**Supplementary Table 1. Sample information and sequencing statistics**

| Sample | Taxon | Morph | Sex | Collecting location | Raw Reads (Gb) | Filtered Reads (Gb) | Mapped rate (%) | Genotype calls (Qual≥30) | Mean Depth (Qual≥30) |
|---|---|---|---|---|---|---|---|---|---|
| PR345 | *Papilio Polytes* | | male | lab reared | 4.76 | 4.66 | 90.43 | 36236144 | 15.85 |
| PR346 | *Papilio Polytes* | | male | lab reared | 2.40 | 2.35 | 91.07 | 35233509 | 8.01 |
| PR347 | *Papilio Polytes* | | male | lab reared | 3.81 | 3.73 | 90.81 | 36107778 | 12.93 |
| PR348 | *Papilio Polytes* | | male | lab reared | 3.60 | 3.52 | 90.21 | 35719296 | 12.46 |
| PR349 | *Papilio Polytes* | | male | lab reared | 4.55 | 4.45 | 90.95 | 36441209 | 15.01 |
| PR350 | *Papilio Polytes* | *cyrus* | female | lab reared | 2.56 | 2.51 | 90.54 | 35464909 | 8.94 |
| PR351 | *Papilio Polytes* | *cyrus* | female | lab reared | 2.99 | 2.93 | 90.56 | 35858619 | 10.26 |
| PR352 | *Papilio Polytes* | *cyrus* | female | lab reared | 2.71 | 2.66 | 90.38 | 35405401 | 9.41 |
| PR353 | *Papilio Polytes* | *cyrus* | female | lab reared | 2.97 | 2.90 | 90.71 | 35591372 | 10.07 |
| PR354 | *Papilio Polytes* | *cyrus* | female | lab reared | 3.08 | 3.01 | 90.27 | 35602801 | 10.59 |
| PR355 | *Papilio Polytes* | *cyrus* | female | lab reared | 1.80 | 1.74 | 90.41 | 33665981 | 6.44 |
| PR356 | *Papilio Polytes* | *cyrus* | female | lab reared | 3.33 | 3.23 | 81.07 | 35339553 | 10.37 |
| PR357 | *Papilio Polytes* | *cyrus* | female | lab reared | 2.90 | 2.81 | 90.67 | 35516315 | 10.08 |
| PR358 | *Papilio Polytes* | *cyrus* | female | lab reared | 2.44 | 2.38 | 80.62 | 34431188 | 7.74 |
| PR359 | *Papilio Polytes* | *cyrus* | female | lab reared | 2.05 | 1.98 | 90.59 | 34486129 | 7.16 |
| PR360 | *Papilio Polytes* | | male | lab reared | 2.02 | 1.83 | 54.79 | 32745479 | 4.16 |
| PR361 | *Papilio Polytes* | | male | lab reared | 3.30 | 3.20 | 90.51 | 35457278 | 11.54 |
| PR362 | *Papilio Polytes* | | male | lab reared | 2.00 | 1.94 | 90.99 | 34230653 | 7.05 |
| PR363 | *Papilio Polytes* | | male | lab reared | 2.33 | 2.25 | 91.2 | 35041142 | 7.99 |
| PR364 | *Papilio Polytes* | | male | lab reared | 1.61 | 1.56 | 83.43 | 33986445 | 5.28 |
| PR365 | *Papilio Polytes* | *polytes* | female | lab reared | 1.68 | 1.62 | 91.18 | 34199491 | 5.85 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PR366 | *Papilio Polytes* | *polytes* | female | lab reared | 2.09 | 2.02 | 86.17 | 34361994 | 7.19 |
| PR367 | *Papilio Polytes* | *polytes* | female | lab reared | 2.88 | 2.79 | 90.76 | 35732553 | 10.08 |
| PR368 | *Papilio Polytes* | *polytes* | female | lab reared | 1.98 | 1.92 | 91.15 | 34772512 | 6.83 |
| PR369 | *Papilio Polytes* | *polytes* | female | lab reared | 1.99 | 1.92 | 90.88 | 34852610 | 6.99 |
| PR370 | *Papilio Polytes* | *polytes* | female | lab reared | 2.16 | 2.09 | 90.79 | 35056121 | 7.50 |
| PR371 | *Papilio Polytes* | *polytes* | female | lab reared | 2.01 | 1.94 | 91.05 | 34995597 | 6.94 |
| PR372 | *Papilio Polytes* | *polytes* | female | lab reared | 2.90 | 2.81 | 90.58 | 35507931 | 10.03 |
| PR373 | *Papilio Polytes* | *polytes* | female | lab reared | 2.18 | 2.11 | 90.14 | 34345076 | 7.70 |
| PR374 | *Papilio Polytes* | *polytes* | female | lab reared | 2.83 | 2.73 | 90.46 | 35249732 | 9.72 |
| pol_t6 | *Papilio Polytes* | *theseus* | female | lab reared | 8.44 | 7.85 | 89.59 | 37440311 | 23.77 |
| pol_t7 | *Papilio Polytes* | *theseus* | female | lab reared | 2.74 | 2.66 | 89.87 | 36097594 | 8.84 |
| timor1 | *Papilio Polytes* | *polytes* | female | Timor, Indonesia | 3.47 | 3.41 | 35.07 | 32279952 | 4.92 |
| timor2 | *Papilio Polytes* | *cyrus* | female | Timor, Indonesia | 2.78 | 2.69 | 83.94 | 37707690 | 8.83 |
