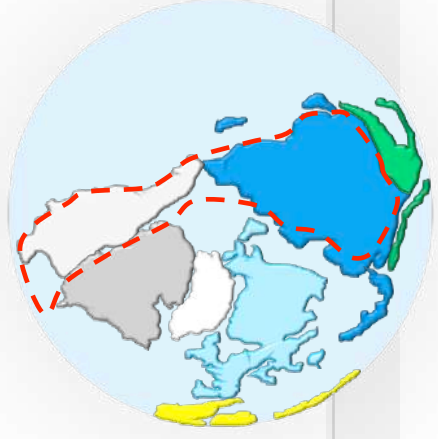
Lue. Zer.

c) Dating with uniform priors (max. 150 Ma) and biogeographic inference with adjacency matrix

Global paleogeography 25 Ma



Papilionidae appeared 67.2 Ma
(95% CI: 47.8-112 Ma)

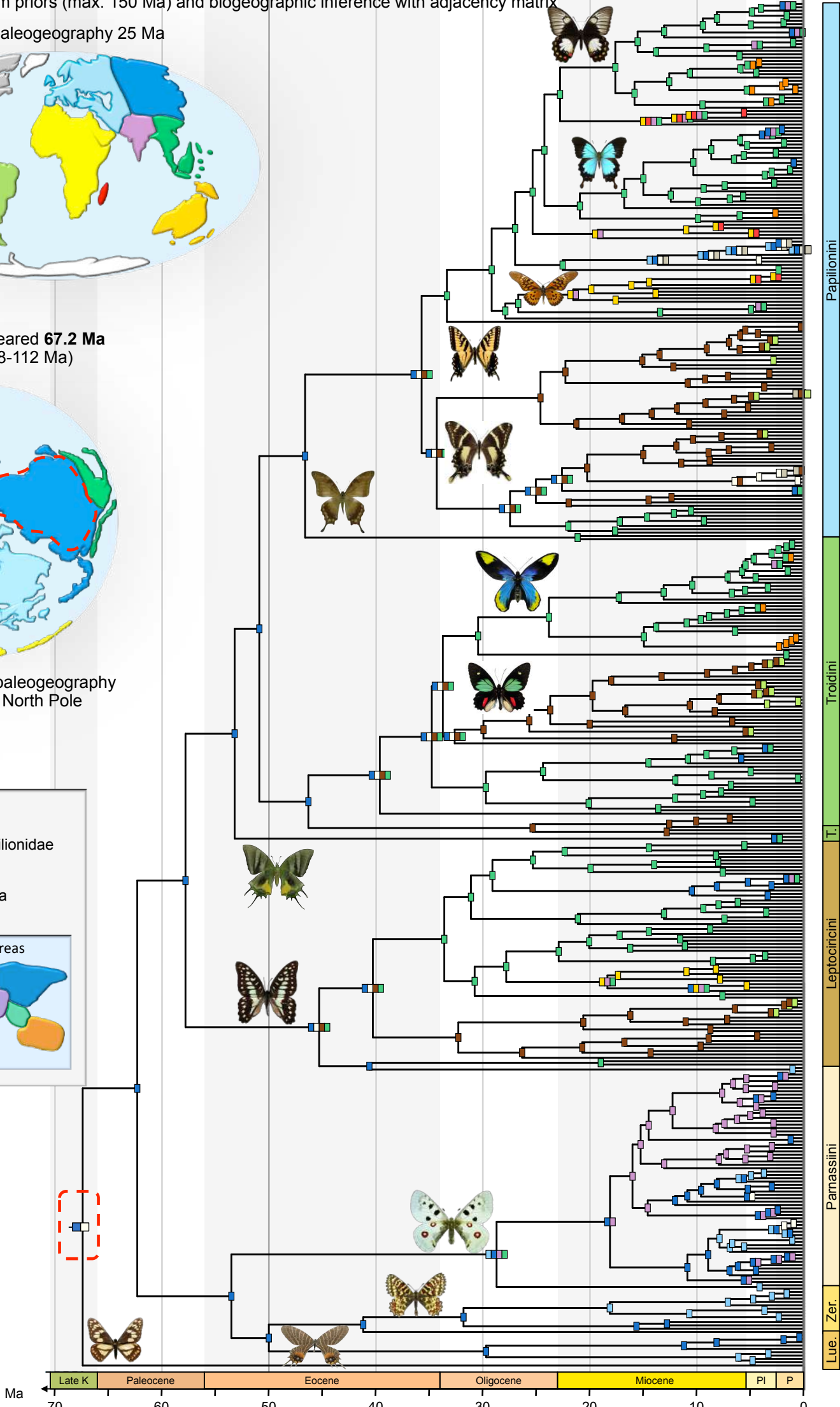


Late Cretaceous paleogeography
Viewed from North Pole

Legend

- Origin of Papilionidae
- Ancestral area

Color code for areas



d) Dating with uniform priors (max. 150 Ma) and biogeographic inference with unconstrained matrix

Global paleogeography 25 Ma

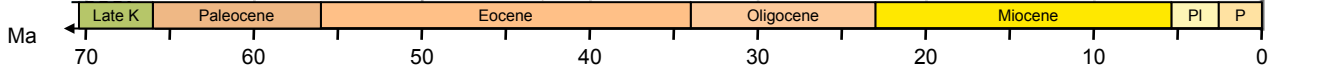
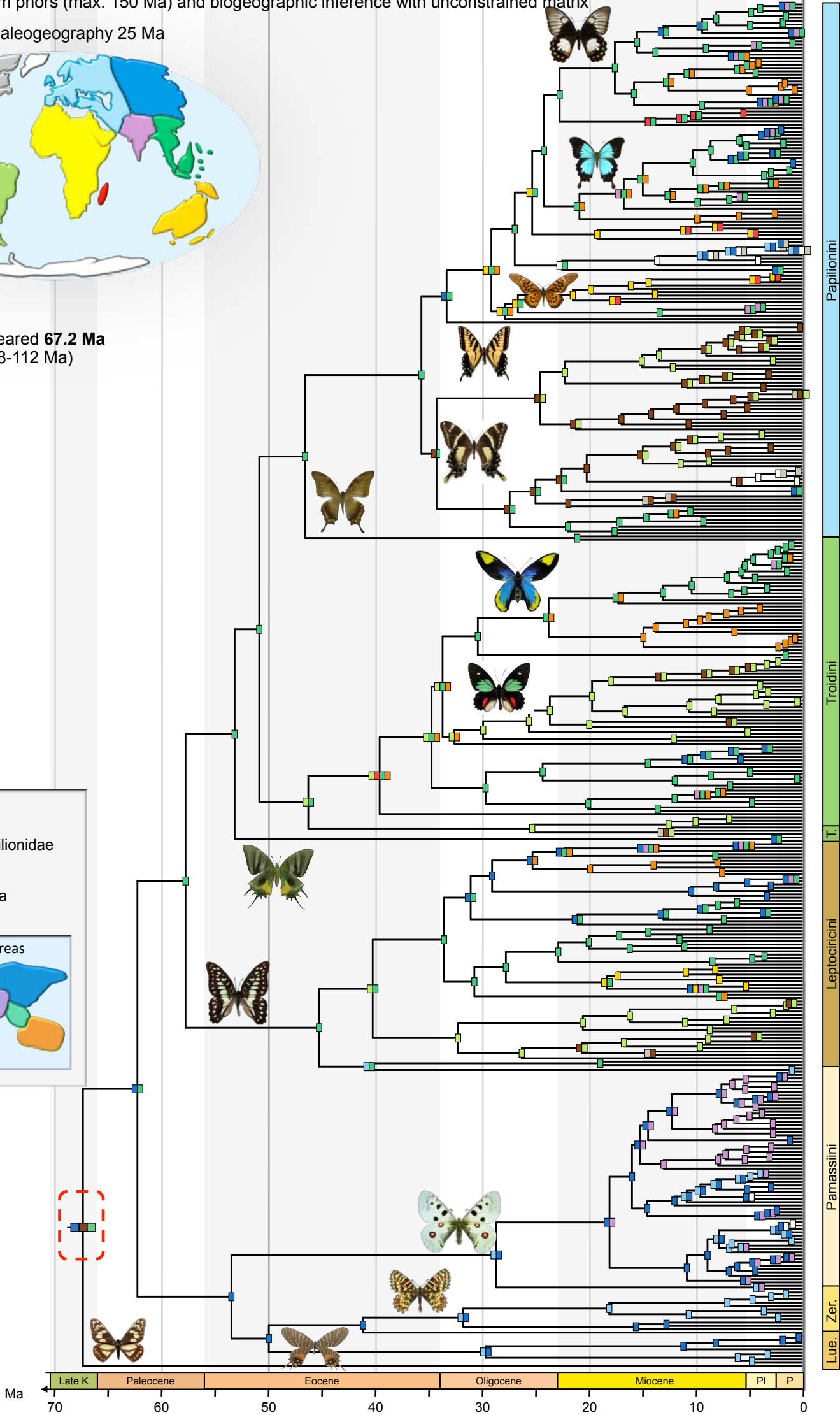


Papilionidae appeared **67.2 Ma**
(95% CI: 47.8-112 Ma)

Legend

- Origin of Papilionidae
- Ancestral area

Color code for areas



Supplementary figure 11. Estimation of the historical biogeography for the four molecular dated trees of Aristolochiaceae with the Dispersal-Extinction-Cladogenesis (DEC) model. For each tree, two DEC analyses were performed: one with time-stratified palaeogeographic constraints, and one without such constraints. The genus *Aristolochia* originated in a northern region centred around the Bering land bridge. J = Jurassic, K = Cretaceous, Pl = Pliocene, P = Pleistocene. Pictures of the plants and the world maps made by Fabien Condamine.

a) Dating with exponential priors (max. 150 Ma) and biogeographic inference with adjacency matrix

Global paleogeography 25 Ma



Early Eocene paleogeography Viewed from North Pole

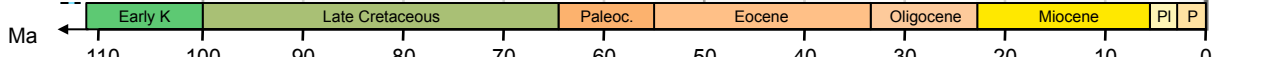
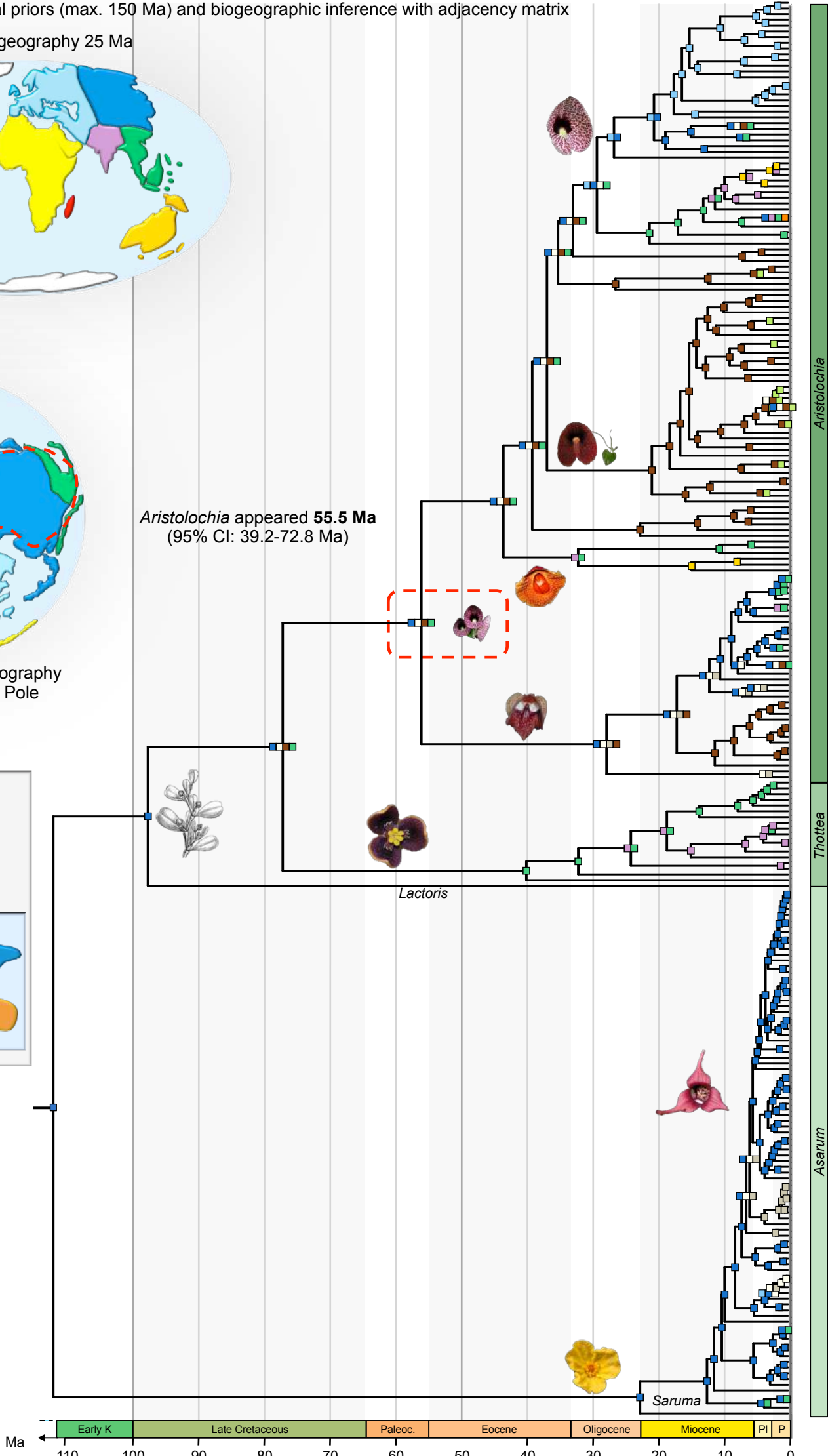
Legend

Origin of *Aristolochia*

Ancestral area

Color code for areas

Aristolochia appeared **55.5 Ma**
(95% CI: 39.2-72.8 Ma)

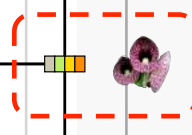


b) Dating with exponential priors (max. 150 Ma) and biogeographic inference with unconstrained matrix


Global paleogeography 25 Ma




Aristolochia appeared **55.5 Ma**
(95% CI: 39.2-72.8 Ma)




Legend

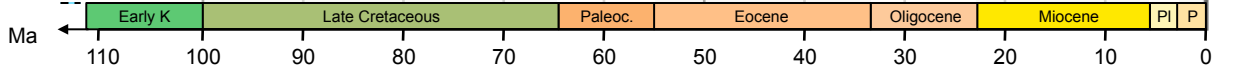
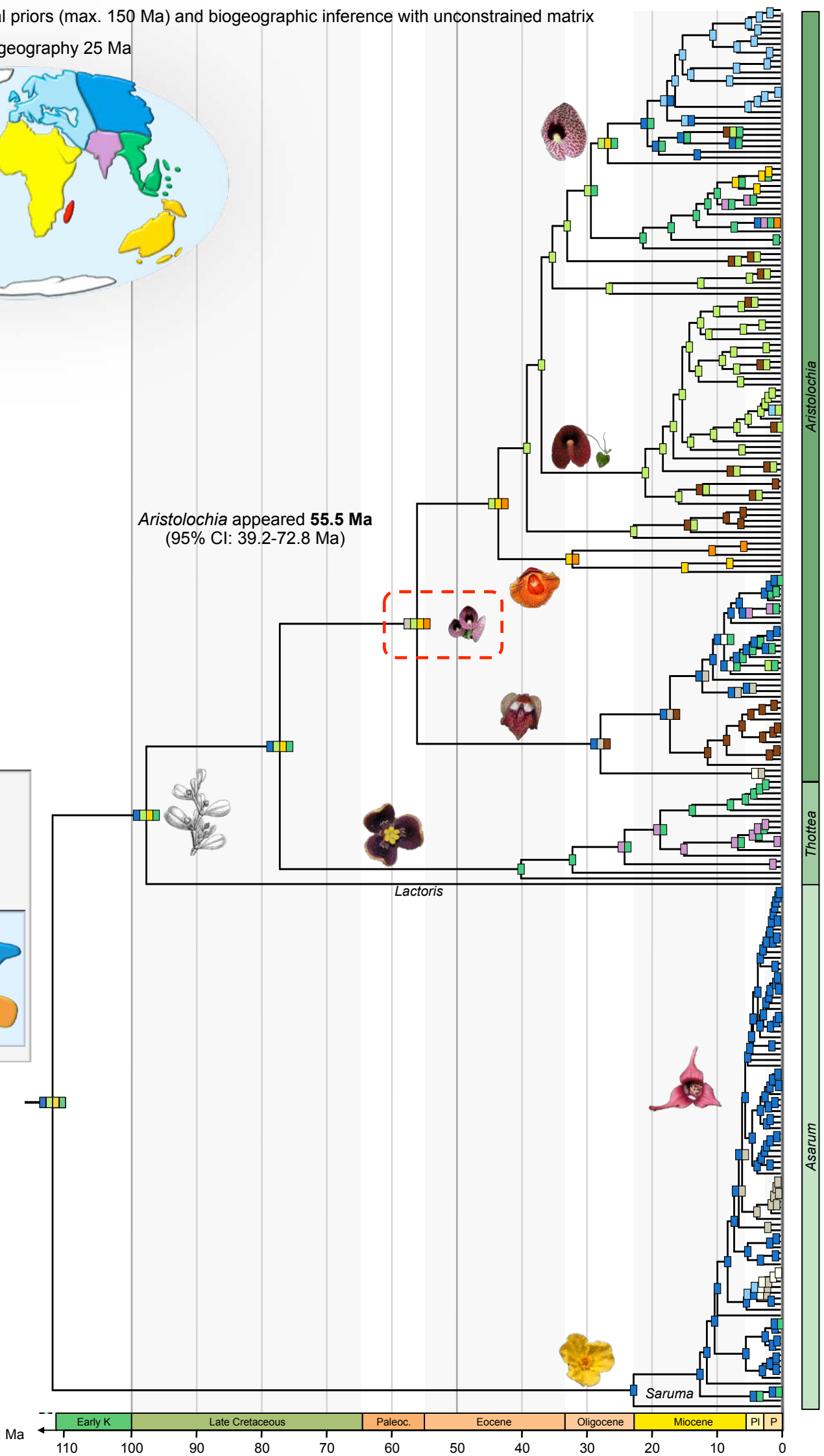
 Origin of *Aristolochia*

 Ancestral area

Color code for areas



The legend includes a color-coded map of the world, where different colors represent the ancestral areas for various clades. The colors correspond to the regions shown in the paleogeography map: light blue, green, yellow, light blue, yellow, and white.



c) Dating with exponential priors (max. 221 Ma) and biogeographic inference with adjacency matrix

