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Article:

Wang, R, Yang, Y, Jing, Y et al. (32 more authors) (2021) Molecular mechanisms of mutualistic and antagonistic interactions in a plant–pollinator association. *Nature Ecology & Evolution*, 5 (7). pp. 974-986. ISSN 2397-334X

<https://doi.org/10.1038/s41559-021-01469-1>

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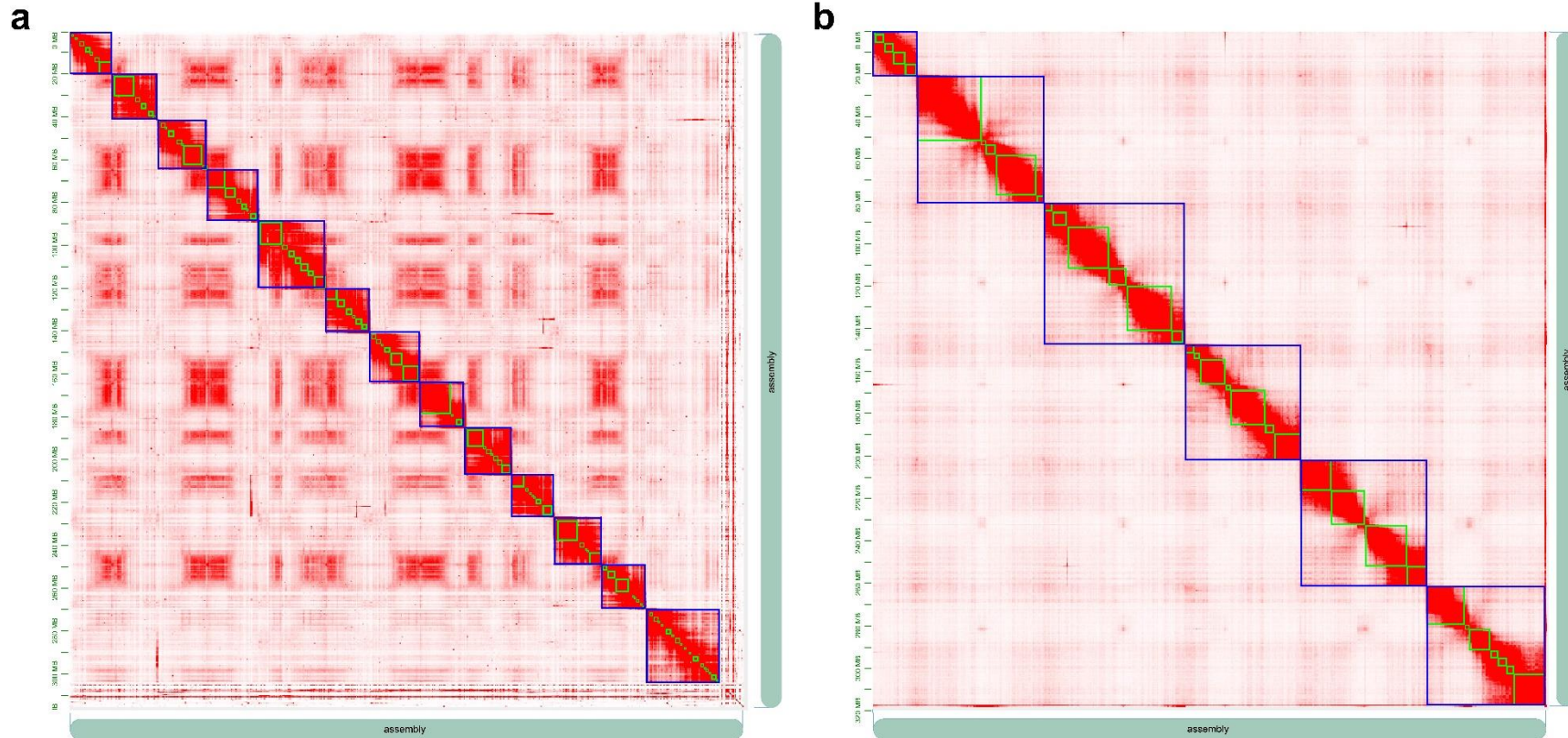
Supplemental information

Title:

Molecular mechanisms of mutualistic and antagonistic interactions in a plant-pollinator association

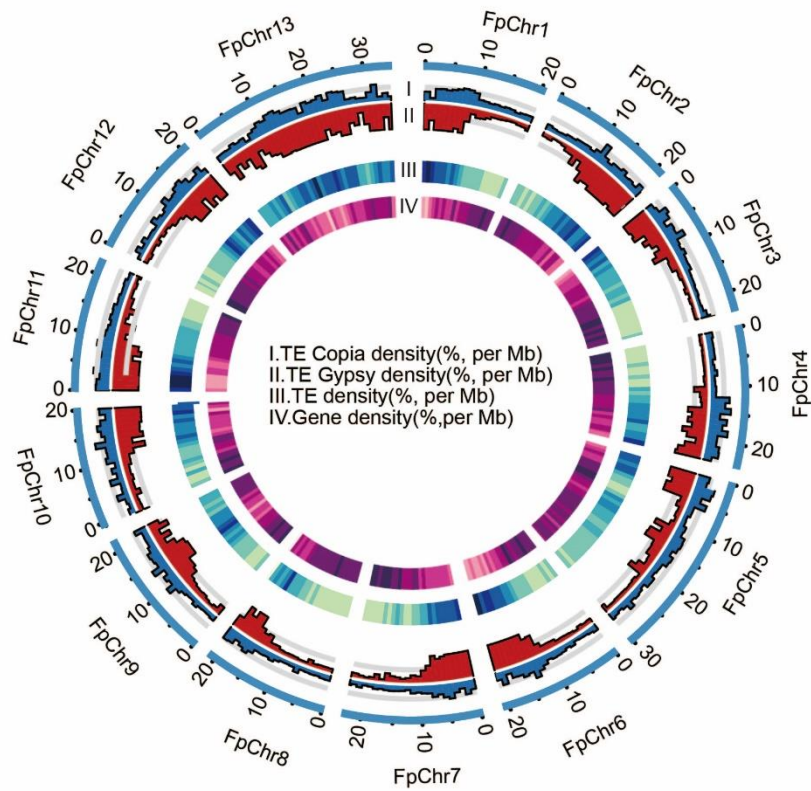
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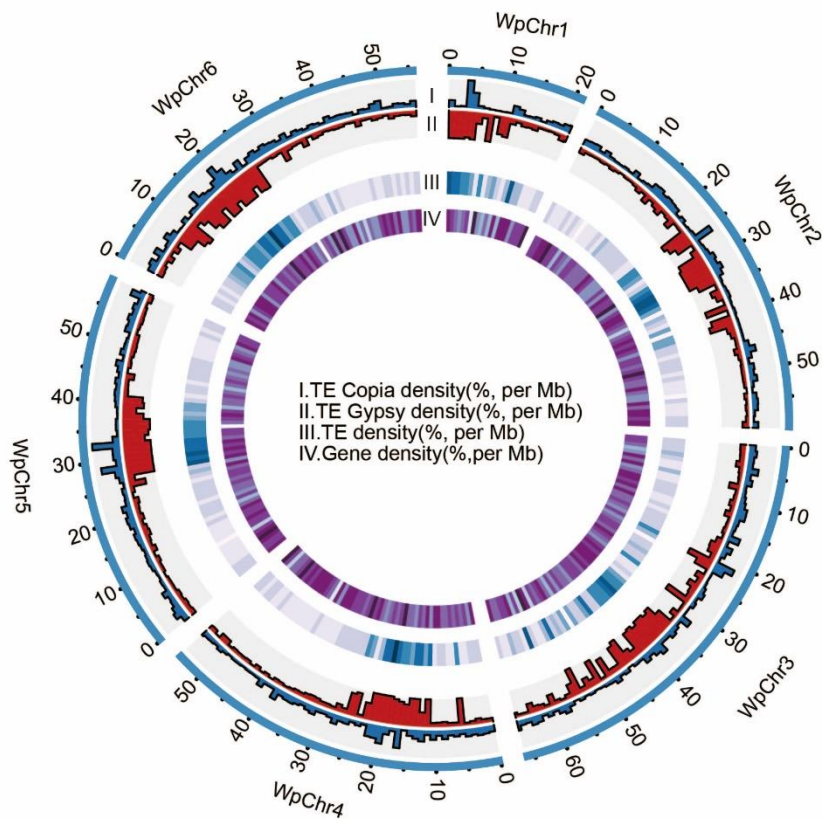


Supplementary Figure 1. Heat map of interaction intensity between any two of the thirteen pseudo-chromosomes clustered by Hi-C data in *Ficus pumila* var. *pumila* (a) and *Wiebesia pumilae* (b) genomes. *Ficus pumila* var. *pumila* has 13 pairs of chromosomes (Ohri, D. & Khoshoo, 1987). Although the chromosome number of *W. pumilae* has not been experimentally checked, a related species *Blastophaga psenes* has been reported to have 6 pairs of chromosomes (Liu et al., 2011).

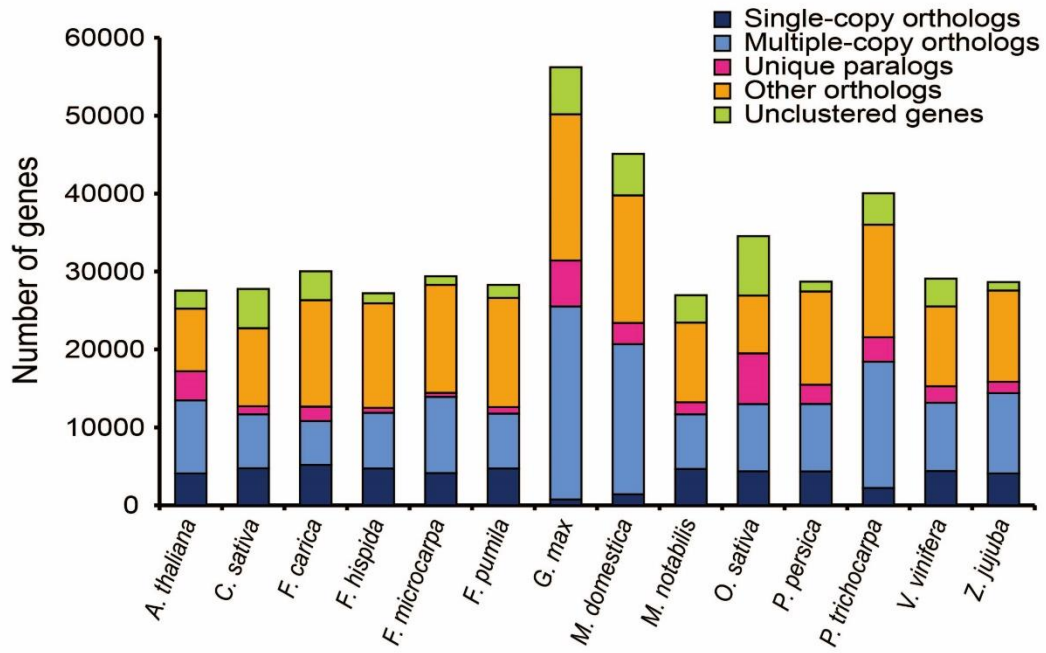
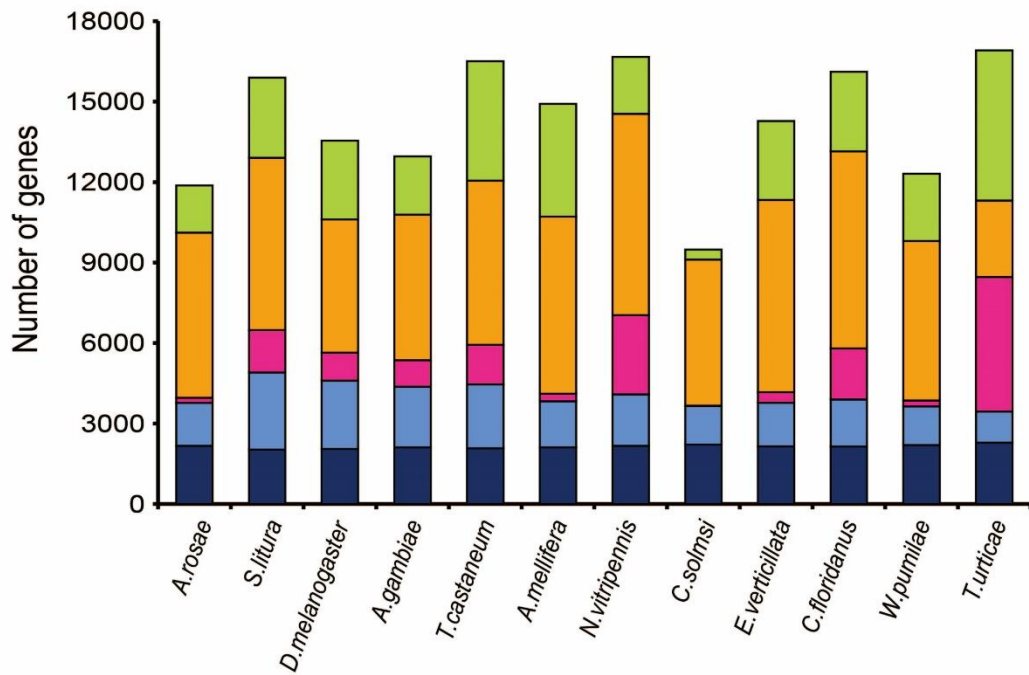
a



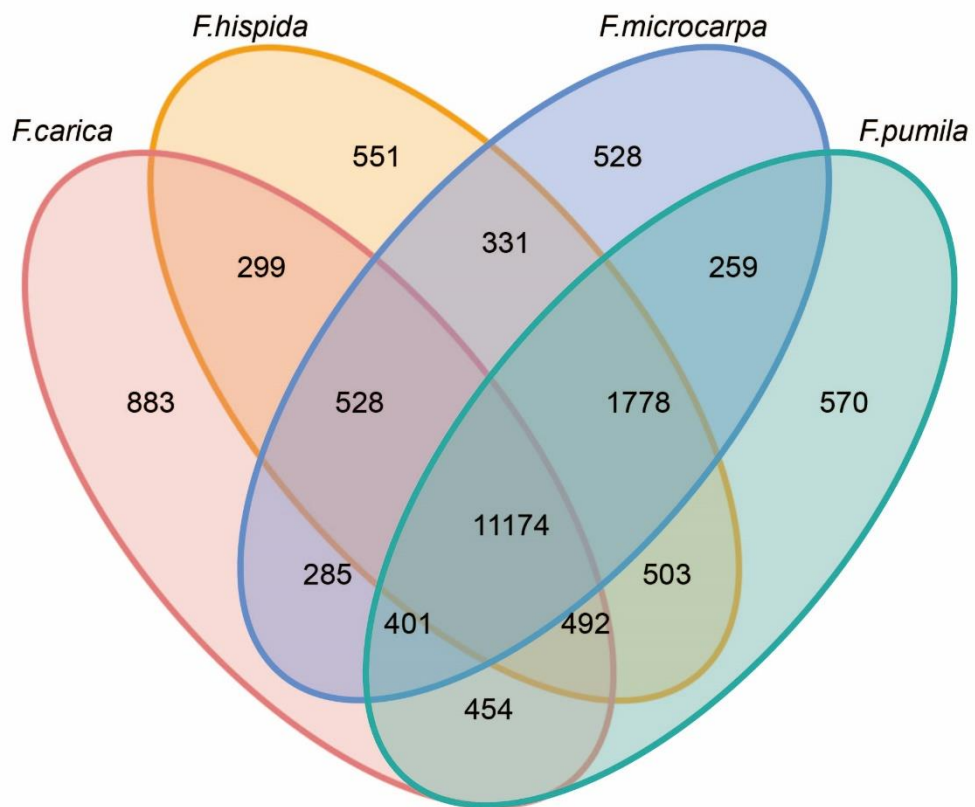
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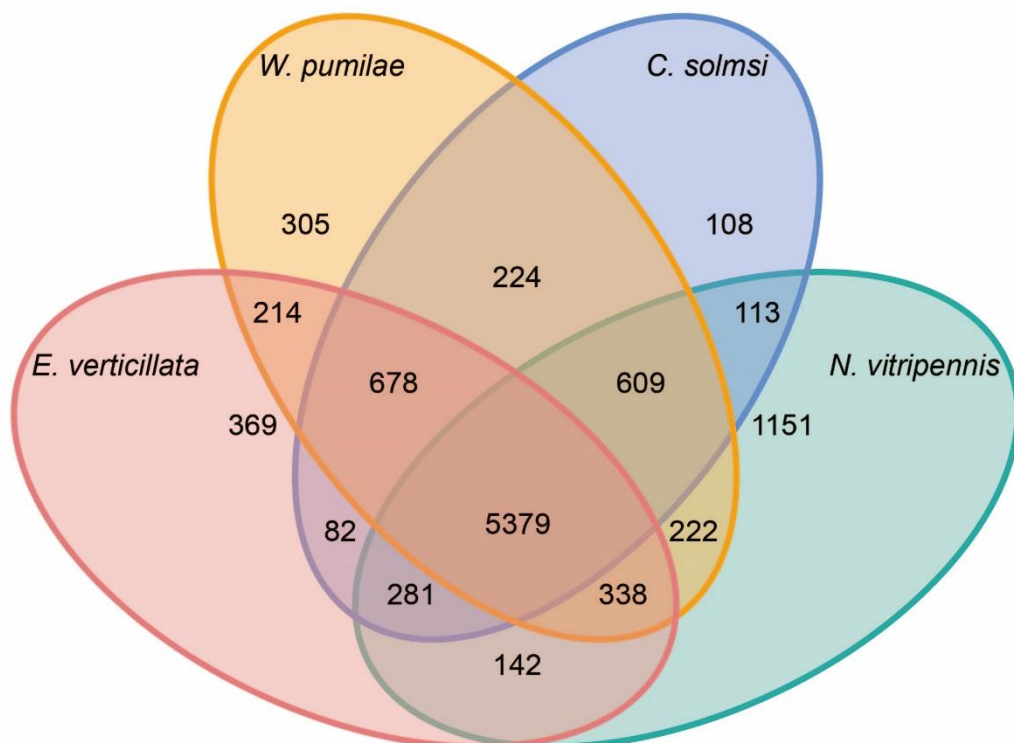
Supplementary Figure 2. Genome features of *F. pumila* var. *pumila* (Fp) (a) and *W. pumilae* (Wp) (b).

a**b**

c

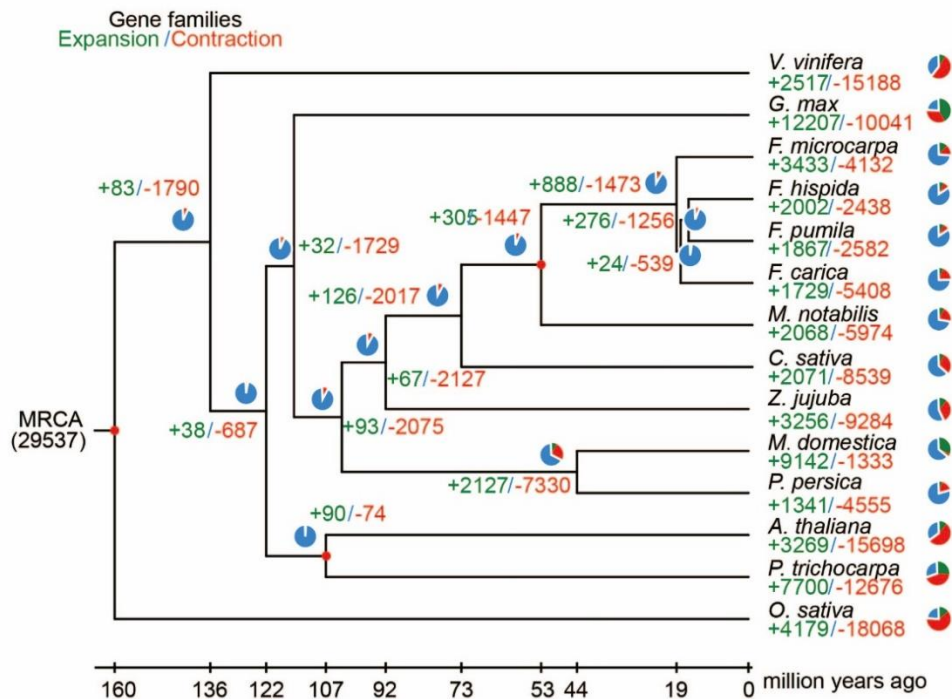


d

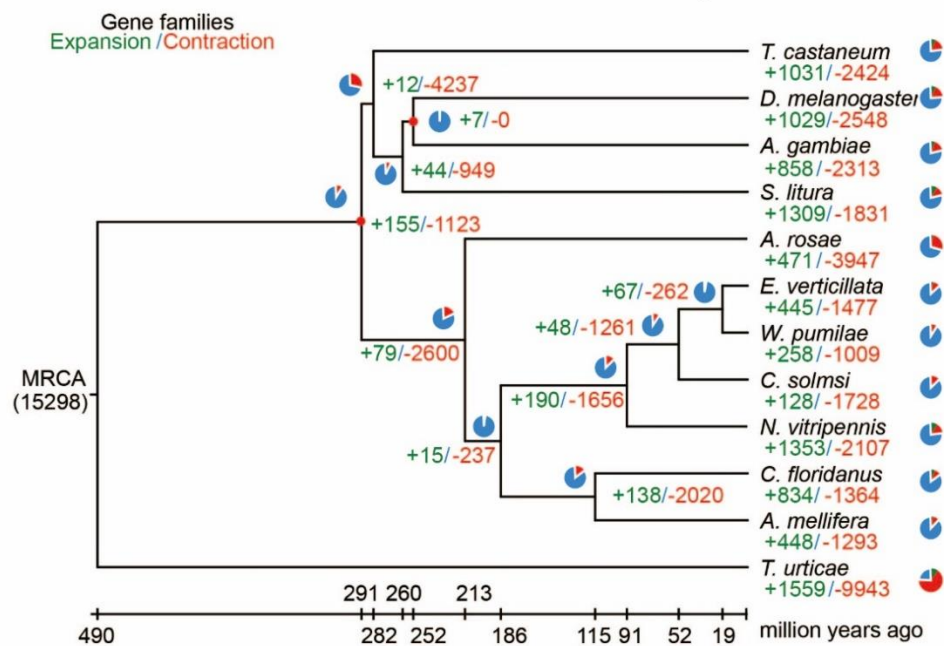


Supplementary Figure 3. Clusters of gene families in the selected angiosperms (a) and arthropods (b) and Venn diagrams showing the number of gene families shared by *F. pumila* var. *pumila* and its related plants (c) and by *W. pumilae* and its related insects (d).