| timor3 | *Papilio Polytes* | *cyrus* | female | Timor, Indonesia | 3.56 | 3.49 | 25.54 | 28239839 | 3.82 |
| landak1 | *Papilio Polytes* | *theseus* | female | Landak, Indonesia | 3.76 | 3.56 | 91.82 | 38555717 | 12.32 |
| lombok1 | *Papilio Polytes* | modified *theseus* | female | Lombok, Indonesia | 5.51 | 5.36 | 92.77 | 38685234 | 17.32 |
| lombok2 | *Papilio Polytes* | modified *theseus* | female | Lombok, Indonesia | 5.18 | 4.98 | 83.32 | 38774944 | 14.87 |
| lombok3 | *Papilio Polytes* | *theseus* | female | Lombok, Indonesia | 3.99 | 3.81 | 92.81 | 38644420 | 13.62 |
| lombok4 | *Papilio Polytes* | *theseus* | female | Lombok, Indonesia | 3.92 | 3.76 | 86.56 | 38170099 | 11.81 |
| sumatra1 | *Papilio Polytes* | | male | Sumatra, Indonesia | 5.75 | 5.63 | 23.22 | 32831474 | 4.98 |
| sumatra2 | *Papilio Polytes* | | male | Sumatra, Indonesia | 2.21 | 2.09 | 95.1 | 37927337 | 8.24 |
| jambi1 | *Papilio Polytes* | *theseus* | female | Jambi, Indonesia | 3.06 | 2.92 | 78.73 | 37794856 | 9.31 |
| bali1 | *Papilio Polytes* | *theseus* | female | Bali, Indonesia | 3.35 | 3.25 | 90.86 | 36880721 | 10.37 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| romulus1 | *Papilio Polytes* | *romulus* | female | Bangarupalyam Mandal, India | 8.73 | 8.02 | 91.14 | 39316440 | 29.22 |
| phestus1 | *Papilio phestus* | | male | Buka, Indonesia | 3.94 | 3.59 | 32.68 | 24285031 | 3.14 |
| phestus2 | *Papilio phestus* | | male | Buka, Indonesia | 3.61 | 2.74 | 60.44 | 31393030 | 5.84 |
| phestus3 | *Papilio phestus* | | male | Buka, Indonesia | 12.24 | 10.38 | 32.51 | 34577294 | 8.82 |
| phestus4 | *Papilio phestus* | | male | Buka, Indonesia | 2.15 | 1.44 | 81.61 | 30199792 | 4.37 |
| arfak1 | *Papilio ambrax* | | female | Arfak, Indonesia | 3.05 | 2.65 | 77.9 | 25730404 | 6.05 |
| arfak2 | *Papilio ambrax* | | female | Arfak, Indonesia | 7.41 | 6.91 | 60.74 | 29512953 | 10.07 |
| arfak3 | *Papilio ambrax* | | female | Arfak, Indonesia | 5.66 | 5.24 | 84.55 | 35013294 | 13.31 |
| arfak4 | *Papilio ambrax* | | female | Arfak, Indonesia | 4.84 | 4.48 | 78.5 | 32887779 | 10.66 |
| timika1 | *Papilio ambrax* | | female | Timika, Indonesia | 1.98 | 1.49 | 87.69 | 28929884 | 4.64 |
| timika2 | *Papilio ambrax* | | female | Timika, Indonesia | 3.43 | 2.48 | 78.15 | 31387988 | 5.89 |
| timika3 | *Papilio ambrax* | | female | Timika, Indonesia | 3.75 | 2.85 | 86.58 | 33186526 | 7.42 |
| timika4 | *Papilio ambrax* | | female | Timika, Indonesia | 3.39 | 2.21 | 87.26 | 30287624 | 5.84 |
| protenor1 | *Papilio protenor* | | female | Guilin, China | 5.36 | 4.40 | 74.93 | 31709831 | 12.65 |
| protenor2 | *Papilio protenor* | | female | Guilin, China | 6.41 | 5.53 | 80.93 | 32590680 | 16.72 |
| protenor3 | *Papilio protenor* | | male | Guilin, China | 6.52 | 5.51 | 56.6 | 31140423 | 11.85 |
| protenor4 | *Papilio protenor* | | male | Guilin, China | 11.83 | 10.44 | 76.57 | 33512723 | 28.49 |

**Supplementary Table 2. Individual genotypes of different species**

|                            | MM | Mm | mm |
|----------------------------|----|----|----|
| *P. polytes polytes*       | 1  | 10 | 2  |
| *P. polytes alphenor*      | 15 | 2  | 15 |
| *P. ambrax* and *P. phestus* | 12 | 0  | 0  |

MM denotes homozygous mimetic

mm denotes homozygous non-mimetic

Mm denotes heterozygous
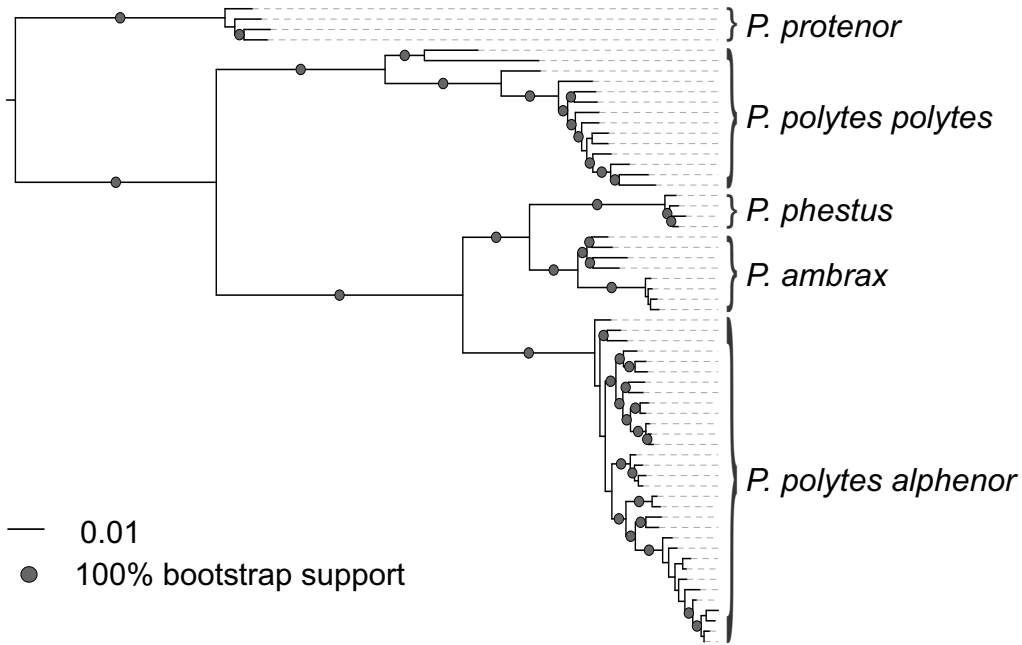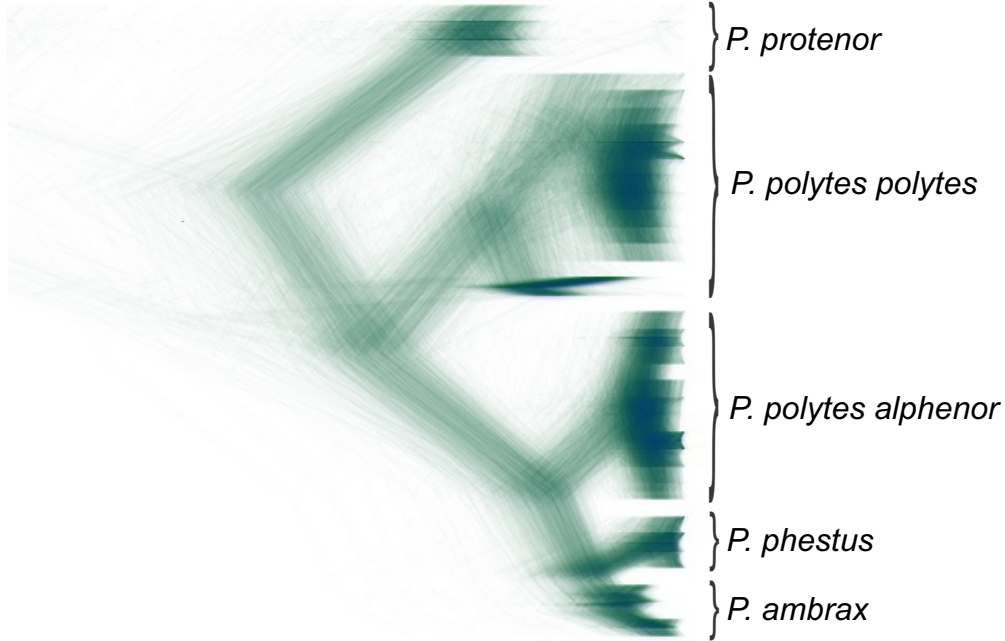
**Supplementary Figure 1. Genome-wide phylogeny of *Papilio* butterflies.**
(a) A maximum-likelihood phylogenetic tree based on 40.2 million genome-wide SNPs. (b) DensiTree of the polytes group produced by overlaying ML trees from 2,134 non-overlapping 100 kbp windows across the genome. 86% of the windows produce an identical tree as the full genome-wide tree, and all trees, except 1, place *P. polytes alphenor* as the sister lineage to *ambrax/phestus*.