Global paleogeography 25 Ma

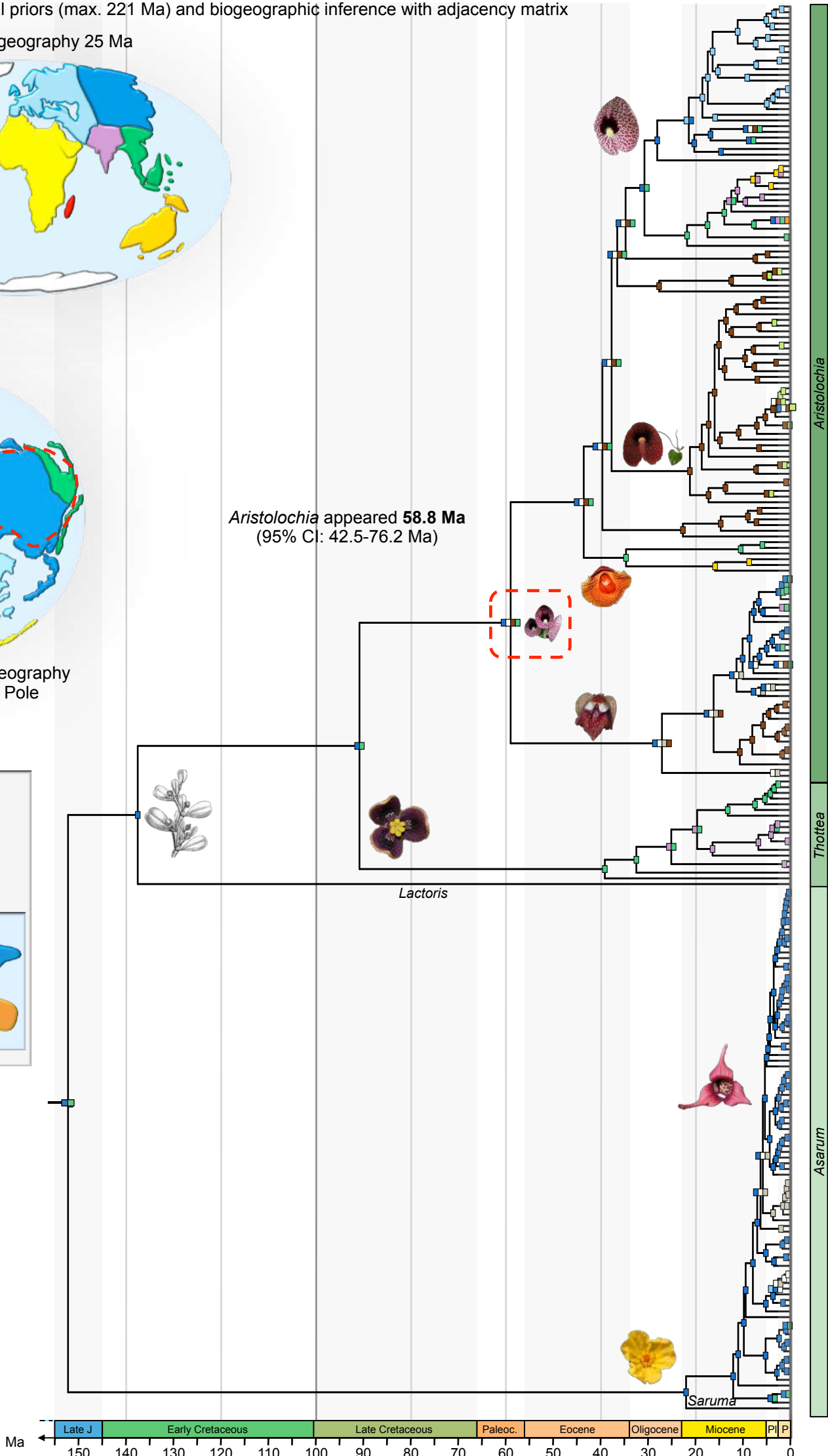


Late Paleocene paleogeography Viewed from North Pole

Legend

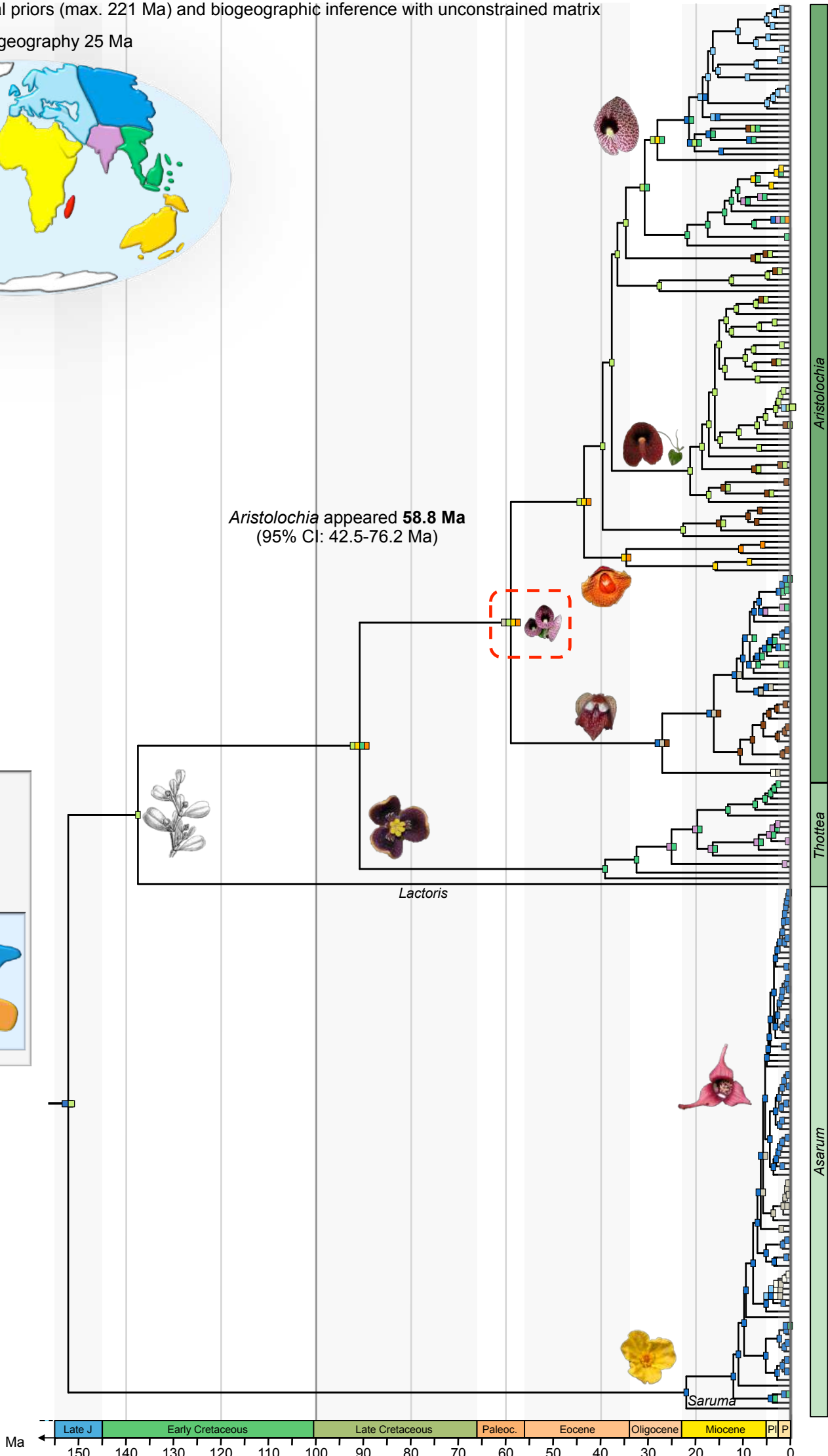
- Origin of *Aristolochia*
- Ancestral area

Color code for areas





d) Dating with exponential priors (max. 221 Ma) and biogeographic inference with unconstrained matrix

Global paleogeography 25 Ma


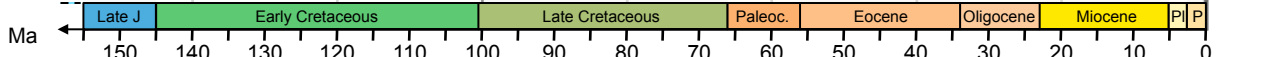


Legend

 Origin of *Aristolochia*

 Ancestral area

Color code for areas

e) Dating with uniform priors (max. 150 Ma) and biogeographic inference with adjacency matrix

Global paleogeography 25 Ma



Late Paleocene paleogeography Viewed from North Pole

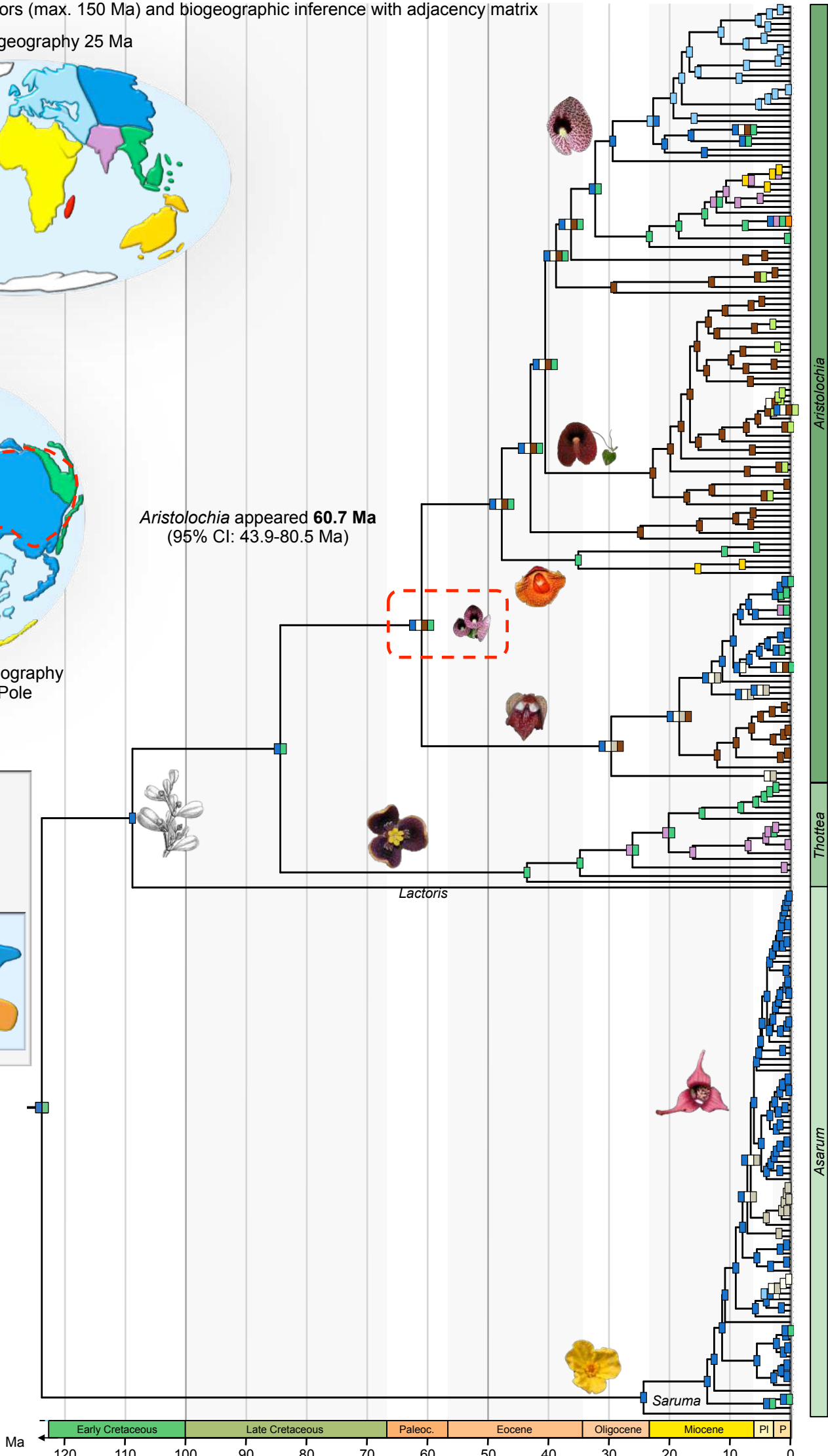
Aristolochia appeared **60.7 Ma**
(95% CI: 43.9-80.5 Ma)

Legend

 Origin of *Aristolochia*

 Ancestral area

Color code for areas

Aristolochia

Thottea

Asarum

Ma 120 110 100 90 80 70 60 50 40 30 20 10 0

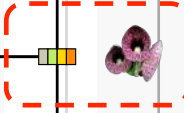
Early Cretaceous Late Cretaceous Paleoc. Eocene Oligocene Miocene PI P

f) Dating with uniform priors (max. 150 Ma) and biogeographic inference with unconstrained matrix


Global paleogeography 25 Ma




Aristolochia appeared **60.7 Ma**
(95% CI: 43.9-80.5 Ma)




Legend

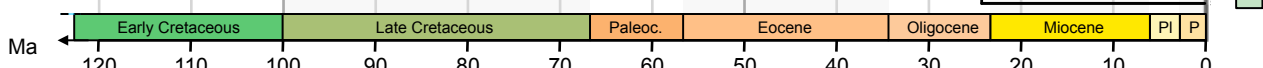
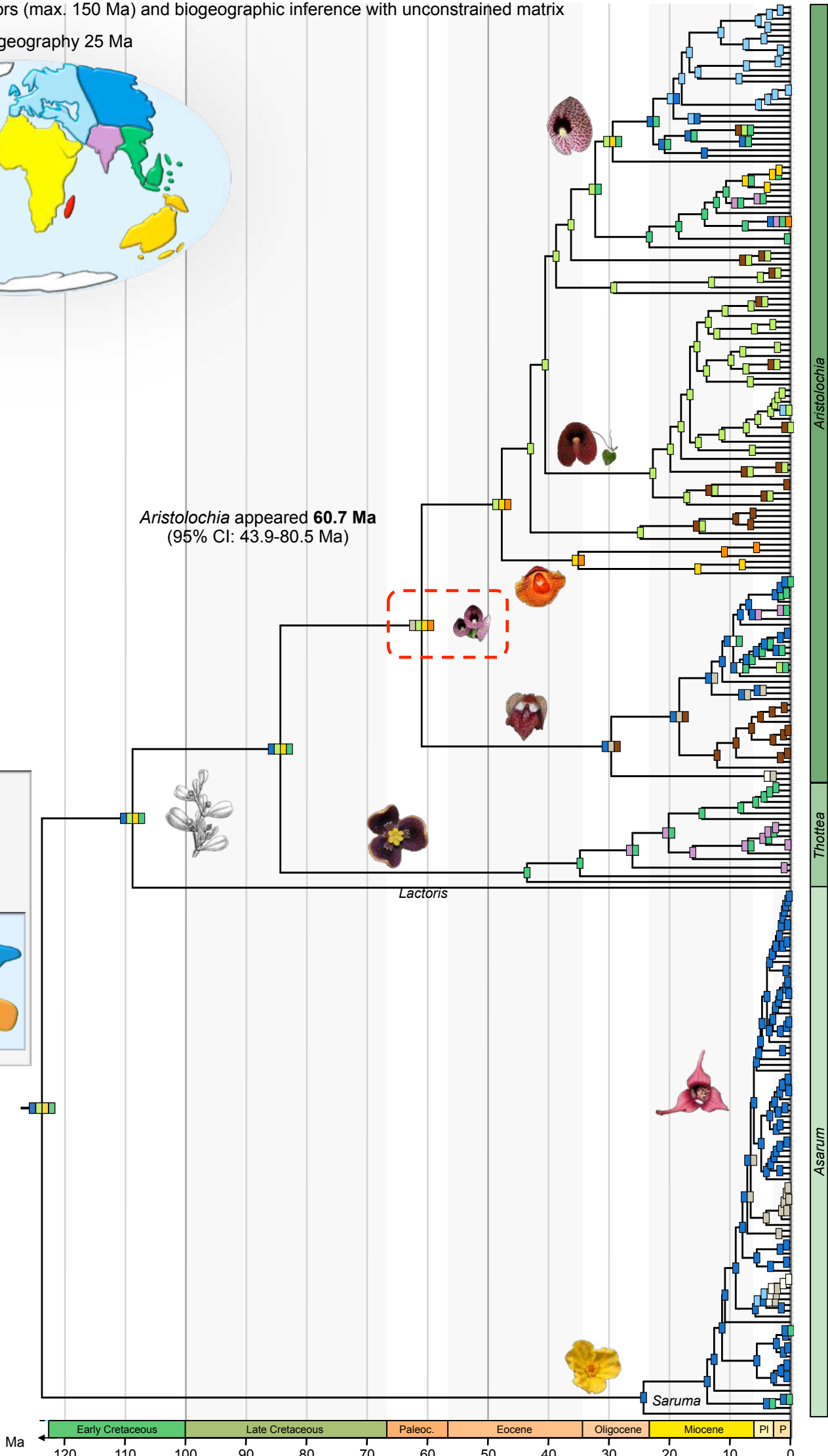
 Origin of *Aristolochia*

 Ancestral area

Color code for areas



A color-coded map of the world showing different geographic areas corresponding to the legend. The colors include light blue, green, yellow, purple, orange, and brown.



g) Dating with uniform priors (max. 221 Ma) and biogeographic inference with adjacency matrix

Global paleogeography 25 Ma



Early Paleocene paleogeography Viewed from North Pole

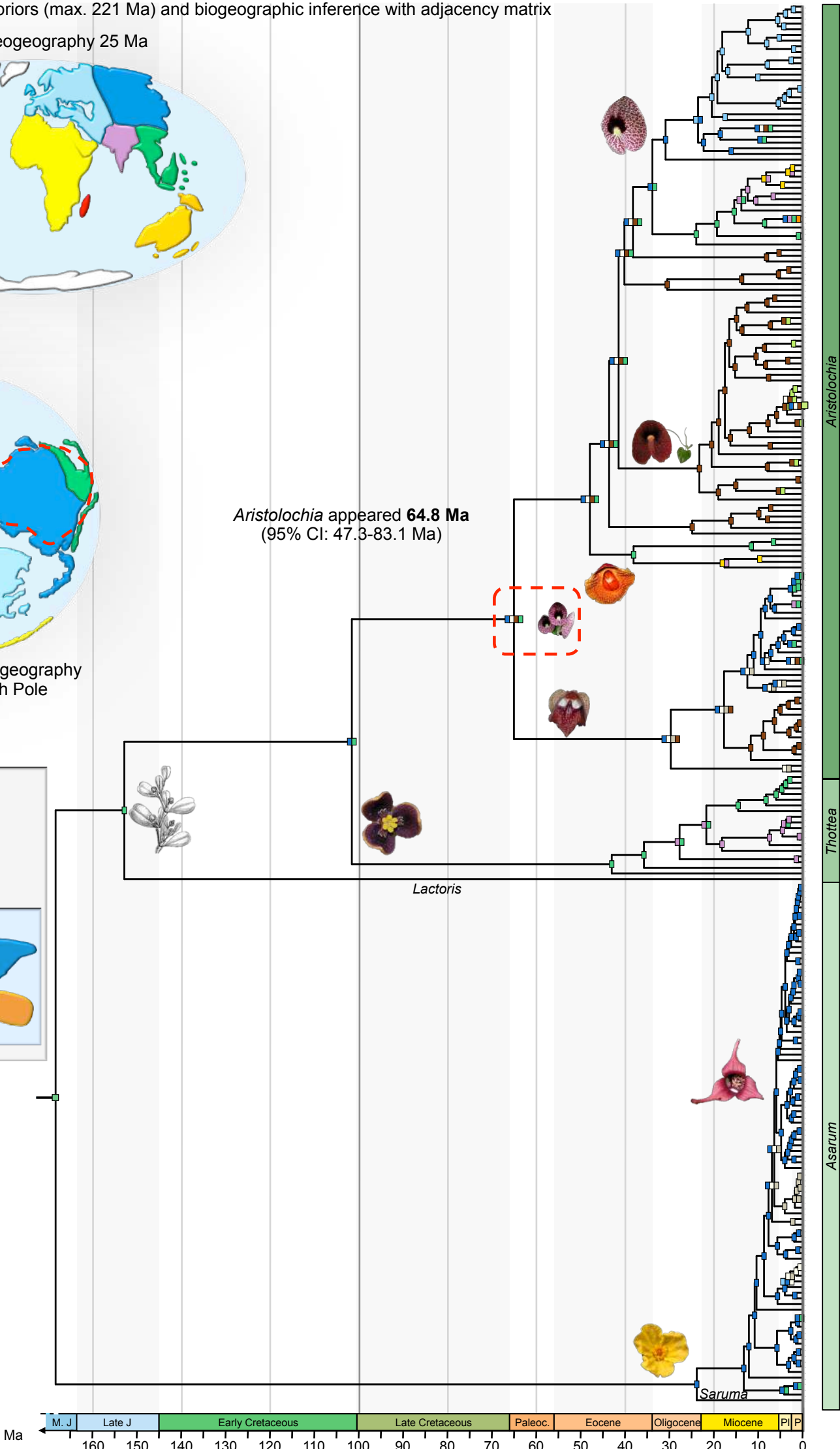
Legend

Origin of *Aristolochia*

Ancestral area

Color code for areas

Aristolochia appeared **64.8 Ma**
(95% CI: 47.3-83.1 Ma)




h) Dating with uniform priors (max. 221 Ma) and biogeographic inference with unconstrained matrix