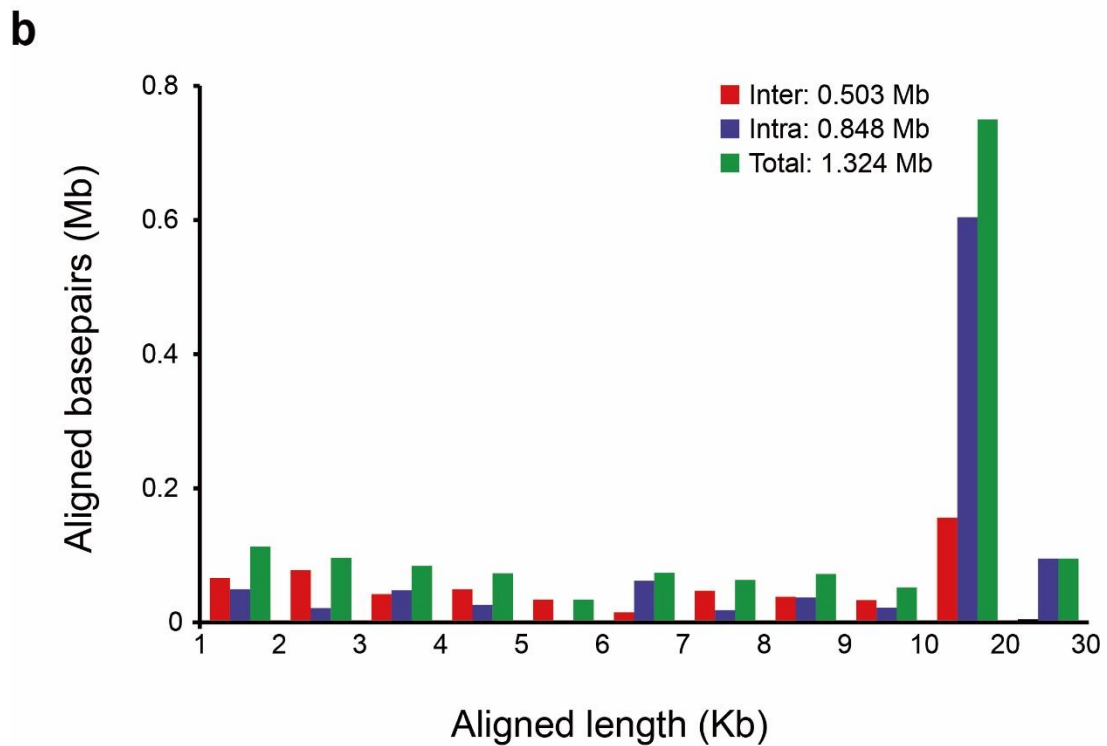
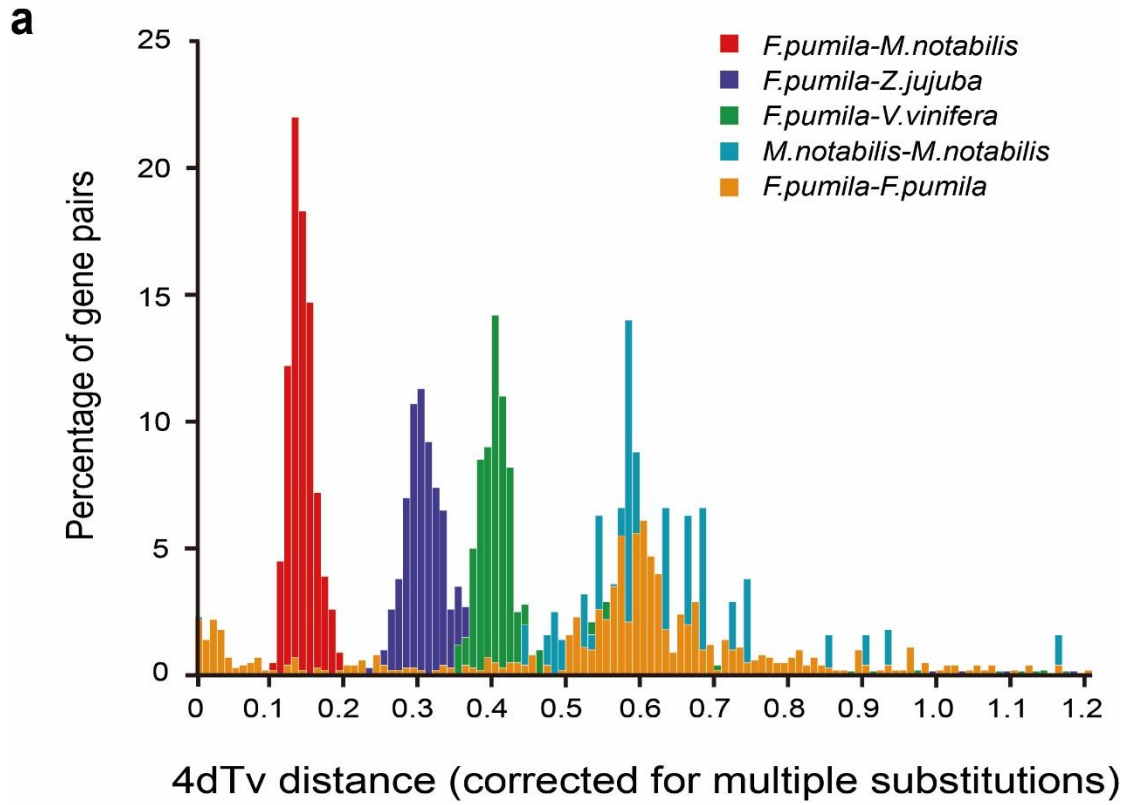
a



b

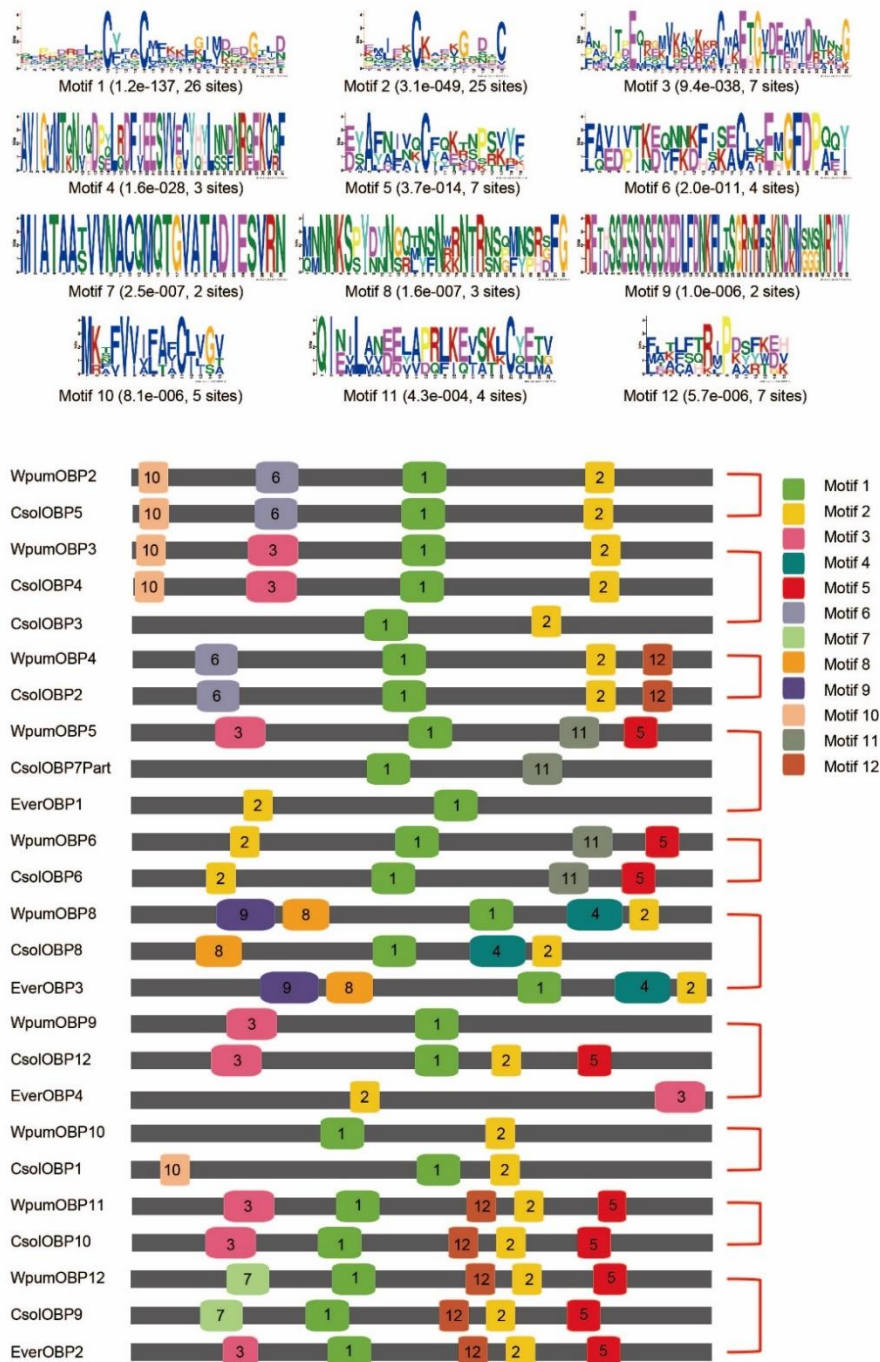


Supplementary Figure 4. The expansion/contraction of gene families in *F. pumila* var. *pumila* (a) and *W. pumilae* (b) genomes. Phylogenetic trees with the results of gene family expansion/contraction analysis. Numbers of expanded (green in pie charts) or contracted (red) gene families are indicated along branches and nodes. Red dots represent the calibrated nodes, based on the fossil evidence and divergence evidence from <http://www.timetree.org/>. Full names of species are shown in Supplementary Table 6.

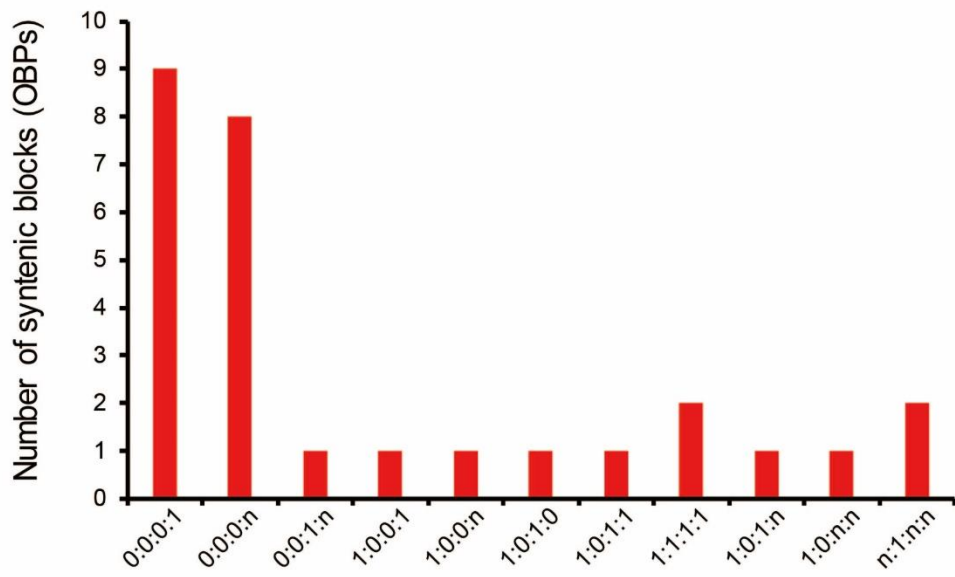
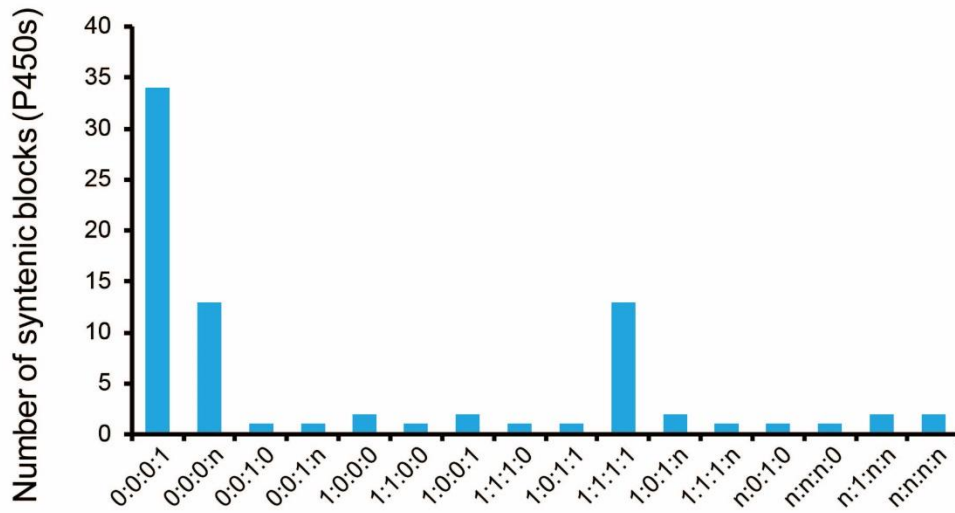
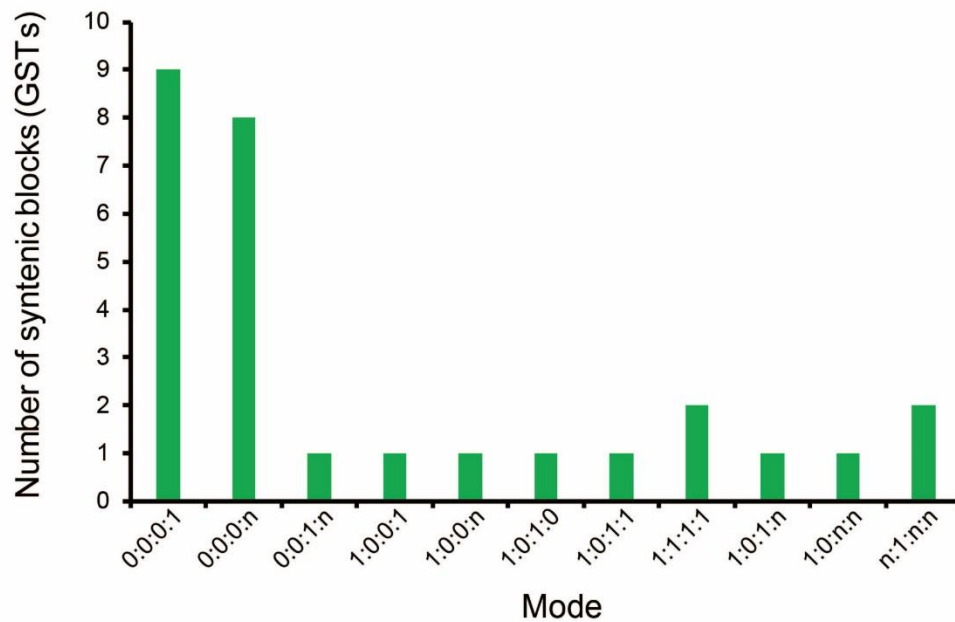


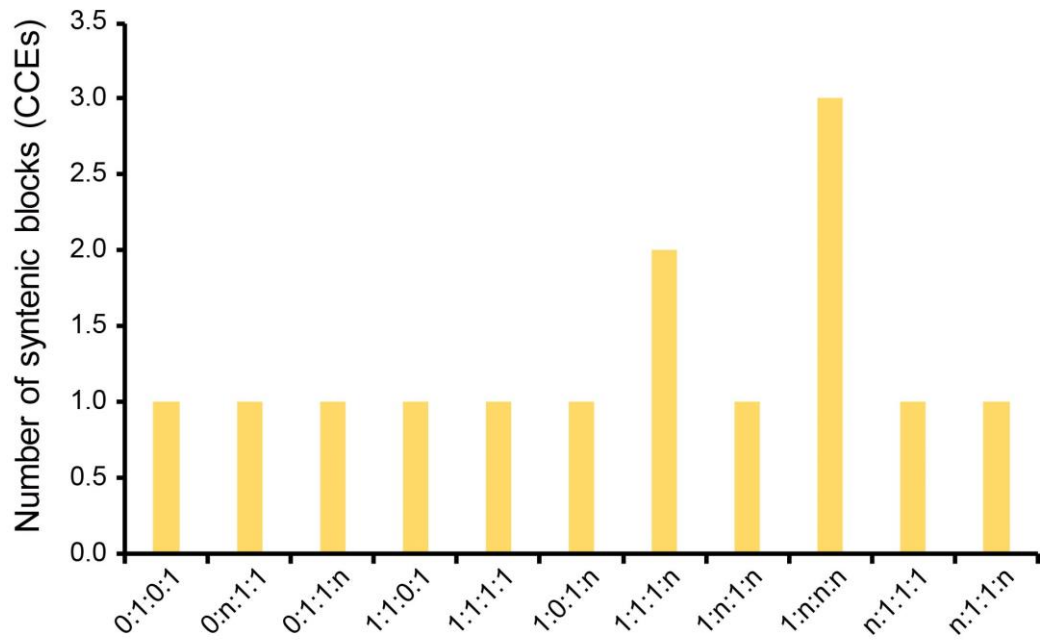
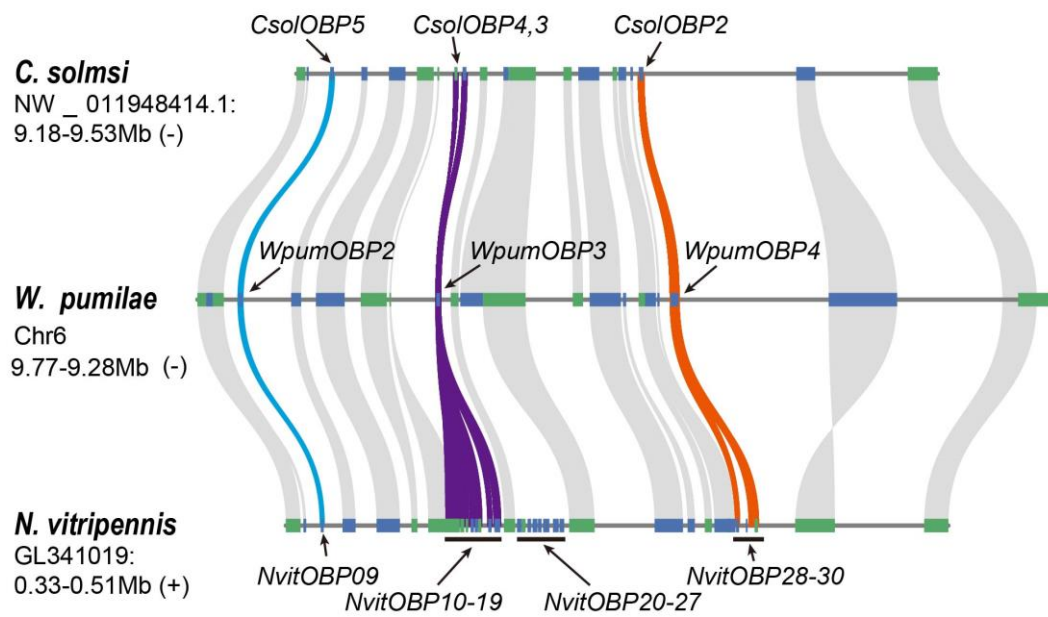
Supplementary Figure 5. Results of 4DTv analysis for *F. pumila* var. *pumila* (a) and segmental duplication analysis for *W. pumilae* (b).

b



Supplementary Figure 6. Phylogenetic trees of OBP genes in *W. pumilae*, *E. verticillata*, *C. solmsi*, *N. vitripennis*, *A. lineolatus* and *C. quinquefasciatus* (a) and results of motif analysis concerning OBPs in *W. pumilae*, *E. verticillata* and *C. solmsi* (b). The trees were constructed in TreeBeST using the neighbor-joining method and setting JTT model with 1000 bootstrapping replicates. OBP names are presented as a four-letter code (first letter of the genus followed by the first three letters of the species name) + OBP + numbers. The OBPs of the three pollinating wasp species are clustered according to their syntenic blocks (see Supplementary Figs. 7a, e).