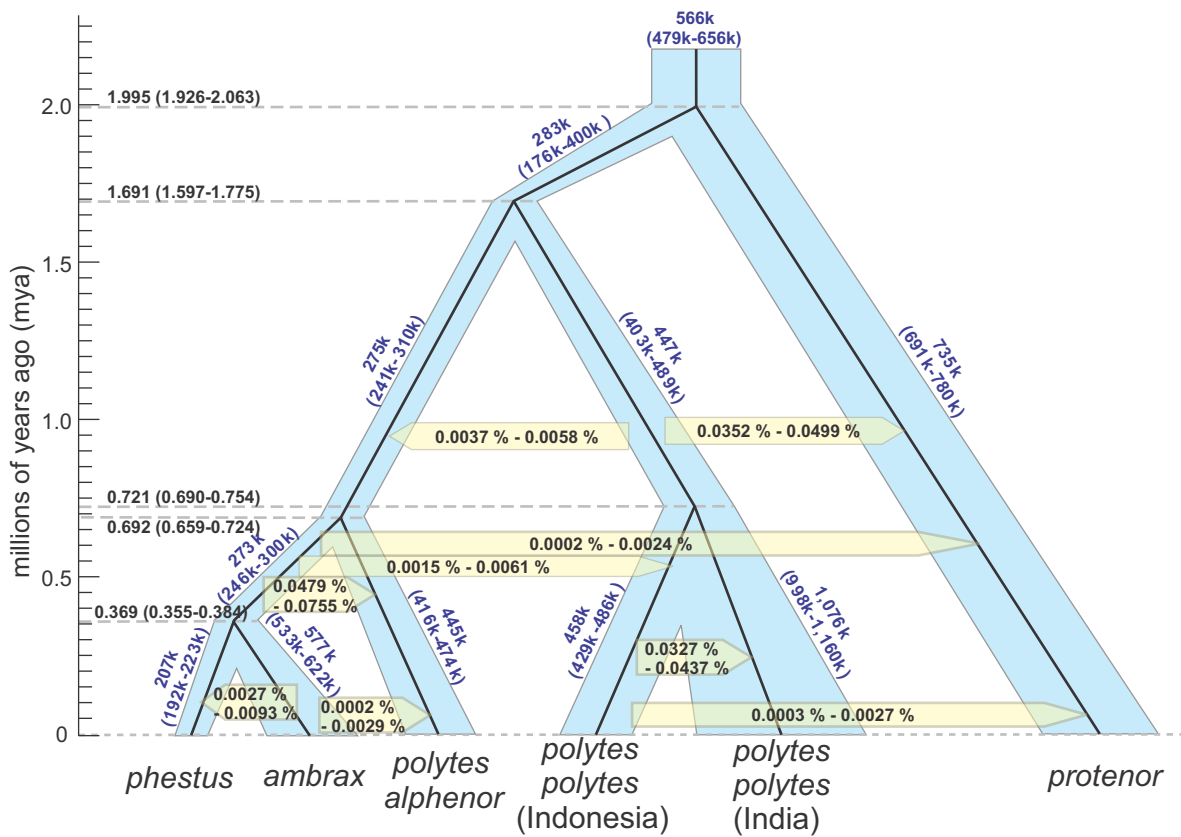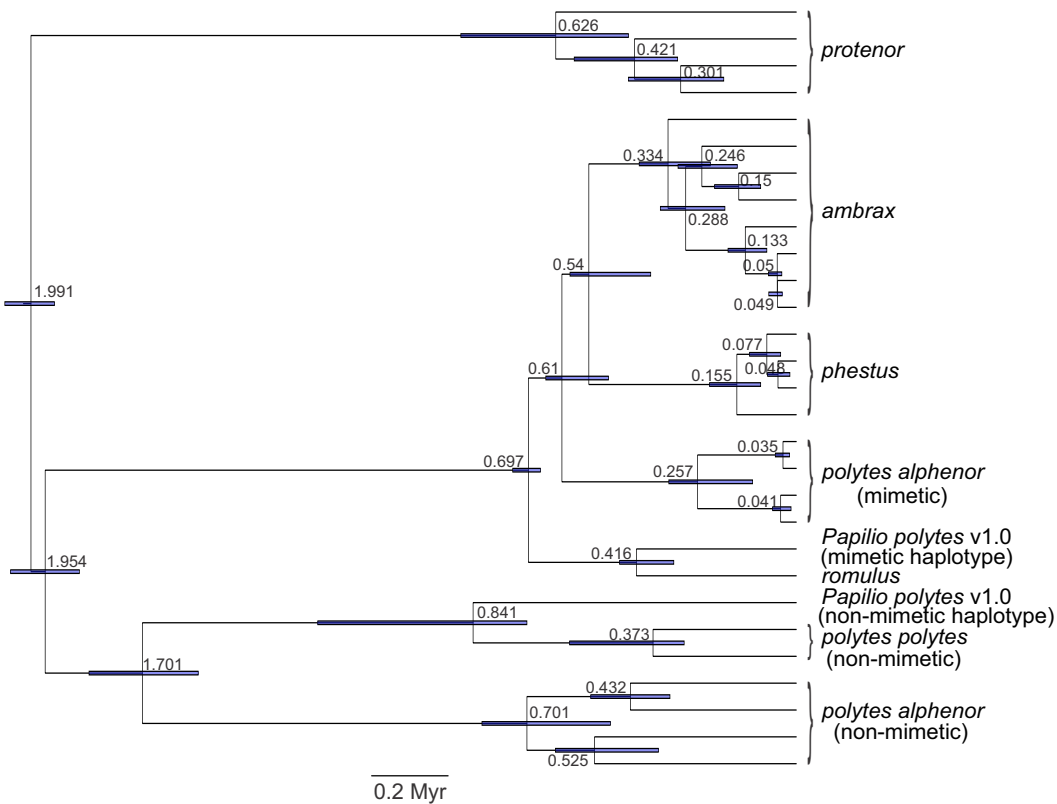
**Supplementary Figure 2. Timing diversification events in the *Papilio polytes* group.**
(a) Divergence times, effective population sizes, and migration rates were inferred among *polytes* group taxa using G-PhoCS. Branch widths are proportional to population size and dashed lines indicate divergence times. Parameter estimates are shown along with 95% Bayesian credible intervals. (b) Maximum-likelihood tree of *doublesex* haplotypes, calibrated using the G-PhoCS estimate of 1.995 ± 0.068 My ago for the common ancestor between *P. protenor* and the *polytes* group. Numbers are in million years and blue bars represent 95% confidence intervals. Comparison of (a) and (b) suggests that divergence between mimetic and non-mimetic *dsx* haplotypes (1.954 My ago) occurred before the radiation of the *polytes* group (1.691 My ago). Data are presented as mean ± SD.
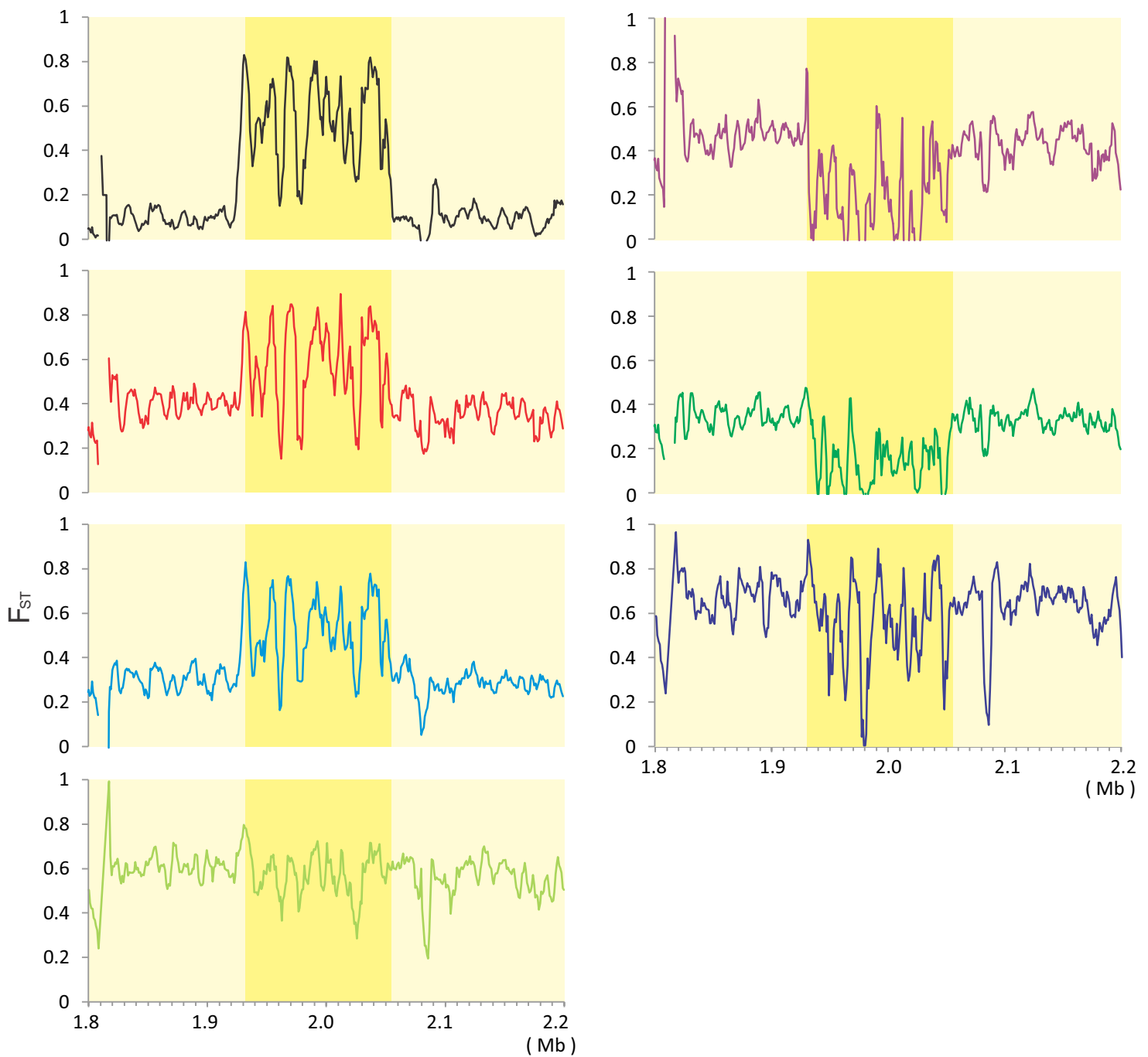
**Supplementary Figure 3. Genetic differentiation (F$_{ST}$) along the *dsx* gene region.**
F$_{ST}$ scans were performed using a 5 kbp window size to infer the breakpoints of the *dsx* inversion in various species comparisons. The entire 130 kbp *dsx* inversion region is colored in darker yellow. Clear deviations, coinciding with inversion breakpoints, are found in the same locations in comparisons between *P. polytes alphenor* non-mimetic and *P. polytes alphenor* mimetic, between *P. polytes alphenor* non-mimetic and *P. ambrax*, between *P. polytes alphenor* non-mimetic and *P. phestus*, between *P. polytes alphenor* mimetic and *P. polytes polytes* mimetic and between *P. polytes alphenor* non-mimetic and *P. polytes polytes* non-mimetic.