Global paleogeography 25 Ma




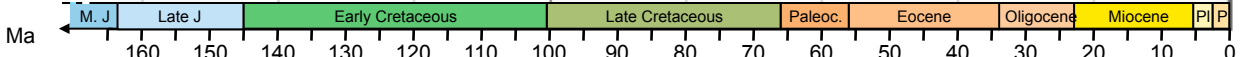
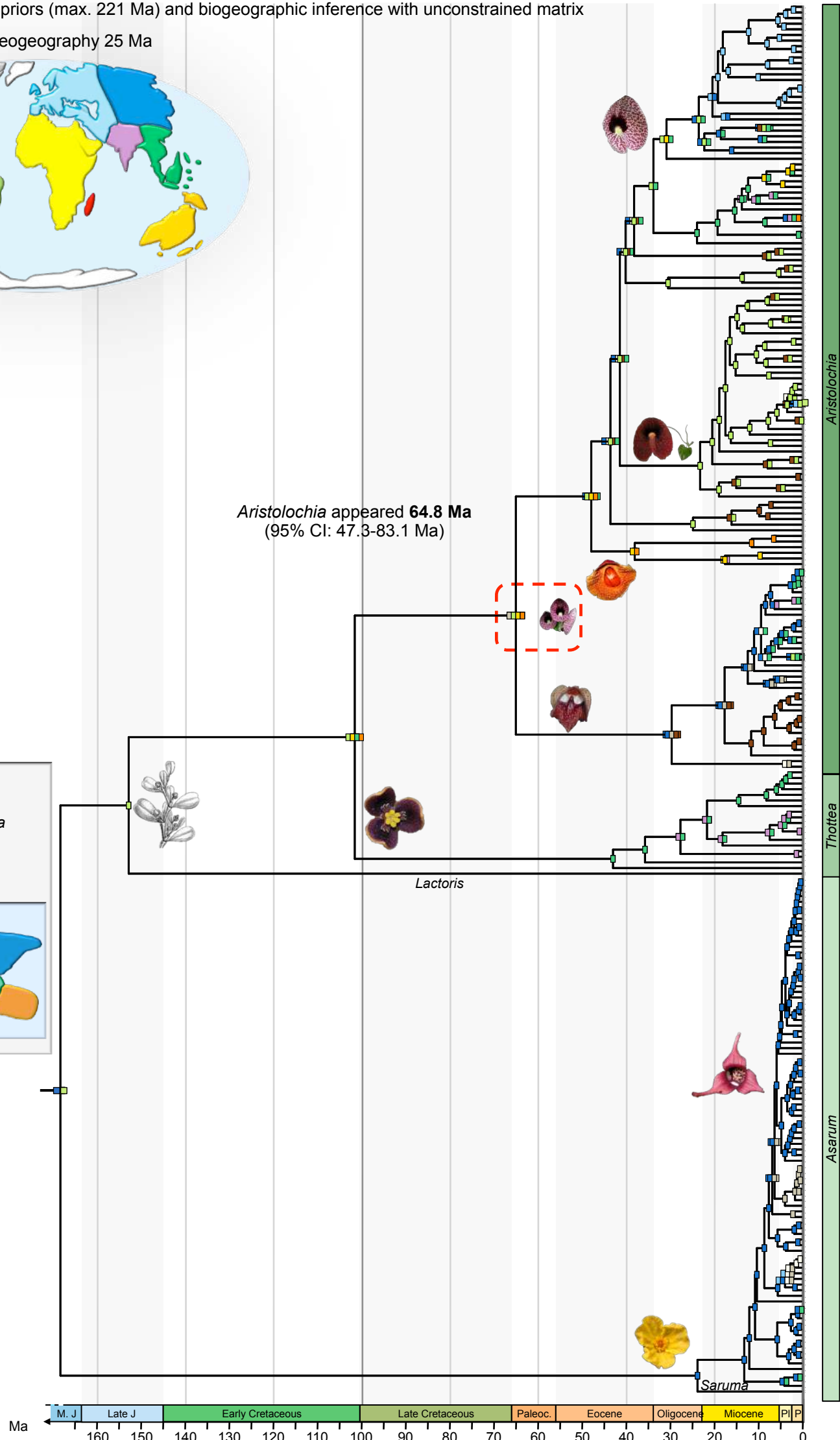
Aristolochia appeared **64.8 Ma**
(95% CI: 47.3-83.1 Ma)

Legend

 Origin of *Aristolochia*

 Ancestral area

Color code for areas

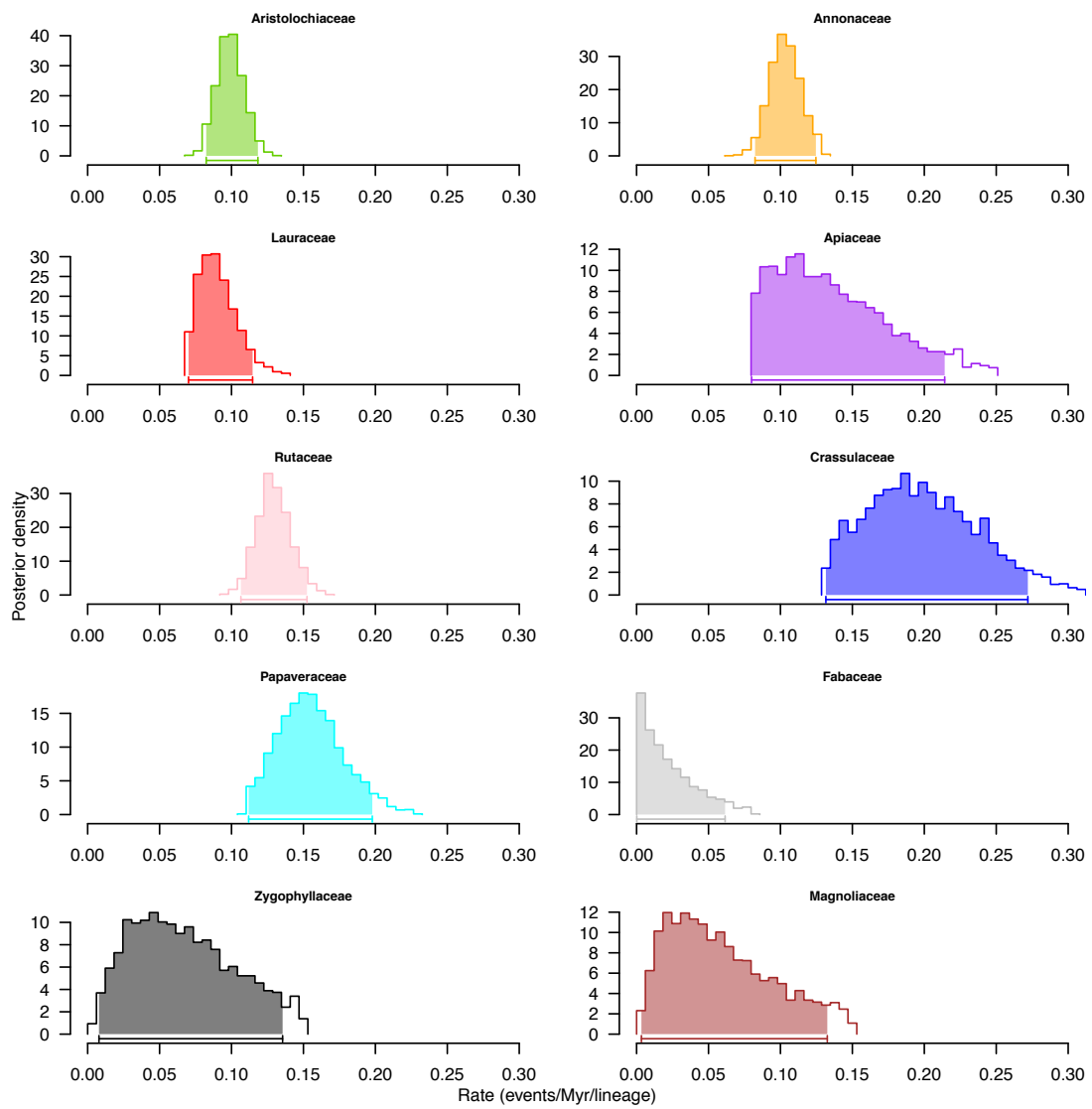
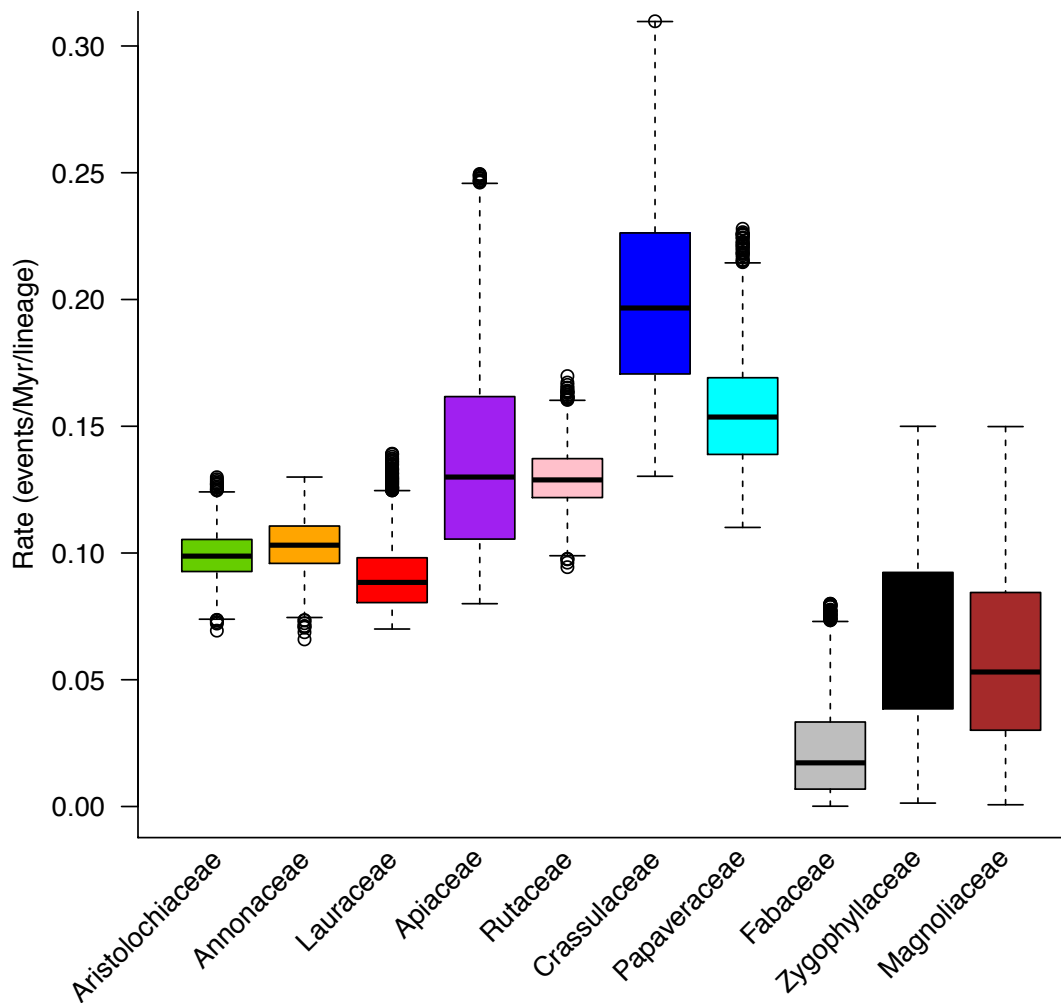
Aristolochia