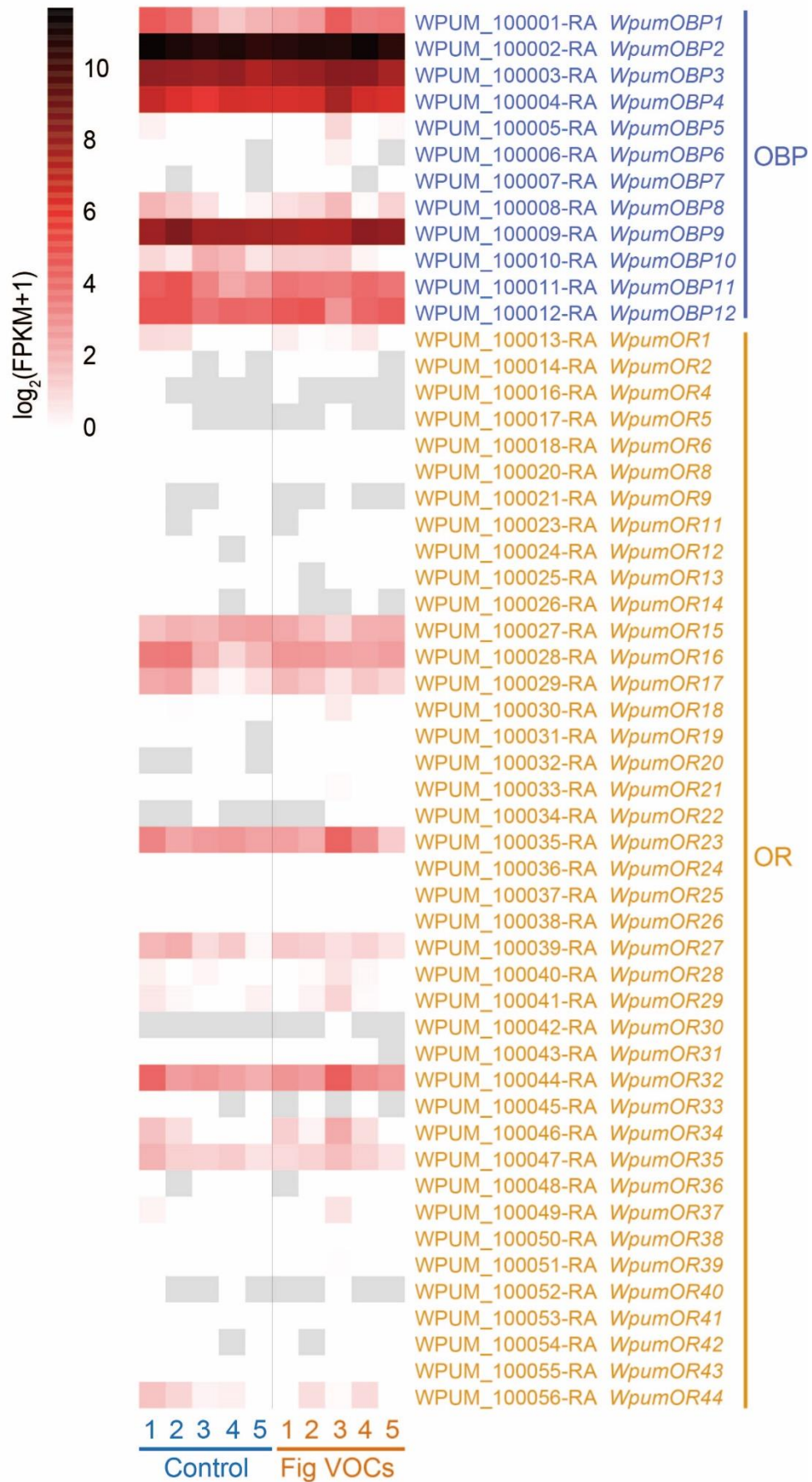
a**b****c**

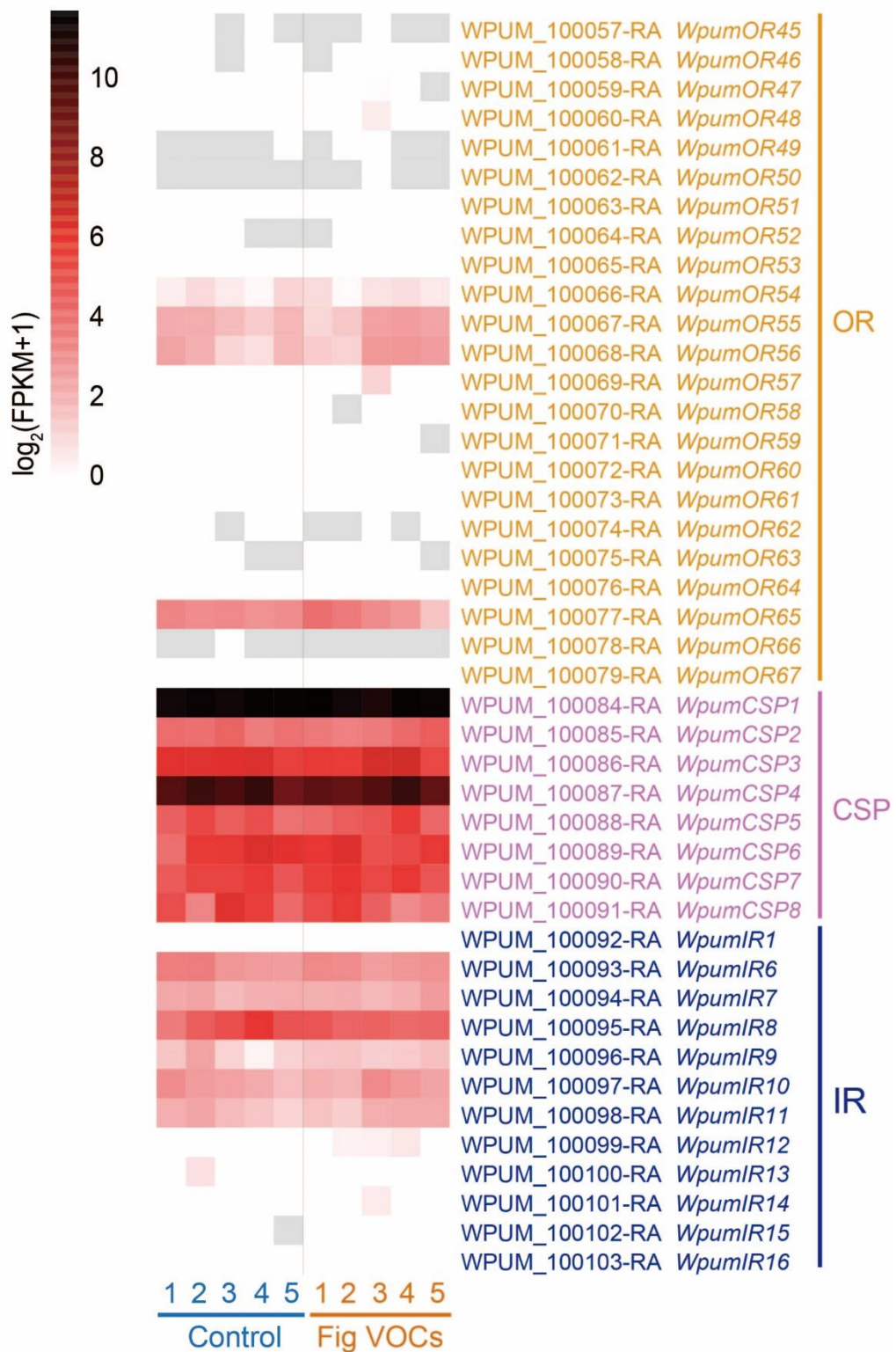
d**e**

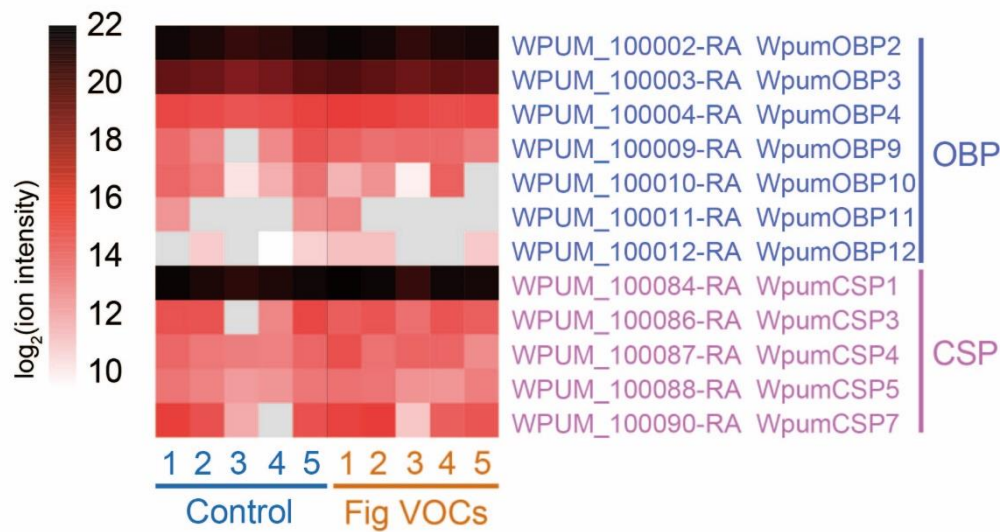
Supplementary Figure 7. Results of synteny analysis of OBPs, CYP450s and GSTs in *W. pumilae*, *E. verticillata*, *C. solmsi* and *N. vitripennis*. Each mode listed in the x-axis represents the number of genes in the three species (*W. pumilae*: *C. solmsi*: *N. vitripennis*) in a syntenic block, for example 1: 1: 1: 1 depicts the situation

where only one gene in each species was detected in a syntenic block, indicating that no tandem duplication event occurred; and 1: 1: 1: n shows a scenario in which a syntenic block contained only one gene in the three pollinating wasp species and at least two genes (n represents gene number ≥ 2) in *N. vitripennis*. The last case is suggestive of a recent gene tandem duplication in *N. vitripennis* but not in the other three species. **(a)** Results of synteny analysis of OBPs. OBPs in *W. pumilae* were highly conservative as gene tandem duplications only happened in 2 syntenic blocks (the frequency of n: 1: n: n) and both of them might have occurred in the common ancestor of the two pollinator, while there were 14 gene tandem duplication events in *N. vitripennis* (the sum of frequencies of n: 1: n: n, 1: 0: 1: n, 1: 0: n: n, 1: 0: 0: n, 0: 0: 1: n and 0: 0: 0: n). The syntenic blocks belonging to 0: 0: 0: 1 and 0: 0: 0: n modes could be caused by species-specific gene duplication in *N. vitripennis* and (or) gene loss in the three pollinating wasp species. **(b)** Results of synteny analysis of CYP450s. CYP450s in *W. pumilae* were highly conservative because gene tandem duplications were only present in 6 syntenic blocks (n: n: n: n + n: 1: n: n + n: 0: 1: 0 + n: n: n: 0) of the total syntenic blocks with at least one gene in this species (29 syntenic blocks). **(c)** Results of synteny analysis of GSTs. GSTs in *W. pumilae* were highly conservative because gene tandem duplications only occurred in 2 (n: 1: n: n) out of the 10 syntenic blocks with at least one gene in this species. **(d)** Results of synteny analysis of CCEs. CCEs in *W. pumilae* were also highly conservative because gene tandem duplications only occurred in 2 (n: 1: 1: n + n: 1: 1: 1) out of the 11 syntenic blocks. **(e)** Schematic representation of OBPs synteny among *W. pumilae*, *E. verticillata* (no OBP genes in these syntenic blocks), *C. solmsi* and *N. vitripennis*. Each line connects a pair of orthologous genes.

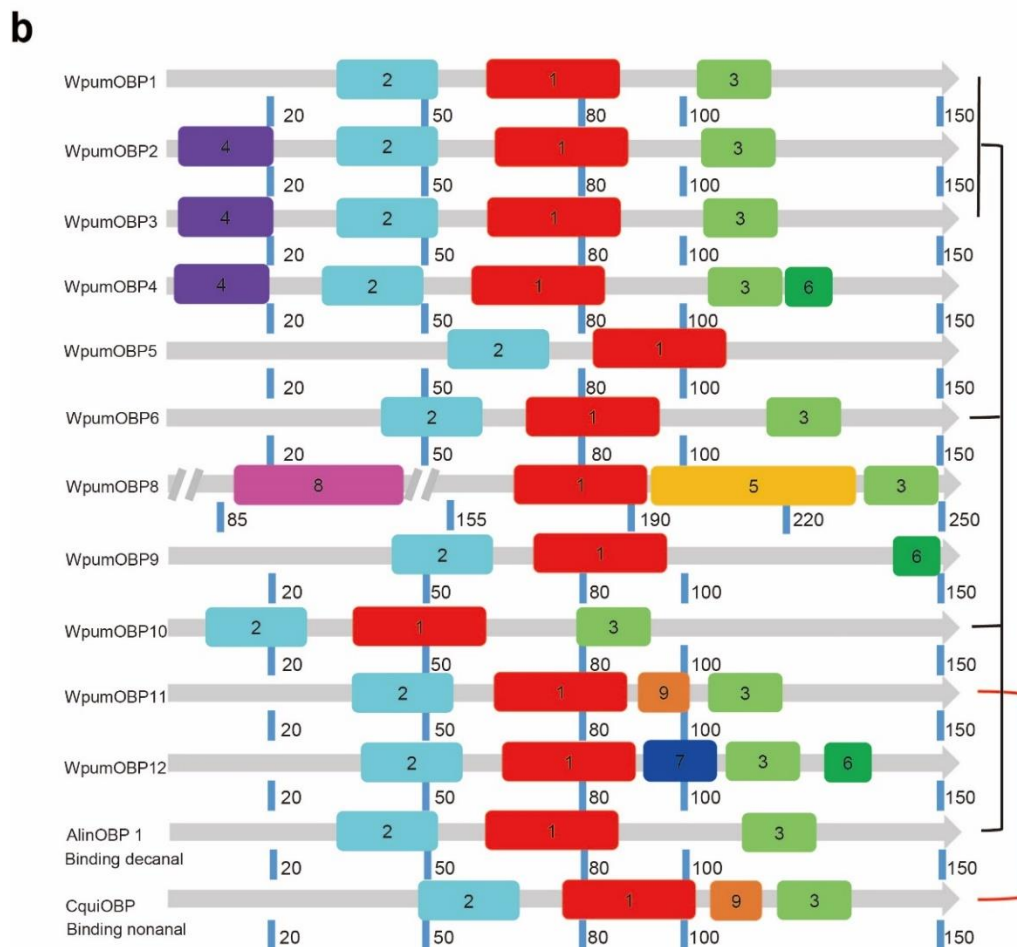
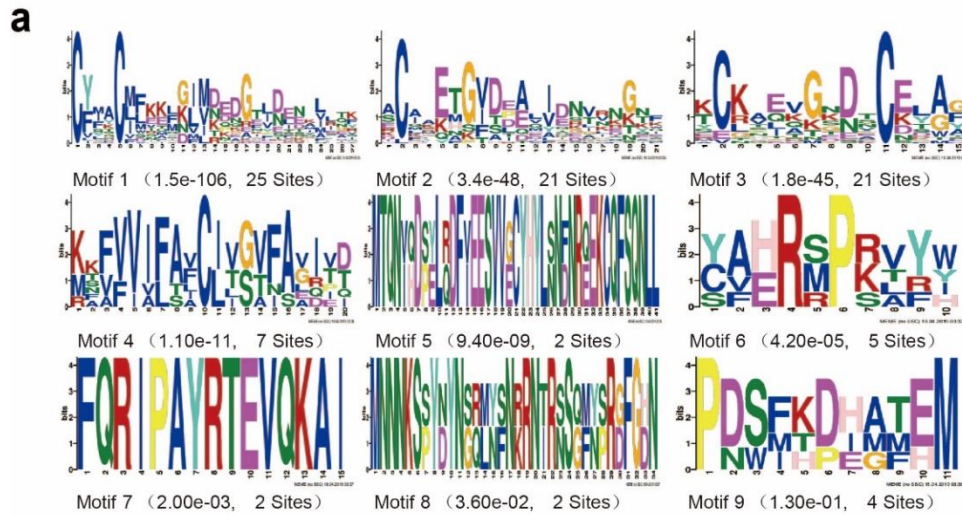
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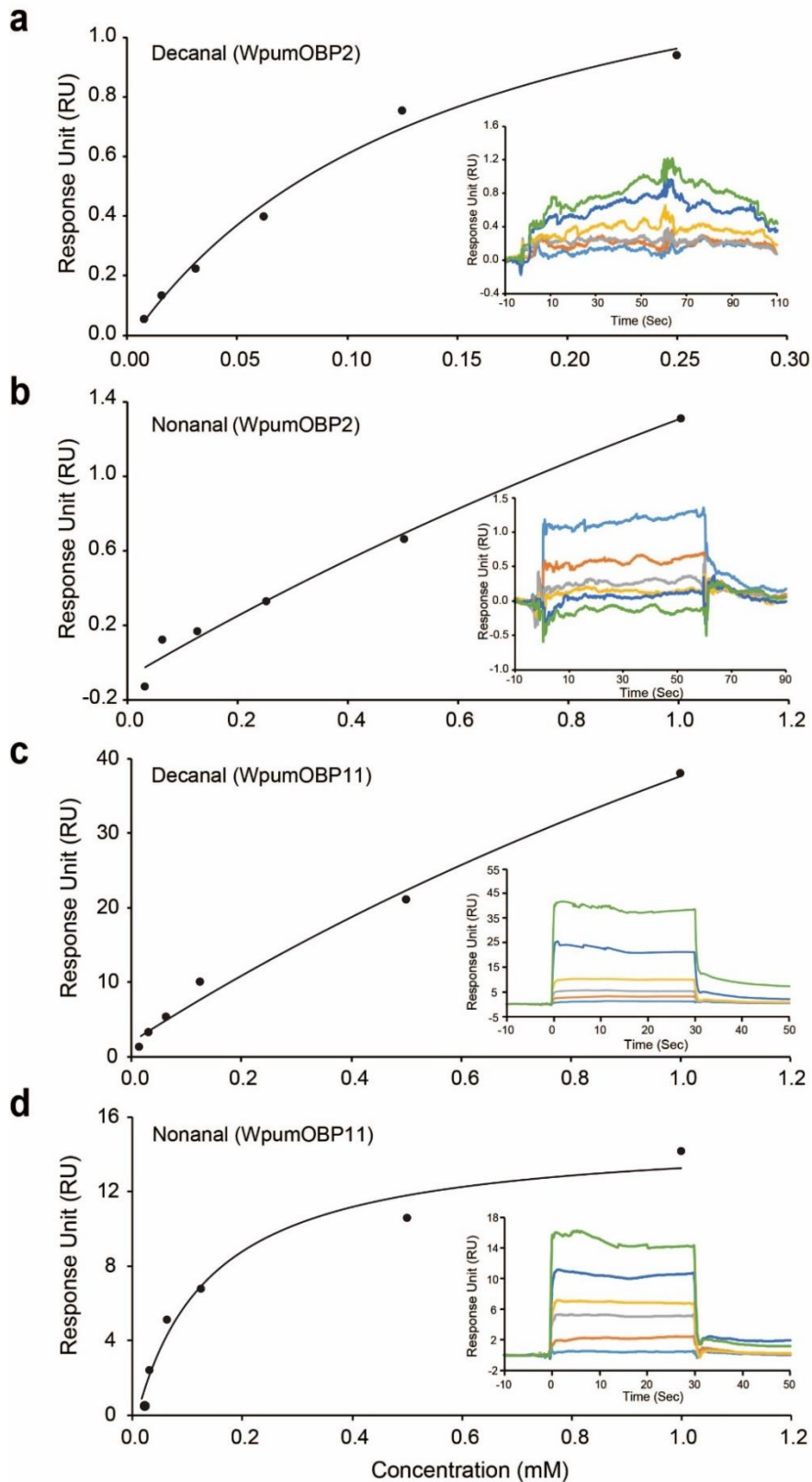


b

Supplementary Figure 8. Heat map of gene expression in transcriptomes (a) and protein quantity in proteomes (b) in OBPs, CSPs, ORs, GRs and IRs in the adult females of *W. pumilae* not contacting and contacting the VOCs emitted by *E. pumila* var. *pumila* figs at receptive stage. Gene expression pattern are consistent no matter whether adult female pollinators contacted with the VOCs emitted by the receptive figs or not ($p > 0.05$ in all analyses, Supplementary Table 10).