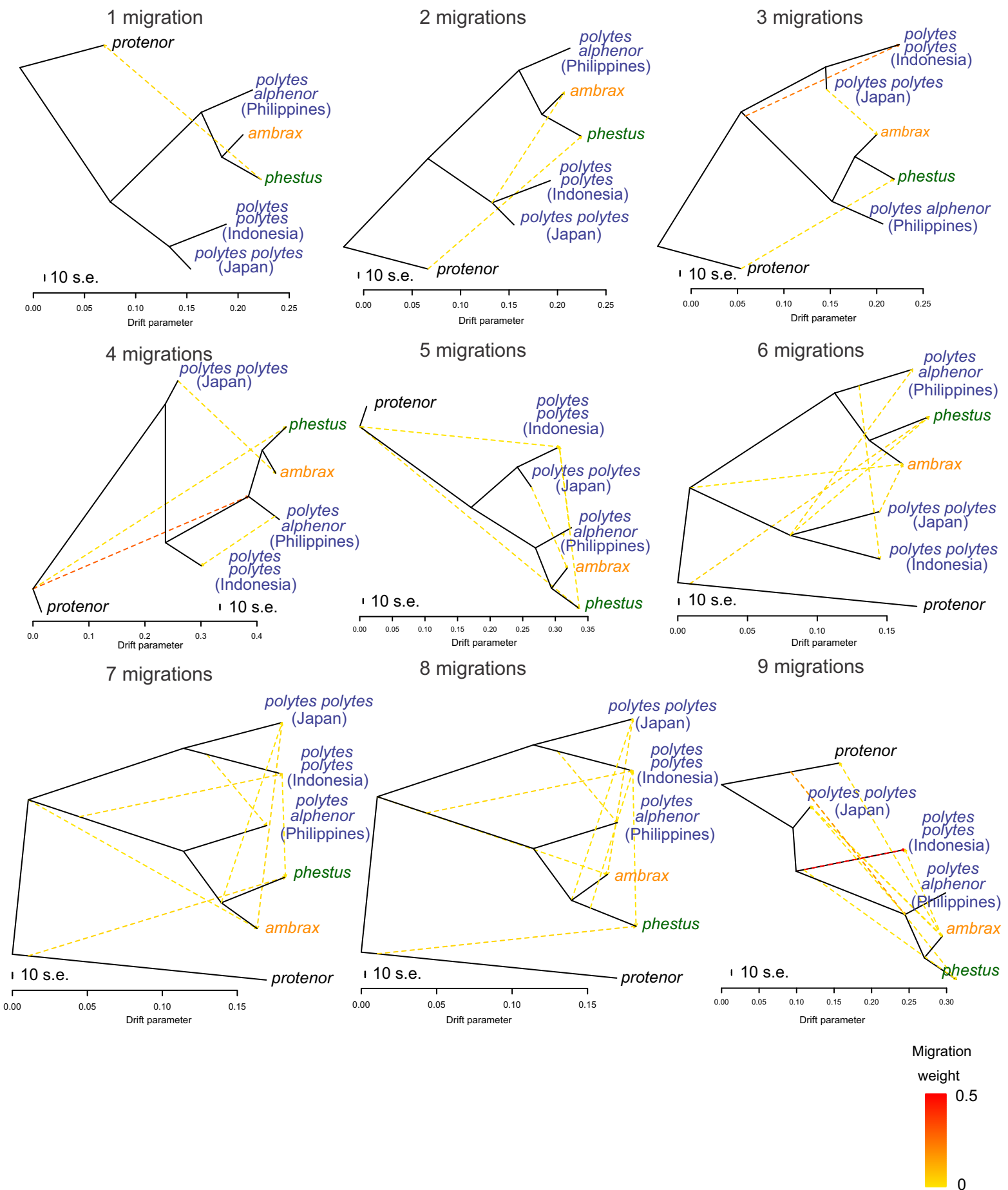
**Supplementary Figure 4. Inferences of relationships and migration among *Papilio* species using Treemix.** In each case, a maximum-likelihood tree was inferred among five species/populations in the *polytes* group, as well as the outgroup species *P. protenor*, based on genome-wide SNP allele frequency data. Migration was explored by assuming 1 to 9 migration edges.