Thottea

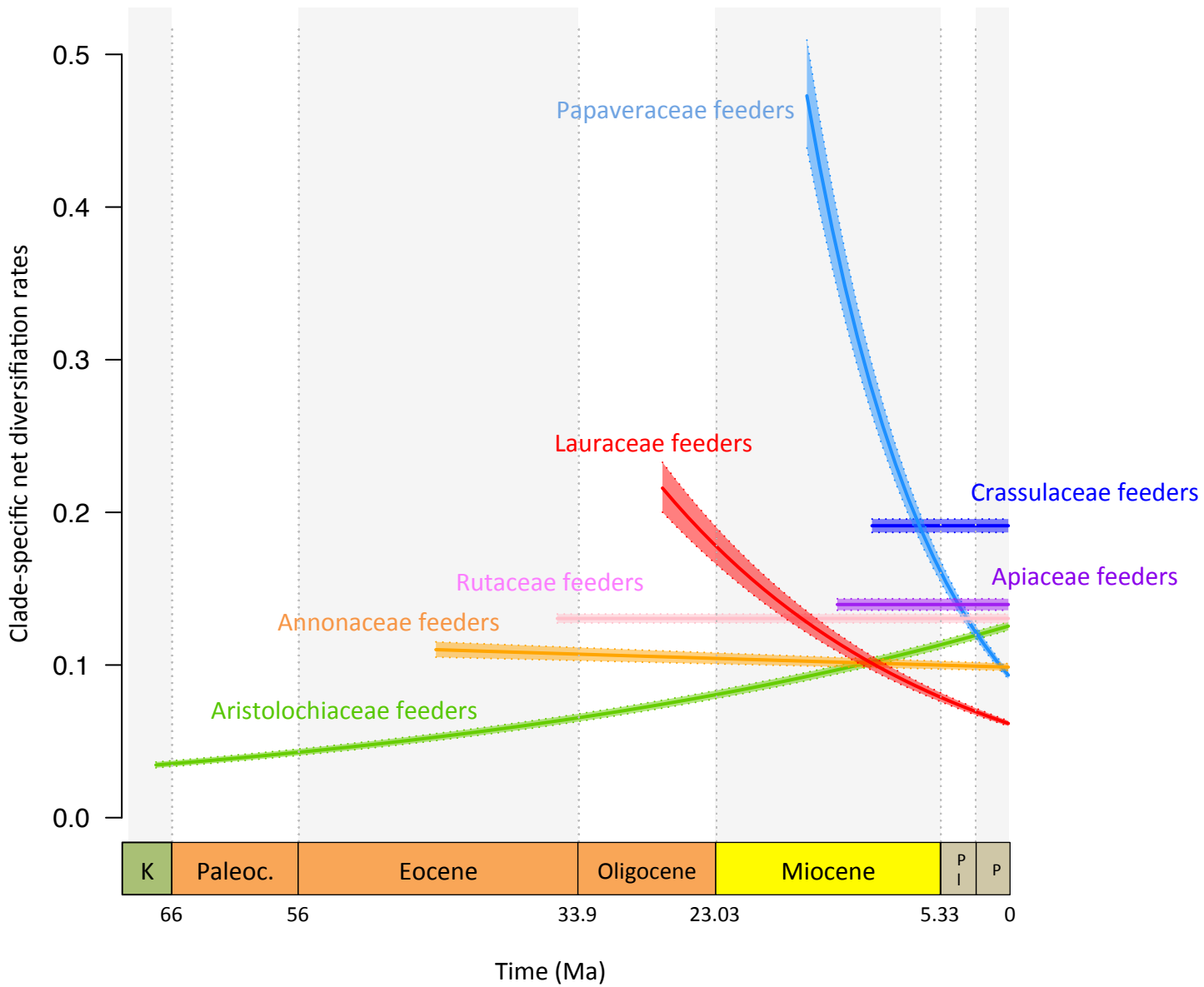
Saruma

Ma

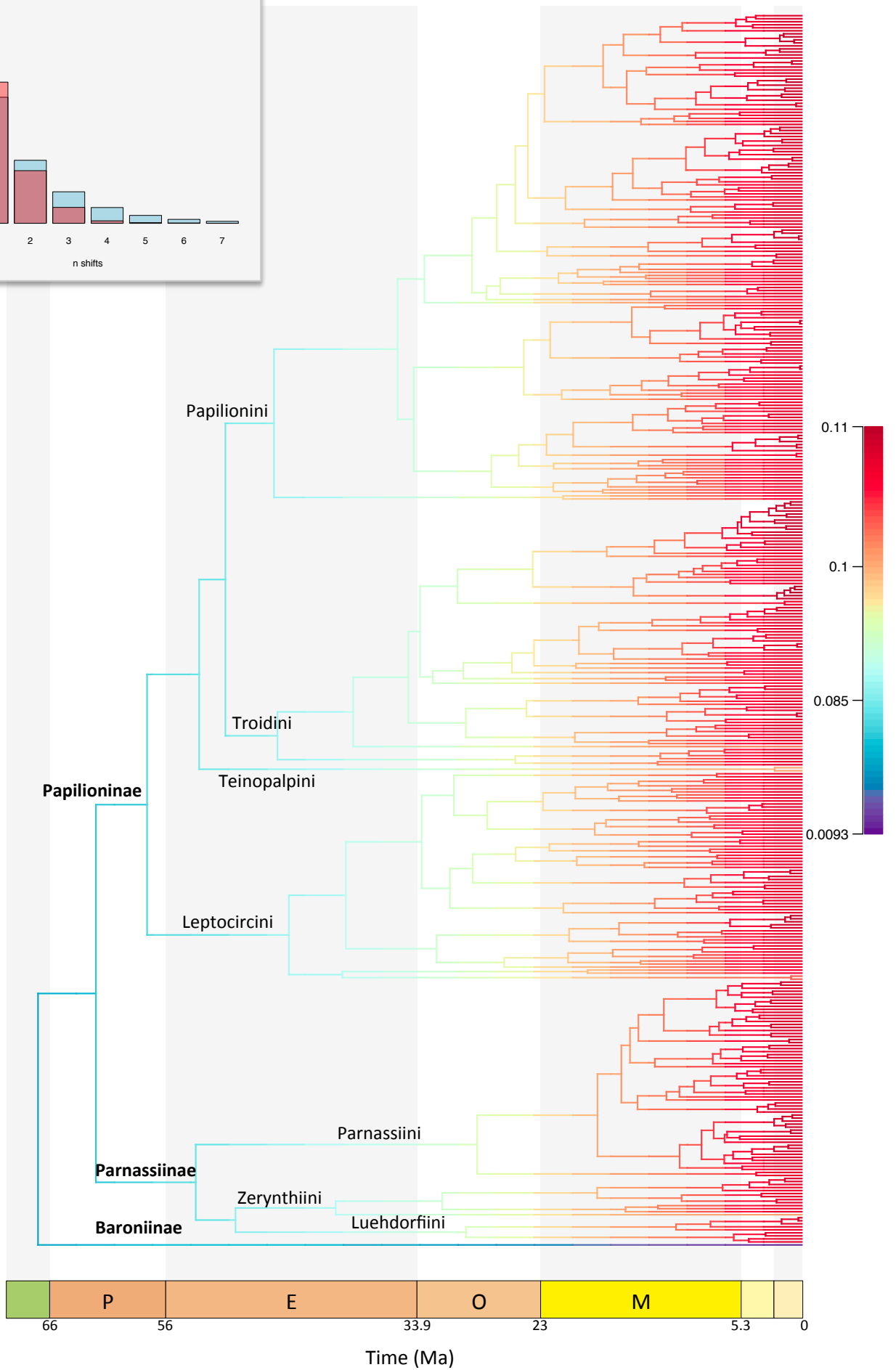
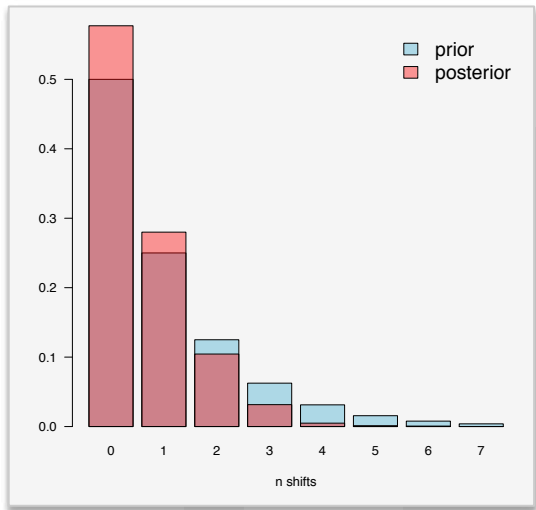
Supplementary figure 12. Trait-dependent diversification of Papilionidae linked to their host-plant. **a**, Bayesian inferences made with the full MuSSE model showed that speciation rates vary according to the host-plant trait. **b**, Boxplots showing the increase of diversification rates following host-plant shifts from the ancestral state (Aristolochiaceae). Only the species-poor swallowtail lineages feeding on Fabaceae, Zygophyllaceae and Magnoliaceae show decrease of diversification rates.

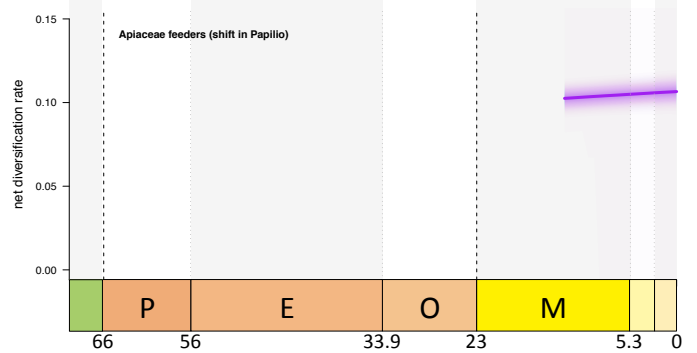
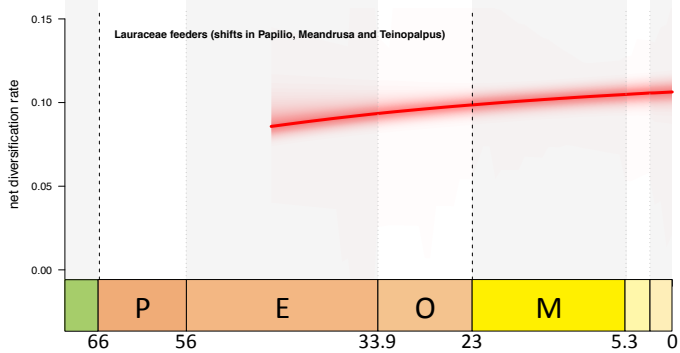
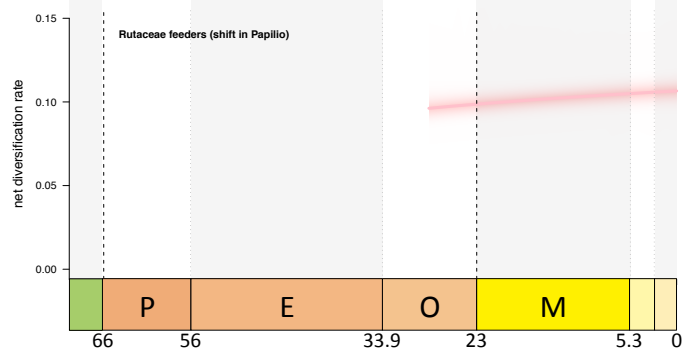
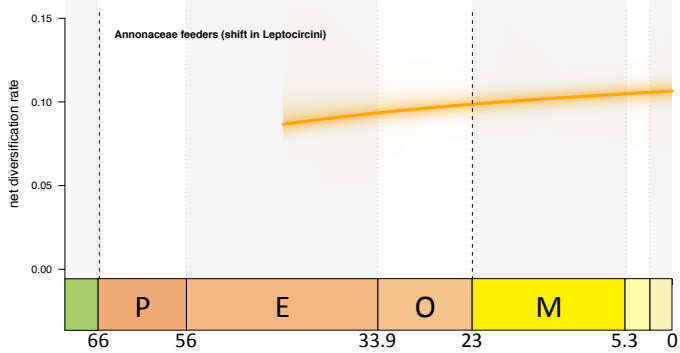
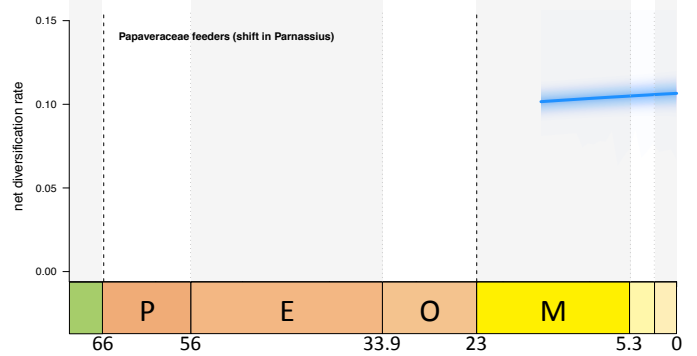
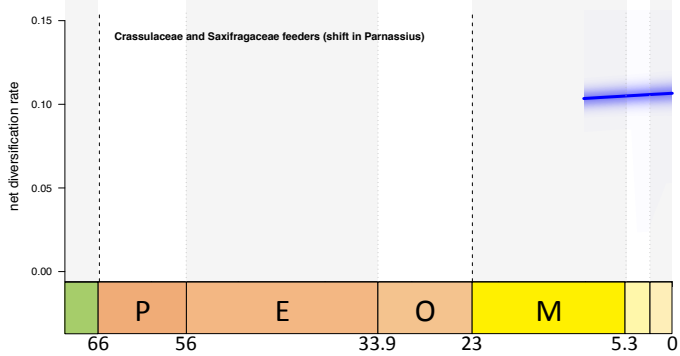
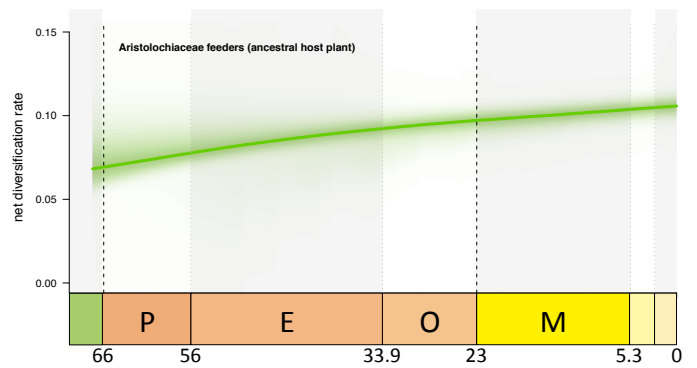
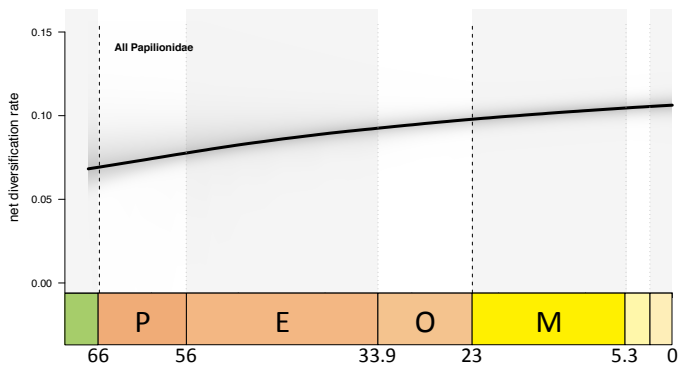
a**b**

Supplementary figure 13. Time-dependent diversification of Papilionidae after shifting to new host-plants. Diversification is inferred with the RPANDA models, and the best-fit model is plotted showing rates through time for each clade. A model with increasing diversification over time best fits the Aristolochiaceae feeders. A model with a slowdown of diversification through time explained the diversification of Annonaceae feeders, Lauraceae feeders, and Papaveraceae feeders. A model with constant rates through time best fits the diversification of Apiaceae feeders, Crassulaceae feeders, and Rutaceae feeders. Solid lines indicate mean rates, and the shaded areas show 95% confidence intervals. K = Cretaceous, Pl = Pliocene, P = Pleistocene.



Supplementary figure 14. Bayesian analysis of clade-specific and time-dependent diversification of Papilionidae obtained with BAMM. a, Phylorate plot showing that global diversification rates increase through time in Papilionidae with no significant rate shifts detected by BAMM (the inset plot indicates the posterior probability for the estimated number of shifts). b, Rate-through-time plots for selected swallowtail lineages feeding on distinct host-plant families. The results also show an overall diversification increase through time for each group of swallowtails. P = Palaeocene, E = Eocene, O = Oligocene, M = Miocene.

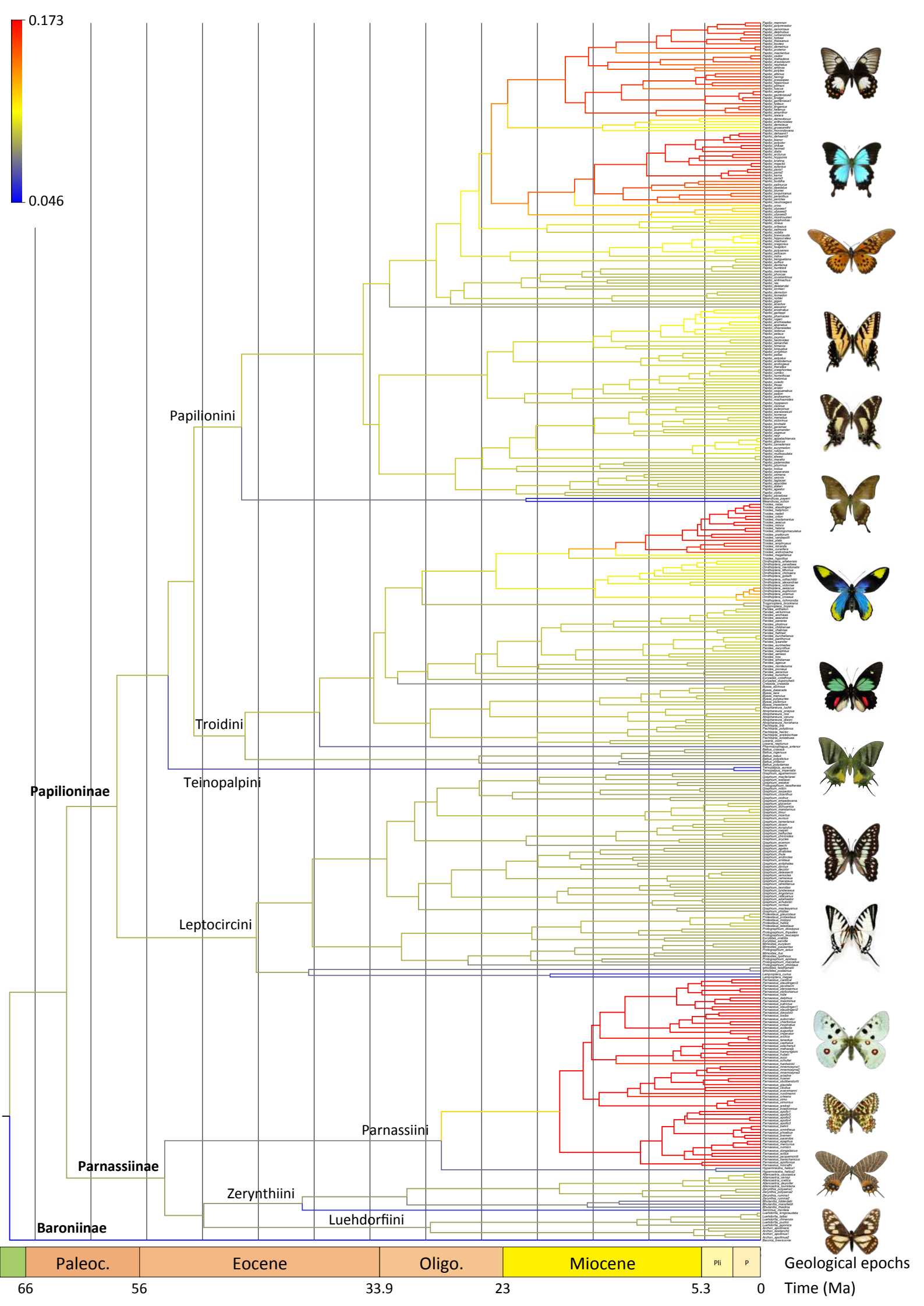




Time (Ma)

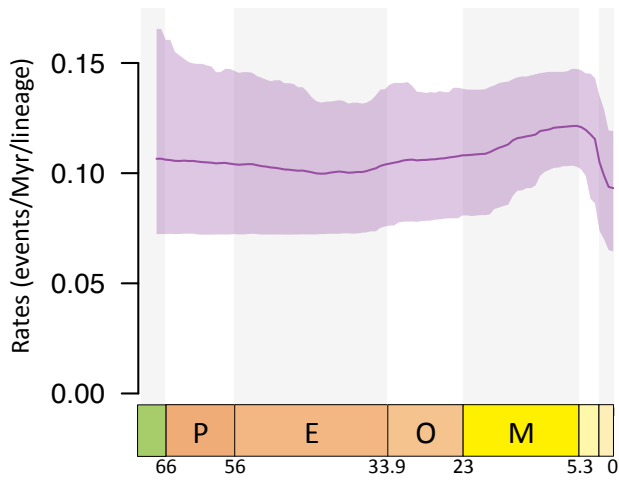
Time (Ma)

Supplementary figure 15. Bayesian analysis of branch-specific and time-dependent diversification of Papilionidae obtained with RevBayes. The median rates of diversification are plotted along each branch of the phylogeny, which shows a global increase of diversification rates through time in Papilionidae. Contrary to BAMM, this approach detected shifts in diversification rates in particular within the genera *Parnassius* and *Papilio* that have both shifted to new host-plant families. Mean posterior branch-specific rates are indicated in the scale bar on the topleft. P = Palaeocene, E = Eocene, O = Oligocene, M = Miocene. Pictures of butterflies made by Fabien Condamine.

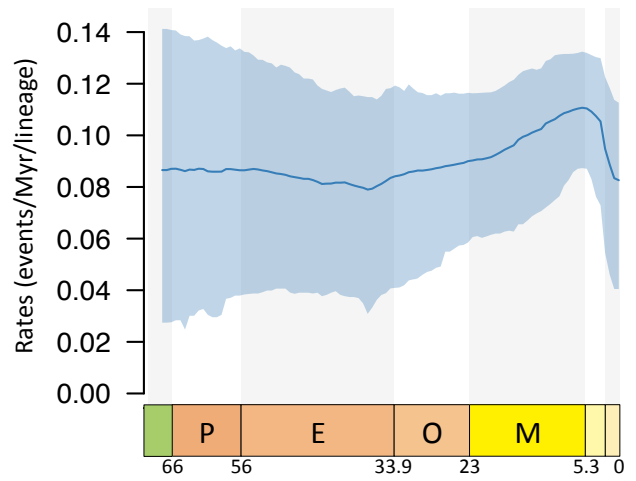


Supplementary figure 16. Bayesian analysis of episodic diversification of Papilionidae obtained with CoMET. The four plots represent speciation, extinction, net diversification, and relative extinction rates through time for the whole family. The result indicates a global increase of diversification rates over time, notably starting ~40 Ma. P = Palaeocene, E = Eocene, O = Oligocene, M = Miocene.