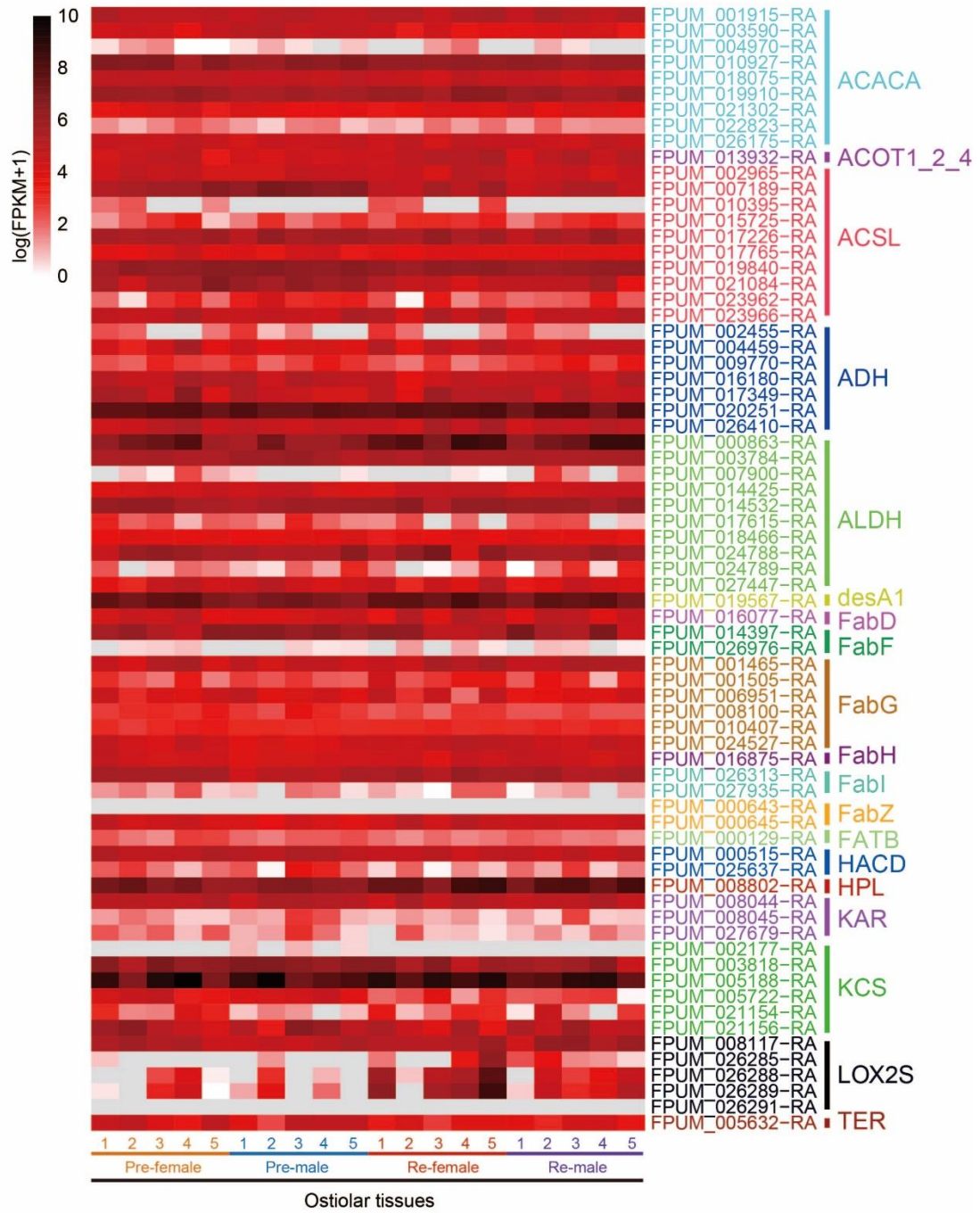


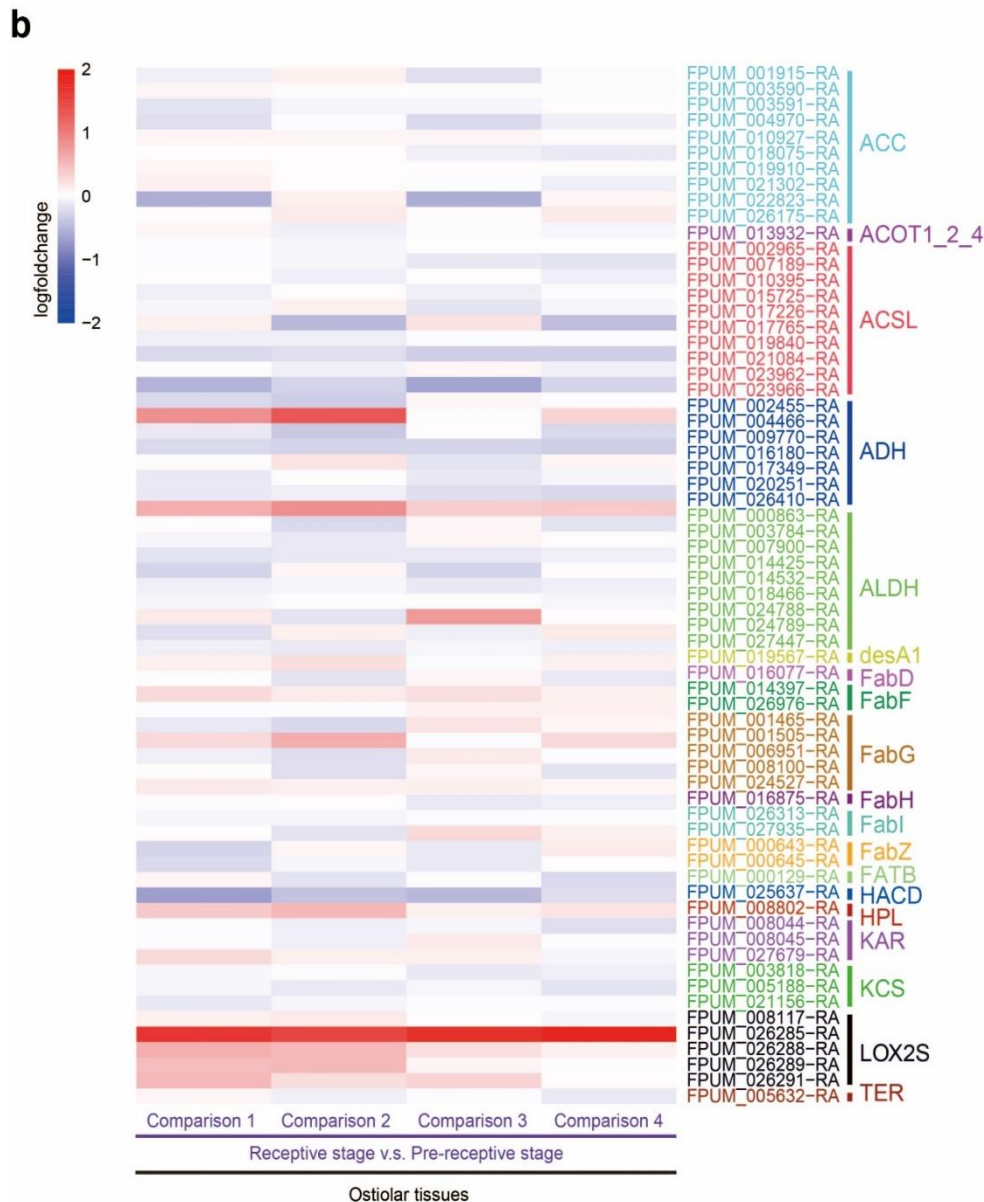
Supplementary Figure 9. Motif analysis of OBPs of *A. lineolatus*, *C. quinquefasciatus* and *W. pumilae*. Motifs in OBPs (E-value and number of sites are shown below each motif) **(a)**. Motif structure in each OBP. The site numbers label the approximate locations of motifs in each OBP starting from the N-terminal **(b)**. We failed to predict the motif structure in WpumOBP7 due to its incomplete sequence.



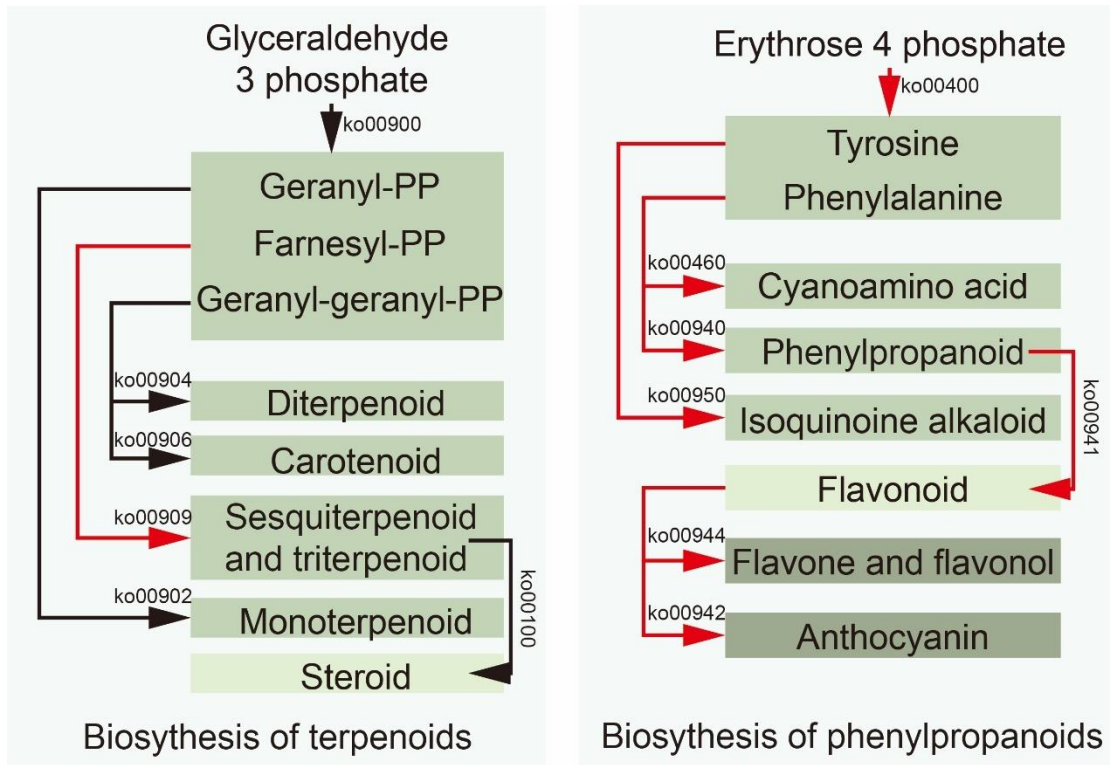
Supplementary Figure 10. Results surface plasmon resonance (SPR) experiments studying the binding affinities of WpumOBP2 (a and b) and WpumOBP11 (c and d) to decanal and nonanal, respectively.

a

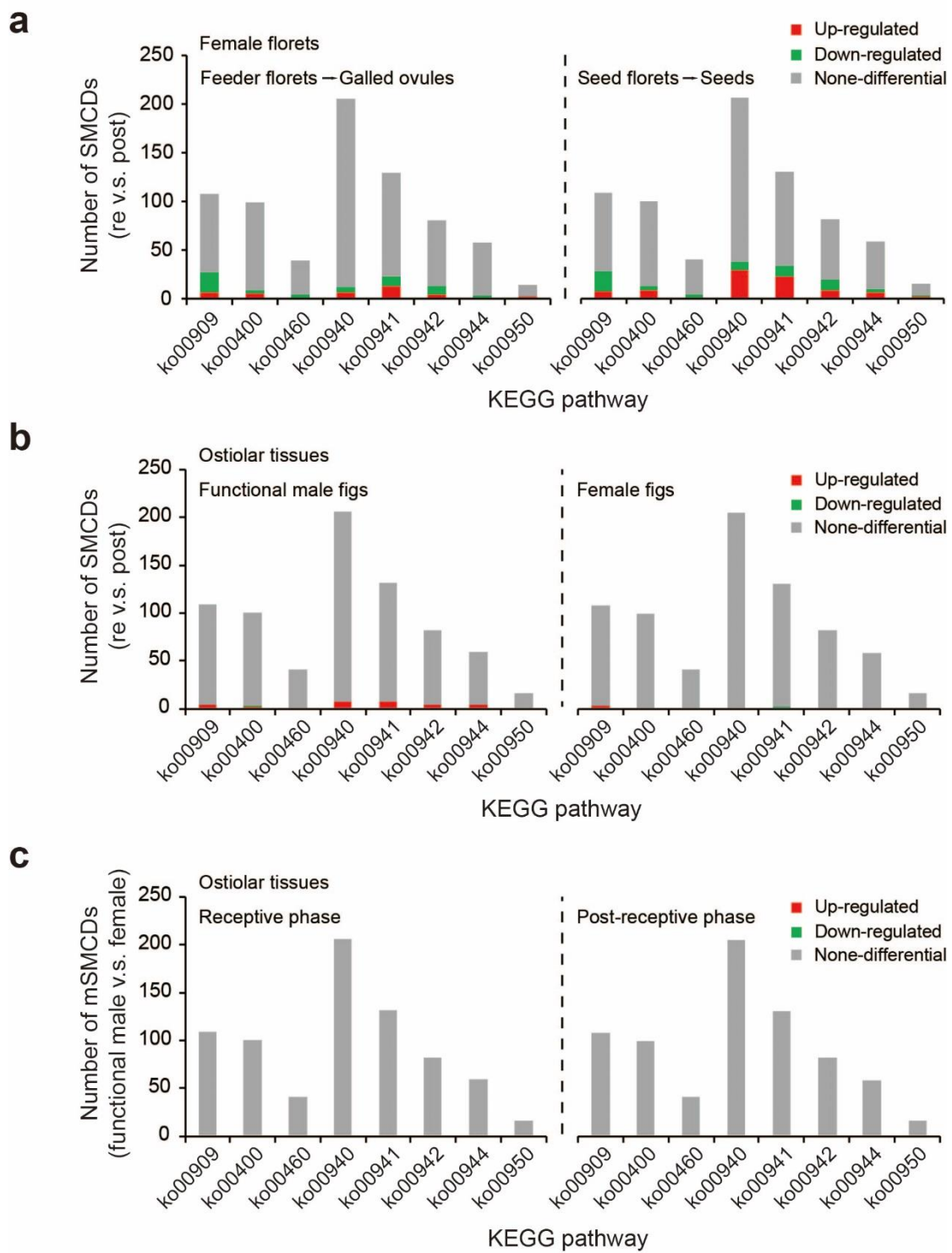




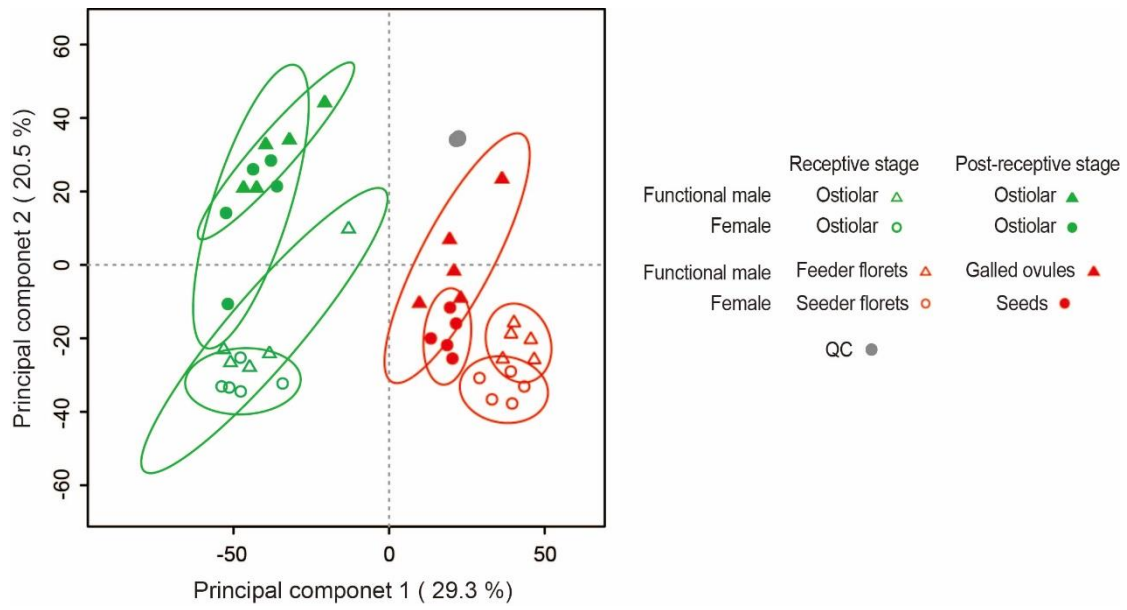
Supplementary Figure 11. Heat map of gene expression in transcriptomes (a) and changes in proteomes (b) in the pathways associated with biosynthesis of decanal and nonanal, at both the pre-receptive and the receptive stages in ostiolar tissues. In proteomes, figs at both stages from 5 individual pairs (one female and one functional male) were used to form 5 patches (one individual pair in one patch) of protein detection. In each patch, there were four comparisons between the two fig development stages (comparison 1: individual 1 stage receptive vs. individual 1 stage pre-receptive, comparison 2: individual 2 stage receptive vs. individual 2 stage pre-receptive, comparison 3: individual 1 stage receptive vs. individual 2 stage pre-receptive, comparison 4: individual 2 stage receptive vs. individual 1 stage pre-receptive), and the mean of each comparison across the five patches were used to test PSDs because direct inter-patch comparison is not available for the iTRAQ-based method. Statistical results are shown in Supplementary Table 12.