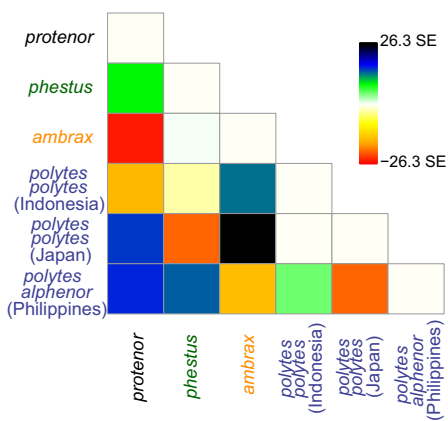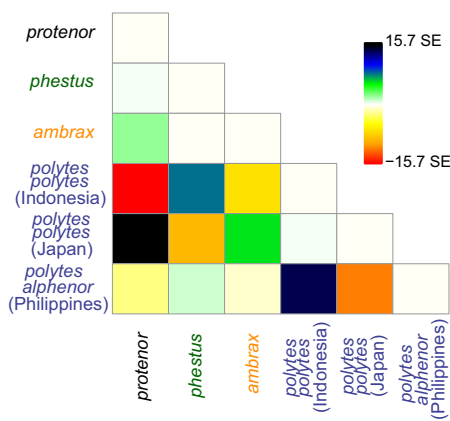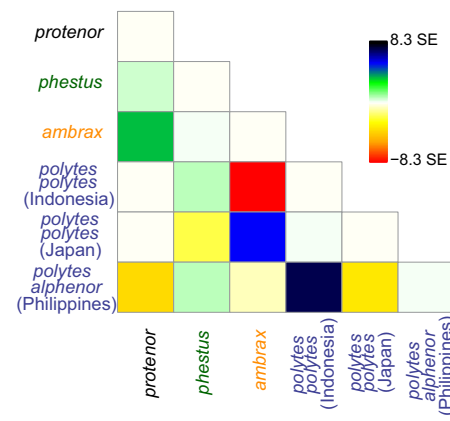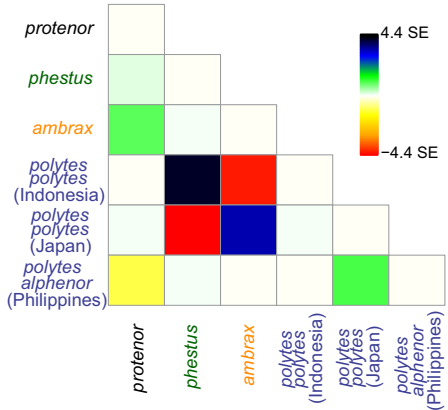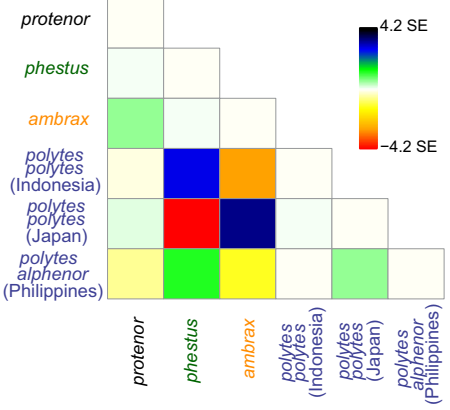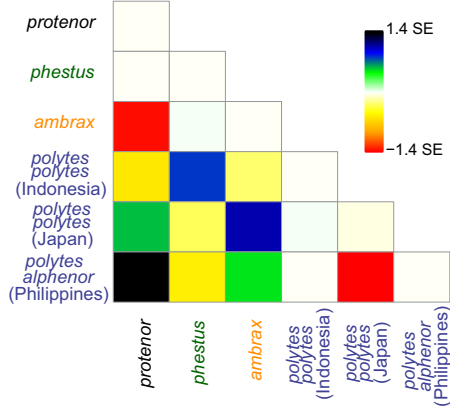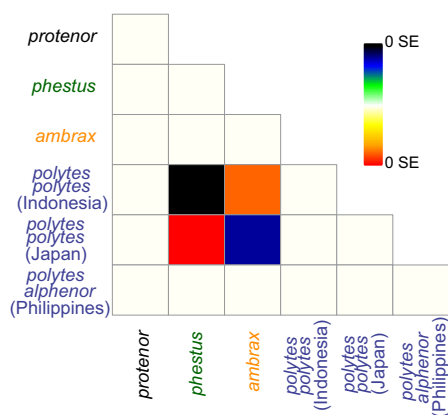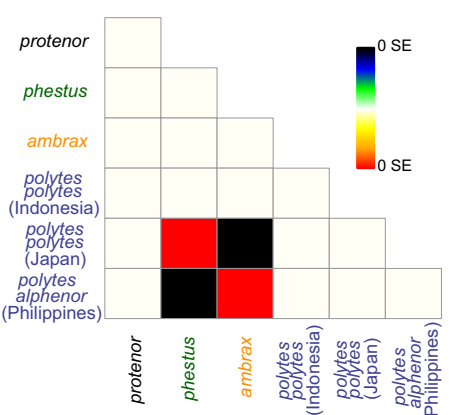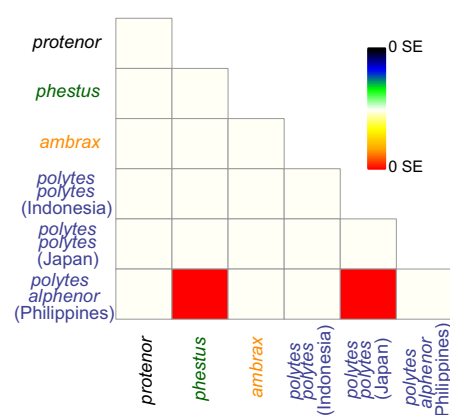
**Supplementary Figure 5. Residue fit from the trees generated using Treemix.**
Each residue fit matrix is generated by dividing the residual covariance of pairwise populations by the average standard error using Treemix. Residues above zero indicate pairs of populations that are closer to each other and could be candidates for migration events. Migration was explored by assuming 1 to 9 migration edges.
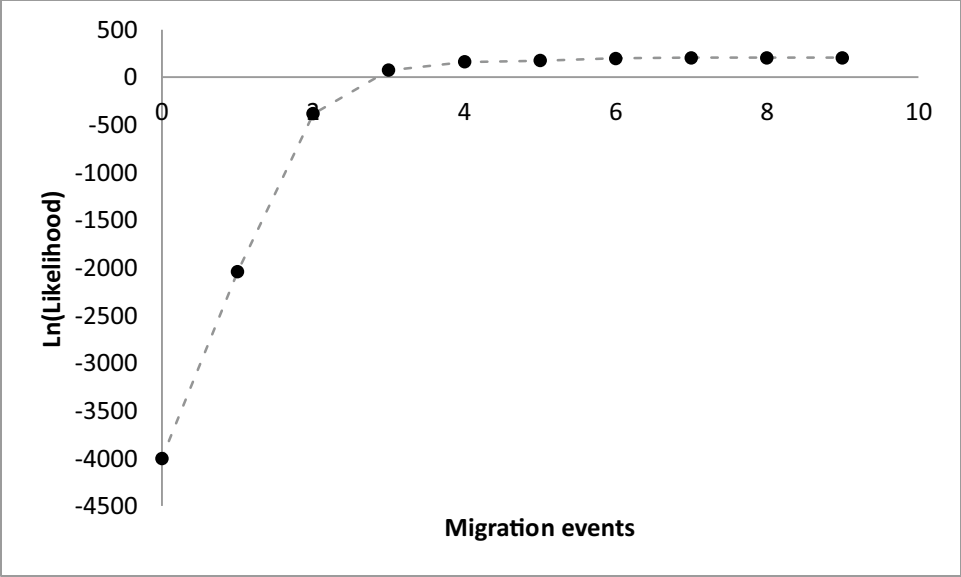
**Supplementary Figure 6. Log-likelihood values for Treemix trees.**
The Ln-likelihood values are calculated for Treemix trees by assuming 1 to 9 migration edges.