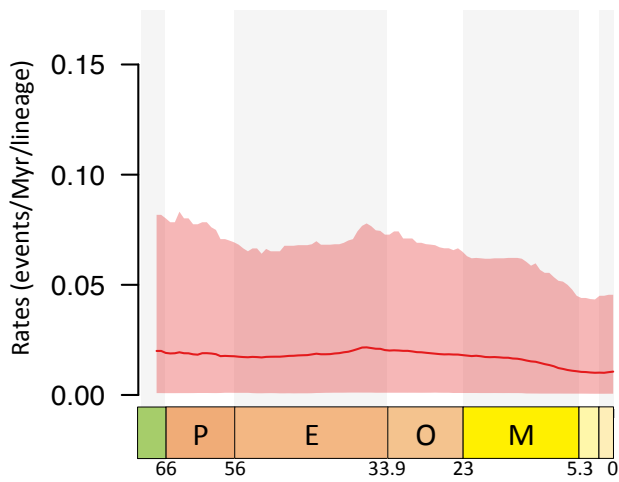
Speciation rates



Net diversification rates

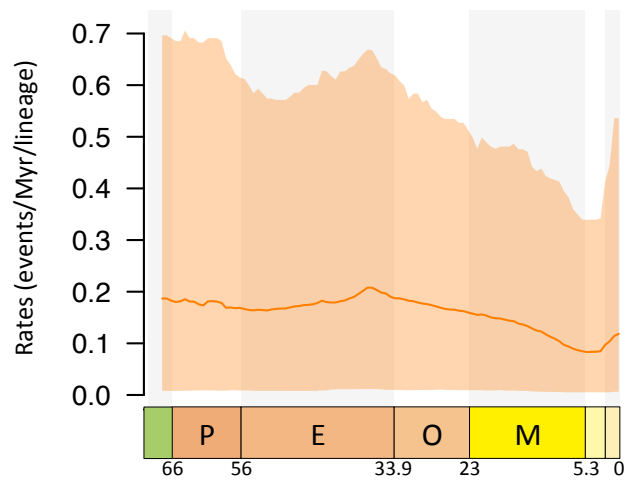


Extinction rates



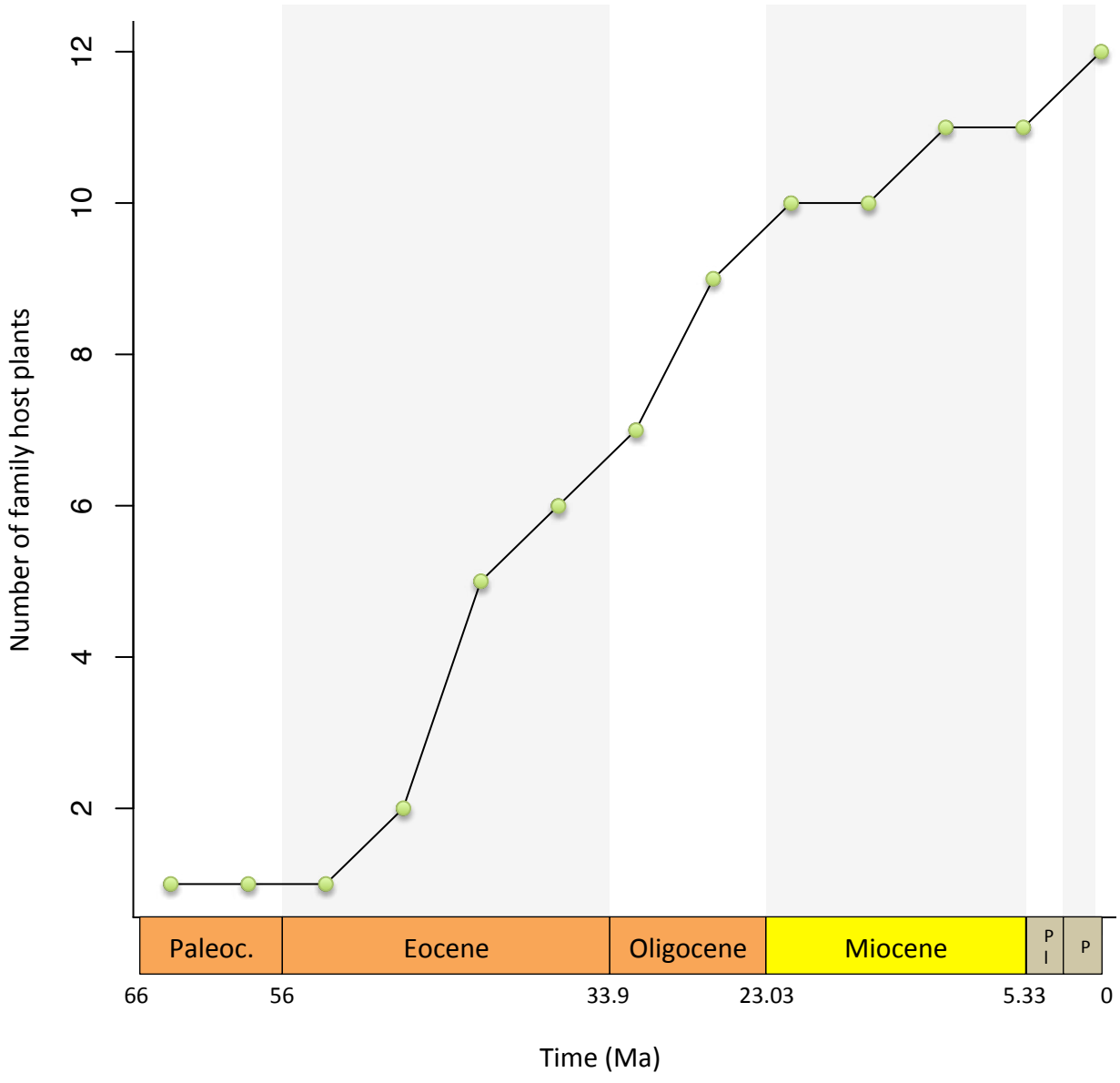
Time (Ma)

Relative extinction rates

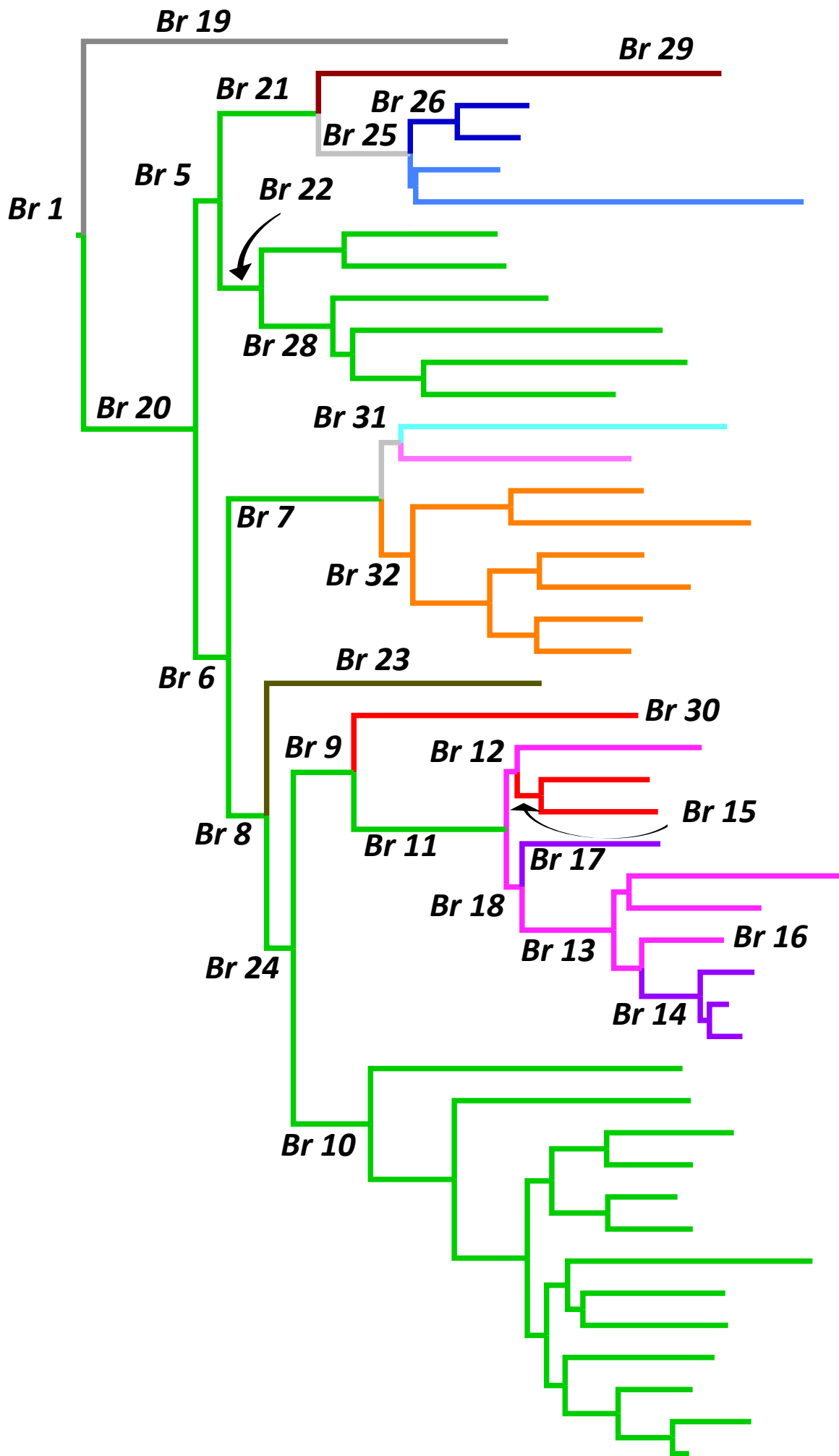


Time (Ma)

Supplementary figure 17. Number of host- plants consumed through time by Papilionidae. Using the estimation of ancestral host-plant preferences (Supplementary Fig. 4), we plotted the time at which a new host-plant family was colonised. This result shows that the swallowtail butterflies have a steady increase in the number of host families consumed over time. This ecological diversification can be paralleled with the global increase in diversification rates estimated by birth-death models (Supplementary Figs. 13-16). K = Cretaceous, Pl = Pliocene, P = Pleistocene.

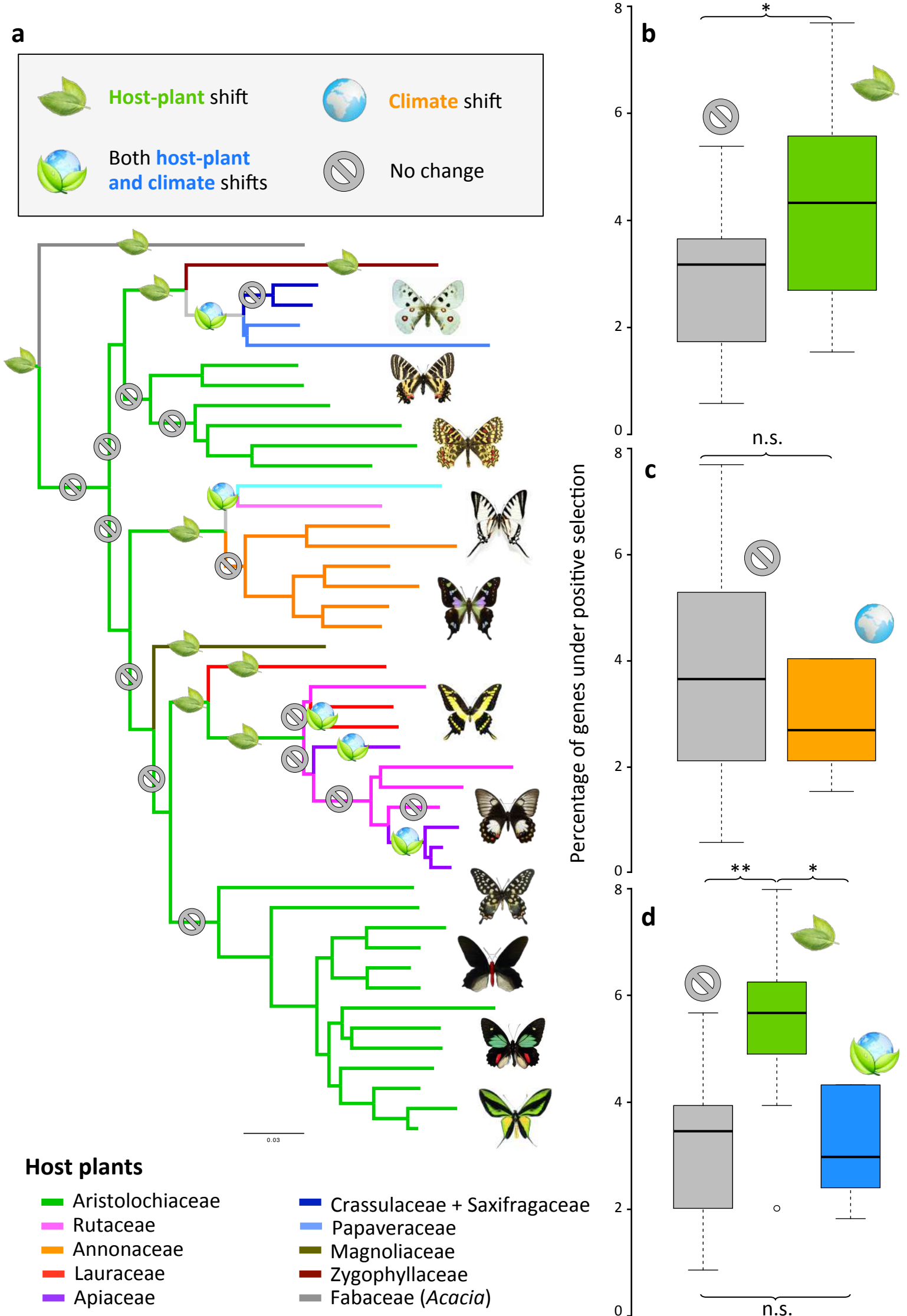


Supplementary figure 18. Genus-level phylogenomic tree of Papilionidae showing the 14 selected branches with host-plant shifts and the 14 selected branches without host-plant shifts (control branches). The selection of these branches is based on the estimation of ancestral state models using the species-level phylogenies and current host-plant preferences (Supplementary Figs. 4, 5).



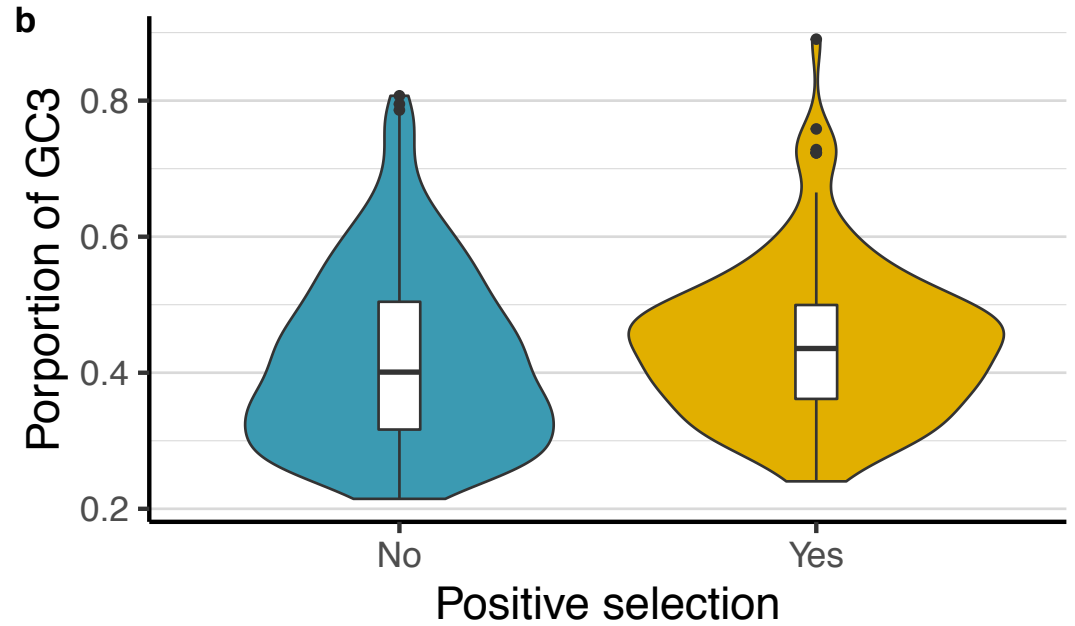
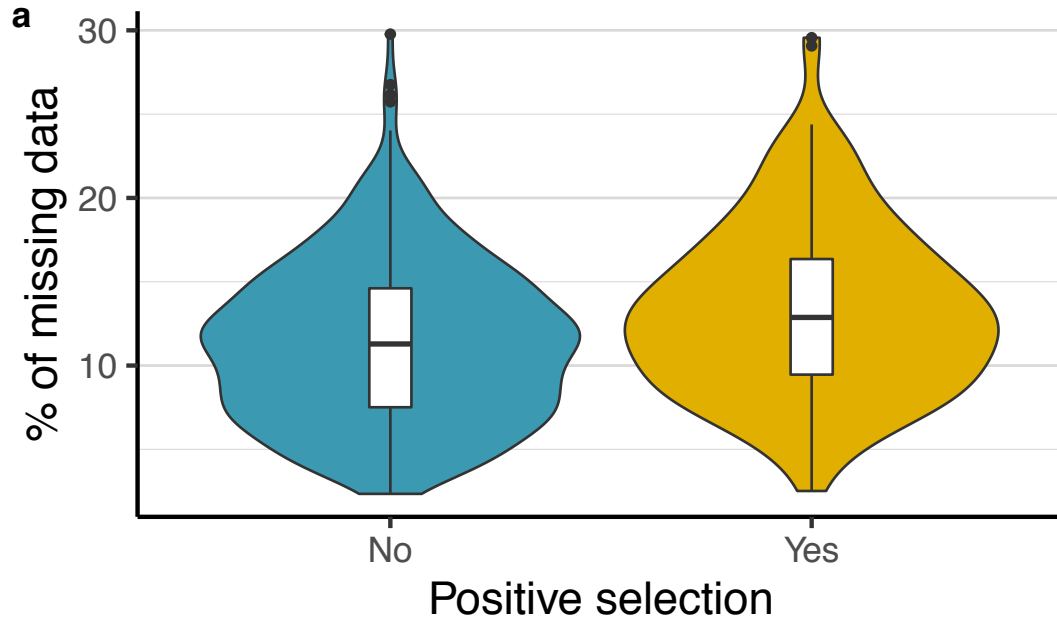
<i>Branch ID</i>	<i>Plant shift</i>	<i>Climate shift</i>	<i>Plant and climate shifts</i>
Branch1	Host-plant shift	No shift	Host shift only
Branch5	No shift	No shift	No shift
Branch6	No shift	No shift	No shift
Branch7	Host-plant shift	No shift	Host shift only
Branch8	No shift	No shift	No shift
Branch9	Host-plant shift	No shift	Host shift only
Branch10	No shift	No shift	No shift
Branch11	Host-plant shift	No shift	Host shift only
Branch12	No shift	No shift	No shift
Branch13	No shift	No shift	No shift
Branch14	Host-plant shift	Climate shift	Host and climate shifts
Branch15	Host-plant shift	Climate shift	Host and climate shifts
Branch16	No shift	No shift	No shift
Branch17	Host-plant shift	Climate shift	Host and climate shifts
Branch18	No shift	No shift	No shift
Branch19	Host-plant shift	No shift	Host shift only
Branch20	No shift	No shift	No shift
Branch21	Host-plant shift	No shift	Host shift only
Branch22	No shift	No shift	No shift
Branch23	Host-plant shift	No shift	Host shift only
Branch24	No shift	No shift	No shift
Branch25	Host-plant shift	Climate shift	Host and climate shifts
Branch26	No shift	No shift	No shift
Branch28	No shift	No shift	No shift
Branch29	Host-plant shift	No shift	Host shift only
Branch30	Host-plant shift	No shift	Host shift only
Branch31	Host-plant shift	Climate shift	Host and climate shifts
Branch32	No shift	No shift	No shift

Supplementary figure 19. a, Genus-level phylogenomic tree displaying branches with and without host-plant shifts, on which genome-wide analyses of molecular evolution are performed. **b**, Proportion of genes under positive selection ($dN/dS > 1$) for swallowtail lineages shifting to new host-plant families ($n=14$, green) or not ($n=14$, grey). **c**, Proportion of genes under positive selection for swallowtail lineages undergoing climate shifts ($n=5$, orange) or not ($n=23$, grey). **d**, Proportion of genes under positive selection for swallowtail lineages shifting to new host-plants ($n=9$, green), shifting both host-plant and climate ($n=5$, blue) or not ($n=14$, grey). The proportion of genes was estimated with *Dataset 1* (520 genes). This demonstrates genome-wide signatures of adaptations in swallowtail lineages shifting to new host-plant families. Genes under positive selection did not contain over- or under-represented functional GO categories (Supplementary data file 2). Wilcoxon rank-sum test: n.s. = not significant ($P > 0.05$), * = $P \leq 0.05$, ** = $P \leq 0.01$. Pictures and icons made by Fabien Condamine.

