## EVOLUTIONARY PATHWAYS FOR THE GENERATION OF NEW SELF-INCOMPATIBILITY HAPLOTYPES IN A NON-SELF RECOGNITION SYSTEM

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## Supplemental figures

- Figure S1. Average number/frequency of SI classes for population size N = 200.
- Figure S2. Completeness deficit of an S-allele in time, pathways of diversification/disappearance.
- Figure S3. Diversification diagrams for pathway 1.
- Figure S4. Diversification diagrams for pathway 2,3.
- Figure S5. Diversification diagrams for pathway 4.
- Figure S6. Composite diversification diagrams for all pathways for k = 8.



FIGURE S1. The average number (a) and frequency (b) of self-incompatibility types in a non-self recognition system in a finite population (N = 200) as a function of self-pollination rate ( $\alpha$ ) and inbreading depression ( $\delta$ ). Colours in the grid squares represent a gradient from low (green) to high (red) average numbers of SI types (a) and frequency of SI types (b) in the population. Mutation rate  $\mu_R = \mu_F = 0.001$ , Length of the F-box (SLF) sequence L = 15, and the total number of potential SLF and SRNase types  $n_F = n_R = 50$ . The large population size is shown in Figure 5.



FIGURE S2. Completeness deficit of the S-alleles. Example of a completeness deficit dependence on time. The parameters of the simulation correspond to those in Figure 4. We picked the SI class with SRNase  $R_{15}$  from the beginning to the end of the simulation. (A) Light green represents a long event, grey represents a short event. The simulation features four long events. Two patterns can be observed: completeness deficit 0 happens almost exclusively during the events with a long lifetime, and the death of a long event is typically associated with a loss of a functional SLF (increase of the completeness deficit before the disappearance of the SI class). (B) The last haplotype of each (of the three studied) SI classes was checked for its ancestors and the resulting pathways are shown in green (leading to diversification) and red (leading to disappearance). The three long events show the following features: (i) Diversification from class 22 (SRNase  $R_{22}$ ) to class 15 leads to a complete haplotype which disappears after losing a functional SLF gene. (ii) The last haplotype of this class had no complete ancestors. The complete haplotypes from this class must have disappeared before the last survivor. (iii) Multiple back-and-forth transitions occured in the lower front edge before the diversification proceeded.



FIGURE S3. Pathway 1. For pathway 1 the ancestral haplotype  $S_k^+$  is assumed complete, implying  $n \ge 1$ , and so we only analyze cases where  $1 \le n \le k$ . Color coding: diversification where intermediate mutant persists in the population (blue), intermediate SC haplotype is not able to invade the initial resident population (brown), intermediate SC haplotype fixes in the population (pink), novel haplotype  $S_{k+1}$  is not able invade into the population (gray), novel haplotype  $S_{k+1}$  is able invade into the population but drives incomplete haplotypes  $S_{\alpha}$  to extinction (white), novel haplotype  $S_{k+1}$  is able invade into the population but drives all but the intermediate self-compatible haplotype to extinction (black; fixation of SC haplotype: "resident strikes back").



FIGURE S4. Pathways 2,3. For pathways 2,3 the ancestral haplotype  $S_k^+$  is complete, and so as in pathway 1, we only analyze cases where  $1 \le n \le k$ . Color coding as in the previous figure, but in addition we have: diversification where intermediate mutant goes extinct (green), novel haplotype  $S_{k+1}$  is able invade into the population but replaces its ancestral haplotype  $S_k$  (red), novel haplotype  $S_{k+1}$  is able invade into the population but slowly drives all the incomplete haplotypes  $S_{\alpha}$  to extinction (light magenta; the extinction boundary has dominant eigenvalue one).



FIGURE S5. Pathway 4. For pathway 4 the ancestral haplotype  $S_k^-$  is incomplete and so we study cases  $0 \le n \le k - 1$  (*n* is never equal to *k* due to at least one incomplete haplotype). Color coding identical to Pathways 1 - 3.

Diversification regions for k=8



FIGURE S6. Diversification in the infinite population model for k = 8. (A) Summary for all pathways 1-5 for the infinite population model as a function of inbreeding depression  $(\delta)$ , proportion of self-pollen  $(\alpha)$ , initial number of SI haplotypes (k = 8) and the level of completeness  $0 \le n \le k$  (n = number of complete haplotypes). The bifurcation plots are superimposed plots of Figures S3-S5 (Supplemental Information). Color coding: diversification with long-term increase in the number of SI haplotypes and a loss of the intermediate mutant (green), short-term diversification (light magenta), no diversification due to exclusion of the novel SI haplotype  $S_{k+1}$  (grey), no diversification because novel SI haplotype  $S_{k+1}$  replaces its ancestral SI haplotype  $S_k$  (red). Below the thick black line is a parameter region where mutations in the SLFs may lead to a complete SC haplotype class  $SC_k$  (pathways 2 - 4), consequently resulting in the fixation of this SC class and a loss of all self-incompatibility from the population. Therefore, diversification is only possible in the region above this line. Long-term stable coexistence after a diversification event is possible only for n = k (green regions). For 1 < n < k, after the invasion of  $S_{k+1}$ , all incomplete haplotype classes will slowly go extinct. An incomplete SI class can be rescued if it gains the missing haplotype before extinction, and diversification happens if all incomplete classes gain the missing SLF. We highlight all feasible pathways for the particular n in the corresponding cube, using the color of the region where diversification via this pathway is possible – either a long-term coexistence of k + 1 SI haplotypes (green), or short-term coexistence (light magenta). For  $k \geq 7$  diversification via pathways 2,3,4 for n = 1 is not possible. For 1 < n < k, the red and brown overlaps with magenta for Pathway 5 (light magenta dots). This implies that as brown and red leaves the number of SI classes intact but pathway 5 modifies the number of SI classes, in this region we expect path 5 to dominate the dynamics (see above).