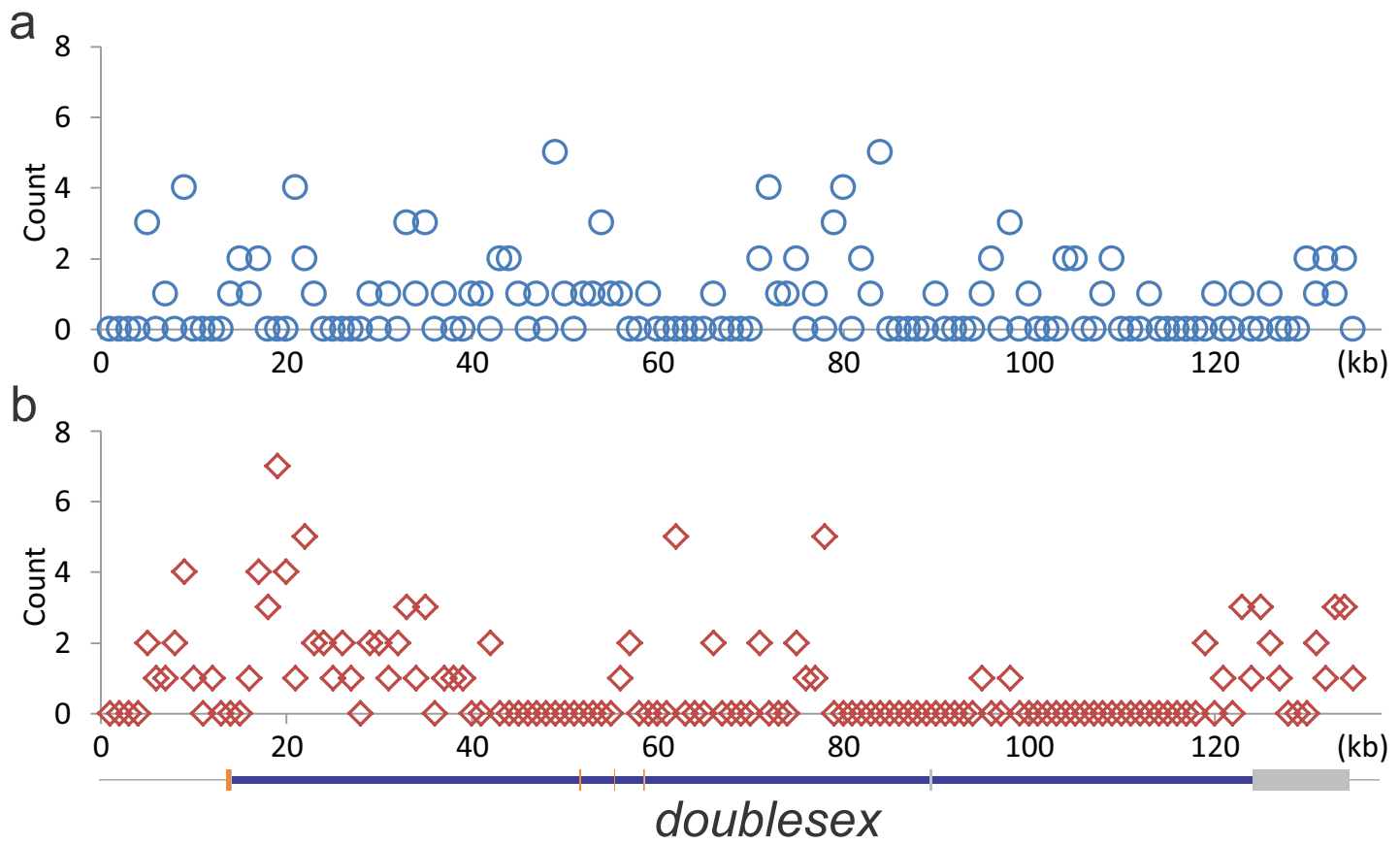
**Supplementary Figure 7. *Theseus* morph SNP counts across *doublesex*.**
The number of *theseus* specific alleles are counted for Philippine group (a) or Indonesia group (b), independently, for each fixed 1 kbp window along the *dsx* gene and neighboring regions. The blue line represents the *dsx* gene. The orange and grey bars represent the coding sequence (CDS) and UTR regions, respectively.

**Supplementary Figure 8. Testing parameter sets for a modified model of negative-frequency-dependent-selection (NFDS).**
A number of *a* and *b* values were selected to model different scenarios, including pure NFDS ($a = b = 1$), modified NFDS with equal benefits to homozygous mimetic and heterozygous genotypes ($a = b = 1.5$, 3 and 5) and modified NFDS with heterozygote advantage ($a = 1.5$ $b = 2$, $a = 2$ $b = 3$, $a = 4$ $b = 5$ and $a = 1.5$ $b = 5$). The starting