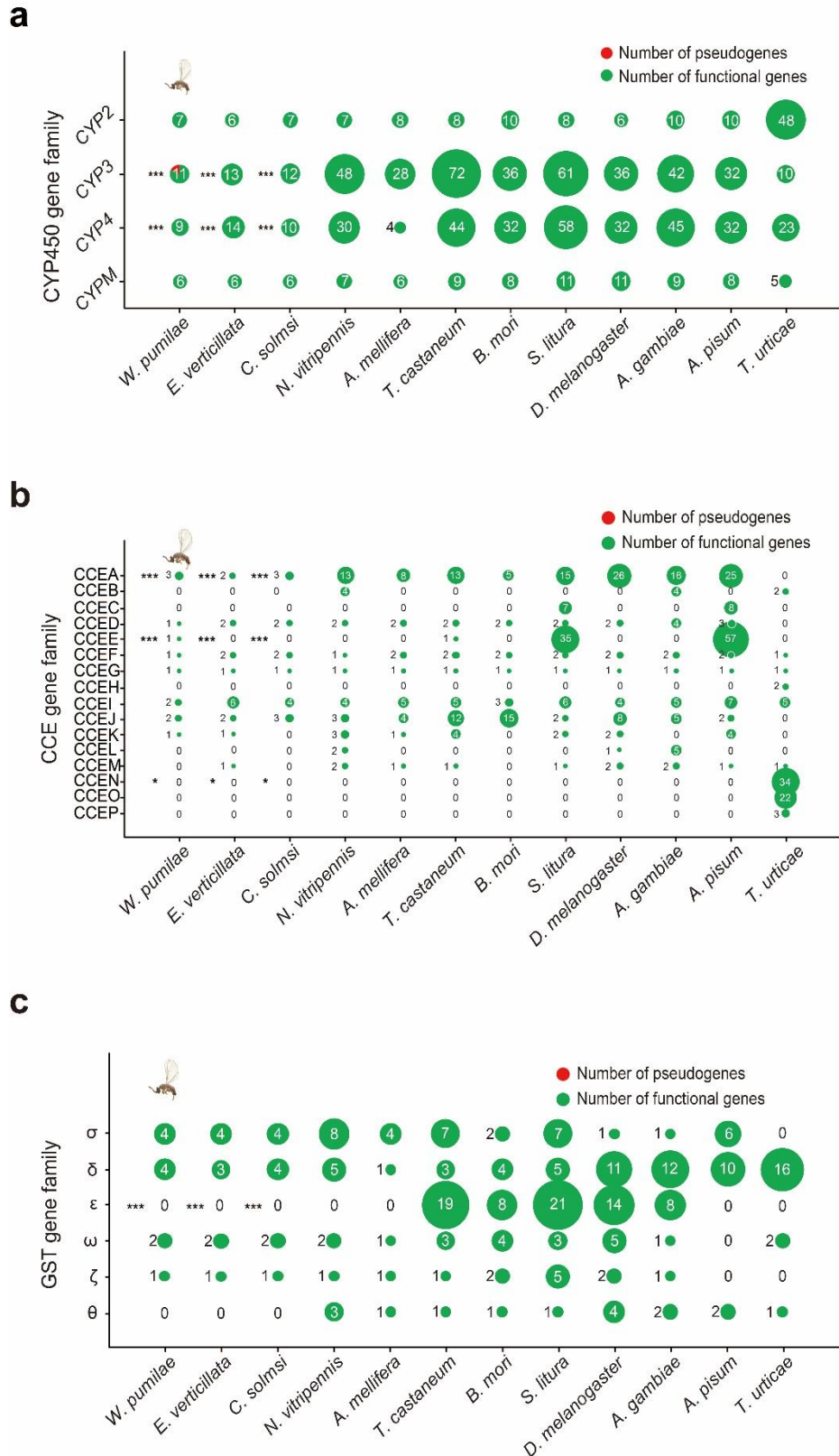
Supplementary Figure 12. Biosynthesis pathways of terpenoids and phenylpropanoids. Pathways labeled with red arrows are used to the analysis of secondary metabolites associated with plant chemical defenses (SMCDs).



Supplementary Figure 13. Distribution of secondary metabolites and those with significant difference in quantity (SMSDs) (a-c) in the pathways associated with biosynthesis of SMCDs.

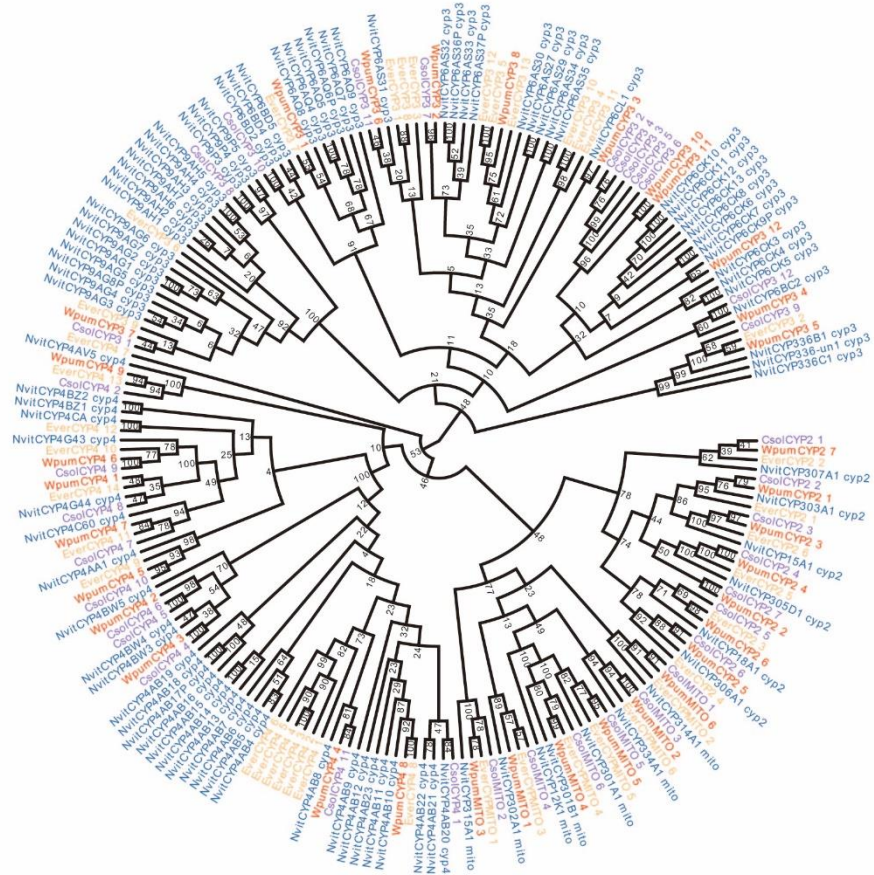


Supplementary Figure 14. Results of PLS-DA for all metabolites found in metabolomes.

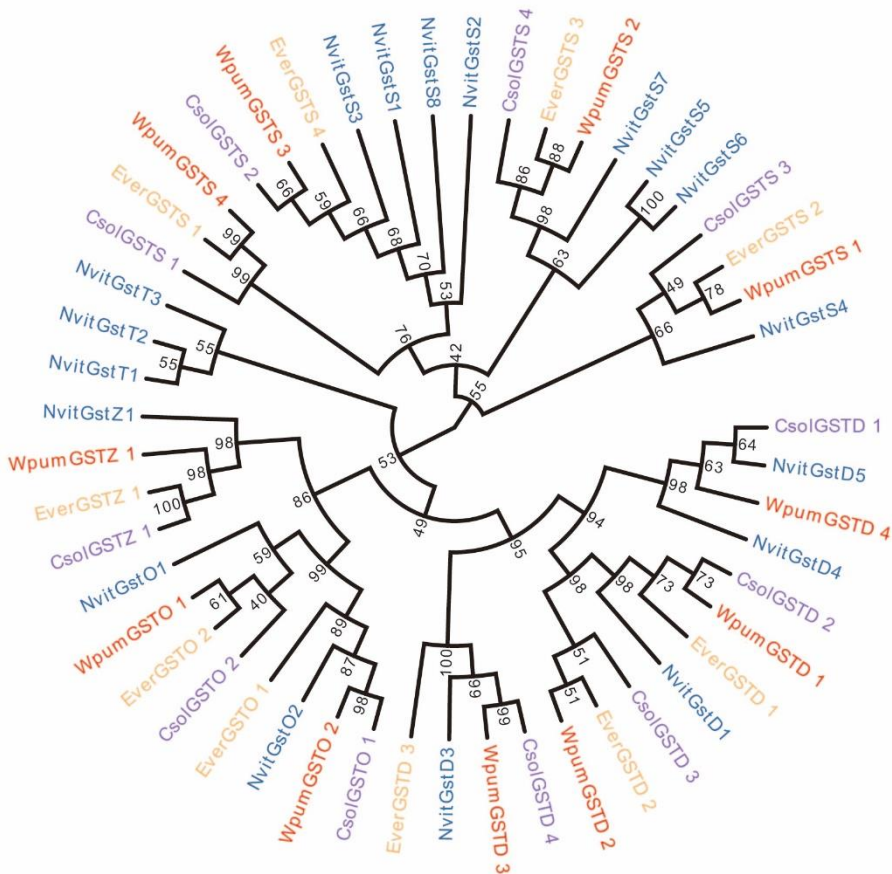


Supplementary Figure 15. Numbers of genes in CYP450, CCE (b) and GST (a) gene families in different insect species. Significantly contracted families (*: $p < 0.01$; *: $p < 0.001$) were shown for *W. pumilae*, *E. verticillata* and *C. solmsi*. The full names of CCE families are shown in Supplementary Table 16.**

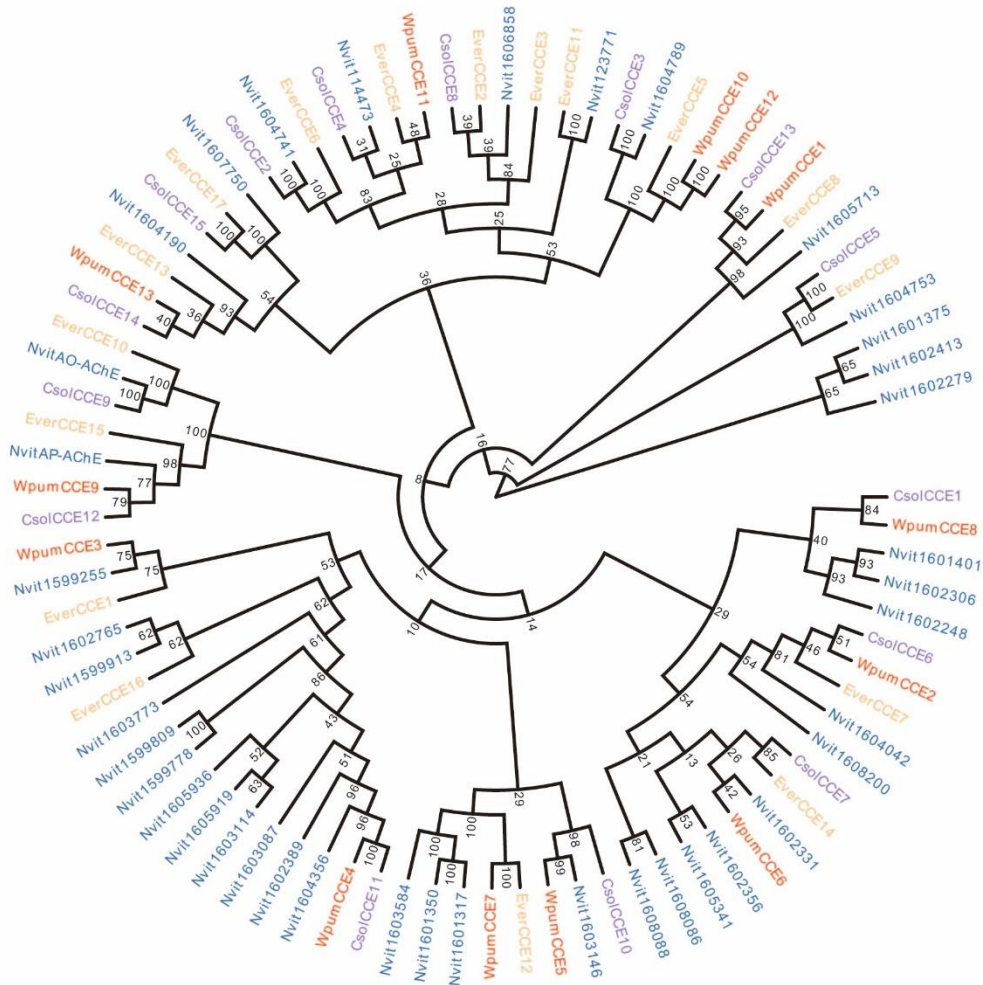
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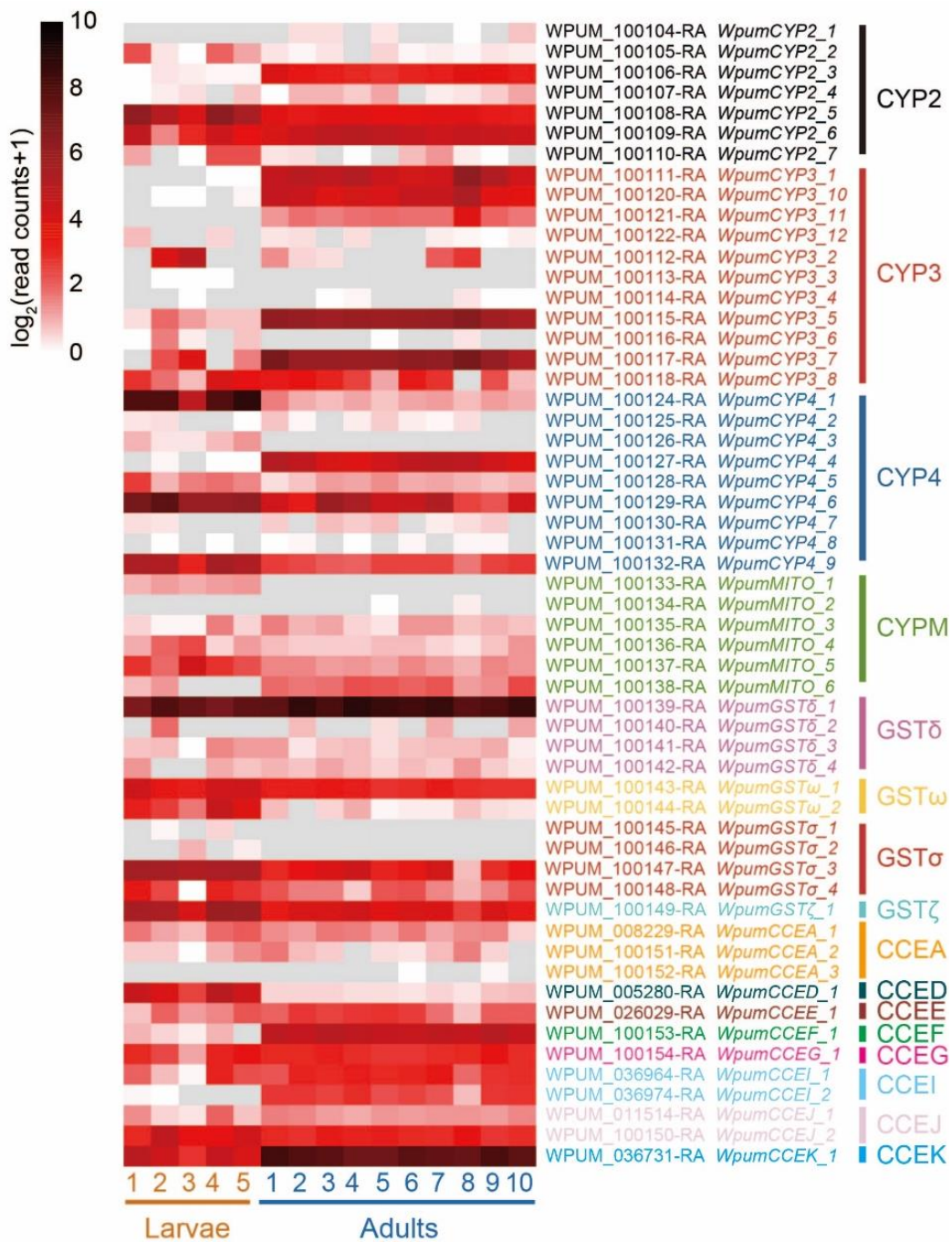
b



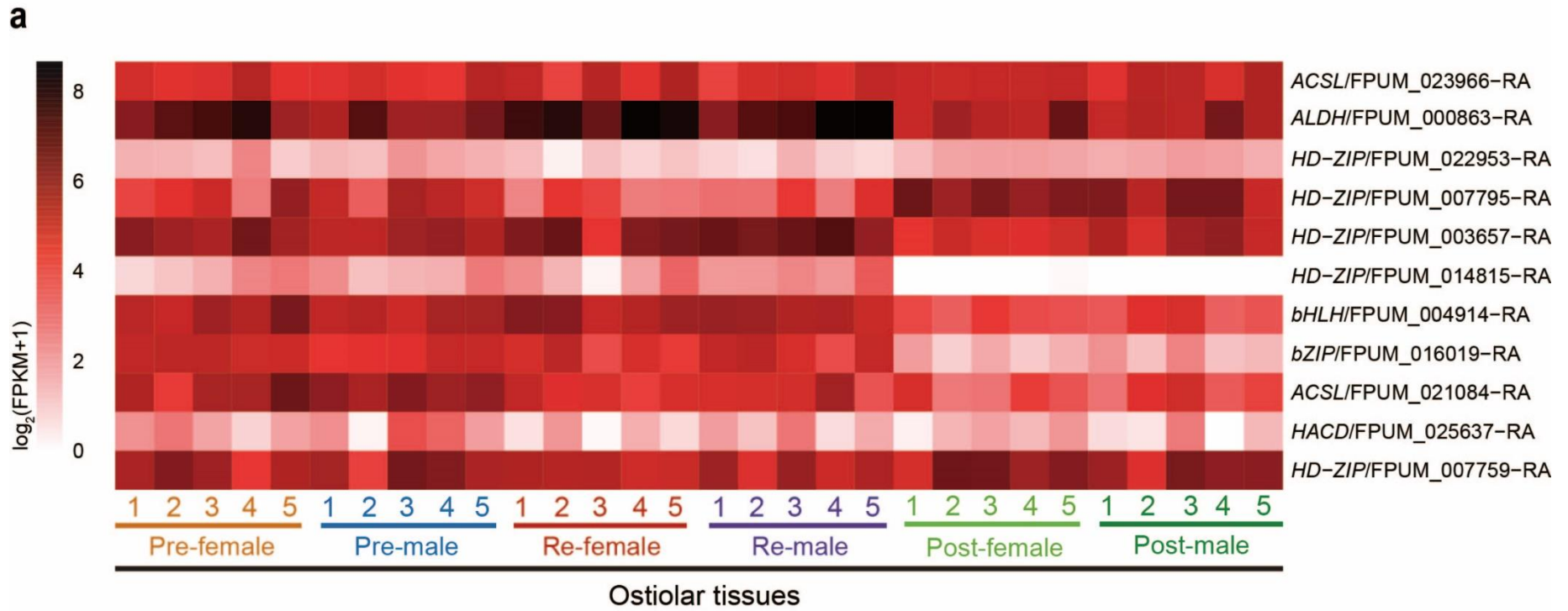
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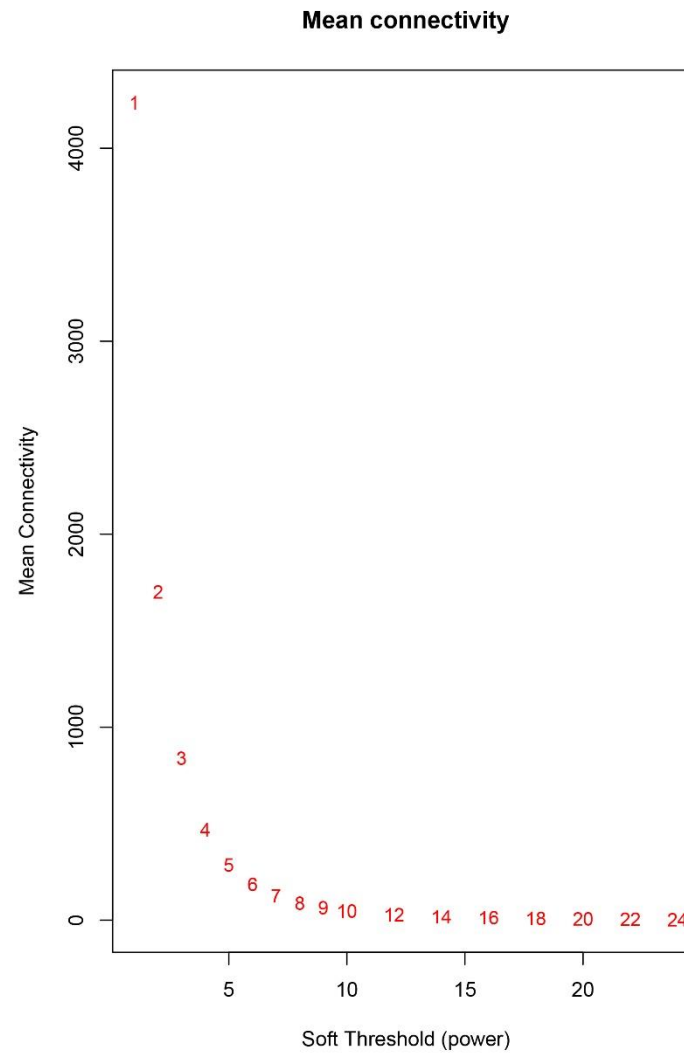
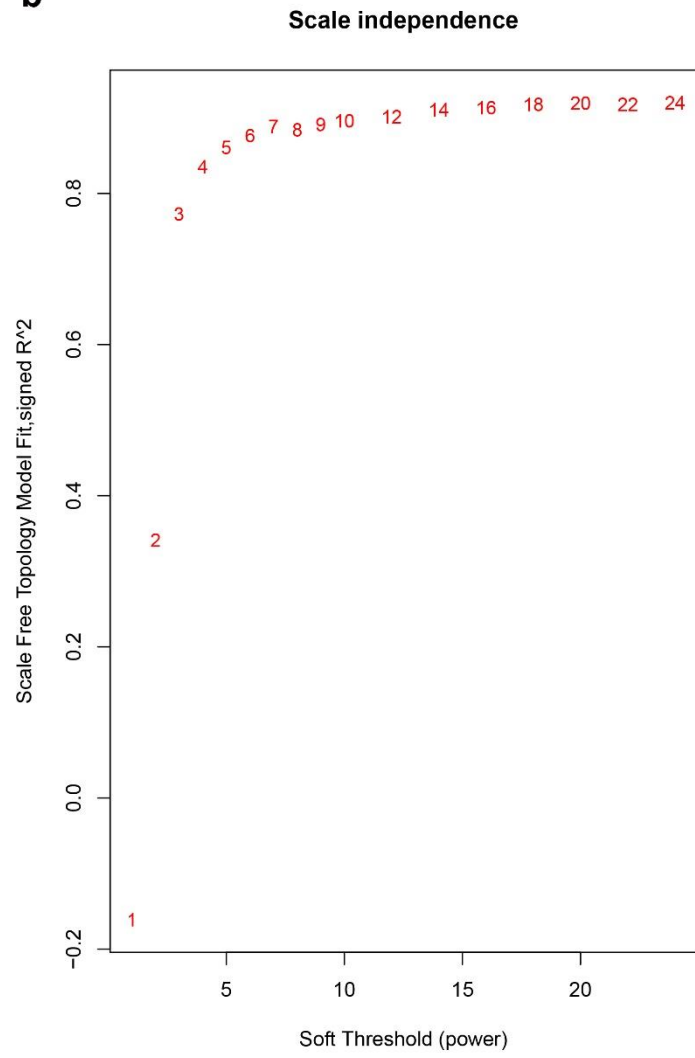
Supplementary Figure 16. Phylogenetic trees of genes in CYP450 (a), GST (b) and CCE (c) families in *W. pumilae*, *E. verticillata*, *C. solmsi* and *N. vitripennis*. The trees were constructed using TreeBeST employing neighbor-joining method and setting JTT model with 1000 bootstrapping replicates. Names of CYP450, GST and CCE genes are presented as a four-letter code (first letter of the genus followed by the first three letters of the species name) + CYP450/GST/CCE + gene numbers.