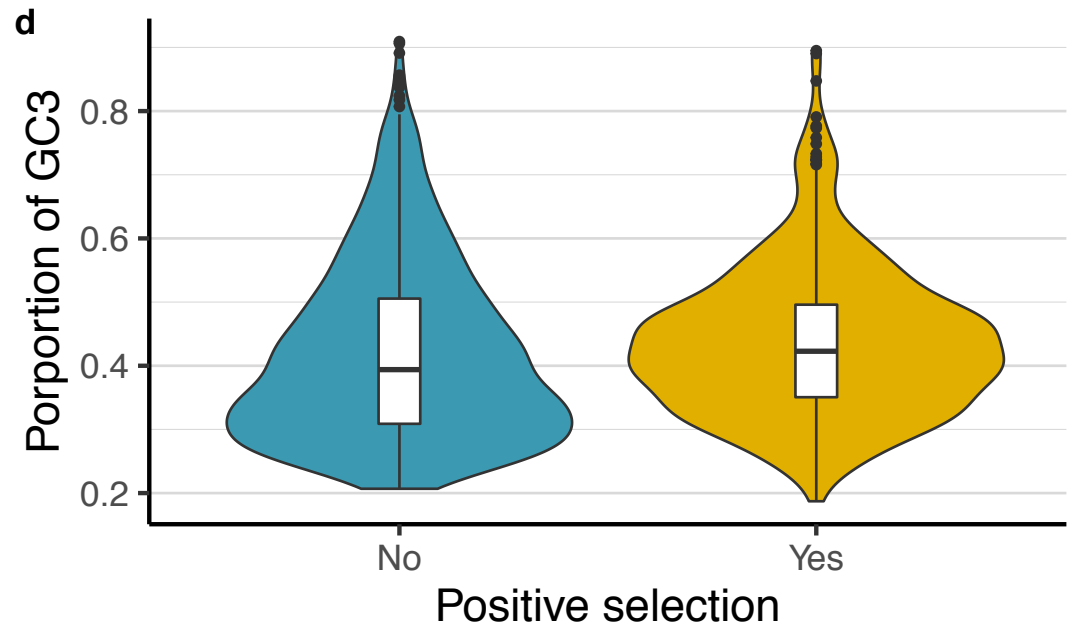
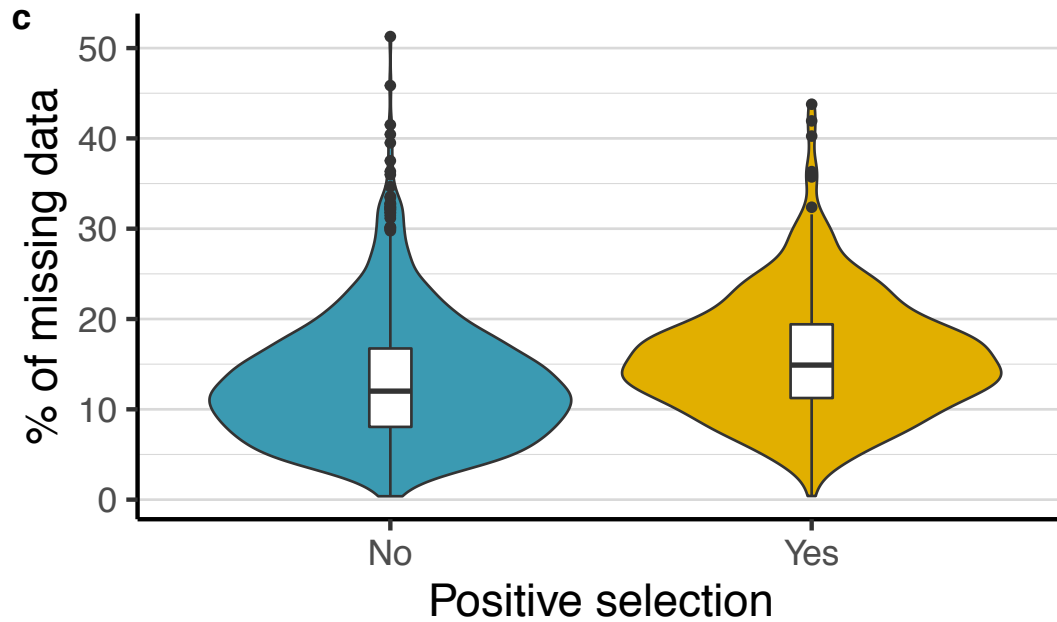


Supplementary figure 20. Violin plots of the percentage of missing data (“N” or “-”) and proportion of GC at third codon position (GC3) in alignment where positive selection have been detected (“Yes”) and positive selection have not been detected (“No”). Panels a and b are *Dataset 1* with 520 genes, and panels c and d are *Dataset 2* with 1,533 genes.

Dataset 1 (n = 520 genes)

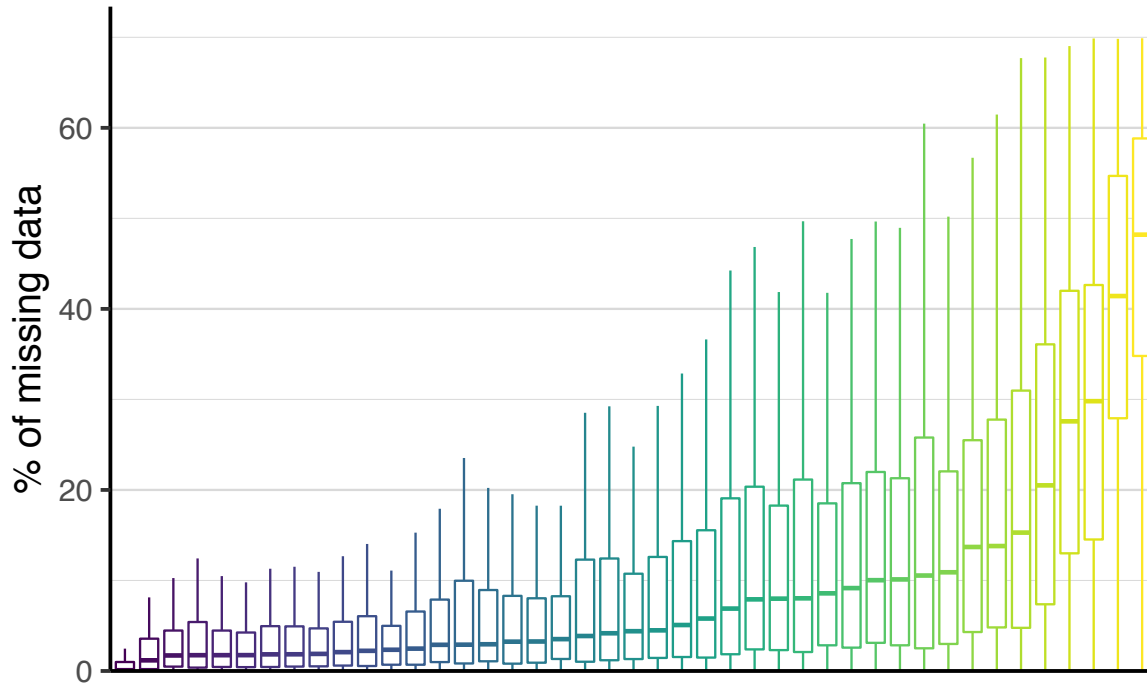


Dataset 2 (n = 1533 genes)

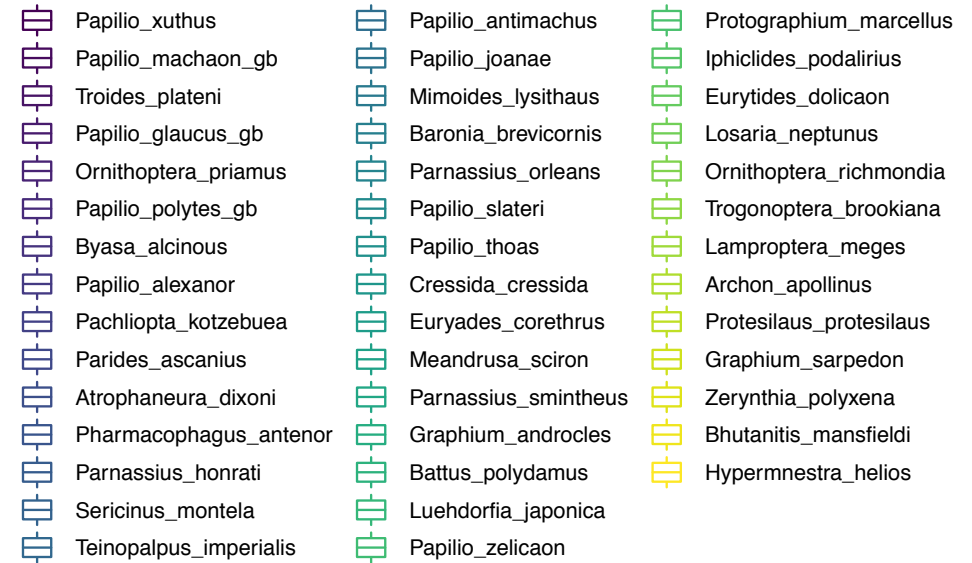


Supplementary figure 21. The percentage of missing data (“N” or “-”) per genes across species computed for *Dataset 1* and *Dataset 2*.

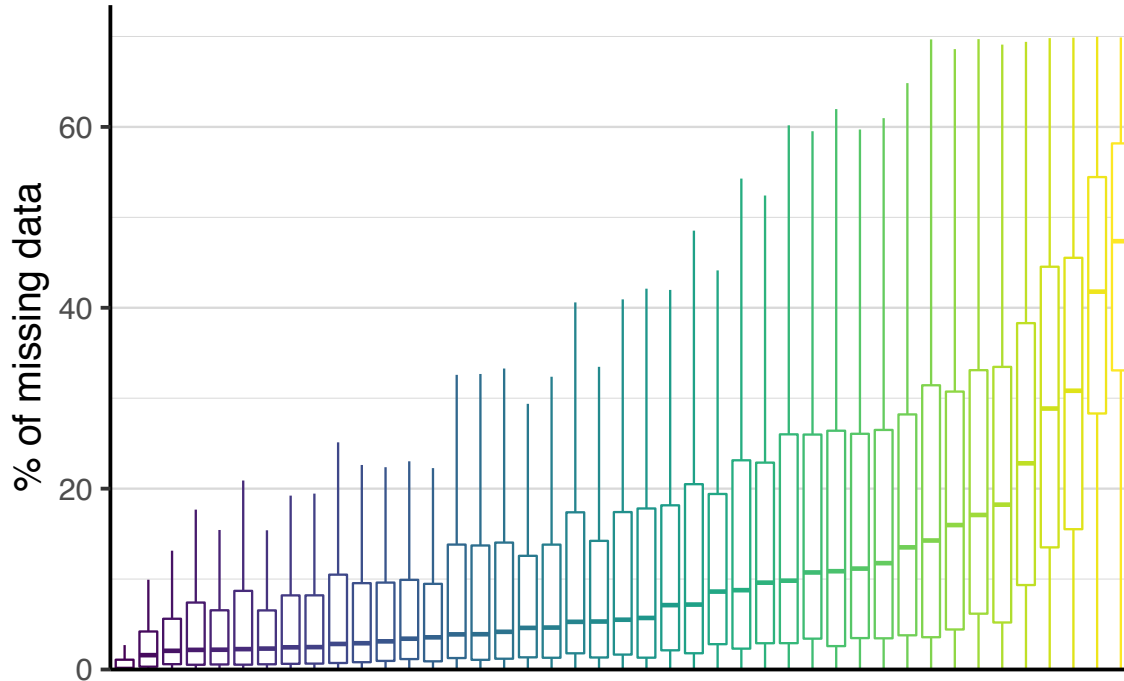
Dataset 1 (n = 520 genes)



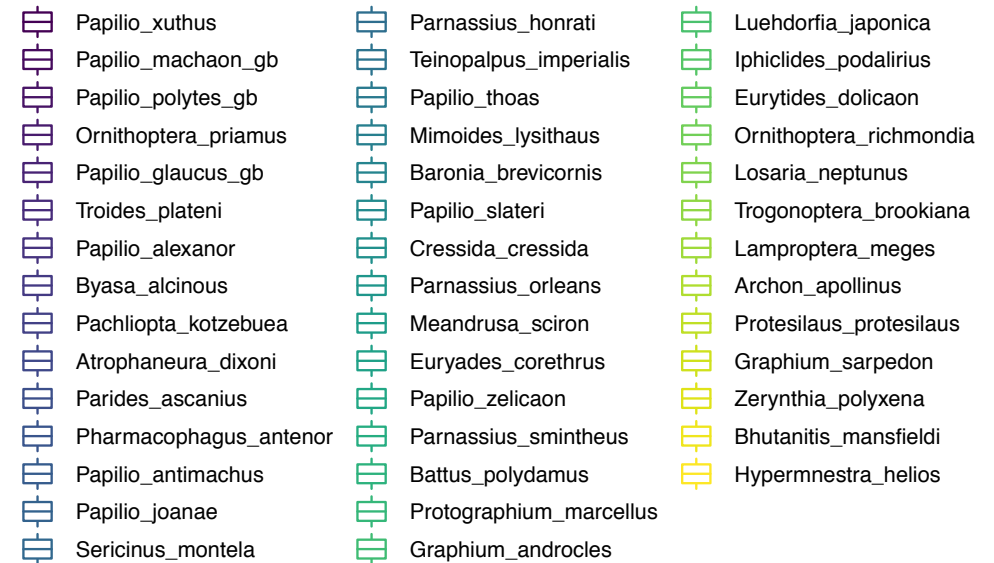
Species



Dataset 2 (n = 1533 genes)

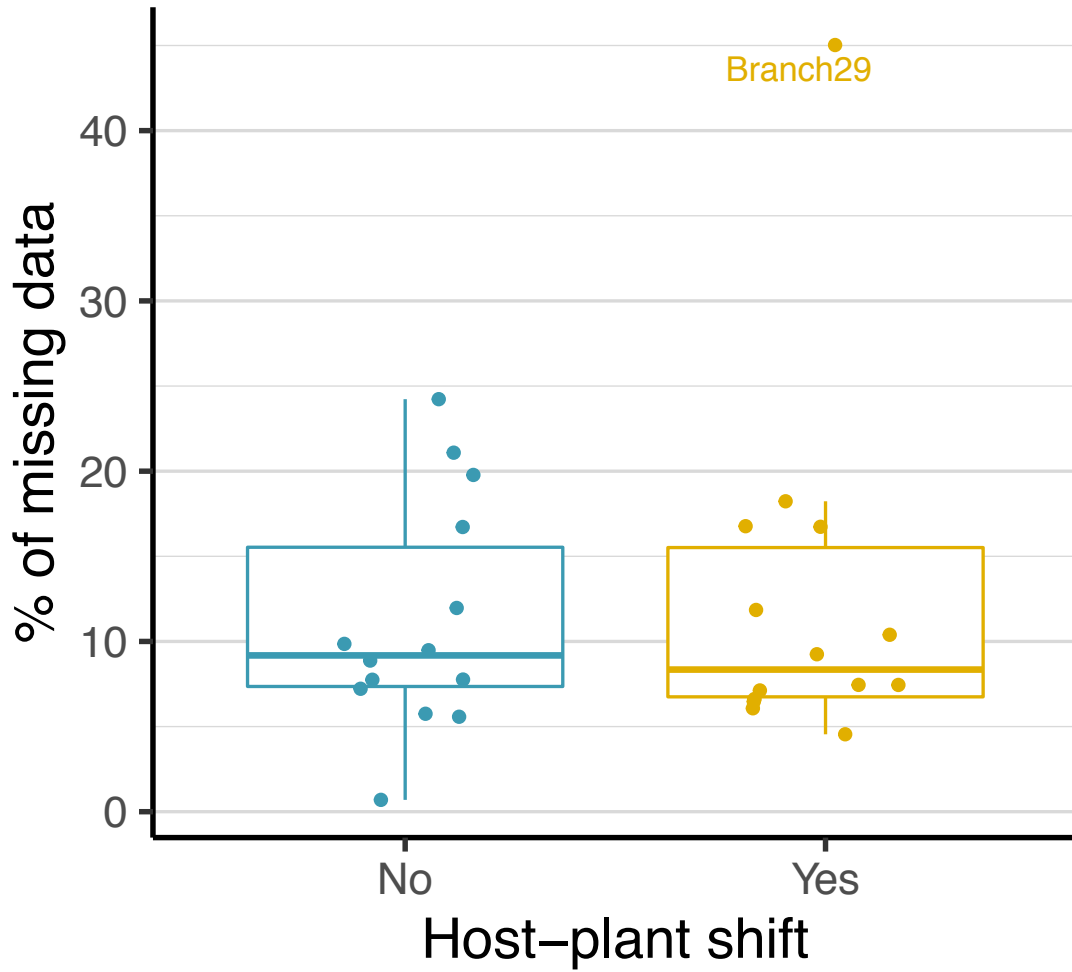


Species

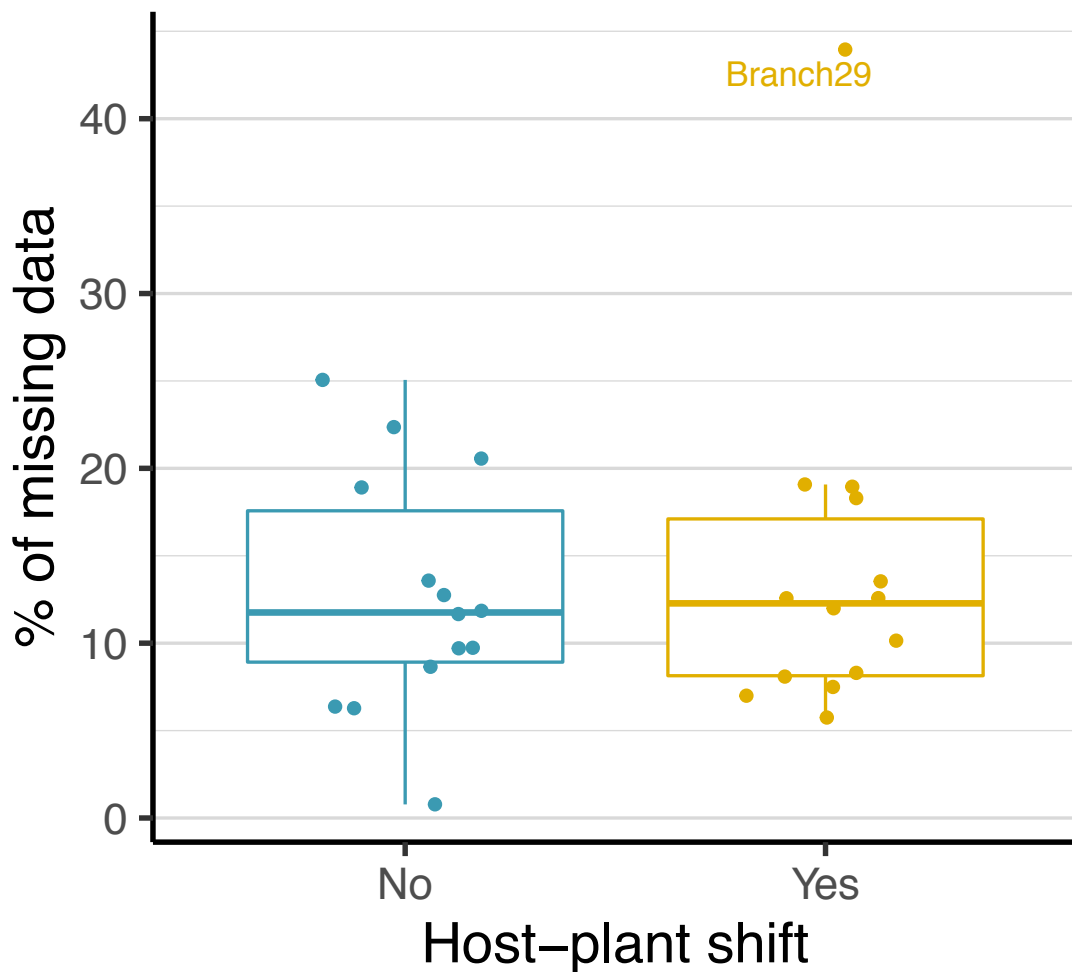


Supplementary figure 22. The percentage of missing data (“N” or “-”) per branch for the branches with (“Yes”, $n = 14$) and without (“No”, $n = 14$) host-plant shift. For a given branch, the percentage of missing data is the mean value of the species of a clade for which the branch is the root.