mimetic allele frequency ranged from 0.05 to 0.95. Different *z* values indicate different strengths of NFDS, from neutral ($z = 0$) to very strong ($z = 0.95$). Each grid represents the mean mimetic allele frequency from 10 separate runs of each model after 100 or 200 generations, with a constant population size Ne = 10,000.
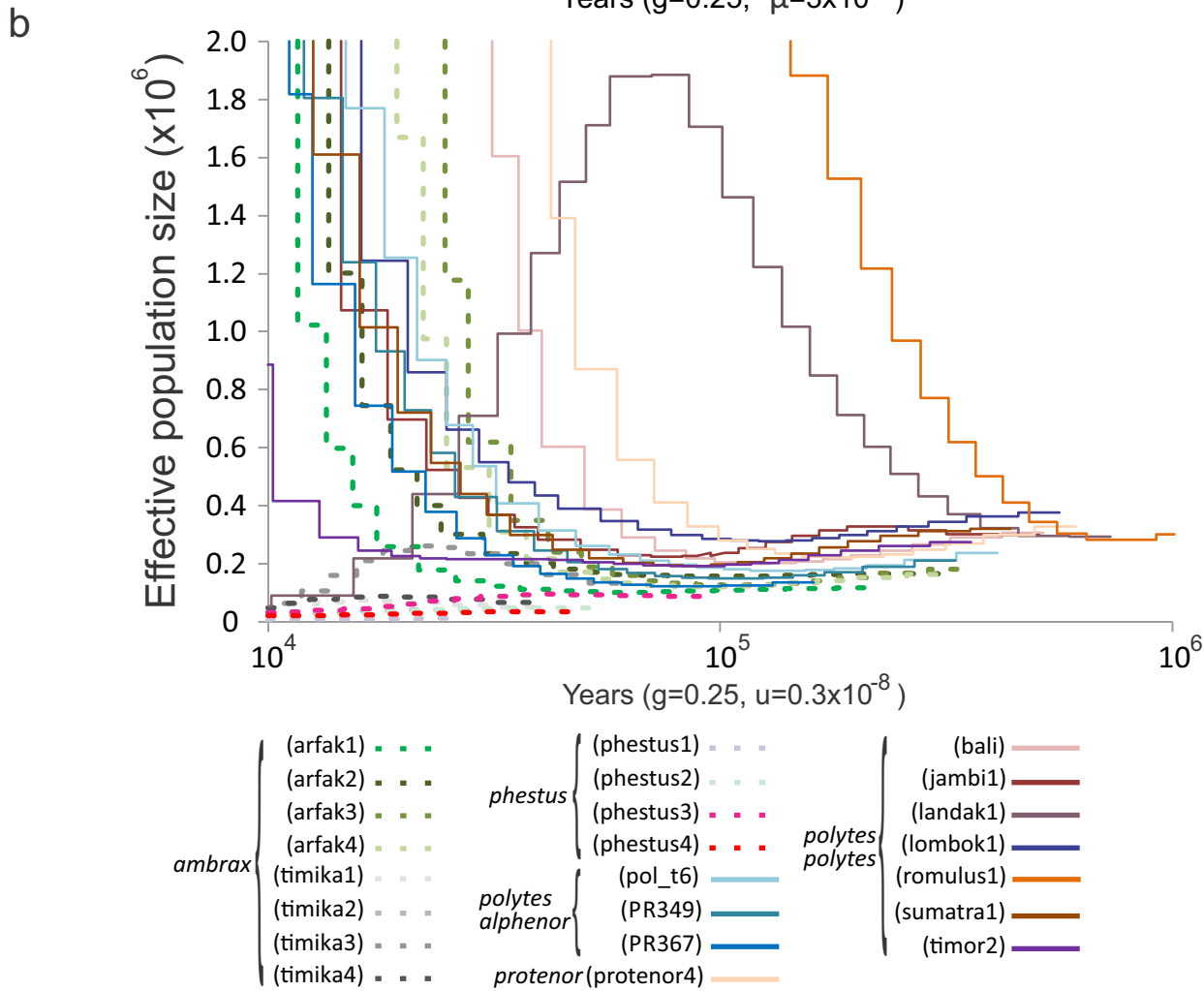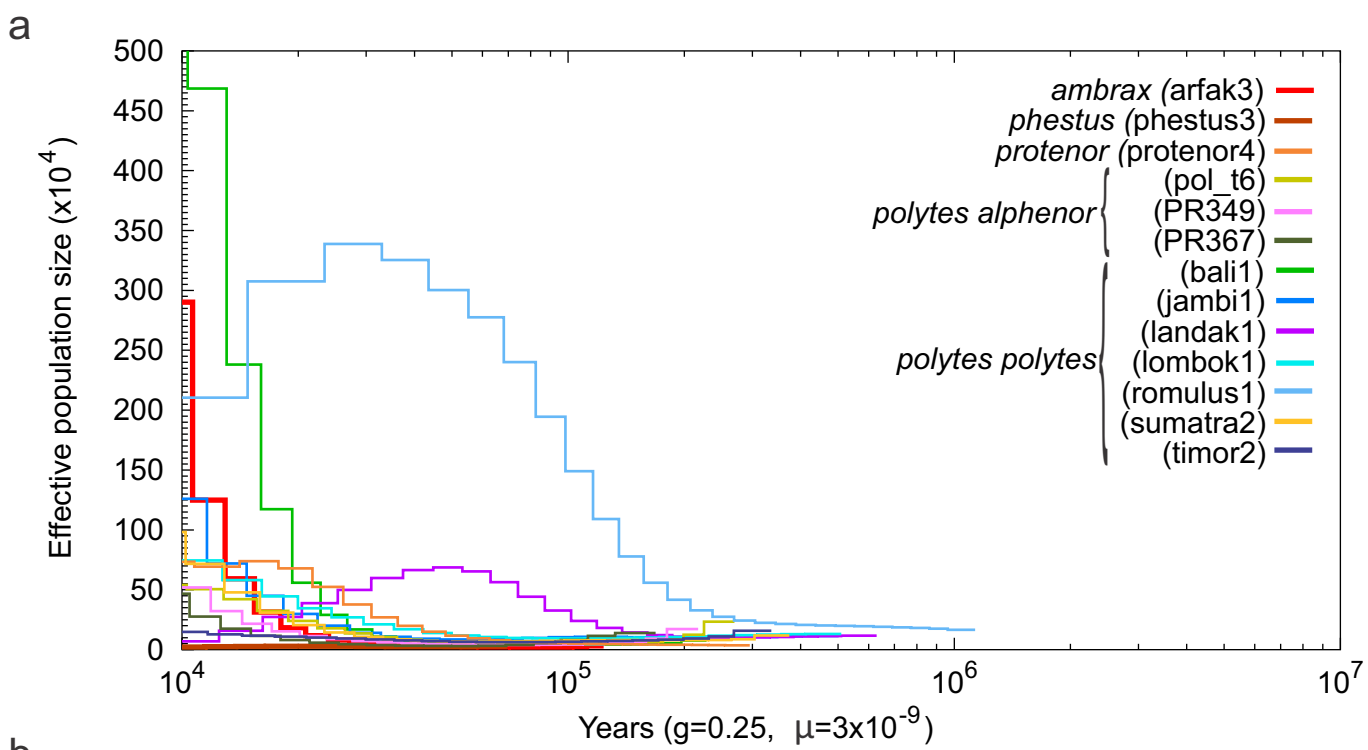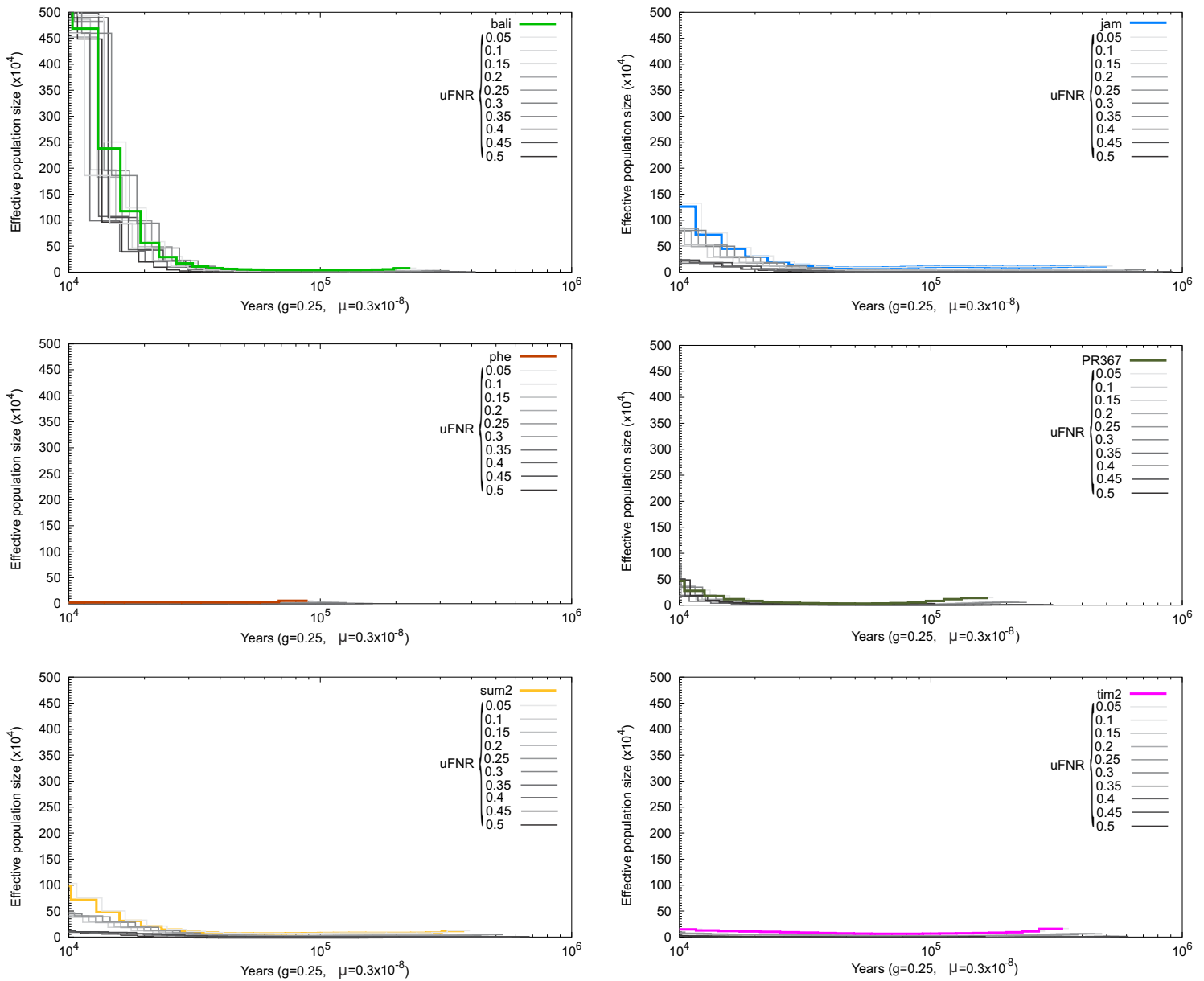
**Supplementary Figure 9. Demographic history of the *polytes* species group.**
(a) Historical effective population sizes were inferred from 13 individual genomes using PSMC, assuming a mutation rate of $\mu = 3.0 \times 10^{-9}$ and an average generation time of g = 0.25 year. (b) Historical effective population sizes were inferred from 23 individual genomes using MSMC, using a mutation rate of $\mu = 3.0 \times 10^{-9}$ and an average generation time of g = 0.25 year.