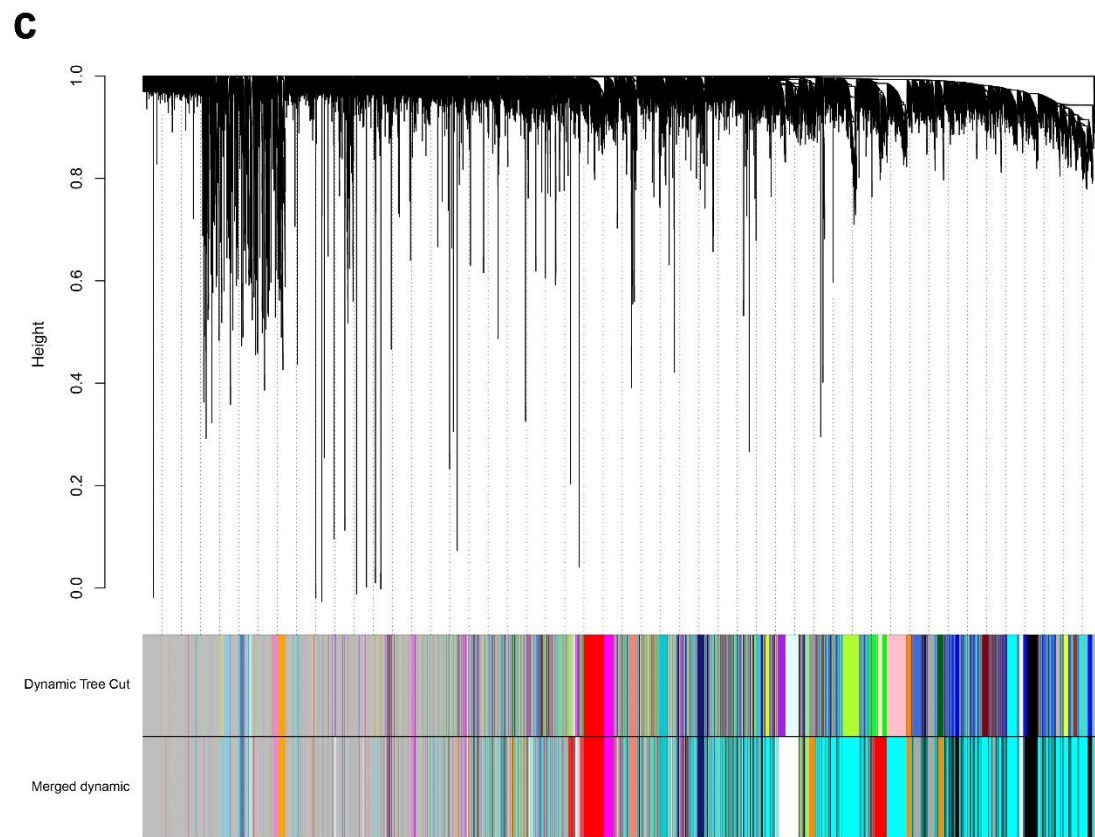


Supplementary Figure 17. Heat maps of transcriptomic expression of both adults and larvae of *W. pumilae* in CYP450, GST and CCE families. Statistical results are shown in Supplementary Table 16.



b





Supplementary Figure 18. Results of co-expression network analysis. (a) Heat map of gene expression of HD-Zip, bHLH and bZIP transcription factors and some key PSDs related to the biosynthesis of decanal and nonanal in ostiolar tissues at different fig developmental stages in transcriptomes. (b) Parameter estimations of co-expression network analysis. (c) Results of co-expression network analysis. The main results are shown in Supplementary Table 14.

Supplementary Table 1. Statistics of sequencing data.

Species	Platform	Insert size (bp)	Average Reads Length (bp)	Sequencing data (Gb)
<i>F. pumila</i>	Illumina	270	150	23.99
		350	150	40.30
		2,000	100	9.62
		5,000	100	7.79
		10,000	100	19.14
		20,000	100	14.76
	Total			115.60
	Pacbio Sequel	20,000	7,903 (N50: 14,270)	65.65
	Illumina (Hi-C)	350	300	43.00
<i>W. pumilae</i>	Illumina	350	150	29.43
		2,000	100	3.66
		5,000	100	3.33
		10,000	100	4.33
		20,000	100	4.14
		Total		
		Pacbio Sequel	20,000	8,033 (N50: 11,990)
	Illumina (Hi-C)	350	300	25.20

Supplementary Table 2. Summary of genome assemblies for both species and results of statistics assessing the quality of genome assemblies.

		<i>Ficus pumila</i> var. <i>pumila</i>	<i>Wiebesia pumilae</i>
Total length of contigs (bp)		315,674,938	318,185,153
Number of contigs		543	102
Contig N50 (bp)		2,293,275	10,940,970
Total length of scaffolds (bp)		315,725,595	318,278,179
Number of scaffolds (>2000 bp)		457	41
K-mer estimated genome size (Mb)		325.07	302.99
Genome heterozygosity		1.39%	0.24%
GC content		33.61	30.33
Repeat density		45.70%	7.72%
Hi-C	Total reads	168,180,953	84,033,799
	Uniquely mapped reads	106,478,957	71,084,500
	Hi-C contacts	85,704,535	66,300,893
	Anchored genome content (Mb)	304.82	317.54
	Anchored rate	96.56%	99.77%
	Scaffold N50 (bp)	22,360,920	59,419,729
	BUSCO	Total Number	1,440
	Complete	94.30%	94.10%
	Single-copy	89.70%	93.50%
	Duplicated	4.60%	0.60%
	Fragmented	1.70%	3.20%
	Missing	4.00%	2.70%
350bp insert size library	Total reads	271,849,877	196,985,530
	Total mapping ratio	96.93%	96.72%
	Properly paired mapping ratio	90.51%	93.03%
	Genome coverage	95.20%	99.71%
RNA-seq data	Total mapping ratio	90.14%-94.60%	71.09%-80.80%
	Uniquely mapping ratio	58.70%-78.93%	52.39%-58.34%
Iso-seq data	Total high-quality isoforms	158,620	201,648
	Mapping ratio	95.07%	93.34%

Supplementary Table 3. Results of gene structure analysis, BUSCO assessments and gene function annotation.

		<i>F. pumila</i> var. <i>pumila</i>	<i>W. pumilae</i>
Gene	Number of genes	28,187	12,316
structure	Average transcript length (bp)	4,277	10,250
	Average CDS* length (bp)	1,267	3,584
	Average exon per gene	6.00	13.46
	Average exon length (bp)	226	266
	Average intron length (bp)	473	517
BUSCO assessment†	Complete BUSCOs	1,271 (92.4%)	4,028 (91.3%)
	Single-copy BUSCOs	1227(89.2%)	4,007 (90.8%)
	Duplicated BUSCOs	44 (3.2%)	21 (0.5%)
	Fragmented BUSCOs	60 (4.4%)	192 (4.3%)
	Missing BUSCOs	44 (3.2%)	195 (4.4%)
Functional annotation	Nr	25,815 (91.6%)	10,671 (86.7%)
	Swissprot	18,988 (67.4%)	8,942 (72.6%)
	KEGG	19,267 (68.4%)	5,435 (44.2%)
	Interpro	23,635 (83.9%)	9,249 (75.1%)
	GO	16,703 (59.3%)	3,030 (24.6%)
	Overall	25,9051 (91.9%)	12,305 (99.9%)

Footnotes:

* Coding sequence.

† BUSCO assessments were conducted in protein model with 1375 and 4415 conserved genes for the plant and the pollinator.

Supplementary Table 4. Annotation of non-coding RNA.

Species	Characters	miRNA	tRNA	rRNA	snRNA
<i>F. pumila</i> var. <i>pumila</i>	N copies	96	567	303	486
	Average length (bp)	131.55	75.09	141.43	110.41
	Total length (bp)	12,629	42,575	42,853	53,659
	% of genome	0.0040	0.0135	0.0136	0.0170
<i>W. pumilae</i>	N copies	44	108	42	42
	Average length (bp)	82.82	76.45	148.62	157.81
	Total length (bp)	3,644	8,257	6,242	6,628
	% of genome	0.00115	0.00260	0.00196	0.00208

Supplementary Table 5. Results of transposable element analysis using Tandem Repeats Finder (TRF), RepeatMasker, RepeatProteinMask and *de novo* approaches (LTR_Finder, PILER and RepeatScout).

Type	<i>F. pumila</i> var. <i>pumila</i>		<i>W. pumilae</i>	
	Repeat size (Mb)	% of genome	Repeat size (Mb)	% of genome
TRF	14.60	4.62	6.22	1.95
RepeatMasker	27.11	8.59	8.44	2.65
RepeatProteinMask	16.19	5.13	1.32	0.41
<i>De novo</i>	134.91	42.73	14.04	4.41
Total	144.29	45.70	24.56	7.72

Supplementary Table 6. Results of gene family clustering based on genome assemblies of other angiosperms and arthropods.

Taxa	Species	Gene number	Genes in families	Family number	Unique families	Average gene number per family	UTL for genome sequences
Angiosperm	<i>Ficus pumila</i>	28,289	26,608	15,631	249	1.70	--
	<i>Arabidopsis thaliana</i>	27,557	25,239	13,205	739	1.91	https://www.arabidopsis.org/download/index-auto.jsp?dir=%2Fdownload_files%2FSequences%2FAraport11_blastsets
	<i>Cannabis sativa</i>	27,764	22,728	13,795	384	1.65	ftp://ftp.ncbi.nlm.nih.gov/genomes/all/GCA/000/230/575/GCA_000230575.1_canSat3
	<i>Ficus carica</i>	30,027	26,330	14,516	516	1.81	https://www.nature.com/articles/srep41124
	<i>Ficus hispida</i>	27,210	25,927	15,656	229	1.66	https://bigd.big.ac.cn/gwh/Assembly/7807/show
	<i>Ficus microcarpa</i>	29,390	28,289	15,284	182	1.85	https://bigd.big.ac.cn/gwh/Assembly/963/show
	<i>Glycine max</i>	56,223	50,182	15,665	1,559	3.20	ftp://ftp.ensemblgenomes.org/pub/plants/release-38/fasta/glycine_max
	<i>Malus domestica</i>	45,104	39,776	15,576	846	2.55	https://www.rosaceae.org/analysis/242
	<i>Morus notabilis</i>	26,965	23,458	14,910	519	1.57	http://morus.swu.edu.cn/morusdb/datasets
	<i>Oryza sativa</i>	34,549	26,920	13,602	1,710	1.98	https://rapdb.dna.affrc.go.jp/download/irgsp1.html
	<i>Populus trichocarpa</i>	40,040	36,020	15,092	785	2.39	ftp://ftp.ensemblgenomes.org/pub/plants/release-38/fasta/populus_trichocarpa
	<i>Prunus persica</i>	28,702	27,454	14,316	262	1.92	ftp://ftp.bioinfo.wsu.edu/species/Prunus_persica/Prunus_persica-genome.v1.0
	<i>Vitis vinifera</i>	29,082	25,519	14,516	611	1.76	ftp://ftp.ensemblgenomes.org/pub/plants/release-38/fasta/vitis_vinifera
<i>Ziziphus jujuba</i>	28,643	27,567	13,920	394	1.98	ftp://ftp.ncbi.nlm.nih.gov/genomes/all/GCF/000/826/755/GCF_000826755.1_ZizJuj_1.1	
Arthropod	<i>Wiebesia pumilae</i>	12,316	9,800	7,969	46	1.23	--
	<i>Anopheles gambiae</i>	12,957	10,787	7,048	254	1.53	ftp://ftp.ensemblgenomes.org/pub/metazoa/release-38/fasta/anopheles_gambiae
	<i>Apis mellifera</i>	14,920	10,710	8,607	105	1.24	http://hymenopteragenome.org/beebase/?q=download_sequences
	<i>Athalia rosae</i>	11,875	10,117	8,194	77	1.23	http://hymenopteragenome.org/beebase/?q=download_sequences
	<i>Camponotus floridanus</i>	16,115	13,145	8,543	387	1.54	http://hymenopteragenome.org/camponotus/?q=genome_consortium_datasets
	<i>Ceratosolen solmsi</i>	9,486	9,111	7,474	7	1.22	ftp://ftp.ncbi.nlm.nih.gov/genomes/all/GCF/000/503/995/GCF_000503995.1_CerSol_1.0

<i>Drosophila melanogaster</i>	13,550	10,607	6,814	334	1.56	ftp://ftp.ensemblgenomes.org/pub/metazoa/release-38/fasta/drosophila_melanogaster
<i>Eupristina verticillata</i>	14,280	11,334	7,483	95	1.51	https://bigd.big.ac.cn/search/?dbId=gwh&q=Eupristina%20verticillata%20&page=1
<i>Nasonia vitripennis</i>	16,669	14,542	8,235	723	1.77	ftp://ftp.ensemblgenomes.org/pub/metazoa/release-38/fasta/nasonia_vitripennis
<i>Spodoptera litura</i>	15,899	12,906	7,475	404	1.73	ftp://ftp.ncbi.nlm.nih.gov/genomes/all/GCF/002/706/865/GCF_002706865.1_ASM270686v1
<i>Tetranychus urticae</i>	16,911	11,314	5,894	973	1.92	ftp://ftp.ensemblgenomes.org/pub/metazoa/release-38/fasta/tetranychus_urticae
<i>Tribolium castaneum</i>	16,507	12,056	7,842	379	1.54	ftp://ftp.ensemblgenomes.org/pub/metazoa/release-38/fasta/tribolium_castaneum

Supplementary Table 7. Locations of the selected mature individuals of *F. pumila* var. *pumila* for attractive VOC(s) identification and comparative transcriptomes, proteomes and metabolomes.

Attractant identification, comparative transcriptomes, proteomes and metabolomes of fig tissues		Comparative transcriptomes and proteomes of adult female pollinators	
Sample ID	Location	Sample ID	Location
Female 1	N29°46'22.99"	--	--
	E121°41'14.46"		
Female 2	N29°47'41.31"	--	--
	E121°44'54.17"		
Female 3	N29°48'30.17"	--	--
	E121°47'24.57"		
Female 4	N29°49'58.09"	--	--
	E121°42'45.41"		
Female 5	N29°50'48.69"	--	--
	E121°42'07.30"		
Male 1	N29°47'39.71"	Male 1	N29°47'39.71"
	E121°48'23.08"		E121°48'23.08"
Male 2	N29°47'44.03"	Male 2	N29°47'44.03"
	E121°44'56.35"		E121°44'56.35"
Male 3	N29°47'40.68"	Male 3	N29°47'40.68"
	E121°43'53.76"		E121°43'53.76"
Male 4	N29°49'42.75"	Male 4	N29°49'42.75"
	E121°43'08.53"		E121°43'08.53"
Male 5	N29°50'48.28"	Male 5	N29°50'48.28"
	E121°44'05.13"		E121°44'05.13"

Supplementary Table 8. Components in VOCs emitted by female and functional male figs of *F. pumila* var. *pumila* at pre-receptive and receptive stages.

Volatile compound	Relative concentration (%)			
	FP*	MP†	FR‡	MR§
Linalool	53.47	0	11.54	44.34
Nonanal	1.55	2.66	3.75	1.52
Decanal	0	0	1.44	1.10
2-Phenyl-2-butanol	0	0	14.71	0
Isophorone	8.85	46.80	9.38	6.51
Acetophenone	7.30	3.67	9.28	6.21
2-Ethylhexanol	0	0	7.69	3.42
Dodecane	1.11	0	5.52	3.50
Tetradecane	0	0	2.56	2.51
4-Ethylacetophenone	0	0	3.82	3.82
6-Methyl-5-nonen-4-one	0	0	2.01	1.76
Diethylene glycol dibutyl ether	0	0	1.78	0
1,2,3-trimethyl-Benzene	0	0	2.54	0.48
2-Propensyre, 6-methylheptylester	0	0	1.51	0
Phenylethylene	2.65	0	1.41	0.40
Benzaldehyde	0	0	1.23	0.68
Tridecane	0	0	1.11	1.36
Decane	0.67	0	0.94	0
1,4-Xylene	0	0	0.94	0.23
Isopropenylbenzene	4.81	9.36	0.94	0.34
d-Longifolene	0	0	0.91	0.86
Diisobutyl phthalate	0	0	0.80	0
1,3-Xylene	0	0	0.78	0
Dimethyl glutarate	0	4.50	0.74	0.33
alpha-Cedrene	0	0	0.72	0.80
(1r,4r)-(+)-campho	0	0	0.63	0
Pentadecane	0	0	0.63	0.57
(+)-Dipentene	0	0	0.59	0
1-Dodecene	0	0	0.56	0
2-Ethylhexyl 2-ethylhexanonate	0	0	0.55	0.35
1-ethyl-2-methyl-Benzene	0	0	0.97	0
6-Methyl-5-hepten-2-one	0	0	0.53	0
2,6,10-Trimethyldecane	0	0	0.53	0
2-ethylhexyl acetate	0	0	0.51	0
Dimethyl succinate	0	0	0.51	0.64
Butyl butyrate	0	0	0.50	0
4,7-Dimethylundecane	0	0	0.50	0
(1-Butenyl)benzene	0	0	0.50	0
4-Methylindan	0	0	0.50	0
(Z)-3-Tetradecene	0	0	0.48	0
p-sec-Butyltoluene	0	0	0.46	0
Pentamethyl phenyl	0	0	0.44	0
Tetratriacontane	0	0	0.37	0
Hexadecane	0	0	0.36	0.33
Mesitylene	0	0	0.32	0
2,2,6,6-tetramethyl-4-methylene-Heptane	0	0	0.31	0
Benzoic acid,2-ethylhexyl ester	0	0	0.28	0
2,5-dimethyl-tetrahydro-furan	0	0	0.27	0.12
1-isopropyl-2-methylbenzene	0	0	0.24	0
Ethylbenzene	0	0	0.22	0
4-Octadecenal	0	0	0.20	0
1-Methoxy-4-ethylbenzene	0	0	0	7.77
2,6-Dimethylocta-1,7-dien-3,6-diol	0	0	0	2.43
(E)-2,6-Dimethyl-3,7-octadiene-2,6-diol	0	0	0	2.02

alpha-Terpineol	0	0	0	1.34
Azulene	0	13.00	0	1.23
Indole	0	0	0	0.38
1-Eicosanol	0	0	0	0.56
2-Ethylhexyl acrylate	0	5.59	0	0.27
1,2-xylene	0	0	0	0.24
Biphenyl	0	0	0	0.15
Methylcyclohexane	0	0	0	0.12
Butyl octyl phthalate	0	0	0	0.45
3,5-Dimethylcumene	0	1.53	0	0.42
Cystophorene	0	0	0	0.42
2-phenyl-2-propanol	14.31	6.40	0	0
2-Ethylhexanol	3.52	0	0	0
Undecane	1.77	0	0	0
Isodurene	0	4.61	0	0
1,2,4,5-Tetramethylbenzene	0	1.89	0	0

Footnotes:

* Female figs at pre-receptive stage;

† Functional male figs at pre-receptive stage;

‡ Female figs at receptive stage;

§ Functional male figs at receptive stage.