Dataset 1 (n = 520 genes)

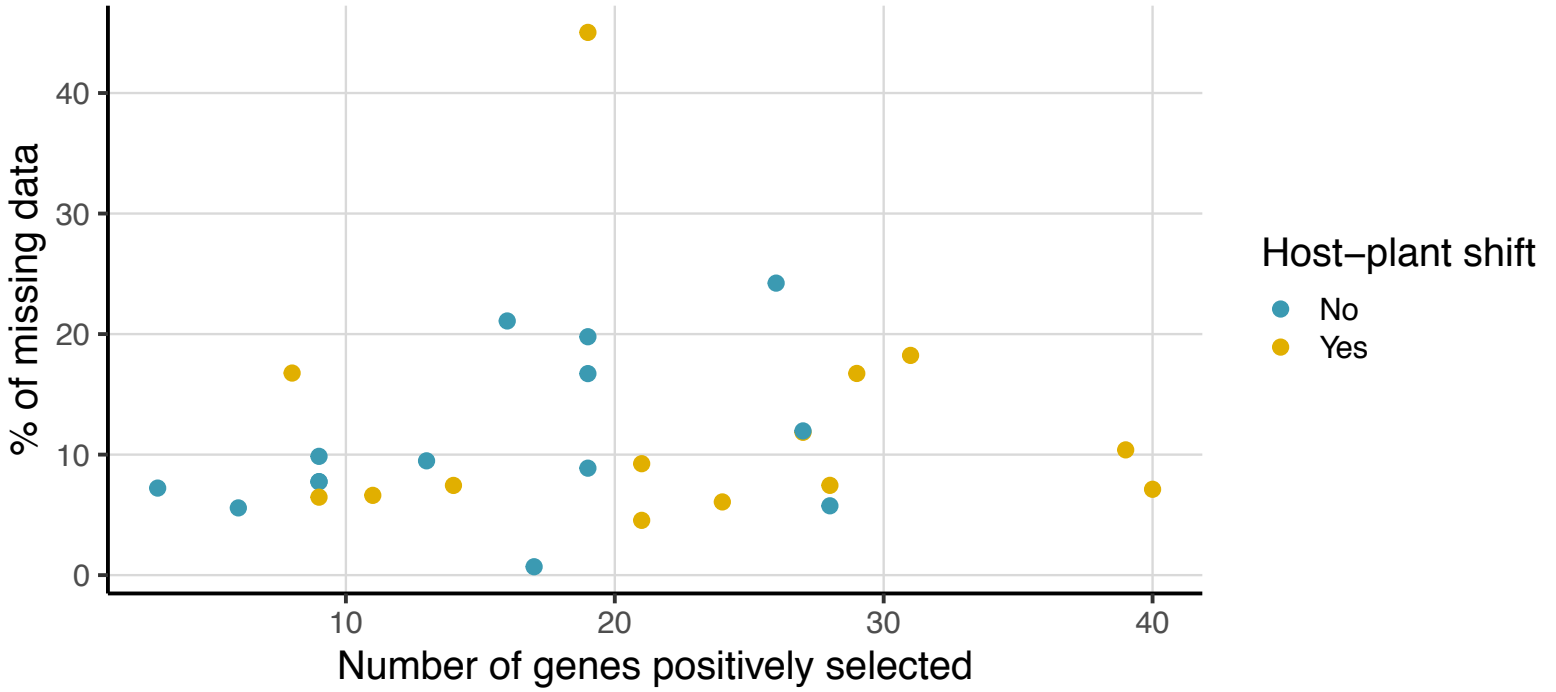


Dataset 2 (n = 1533 genes)

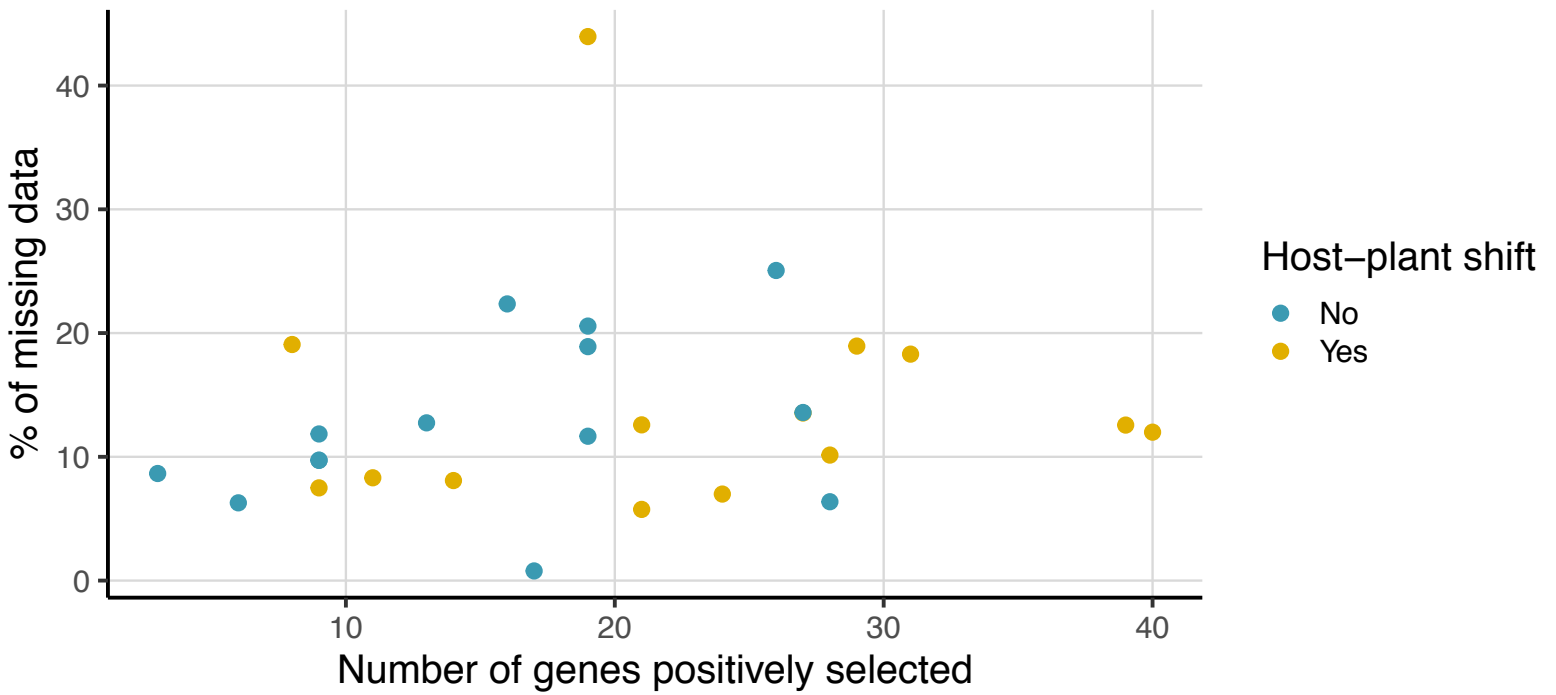


Supplementary figure 23. Relationship between the percentage of missing data (“N” or “-”) and the number of positively selected genes per branch. For a given branch, the percentage of missing data is the mean value of the species of a clade for which the branch is the root.

Dataset 1 (n = 520 genes)

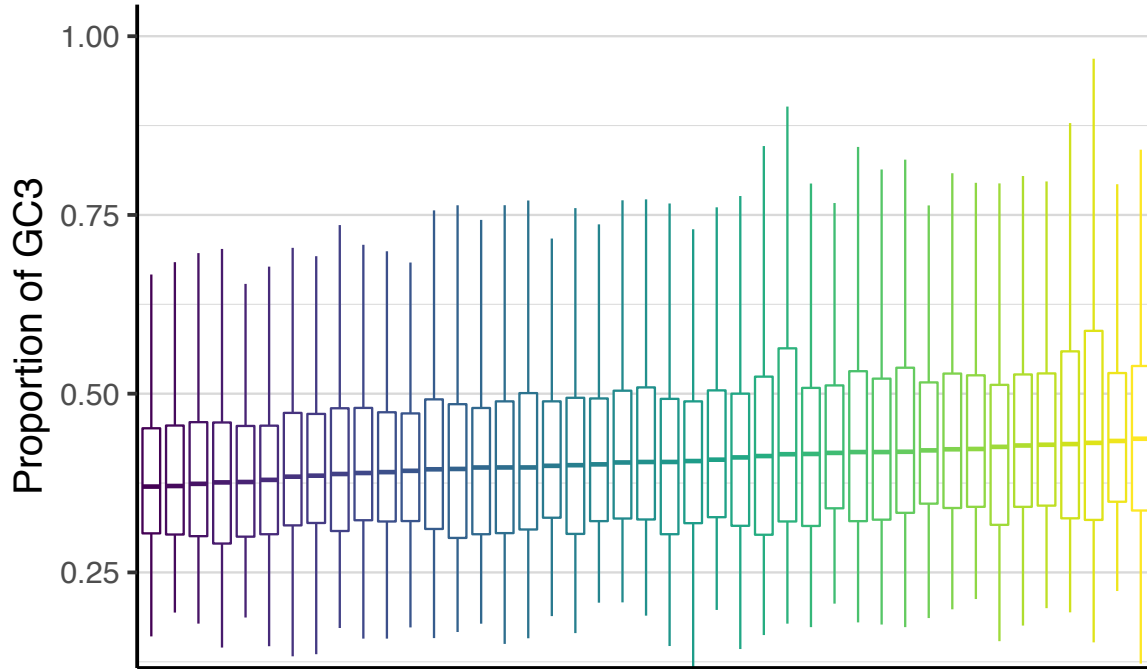


Dataset 2 (n = 1533 genes)



Supplementary figure 24. The percentage of GC at third codon position (GC3) per gene across species computed for *Dataset 1* and *Dataset 2*.

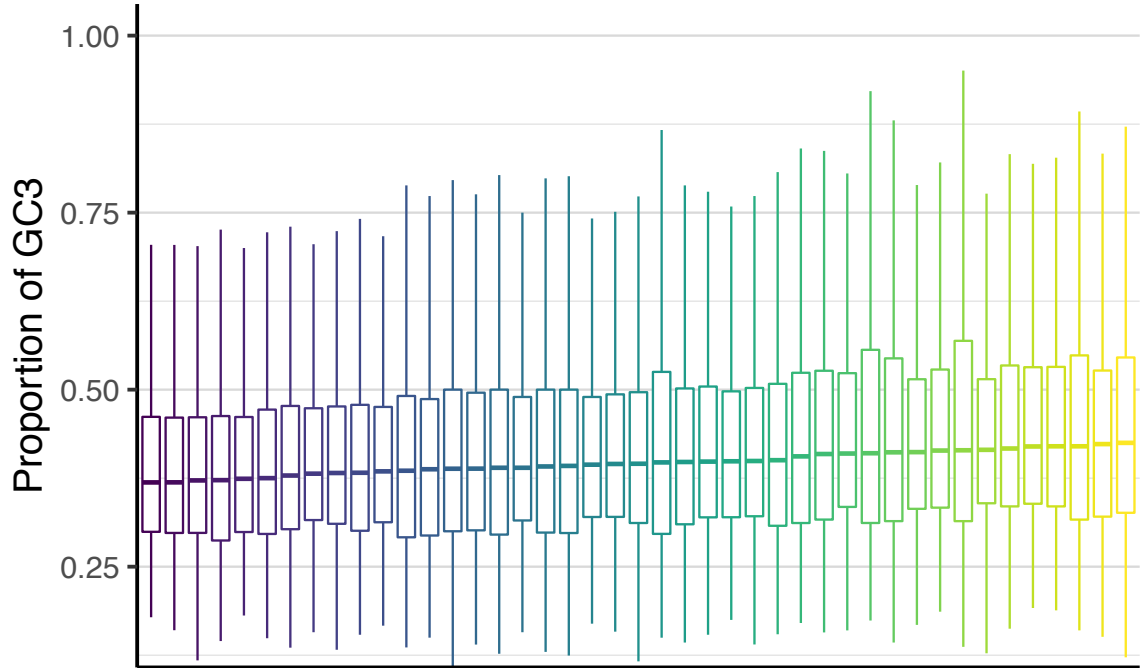
Dataset 1 (n = 520 genes)



Species

- | | | |
|------------------------|-------------------------|-------------------------|
| Parnassius_honrati | Ornithoptera_richmondia | Eurytides_doliceon |
| Parnassius_smintheus | Trogonoptera_brookiana | Graphium_androcles |
| Hypermnestra_helios | Papilio_polytes_gb | Protesilaus_protesilaus |
| Baronia_brevicornis | Troides_plateni | Meandrusa_sciron |
| Parnassius_orleans | Papilio_xuthus | Papilio_alexanor |
| Zerynthia_polyxena | Papilio_zelicaon | Lamproptera_meges |
| Cressida_cressida | Papilio_joanae | Losaria_neptunus |
| Bhutanitis_mansfieldi | Pachliopta_kotzebuea | Papilio_thoas |
| Sericinus_montela | Battus_polydamus | Papilio_slateri |
| Archon_apollinus | Papilio_machaon_gb | Protographium_marcellus |
| Luehdorfia_japonica | Atrophaneura_dixoni | Iphiclides_podalirius |
| Teinopalpus_imperialis | Pharmacophagus_antenor | Papilio_antimachus |
| Parides_ascanius | Mimoides_lysitheus | Graphium_sarpedon |
| Ornithoptera_priamus | Byasa_alcinous | |
| Euryades_corethrus | Papilio_glaucus_gb | |

Dataset 2 (n = 1533 genes)