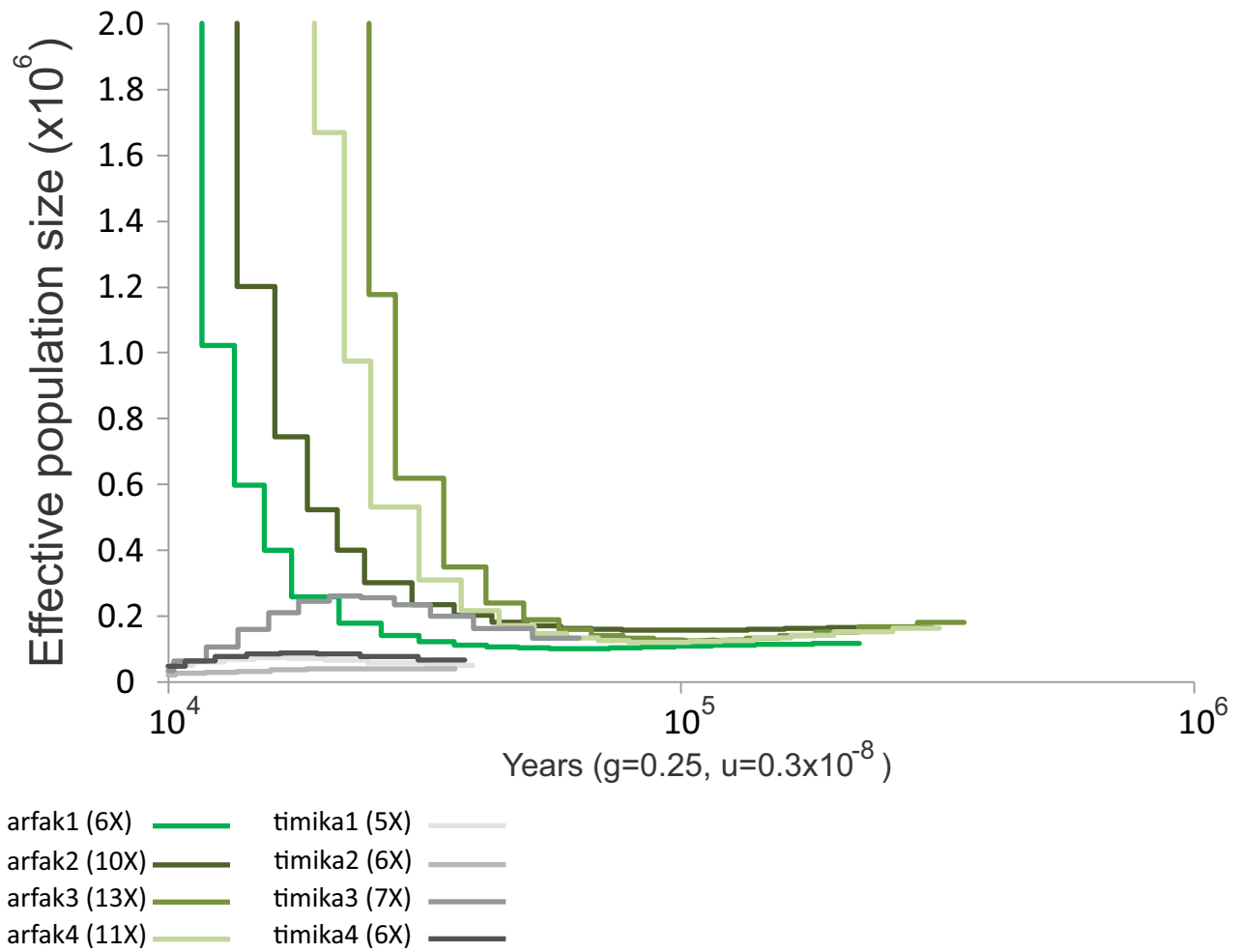
**Supplementary Figure 10. Demographic history of P. *ambrax* inferred using MSMC.**
Historical effective population sizes were inferred from eight *P. ambrax* genomes using MSMC, using a mutation rate of $\mu = 3.0 \times 10^{-9}$ and an average generation time of $g = 0.25$ year. The sequencing depth (X) is indicated for each individual.

**Supplementary Figure 11. Demographic history inferred using PSMC with false negative rate corrected.**
Historical effective population sizes were inferred from 6 individual genomes with sequencing coverage lower than 10X using PSMC, assuming a mutation rate of $\mu = 3.0 \times 10^{-9}$ and an average generation time of $g = 0.25$ year. Different values of uniform False Negative Rate (uFNR) from 0.05 to 0.5. For each individual, the original inference is plotted as a colorful line and the uFNR corrected results are plotted in grayscale.
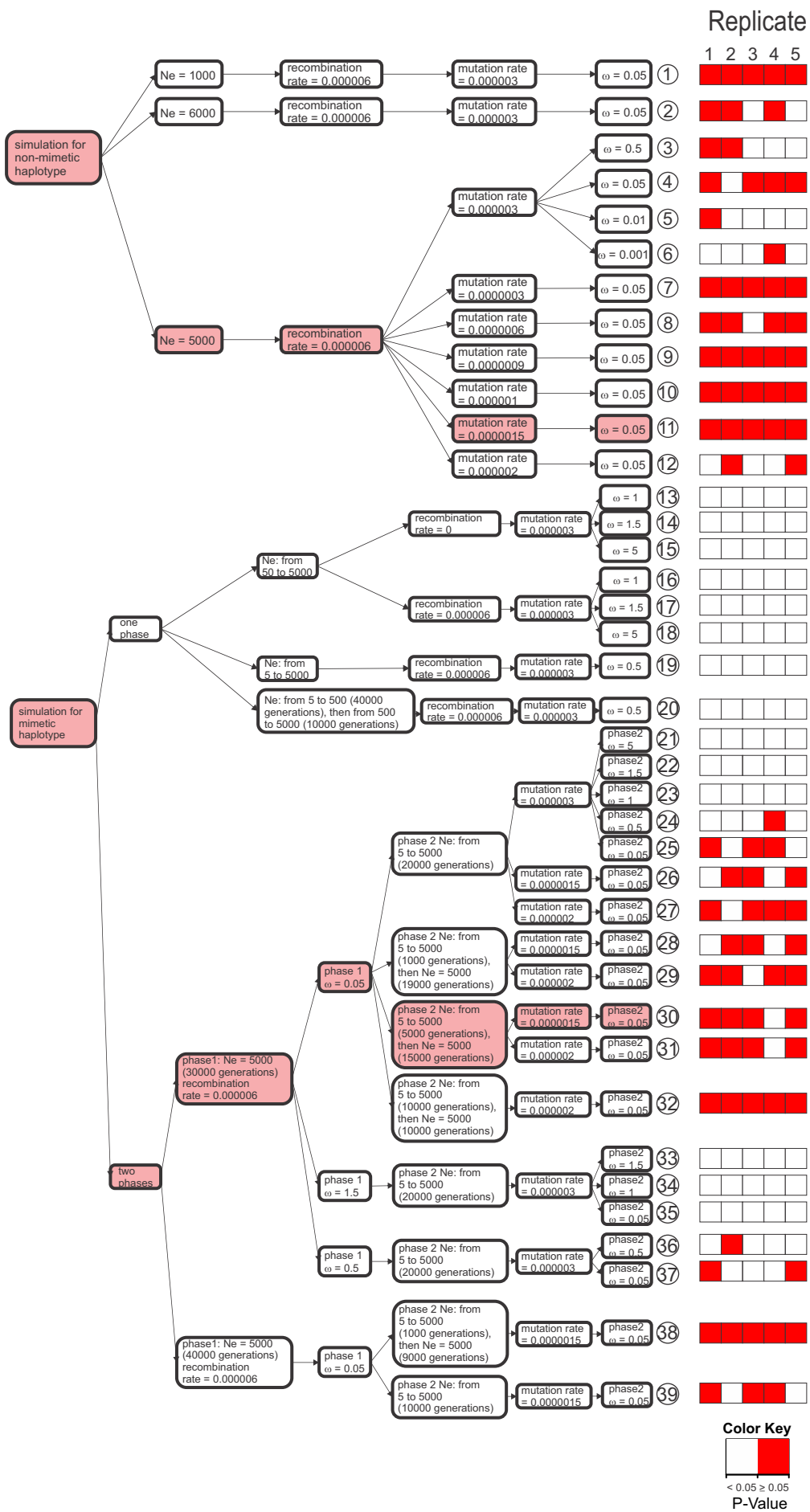
**Supplementary Figure 12. Workflow for simulating the molecular evolution of the non-mimetic and mimetic *doublesex* haplotypes.**

Scenario 11 and 30, which are highlighted, were selected because they yielded results most similar to our observed data. We compared empirical and simulated DNA sequence variations in *P. polytes*. Each grid represents a Fisher's exact test result from comparing a set of simulation counts with the observed variation from Fig. 4a.