Supplementary Table 9. Results of behavioral preference tests of female pollinators examined by Y-tube olfactometer using GLMs assuming binomial distribution of residuals.

Year	Treatment	Control	NP* toward treatment	NP toward control	NP no choice	GLMs	
						z-value	p-value
2020	Decanal (0.8 ug)	Hexane	41	9	0	-5.83	<0.001
	Nonanal (0.8 ug)	Hexane	15	35	0	3.88	<0.001
	Linalool (0.8 ug)	Hexane	26	22	2	-0.82	0.415
	Decanal (0.8 ug)	DN† (0.8ug)	23	27	0	0.799	0.424
2019	Decanal (0.8 ug)	Hexane	41	17	0	-4.32	<0.001
	Nonanal (0.8 ug)	Hexane	7	26	0	4.36	<0.001
	Linalool (0.8 ug)	Hexane	19	24	4	1.08	0.282
	Decanal (0.8 ug)	DN† (0.8ug)	18	13	0	-1.26	0.206

Footnotes:

* Number of female pollinators.

† Decanal and nonanal;

Supplementary Table 10. Comparisons of gene expression and protein quantity of OBPs, CSPs, ORs, GRs and IRs between the adult females of *W. pumilae* that had or had not been in contact with the VOCs emitted by *F. pumila* var. *pumila* figs at receptive stage using DEseq2 for transcriptomes and MSstats for proteomes.

Transcriptomes		Average expression*		Log ₂ (fold change)	Adjusted p-value
Gene ID	Gene name	Control (FPKM)	fig VOCs (FPKM)		
WPUM_100001-RA	<i>WpumOBP1</i>	10.85	11.82	0.44 ± 0.97	0.999
WPUM_100002-RA	<i>WpumOBP2</i>	2143.34	2058.94	-0.04 ± 0.20	0.999
WPUM_100003-RA	<i>WpumOBP3</i>	255.83	280.18	0.12 ± 0.14	0.999
WPUM_100004-RA	<i>WpumOBP4</i>	87.39	113.26	0.31 ± 0.40	0.999
WPUM_100005-RA	<i>WpumOBP5</i>	0.56	0.846	0.53 ± 0.91	0.999
WPUM_100006-RA	<i>WpumOBP6</i>	0.30	0.41	0.53 ± 1.37	0.999
WPUM_100007-RA	<i>WpumOBP7Part</i>	0.08	0.18	1.26 ± 1.45	0.999
WPUM_100008-RA	<i>WpumOBP8</i>	2.06	2.10	0.11 ± 0.41	0.999
WPUM_100009-RA	<i>WpumOBP9</i>	260.13	234.18	-0.14 ± 0.30	0.999
WPUM_100010-RA	<i>WpumOBP10</i>	2.64	1.87	-0.49 ± 0.43	0.999
WPUM_100011-RA	<i>WpumOBP11</i>	14.97	13.66	0.19 ± 0.55	0.999
WPUM_100012-RA	<i>WpumOBP12</i>	21.96	20.26	-0.20 ± 0.24	0.999
WPUM_100013-RA	<i>WpumOR1</i>	1.15	1.08	-0.02 ± 0.41	0.999
WPUM_100014-RA	<i>WpumOR2</i>	0.06	0.05	0.50 ± 0.96	0.999
WPUM_100016-RA	<i>WpumOR4</i>	0.02	0.01	-0.87 ± NA	0.999
WPUM_100017-RA	<i>WpumOR5</i>	0.16	0.30	0.72 ± 0.75	0.999
WPUM_100018-RA	<i>WpumOR6</i>	0.02	0.02	-0.44 ± 1.88	0.999
WPUM_100020-RA	<i>WpumOR8</i>	0.15	0.20	0.35 ± 0.83	0.999
WPUM_100021-RA	<i>WpumOR9</i>	0.04	0.01	-1.56 ± 1.07	0.999
WPUM_100023-RA	<i>WpumOR11Pseu</i>	0.11	0.11	0.24 ± 1.53	0.999
WPUM_100024-RA	<i>WpumOR12</i>	0.16	0.23	0.91 ± 0.93	0.999
WPUM_100025-RA	<i>WpumOR13</i>	0.18	0.18	-0.55 ± 0.88	0.999
WPUM_100026-RA	<i>WpumOR14</i>	0.10	0.03	-1.60 ± 1.38	0.999
WPUM_100027-RA	<i>WpumOR15</i>	4.34	3.79	-0.22 ± 0.24	0.999
WPUM_100028-RA	<i>WpumOR16</i>	7.02	6.03	0.12 ± 0.44	0.999
WPUM_100029-RA	<i>WpumOR17Part</i>	2.93	2.56	0.05 ± 0.38	0.999
WPUM_100030-RA	<i>WpumOR18</i>	0.40	0.51	0.26 ± 0.91	0.999
WPUM_100031-RA	<i>WpumOR19</i>	0.25	0.29	0.75 ± 0.89	0.999
WPUM_100032-RA	<i>WpumOR20</i>	0.03	0.13	1.91 ± 1.12	0.999
WPUM_100033-RA	<i>WpumOR21</i>	0.46	0.56	-0.03 ± 0.54	0.999
WPUM_100034-RA	<i>WpumOR22</i>	0.01	0.08	3.03 ± 0.67	0.999
WPUM_100035-RA	<i>WpumOR23</i>	6.79	8.25	-0.03 ± 0.48	0.999
WPUM_100036-RA	<i>WpumOR24</i>	0.18	0.24	0.61 ± 0.32	0.999
WPUM_100037-RA	<i>WpumOR25</i>	0.53	0.59	0.25 ± 0.37	0.999
WPUM_100038-RA	<i>WpumOR26</i>	0.23	0.27	0.10 ± 0.36	0.999
WPUM_100039-RA	<i>WpumOR27</i>	2.77	2.10	-0.26 ± 0.23	0.999
WPUM_100040-RA	<i>WpumOR28</i>	0.82	0.978	0.20 ± 0.34	0.999
WPUM_100041-RA	<i>WpumOR29</i>	1.11	1.18	-0.01 ± 0.45	0.999
WPUM_100042-RA	<i>WpumOR30</i>	0.00	0.01	1.58 ± NA	0.999
WPUM_100043-RA	<i>WpumOR31</i>	0.10	0.12	-0.41 ± 1.07	0.999

WPUM_100044-RA	<i>WpumOR32</i>	8.48	10.38	0.30 ± 0.51	0.999
WPUM_100045-RA	<i>WpumOR33</i>	0.10	0.04	-1.63 ± 1.38	0.999
WPUM_100046-RA	<i>WpumOR34Part</i>	1.36	2.10	0.59 ± 0.58	0.999
WPUM_100047-RA	<i>WpumOR35Pseu</i>	2.51	2.23	-0.15 ± 0.26	0.999
WPUM_100048-RA	<i>WpumOR36</i>	0.19	0.22	-0.39 ± 1.45	0.999
WPUM_100049-RA	<i>WpumOR37Part</i>	0.81	0.80	-0.28 ± 0.71	0.999
WPUM_100050-RA	<i>WpumOR38</i>	0.16	0.25	0.91 ± 0.62	0.999
WPUM_100051-RA	<i>WpumOR39</i>	0.25	0.51	0.87 ± 0.72	0.999
WPUM_100052-RA	<i>WpumOR40</i>	0.06	0.07	-0.79 ± 2.97	0.999
WPUM_100053-RA	<i>WpumOR41</i>	0.17	0.16	-0.09 ± 0.54	0.999
WPUM_100054-RA	<i>WpumOR42</i>	0.05	0.10	0.67 ± 0.95	0.999
WPUM_100055-RA	<i>WpumOR43</i>	0.01	0.05	1.48 ± 0.94	0.999
WPUM_100056-RA	<i>WpumOR44</i>	1.69	1.28	-0.39 ± 0.35	0.999
WPUM_100057-RA	<i>WpumOR45Pseu</i>	0.10	0.10	-1.49 ± 2.40	0.999
WPUM_100058-RA	<i>WpumOR46</i>	0.24	0.34	0.12 ± 1.90	0.999
WPUM_100059-RA	<i>WpumOR47</i>	0.41	0.35	-1.08 ± 1.09	0.999
WPUM_100060-RA	<i>WpumOR48</i>	0.34	0.49	0.61 ± 0.69	0.999
WPUM_100061-RA	<i>WpumOR49</i>	0.01	0.03	0.98 ± 1.90	0.999
WPUM_100062-RA	<i>WpumOR50</i>	0.00	0.02	3.32 ± NA	0.999
WPUM_100063-RA	<i>WpumOR51</i>	0.43	0.29	-0.78 ± 0.79	0.999
WPUM_100064-RA	<i>WpumOR52</i>	0.05	0.16	1.34 ± 1.41	0.999
WPUM_100065-RA	<i>WpumOR53</i>	0.39	0.37	0.06 ± 0.63	0.999
WPUM_100066-RA	<i>WpumOR54</i>	1.59	1.57	0.00 ± 0.30	0.999
WPUM_100067-RA	<i>WpumOR55</i>	3.72	4.30	0.11 ± 0.46	0.999
WPUM_100068-RA	<i>WpumOR56</i>	3.40	4.85	0.47 ± 0.65	0.999
WPUM_100069-RA	<i>WpumOR57</i>	0.60	0.81	-0.04 ± 0.60	0.999
WPUM_100070-RA	<i>WpumOR58Pseu</i>	0.33	0.20	-1.11 ± 1.31	0.999
WPUM_100071-RA	<i>WpumOR59Part</i>	0.27	0.23	-0.94 ± 1.32	0.999
WPUM_100072-RA	<i>WpumOR60Part</i>	0.47	0.28	-0.92 ± 0.73	0.999
WPUM_100073-RA	<i>WpumOR61</i>	0.12	0.19	0.60 ± 0.80	0.999
WPUM_100074-RA	<i>WpumOR62Pseu</i>	0.07	0.05	-1.16 ± 1.22	0.999
WPUM_100075-RA	<i>WpumOR63</i>	0.16	0.12	0.37 ± 1.070	0.999
WPUM_100076-RA	<i>WpumOR64</i>	0.19	0.33	1.16 ± 0.57	0.999
WPUM_100077-RA	<i>WpumOR65</i>	8.72	9.27	-0.12 ± 0.40	0.999
WPUM_100078-RA	<i>WpumOR66</i>	0.01	0.00	-1.58 ± NA	0.999
WPUM_100079-RA	<i>WpumOR67</i>	0.49	0.37	-0.25 ± 0.40	0.999
WPUM_100080-RA	<i>WpumCSP1</i>	2963.47	2850.88	-0.07 ± 0.13	0.999
WPUM_100081-RA	<i>WpumCSP2</i>	15.57	15.18	-0.07 ± 0.27	0.999
WPUM_100082-RA	<i>WpumCSP3</i>	69.40	67.47	-0.10 ± 0.16	0.999
WPUM_100083-RA	<i>WpumCSP4</i>	1022.76	871.64	-0.21 ± 0.21	0.999
WPUM_100084-RA	<i>WpumCSP5</i>	26.09	27.57	0.03 ± 0.27	0.999
WPUM_100085-RA	<i>WpumCSP6</i>	55.94	51.97	0.02 ± 0.56	0.999
WPUM_100086-RA	<i>WpumCSP7</i>	37.98	47.05	0.31 ± 0.21	0.999
WPUM_100087-RA	<i>WpumCSP8</i>	36.43	26.62	-0.43 ± 0.87	0.999
WPUM_100092-RA	<i>WpumIR1</i>	0.27	0.34	0.22 ± 0.48	0.999
WPUM_100093-RA	<i>WpumIR6</i>	8.29	7.65	-0.08 ± 0.15	0.999
WPUM_100094-RA	<i>WpumIR7</i>	4.45	4.54	0.01 ± 0.14	0.999
WPUM_100095-RA	<i>WpumIR8</i>	31.22	20.64	-0.43 ± 0.48	0.999
WPUM_100096-RA	<i>WpumIR9</i>	2.76	2.71	0.14 ± 0.33	0.999

WPUM_100097-RA	<i>WpumIR10</i>	5.53	5.83	0.07 ± 0.36	0.999
WPUM_100098-RA	<i>WpumIR11</i>	3.59	3.84	0.12 ± 0.41	0.999
WPUM_100099-RA	<i>WpumIR12</i>	0.83	1.15	0.44 ± 0.22	0.999
WPUM_100100-RA	<i>WpumIR13</i>	0.87	0.75	-0.04 ± 0.33	0.999
WPUM_100101-RA	<i>WpumIR14</i>	0.55	0.61	-0.21 ± 0.53	0.999
WPUM_100102-RA	<i>WpumIR15</i>	0.07	0.15	1.21 ± 0.69	0.999
WPUM_100103-RA	<i>WpumIR16</i>	0.59	0.38	-0.64 ± 0.47	0.999

Proteomes

Protein ID	Protein name	Average quantification		Log ₂ (fold change)	Adjusted p-value
		Not contacting VOCs (quantified)	Contacting VOCs (quantified)		
WPUM_100002-RA	WpumOBP2	21.23	21.40	0.20 ± 0.12	0.551
WPUM_100003-RA	WpumOBP3	19.30	19.65	0.36 ± 0.18	0.516
WPUM_100004-RA	WpumOBP4	15.04	15.25	0.22 ± 0.15	0.586
WPUM_100009-RA	WpumOBP9	13.67	13.83	0.16 ± 0.40	0.857
WPUM_100010-RA	WpumOBP10	12.67	12.13	-0.44 ± 0.89	0.821
WPUM_100012-RA	WpumOBP12	10.44	11.22	0.30 ± 0.08	0.551
WPUM_100084-RA	WpumCSP1	21.44	21.54	0.09 ± 0.17	0.807
WPUM_100086-RA	WpumCSP3	14.43	14.34	-0.10 ± 0.47	0.915
WPUM_100087-RA	WpumCSP4	13.60	13.92	0.32 ± 0.38	0.700
WPUM_100088-RA	WpumCSP5	13.05	13.15	0.11 ± 0.14	0.727
WPUM_100090-RA	WpumCSP7	14.27	14.20	-0.11 ± 0.28	0.855

Footnote:

* The average expression (or average quantification) was calculated as the sum of gene expression in different samples divided by total sample size.

Supplementary Table 11. The binding affinities (K_D) of WpumOBP2 and WpumOBP11 to decanal and nonanal using surface plasmon resonance (SPR). We calculated K_D values using both steady state affinity (see Supplementary Fig. 10) and 1:1 binding model for the two OBPs.

Gene	Substrate	Fitting model	K_a (1/M/s)	K_d (1/s)	K_D ($M \times 10^{-4}$)	Rmax (RU)	Chi ² (RU ²)
WpumOBP2	Decanal	Steady state affinity	--	--	1.46 ± 0.54	1.58 ± 0.21	0.002
	Nonanal	Steady state affinity	--	--	39.4 ± 5.6	6.80 ± 0.76	0.007
	Decanal	1:1 binding	227.7 ± 2.7	$6.3 \times 10^{-3} \pm 8.0 \times 10^{-5}$	0.28	1.05 ± 0.01	0.008
	Nonanal	1:1 binding	15.1 ± 1.5	$3.0 \times 10^{-2} \pm 5.4 \times 10^{-4}$	20.1	1.64 ± 0.13	0.005
WpumOBP11	Decanal	Steady state affinity	--	--	30.7 ± 3.1	144.76 ± 11.30	3.19
	Nonanal	Steady state affinity	--	--	1.31 ± 0.62	15.86 ± 1.46	1.07
	Decanal	1:1 binding	0.2 ± 0.02	$4.6 \times 10^{-3} \pm 1.9 \times 10^{-4}$	224.3	1148.5 ± 120.0	1.88
	Nonanal	1:1 binding	151.70 ± 6.2	$6.8 \times 10^{-3} \pm 2.9 \times 10^{-4}$	0.45	1.55 ± 0.03	0.12

Supplementary Table 12. Comparisons of gene expression and protein quantity in pathways associated with biosynthesis of decanal and nonanal between pre-receptive and receptive stage in ostiolar tissues using DEseq2 for transcriptomes and IQant (iTRAQ) for proteomes.

Transcriptomes of ostiolar tissues

Gene ID	Enzyme name	Average expression*		Log ₂ (fold change)	Adjusted p-value
		FPKM pre	FPKM re		
FPUM_001915-RA	<i>FpumACC1</i>	31.77	35.51	0.18 ± 0.11	0.456
FPUM_003590-RA	<i>FpumACC2</i>	25.16	15.94	-0.62 ± 0.18	0.015
FPUM_004970-RA	<i>FpumACC3</i>	1.56	1.18	-0.38 ± 0.45	0.703
FPUM_010927-RA	<i>FpumACC4</i>	84.65	70.59	-0.23 ± 0.15	0.353
FPUM_018075-RA	<i>FpumACC5</i>	28.28	23.80	-0.22 ± 0.07	0.136
FPUM_019910-RA	<i>FpumACC6</i>	55.95	64.63	0.22 ± 0.10	0.351
FPUM_021302-RA	<i>FpumACC7</i>	14.56	15.39	0.10 ± 0.11	0.731
FPUM_022823-RA	<i>FpumACC8</i>	2.80	2.86	0.05 ± 0.20	0.904
FPUM_026175-RA	<i>FpumACC9</i>	24.66	24.55	0.04 ± 0.09	0.883
FPUM_013932-RA	<i>FpumACOT1_2_4-1</i>	21.68	31.48	0.54 ± 0.21	0.041
FPUM_002965-RA	<i>FpumACSL1</i>	23.82	24.24	0.03 ± 0.13	0.923
FPUM_007189-RA	<i>FpumACSL2</i>	77.81	35.76	-1.10 ± 0.21	< 0.001
FPUM_010395-RA	<i>FpumACSL3</i>	1.27	1.70	-1.06 ± 0.79	0.296
FPUM_015725-RA	<i>FpumACSL4</i>	5.51	7.19	0.39 ± 0.30	0.409
FPUM_017226-RA	<i>FpumACSL5</i>	51.00	49.42	-0.03 ± 0.11	0.938
FPUM_017765-RA	<i>FpumACSL6</i>	4.81	3.12	-0.53 ± 0.11	0.398
FPUM_019840-RA	<i>FpumACSL7</i>	78.79	69.90	-0.15 ± 0.12	0.413
FPUM_021084-RA	<i>FpumACSL8</i>	60.11	28.47	-1.01 ± 0.28	0.001
FPUM_023962-RA	<i>FpumACSL9</i>	8.15	5.27	-0.57 ± 0.32	0.321
FPUM_023966-RA	<i>FpumACSL10</i>	28.26	30.05	0.11 ± 0.18	0.804
FPUM_002455-RA	<i>FpumADH1</i>	2.49	2.61	0.05 ± 0.45	0.980
FPUM_004466-RA	<i>FpumADH2</i>	0.10	0.13	0.35 ± 0.75	0.760
FPUM_009770-RA	<i>FpumADH3</i>	6.59	6.75	0.08 ± 0.23	0.893
FPUM_016180-RA	<i>FpumADH4</i>	32.92	27.21	-0.24 ± 0.16	0.464
FPUM_017349-RA	<i>FpumADH5</i>	36.27	32.47	-0.12 ± 0.33	0.872
FPUM_020251-RA	<i>FpumADH6</i>	208.21	227.19	0.15 ± 0.18	0.564
FPUM_026410-RA	<i>FpumADH7</i>	27.10	31.09	0.20 ± 0.17	0.468
FPUM_000863-RA	<i>FpumALDH1</i>	111.15	245.52	1.09 ± 0.34	0.015
FPUM_003784-RA	<i>FpumALDH2</i>	48.91	44.51	-0.11 ± 0.12	0.641
FPUM_007900-RA	<i>FpumALDH3</i>	1.61	1.85	0.21 ± 0.64	0.858
FPUM_014425-RA	<i>FpumALDH4</i>	21.00	23.50	0.08 ± 0.12	0.760
FPUM_014532-RA	<i>FpumALDH5</i>	58.12	66.21	0.19 ± 0.18	0.585
FPUM_018466-RA	<i>FpumALDH6</i>	13.87	13.46	-0.02 ± 0.10	0.934
FPUM_024788-RA	<i>FpumALDH7</i>	52.81	60.35	0.19 ± 0.26	0.741
FPUM_024789-RA	<i>FpumALDH8</i>	3.18	3.57	0.16 ± 0.33	0.913
FPUM_024790-RA	<i>FpumALDH9</i>	0.99	1.60	0.47 ± 0.78	0.726