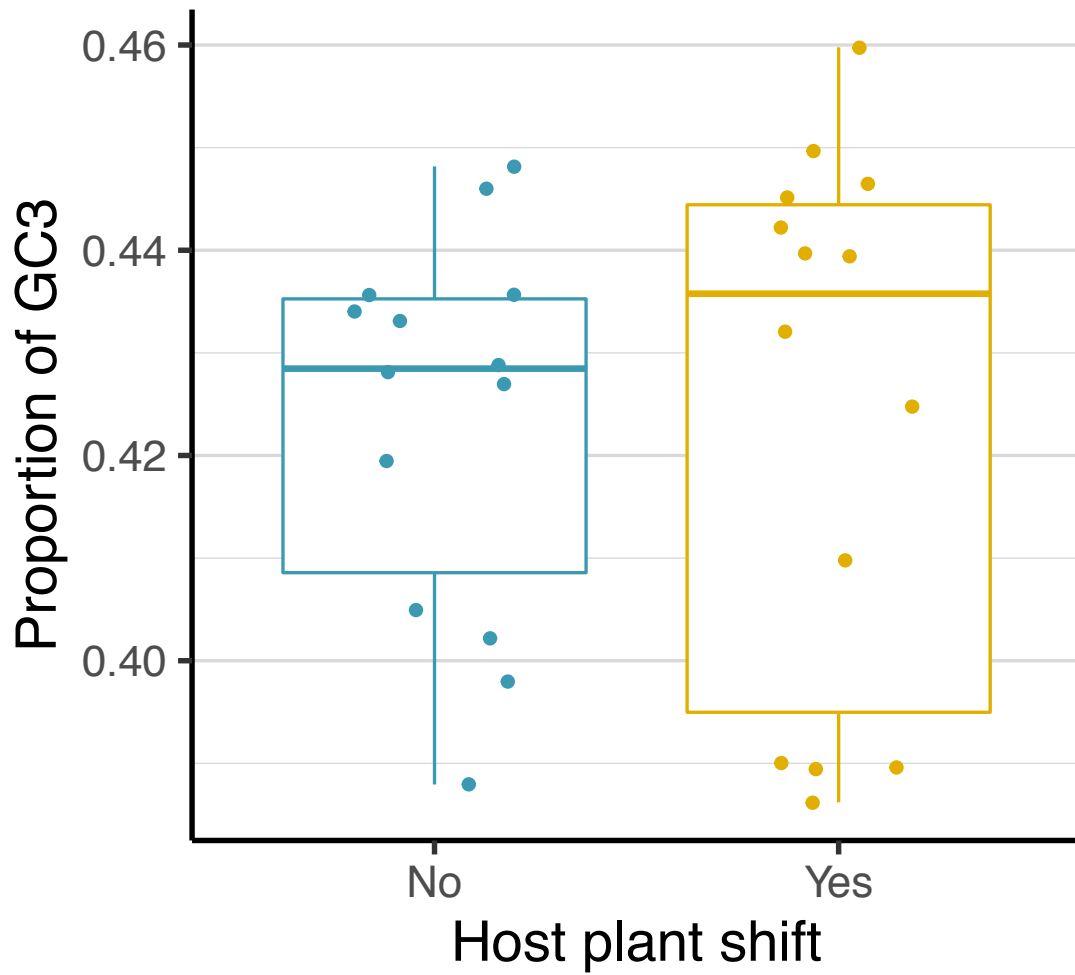


Species

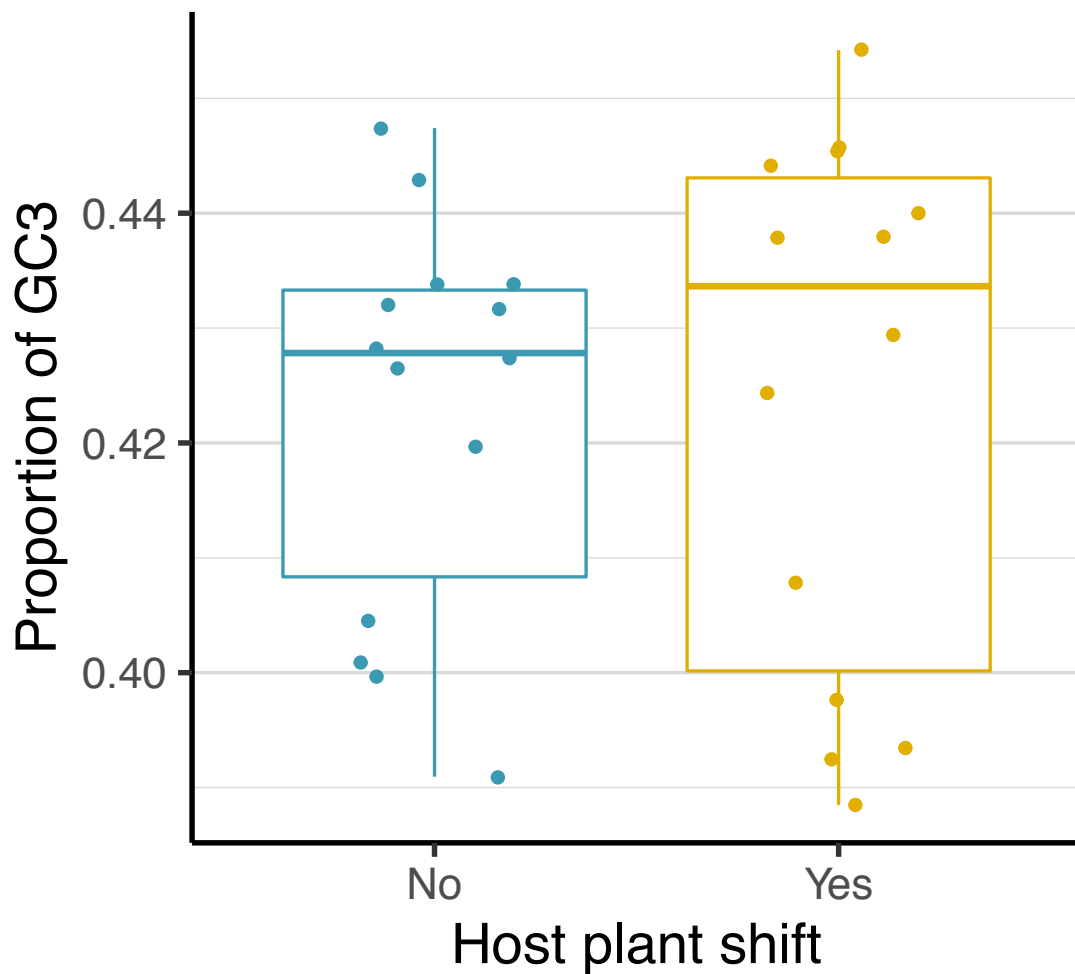
- | | | |
|------------------------|-------------------------|-------------------------|
| Parnassius_smintheus | Troides_plateni | Papilio_alexanor |
| Parnassius_honrati | Archon_apollinus | Mimoides_lysitheus |
| Zerynthia_polyxena | Pachliopta_kotzebuea | Eurytides_doliceon |
| Baronia_brevicornis | Ornithoptera_richmondia | Papilio_glaucus_gb |
| Parnassius_orleans | Papilio_polytes_gb | Lamproptera_meges |
| Hypermnestra_helios | Papilio_xuthus | Iphiclides_podalirius |
| Bhutanitis_mansfieldi | Battus_polydamus | Meandrusa_sciron |
| Luehdorfia_japonica | Pharmacophagus_antenor | Papilio_thoas |
| Cressida_cressida | Atrophaneura_dixoni | Papilio_antimachus |
| Sericinus_montela | Papilio_joanae | Papilio_slateri |
| Teinopalpus_imperialis | Papilio_zelicaon | Protographium_marcellus |
| Ornithoptera_priamus | Papilio_machaon_gb | Losaria_neptunus |
| Euryades_corethrus | Byasa_alcinous | Graphium_sarpedon |
| Trogonoptera_brookiana | Graphium_androcles | |
| Parides_ascanius | Protesilaus_protesilaus | |

Supplementary figure 25. The percentage of GC at third codon position (GC3) per branch for the branches with (“Yes”, $n = 14$) and without (“No”, $n = 14$) host-plant shift. For a given branch, the percentage of GC3 is the mean value of the species of a clade for which the branch is the root.

Dataset 1 (n = 520 genes)

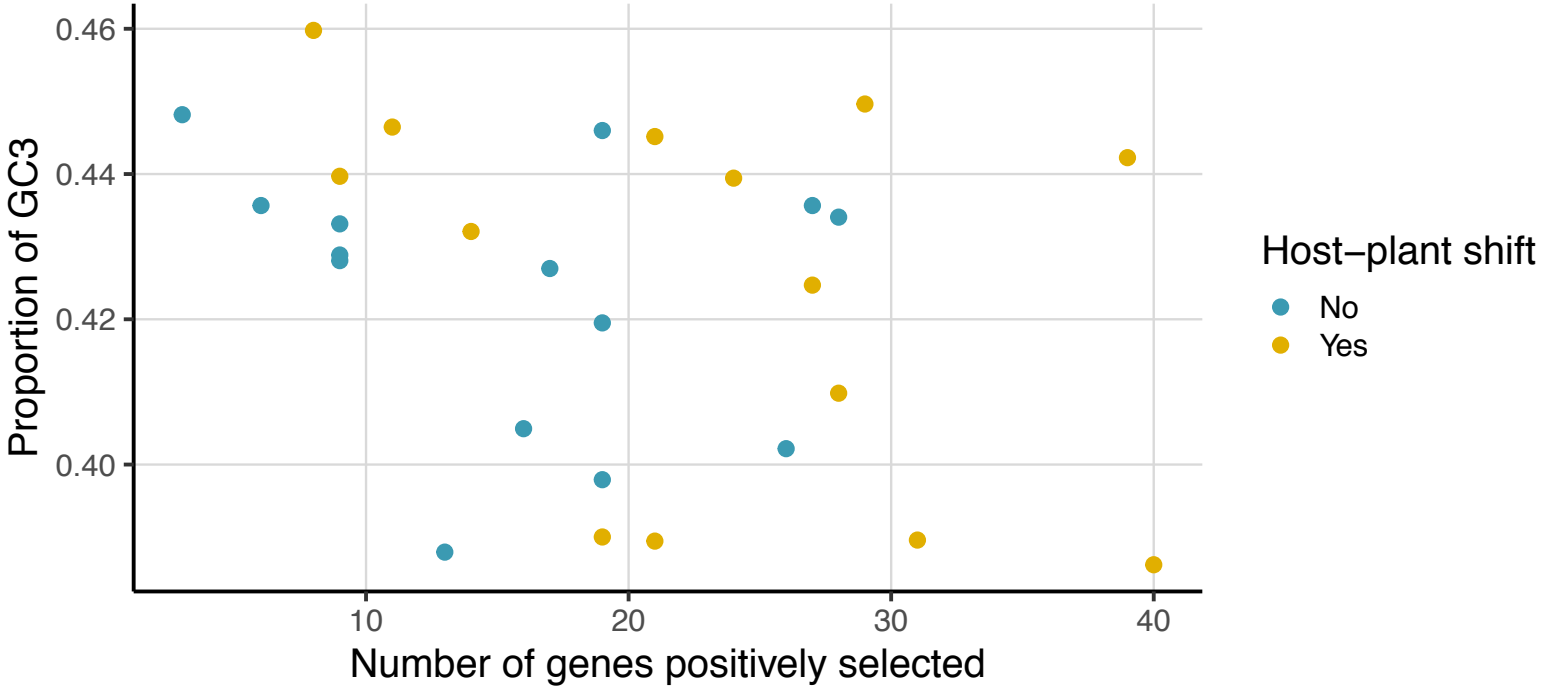


Dataset 2 (n = 1533 genes)

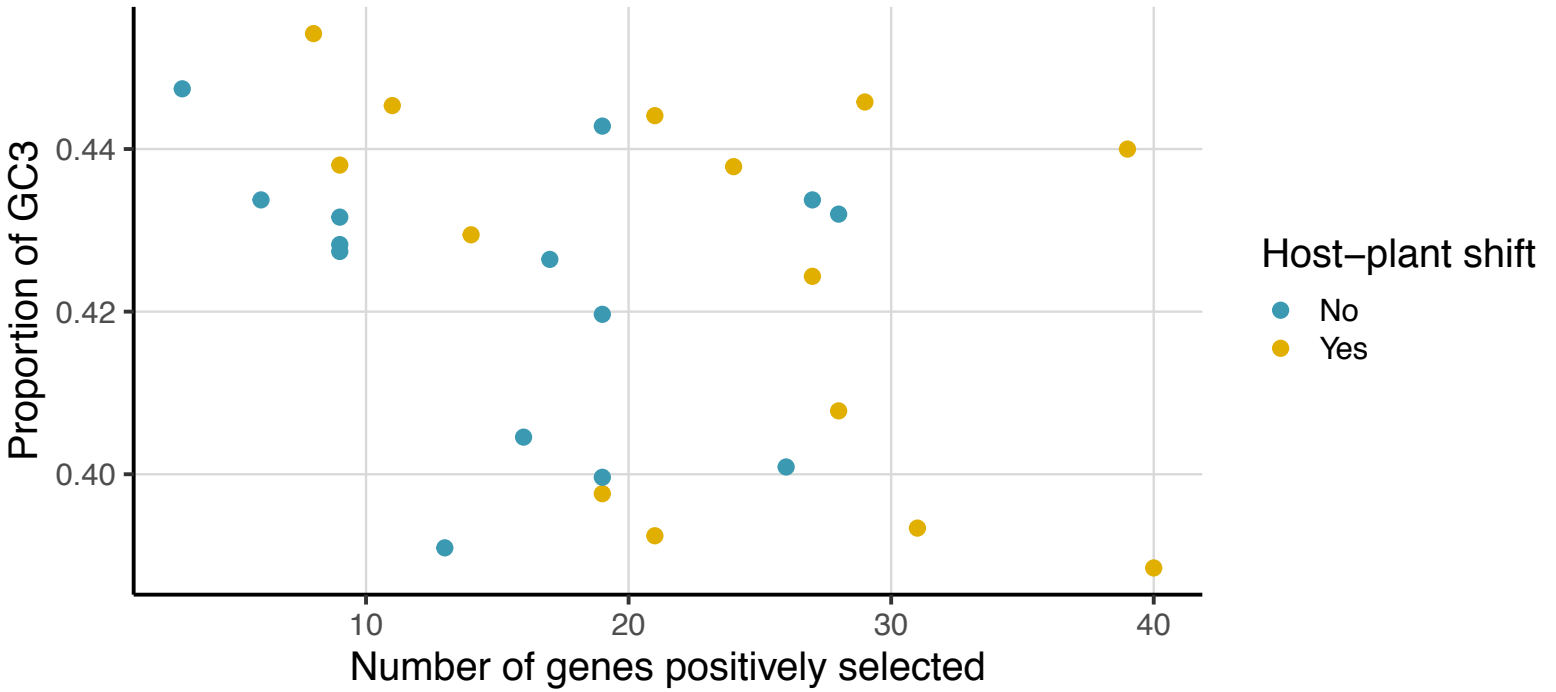


Supplementary figure 26. Relationship between the percentage of GC at third codon position (GC3) and the number of positively selected genes per branch. For a given branch, the percentage of GC3 is the mean value of the species of a clade for which the branch is the root.

Dataset 1 (n = 520 genes)



Dataset 2 (n = 1533 genes)



Supplementary Table 1. Results from analyses of diversification rates performed with LASER. For clades shifting to new host plants, net diversification rates are estimated based on their crown age and extant species diversity using the method of moments. Net diversification rates for shifting clades are higher than the global rates of the family, suggesting that shifting to a new host plant confer higher rates of species diversification. Estimates of expected clade size based on the global diversification rates and crown age of shifting clades show that four clades diversified significantly faster than background diversification rates of non-shifting clades.

Clades	Host plants	Crown age (Ma)	Extant species	Net diversification rate per Myr			Expected clade size			P value		
				$\epsilon=0$	$\epsilon=0.5$	$\epsilon=0.9$	$\epsilon=0$	$\epsilon=0.5$	$\epsilon=0.9$	$\epsilon=0$	$\epsilon=0.5$	$\epsilon=0.9$
Leptocircini	Annonaceae	40.16	132	0.1043	0.0973	0.0646	84.9	112.9	196.7	0.0588	0.1254	0.2899
<i>Papilio</i> subg. <i>Papilio</i>	Apiaceae	13.54	9	0.1111	0.0966	0.0394	9.1	11.8	27.0	0.2166	0.3023	0.5693
<i>Papilio</i> subg. <i>Pterourus</i> , <i>Chilasa</i> and <i>Agehana</i>	Lauraceae	27.35	37	0.1067	0.0970	0.0539	29.0	39.4	82.8	0.1108	0.1980	0.4436
<i>Papilio</i> other subgenera	Rutaceae	35.61	163	0.1236	0.1157	0.0785	57.9	77.9	146.0	0.0023	0.0194	0.1262
<i>Parnassius</i> subg. <i>Parnassius</i>	Crassulaceae	10.77	19	0.2091	0.1866	0.0908	7.2	9.1	20.4	0.0012	0.0145	0.1812
<i>Parnassius</i> other subgenera	Papaveraceae	15.89	35	0.1944	0.1776	0.1016	11.1	14.7	33.6	0.0001	0.0020	0.0873
Papilionidae as a whole	-	67.28	570	0.0840	0.0798	0.0596	-	-	-	-	-	-

Supplementary Table 2. Summary of CodeML analyses for the Dataset 2 (1,533 genes). The ratio of genes under positive selection is reported for each branch. The columns “Plant shift”, “Env. shift” and “Plant/Env. shift” report whether a shift and what type of shift occurred or not along each branch. The columns with “recovering the focal branch” indicate that the gene trees of this dataset recovered the focal branch as in the species tree.

Branch ID	Nb. of genes	Genes recovering the focal branch	Genes under positive selection	Genes under positive selection recovering the focal branch	% positive selection	% positive selection (recovering the focal branch)	Plant/Env. shift	Plant shift	Env. shift
Branch1	1533	1533	69	69	4.5010	4.5010	Host shift only	Host-plant shift	No shift
Branch5	1533	254	42	11	2.7397	4.3307	No shift	No shift	No shift
Branch6	1533	270	19	6	1.2394	2.2222	No shift	No shift	No shift
Branch7	1517	795	81	53	5.3395	6.6667	Host shift only	Host-plant shift	No shift
Branch8	1533	373	20	9	1.3046	2.4129	No shift	No shift	No shift
Branch9	1483	618	19	15	1.2812	2.4272	Host shift only	Host-plant shift	No shift
Branch10	1455	652	43	24	2.9553	3.6810	No shift	No shift	No shift
Branch11	1483	975	59	42	3.9784	4.3077	Host shift only	Host-plant shift	No shift
Branch12	1474	254	13	2	0.8820	0.7874	No shift	No shift	No shift
Branch13	1518	887	59	37	3.8867	4.1714	No shift	No shift	No shift
Branch14	1472	1026	42	25	2.8533	2.4366	Host and climate shifts	Host-plant shift	Climate shift
Branch15	1436	614	25	15	1.7409	2.4430	Host and climate shifts	Host-plant shift	Climate shift
Branch16	1530	1530	45	45	2.9412	2.9412	No shift	No shift	No shift
Branch17	1521	1521	56	56	3.6818	3.6818	Host and climate shifts	Host-plant shift	Climate shift
Branch18	1521	331	17	2	1.1177	0.6042	No shift	No shift	No shift
Branch19	1533	1533	104	104	6.7841	6.7841	Host shift only	Host-plant shift	No shift
Branch20	1533	617	65	38	4.2401	6.1588	No shift	No shift	No shift
Branch21	952	492	55	29	5.7773	5.8943	Host shift only	Host-plant shift	No shift
Branch22	1533	471	38	13	2.4788	2.7601	No shift	No shift	No shift
Branch23	1533	1533	80	80	5.2185	5.2185	Host shift only	Host-plant shift	No shift
Branch24	1533	314	22	11	1.4351	3.5032	No shift	No shift	No shift
Branch25	1325	958	61	43	4.6038	4.4885	Host and climate shifts	Host-plant shift	Climate shift
Branch26	1248	864	32	23	2.5641	2.6620	No shift	No shift	No shift
Branch28	1343	634	52	25	3.8719	3.9432	No shift	No shift	No shift
Branch29	952	952	30	30	3.1513	3.1513	Host shift only	Host-plant shift	No shift
Branch30	1483	1483	79	79	5.3270	5.3270	Host shift only	Host-plant shift	No shift
Branch31	1349	269	21	8	1.5567	2.9740	Host and climate shifts	Host-plant shift	Climate shift
Branch32	1330	321	32	10	2.4060	3.1153	No shift	No shift	No shift

Supplementary Table 3. Summary of diversification models in BAMM compared across a gradient of values for the Poisson process governing the number of rate shifts. The analyses show that a scenario with no shift of diversification best explained the macroevolution of Papilionidae. Although it might suggest that the Poisson prior has some effect on the analyses, it is important to note that all shifts are in common between the analyses. Based on the effective sample size (ESS) and the highest posterior distribution per number of shifts for the Poisson rate prior, we selected the model with a Poisson prior of 1. In addition this model did not favour a model with more shifts.

Poisson prior	ESS $\log L$	ESS <i>Nb. shifts</i>	<i>Posterior distribution of the number of shifts</i>							
			0	1	2	3	4	5	6	7
1	403.5	501.0	0.60*	0.28	0.091	0.026	0.007	0.002	<0.001	<0.001
5	398.5	462.8	0.38*	0.31	0.17	0.083	0.031	0.014	0.005	<0.001
10	385.6	282.9	0.34*	0.3	0.19	0.093	0.045	0.019	0.006	0.004

Note: for each model, the asterisk () denotes the highest posterior probability for the number of shifts.*

Supplementary Table 4. Comparison of the gene-tree inferences with the species tree to define the control and focal branches. The ‘Branch recovered’ column reports the number of gene trees (gene trees were inferred in Allio *et al.* 2020) showing the focal branch as monophyletic (i.e. including all genera for the focal clade), and the ‘Branch not recovered’ column indicates the number of gene trees for which the focal branch is not recovered. Overall, gene trees are more often in agreement with the species tree for the branches with a host-plant shift than without shift ($P = 0.03$, Wilcoxon-rank test).

Branch	Nb. genes	Branch not recovered	Branch recovered	Ratio	Plant/Env. shift	Plant shift	Env. shift
branch1	1528	665	863	0.77057	Host shift only	Host-plant shift	No shift
branch5	1528	1274	254	5.01575	No shift	No shift	No shift
branch6	1528	1258	270	4.65926	No shift	No shift	No shift
branch7	1528	725	803	0.90286	Host shift only	Host-plant shift	No shift
branch8	1528	1155	373	3.09651	No shift	No shift	No shift
branch9	1480	862	618	1.39482	Host shift only	Host-plant shift	No shift
branch10	1451	799	652	1.22546	No shift	No shift	No shift
branch11	1480	505	975	0.51795	Host shift only	Host-plant shift	No shift
branch12	1469	1215	254	4.78346	No shift	No shift	No shift
branch13	1513	626	887	0.70575	No shift	No shift	No shift
branch14	1467	441	1026	0.42982	Host and climate shifts	Host-plant shift	Climate shift
branch15	1431	817	614	1.33062	Host and climate shifts	Host-plant shift	Climate shift
branch18	1516	1185	331	3.58006	No shift	No shift	No shift
branch20	1528	911	617	1.47650	No shift	No shift	No shift
branch21	952	460	492	0.93496	Host shift only	Host-plant shift	No shift
branch22	1528	1057	471	2.24416	No shift	No shift	No shift
branch24	1528	1214	314	3.86624	No shift	No shift	No shift
branch25	1322	364	958	0.37996	Host and climate shifts	Host-plant shift	Climate shift
branch26	1319	383	936	0.40919	No shift	No shift	No shift
branch28	1341	707	634	1.11514	No shift	No shift	No shift
branch31	1347	1078	269	4.00743	Host and climate shifts	Host-plant shift	Climate shift
branch32	1328	1007	321	3.13707	No shift	No shift	No shift