FPUM_027447-RA	<i>FpumALDH10</i>	21.37	19.26	-0.12 ± 0.25	0.827
FPUM_019567-RA	<i>FpumdesA1-1</i>	147.50	193.20	0.41 ± 0.11	0.161
FPUM_016077-RA	<i>FpumFabD1</i>	20.61	24.68	0.29 ± 0.21	0.494
FPUM_014397-RA	<i>FpumFabF1</i>	69.70	61.86	-0.18 ± 0.25	0.823
FPUM_026976-RA	<i>FpumFabF2</i>	1.16	1.37	0.27 ± 0.29	0.655
FPUM_001465-RA	<i>FpumFabG1</i>	26.36	35.79	0.46 ± 0.19	0.095
FPUM_001505-RA	<i>FpumFabG2</i>	5.66	9.05	0.67 ± 0.30	0.138
FPUM_006951-RA	<i>FpumFabG3</i>	17.99	17.13	-0.04 ± 0.27	0.959
FPUM_008100-RA	<i>FpumFabG4</i>	8.02	5.41	-0.31 ± 0.10	0.083
FPUM_024527-RA	<i>FpumFabG5</i>	19.63	26.66	0.46 ± 0.12	0.021
FPUM_016875-RA	<i>FpumFabH1</i>	19.83	22.36	0.19 ± 0.12	0.370
FPUM_026313-RA	<i>FpumFabI1</i>	41.35	48.98	0.23 ± 0.16	0.403
FPUM_027935-RA	<i>FpumFabI2</i>	2.59	2.22	-0.16 ± 0.36	0.839
FPUM_000643-RA	<i>FpumFabZ1</i>	0.38	0.22	-0.68 ± 0.89	0.457
FPUM_000645-RA	<i>FpumFabZ2</i>	18.98	24.57	0.40 ± 0.17	0.086
FPUM_000129-RA	<i>FpumFATB1</i>	4.45	3.40	-0.36 ± 0.17	0.071
FPUM_025637-RA	<i>FpumHACD1</i>	5.22	2.89	-0.75 ± 0.34	0.186
FPUM_008802-RA	<i>FpumHPL1</i>	106.44	239.95	1.13 ± 0.27	< 0.001
FPUM_008044-RA	<i>FpumKAR1</i>	34.42	31.99	-0.08 ± 0.14	0.852
FPUM_008045-RA	<i>FpumKAR2</i>	3.00	2.34	-0.31 ± 0.18	0.581
FPUM_027679-RA	<i>FpumKAR3</i>	3.63	2.28	-0.60 ± 0.41	0.238
FPUM_003818-RA	<i>FpumKCS1</i>	87.67	60.89	-0.48 ± 0.26	0.222
FPUM_005188-RA	<i>FpumKCS2</i>	467.89	407.78	-0.15 ± 0.48	0.868
FPUM_005722-RA	<i>FpumKCS3</i>	18.46	5.75	-1.59 ± 0.27	< 0.001
FPUM_021156-RA	<i>FpumKCS4</i>	47.15	32.85	-0.46 ± 0.34	0.472
FPUM_008117-RA	<i>FpumLOX2S1</i>	35.52	48.53	0.44 ± 0.28	0.247
FPUM_026285-RA	<i>FpumLOX2S2</i>	0.79	11.91	2.00 ± 0.81	0.002
FPUM_026288-RA	<i>FpumLOX2S3</i>	3.51	43.36	1.99 ± 0.90	0.011
FPUM_026289-RA	<i>FpumLOX2S4</i>	5.32	67.72	1.95 ± 0.91	0.015
FPUM_026291-RA	<i>FpumLOX2S5</i>	0.00	0.04	0.75 ± 0.58	NA
FPUM_005632-RA	<i>FpumTER1</i>	21.84	13.86	-0.60 ± 0.22	0.137

Proteomes of ostiolar tissues

Protein ID	Protein name	Mean fold change	p-value
FPUM_001915-RA	FpumACC1	0.98 ± 0.05	0.606
FPUM_003590-RA	FpumACC2	1.03 ± 0.01	0.149
FPUM_004970-RA	FpumACC3	0.92 ± 0.04	0.099
FPUM_010927-RA	FpumACC4	1.05 ± 0.01	0.002
FPUM_018075-RA	FpumACC5	0.98 ± 0.02	0.390
FPUM_019910-RA	FpumACC6	1.03 ± 0.01	0.014
FPUM_021302-RA	FpumACC7	1.01 ± 0.03	0.790
FPUM_022823-RA	FpumACC8	0.88 ± 0.12	0.320
FPUM_026175-RA	FpumACC9	1.08 ± 0.03	0.070
FPUM_003591-RA	FpumACC10	0.97 ± 0.03	0.343
FPUM_013932-RA	FpumACOT1_2_4-1	1.00 ± 0.02	0.845
FPUM_002965-RA	FpumACSL1	1.01 ± 0.01	0.519
FPUM_007189-RA	FpumACSL2	0.94 ± 0.02	0.074
FPUM_010395-RA	FpumACSL3	0.98 ± 0.02	0.459
FPUM_015725-RA	FpumACSL4	0.98 ± 0.02	0.390
FPUM_017226-RA	FpumACSL5	0.98 ± 0.04	0.645
FPUM_017765-RA	FpumACSL6	0.92 ± 0.12	0.479
FPUM_019840-RA	FpumACSL7	0.97 ± 0.02	0.165
FPUM_021084-RA	FpumACSL8	0.83 ± 0.02	0.003
FPUM_023962-RA	FpumACSL9	1.00 ± 0.03	0.865
FPUM_023966-RA	FpumACSL10	0.75 ± 0.04	0.016
FPUM_002455-RA	FpumADH1	0.94 ± 0.07	0.371
FPUM_004466-RA	FpumADH2	1.65 ± 0.34	0.126
FPUM_009770-RA	FpumADH3	0.89 ± 0.06	0.134
FPUM_016180-RA	FpumADH4	0.82 ± 0.01	0.001
FPUM_017349-RA	FpumADH5	1.03 ± 0.05	0.700
FPUM_020251-RA	FpumADH6	0.96 ± 0.03	0.194
FPUM_026410-RA	FpumADH7	0.90 ± 0.02	0.025
FPUM_000863-RA	FpumALDH1	1.49 ± 0.12	0.017
FPUM_003784-RA	FpumALDH2	0.96 ± 0.05	0.456
FPUM_007900-RA	FpumALDH3	0.99 ± 0.03	0.770
FPUM_014425-RA	FpumALDH4	0.92 ± 0.01	0.004
FPUM_014532-RA	FpumALDH5	0.94 ± 0.07	0.388
FPUM_018466-RA	FpumALDH6	0.94 ± 0.01	0.021
FPUM_024788-RA	FpumALDH7	0.98 ± 0.01	0.177
FPUM_024789-RA	FpumALDH8	1.19 ± 0.18	0.374
FPUM_024790-RA	FpumALDH9	1.00 ± 0.06	0.968
FPUM_027447-RA	FpumALDH10	0.95 ± 0.01	0.032
FPUM_019567-RA	FpumdesA1-1	1.09 ± 0.03	0.060
FPUM_016077-RA	FpumFabD1	0.98 ± 0.04	0.580
FPUM_014397-RA	FpumFabF1	1.15 ± 0.02	0.006
FPUM_026976-RA	FpumFabF2	1.04 ± 0.03	0.202

FPUM_001465-RA	FpumFabG1	0.99 ± 0.07	0.798
FPUM_001505-RA	FpumFabG2	1.23 ± 0.11	0.107
FPUM_006951-RA	FpumFabG3	0.98 ± 0.05	0.717
FPUM_008100-RA	FpumFabG4	0.96 ± 0.05	0.461
FPUM_024527-RA	FpumFabG5	1.09 ± 0.01	0.004
FPUM_016875-RA	FpumFabH1	0.97 ± 0.02	0.283
FPUM_026313-RA	FpumFabI1	0.98 ± 0.01	0.160
FPUM_027935-RA	FpumFabI2	1.06 ± 0.07	0.510
FPUM_000643-RA	FpumFabZ1	0.98 ± 0.06	0.761
FPUM_000645-RA	FpumFabZ2	0.94 ± 0.04	0.218
FPUM_000129-RA	FpumFATB1	0.95 ± 0.05	0.336
FPUM_025637-RA	FpumHACD1	0.74 ± 0.05	0.019
FPUM_008802-RA	FpumHPL1	1.25 ± 0.08	0.047
FPUM_008044-RA	FpumKAR1	0.95 ± 0.03	0.154
FPUM_008045-RA	FpumKAR2	1.02 ± 0.03	0.677
FPUM_027679-RA	FpumKAR3	1.09 ± 0.05	0.157
FPUM_003818-RA	FpumKCS1	0.95 ± 0.02	0.092
FPUM_005188-RA	FpumKCS2	0.93 ± 0.02	0.041
FPUM_021156-RA	FpumKCS4	0.97 ± 0.02	0.316
FPUM_008117-RA	FpumLOX2S1	1.05 ± 0.03	0.167
FPUM_026285-RA	FpumLOX2S2	3.21 ± 0.17	< 0.001
FPUM_026288-RA	FpumLOX2S3	1.31 ± 0.10	0.044
FPUM_026289-RA	FpumLOX2S4	1.23 ± 0.11	0.126
FPUM_026291-RA	FpumLOX2S5	1.22 ± 0.09	0.071
FPUM_005632-RA	FpumTER1	0.98 ± 0.03	0.559

Footnotes:

* The average expression (or average quantification) was calculated as the sum of gene expression in different samples divided by total sample size.

Supplementary Table 13. Results of co-expression network analysis showing that two HD-ZIP, one bHLH and one bZIP transcription factors and two functional genes (ACSL and ALDH) were assigned into the same module.

Gene ID	Gene name	Module	k ME	p-value of k ME
FPUM_023966-RA	<i>FpumACSL10</i>	Cyan	-0.45	0.012
FPUM_000863-RA	<i>FpumALDH1</i>	Cyan	0.59	0.001
FPUM_003657-RA	<i>FpumHD-ZIP1</i>	Cyan	0.68	0.000
FPUM_007795-RA	<i>FpumHD-ZIP2</i>	Cyan	-0.68	0.000
FPUM_004914-RA	<i>FpumbHLH1</i>	Cyan	0.88	0.000
FPUM_016019-RA	<i>FpumbZIP1</i>	Cyan	0.98	0.000

Supplementary Table 14. Binding motifs located on 2-kb promoter sequences upstream of four key functional genes involved in biosynthesis of nonanal and decanal in figs of *F. pumila* var. *pumila* and prediction of functions of these motifs using cis-element detection in MEME Suite 5.0.4. The ACSL gene (FPUM_023966-RA) has G-box binding motif that can be bound by both bHLH and bZIP transcription factors. The ALDH gene (FPUM_000863-RA) has both G-box and HD-Zip binding motifs and the latter can be bound by HD-ZIP transcription factors. The ADH gene (FPUM_016180-RA) has G-box binding motif that can be bound by bZIP transcription factor.

Binding motif	<i>FpumACSL8</i>	<i>FpumACSL10</i>	<i>FpumALDH1</i>	<i>FpumADH4</i>	Predicted function
G-box	0	1	6	5	cis-acting regulatory element involved in light responsiveness
HD-Zip	0	0	1	1	element involved in differentiation of the palisade mesophyll cells
ACE	2	0	0	0	cis-acting element involved in light responsiveness
box 4	4	2	4	2	part of a conserved DNA module involved in light responsiveness
Gap-box	0	1	0	0	part of a light responsive element
ATC-motif	0	0	1	0	part of a conserved DNA module involved in light responsiveness
GT1-motif	0	0	2	0	light responsive element
I-box	0	0	0	0	part of a light responsive element
GTGGC-motif	1	0	0	0	part of a light responsive element
Sp1	0	0	0	0	light responsive element
GATA-motif	2	1	0	0	part of a light responsive element
chs-CMA2a	0	5	1	0	part of a light responsive element
TCT-motif	0	0	1	1	part of a light responsive element

Supplementary Table 15. The dominant (top 10% based on ion intensities) secondary metabolites associated with plant chemical defenses (SMCDs) in ostiolar tissues and female florets (including galled ovules and seeds).

Phenylpropanoids

Compound.ID	Average ion intensity (TIC × 100,000)		Pathway	KEGG.ID	Description
	Ostiolar tissues	Female florets			
8.20_163.0390m/z	864.20	800.16	ko00400, ko00940, ko00950	C01179, C01197	3-(4-Hydroxyphenyl)pyruvate; 4-Hydroxyphenylpyruvate; p-Hydroxyphenylpyruvicacid; Caffeate; Caffeicacid; 3,4-Dihydroxy-trans-cinnamate; trans-Caffeate; (2E)-3-(3,4-Dihydroxyphenyl)prop-2-enoate; 4-Hydroxyphenylpyruvicacid
6.19_177.0540m/z	452.96	459.33	ko00400, ko00940	C02666, C12205, C20327	Coniferylaldehyde; Coniferaldehyde; 4-Hydroxy-3-methoxycinnamaldehyde; Ferulaldehyde; 5-Hydroxyconiferylalcohol; 2-Oxo-4-phenylbutyricacid; 2-Oxo-4-phenylbutanoicacid; 2-Oxo-4-phenylbutanoate; (2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal
0.75_130.0862m/z	641.18	587.37	ko00460	C20310	N-Hydroxy-L-isoleucine;
7.57_281.0444m/z	289.22	291.82	ko00944	C04293, C10098	Chrysoeriol; 5,7,4'-Trihydroxy-3'-methoxyflavone; 3'-O-Methyluteolin; Kaempferide; Kempferide; Kaempferol4'-methylether;
12.97_140.0685m/z	278.08	258.03	ko00460	C00183	L-Valine; 2-Amino-3-methylbutyricacid;
4.06_203.0820m/z	95.89	70.60	ko00400	C00078	L-Tryptophan; Tryptophan; (S)-alpha-Amino-beta-(3-indolyl)-propionicacid;
0.62_260.0287n	89.54	72.41	ko00400	C01094	D-Fructose1-phosphate;
3.61_120.0806m/z	92.98	95.26	ko00950	C00483	Tyramine; 2-(p-Hydroxyphenyl)ethylamine;

3.61_148.0520n	66.62	63.53	ko00940	C00423, C05608	trans-Cinnamate; trans-Cinnamicacid; (E)-Cinnamate; (2E)-3-Phenylprop-2-enoate; 4-Hydroxycinnamylaldehyde; p-Coumaraldehyde; (E)-3-(4-Hydroxyphenyl)-2-propenal
9.60_337.1680m/z	62.17	48.88	ko00950	C02915	(S)-cis-N-Methylcanadine;
1.07_84.0801m/z	81.97	77.91	ko00460	C19491, C20312	(E)-2-Methylbutanaloxime; (Z)-2-Methylbutanaloxime;
4.07_118.0651m/z	69.22	55.47	ko00400, ko00460	C00463, C16074, C16075, C19714	Indole; 2,3-Benzopyrrole; Phenylacetonitrile; Benzylcyanide; (Z)-Phenylacetaldehydeoxime; Z-Phenylacetaldoxime; (E)-Phenylacetaldoxime; (E)-Phenylacetaldehydeoxime; Benzeneacetonitrile
12.02_223.0944m/z	83.55	77.92	ko00940	C20225	Coniferylacetate;
0.65_261.0370m/z	86.68	85.68	ko00400	C01094	D-Fructose 1-phosphate;
12.07_209.0791m/z	71.20	66.26	ko00940	C05610	Sinapoylaldehyde; Sinapaldehyde;
7.43_149.0961m/z	54.25	49.83	ko00940	C10428, C10452	Anethole; t-Anethole; trans-Anethole; Estragole; 1-Methoxy-4-(2-propenyl)benzene; Methylchavicol;
0.74_84.0802m/z	58.84	53.49	ko00460	C19491, C20312	(E)-2-Methylbutanaloxime; (Z)-2-Methylbutanaloxime;
5.08_443.1552m/z	65.00	51.54	ko00950	C21589	(13S,14R)-1,8-Dihydroxy-13-O-acetyl-N-methylcanadine;
0.59_132.0527n	49.67	39.34	ko00460	C00152	L-Asparagine; 2-Aminosuccinamicacid;
0.73_192.0630n	52.89	44.37	ko00400	C00296	Quinate; Quinicacid; Kinicacid; Chanicacid; L-Quinicacid; L-Quinate; (-)-Quinicacid;
1.74_164.0470n	45.14	61.02	ko00400, ko00940, ko00950	C00166, C00811, C01772, C05838, C10945	Phenylpyruvate; Phenylpyruvicacid; alpha-Ketohydrocinnamicacid; keto-Phenylpyruvate; 3-Phenyl-2-oxopropanoate; 2-Oxo-3-phenylpropanoate; 4-Coumarate; p-Coumaricacid; trans-4-Hydroxycinnamate; trans-p-Hydroxycinnamate; 4-Hydroxycinnamicacid; 4-Hydroxycinnamate; trans-2-Hydroxycinnamate; trans-2-Hydroxycinnamicacid; 2-Hydroxycinnamate; 2-Coumaricacid; o-Coumaricacid; 2-Coumarate;

3.97_205.0854m/z	46.44	43.16	ko00940	C20225	cis-2-Hydroxycinnamate; 2-Coumarinate; Caffeicaldehyde; 3,4-Dihydroxycinnamaldehyde; Caffeylaldehyde; (2E)-3-(3,4-dihydroxyphenyl)prop-2-enal
9.11_371.1631m/z	42.35	38.33	ko00950	C05189	Coniferylacetate; Protopine;
5.30_609.1447m/z	124.28	NA	ko00944	C04858, C05625, C12634, C16490, C19796	Apigenin7-O-[beta-D-aposyl-(1->2)-beta-D-glucoside]; 7-O-(beta-D-Apiofuranosyl-1,2-beta-D-glucosyl)-5,7,4'-trihydroxyflavone; Apiin; 7-[(2-O-D-Apio-beta-D-furanosyl-beta-D-glucopyranosyl)oxy]-5-hydroxy-2-(4-hydroxy-phenyl)-4H-1-benzopyran-4-one; Apioside; Rutin; 3-[[6-O-(6-Deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one; Quercetin3-rutinoside; Rutoside; Phytomelin; Kaempferol3-O-beta-D-glucosyl-(1->2)-beta-D-glucoside; Kaempferol3-O-beta-D-sophoroside; Sophoraflavonololide; Kaempferol3-O-beta-D-glucosylgalactoside; Quercetin3-O-rhamnoside7-O-glucoside;
9.32_335.1521m/z	32.09	24.62	ko00950	C05315	Palmatine; 5,6-Dihydro-2,3,9,10-tetramethoxydibenzo[a,g]quinolizinium;
0.73_156.0424n	39.45	34.56	ko00400	C20710	(4R,5R)-4,5-Dihydroxycyclohexa-1(6),2-diene-1-carboxylate; (3R,4R)-3,4-Dihydroxycyclohexa-1,5-diene-1-carboxylate; DCDC;
4.39_353.0870m/z	30.82	28.86	ko00940, ko00941	C00852, C01527	Chlorogenate; Chlorogenicacid; Caffeoylequinicacid; trans-5-O-Caffeoyle-D-quininate; Scopolin;
4.40_354.0949n	30.65	29.54	ko00940, ko00941	C00852, C01527	Chlorogenate; Chlorogenicacid; Caffeoylequinicacid; trans-5-O-Caffeoyle-D-quininate; Scopolin;
5.31_610.1542n	86.42	NA	ko00944	C05625, C12634, C16490, C19796	Rutin; 3-[[6-O-(6-Deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-

4.48_114.0910m/z	27.32	25.25	ko00460	C00407	benzopyran-4-one; Quercetin3-rutinoside; Rutoside; Phytomelin; Kaempferol3-O-beta-D-glucosyl-(1->2)-beta-D-glucoside; Kaempferol3-O-beta-D-sophoroside; Sophoraflavonolside; Kaempferol3-O-beta-D-glucosylgalactoside; Quercetin3-O-rhamnoside7-O-glucoside;
5.76_428.1679n	175.32	NA	ko00950	C21588	L-Isoleucine; 2-Amino-3-methylvalericacid; 2S-Amino-3S-methylpentanoicacid
3.45_138.0315n	69.99	67.84	ko00400, ko00950	C00587, C16700	(13S,14R)-1-Hydroxy-13-O-acetyl-N-methylcanadine; 3-Hydroxybenzoate; 3-Hydroxybenzoicacid; m-Hydroxybenzoicacid; 3,4-Dihydroxybenzaldehyde; Protocatechualdehyde;
1.99_132.1017m/z	26.83	26.62	ko00460	C00407	L-Isoleucine; 2-Amino-3-methylvalericacid; 2S-Amino-3S-methylpentanoicacid
0.96_174.0520n	24.89	29.41	ko00400	C00493	Shikimate; Shikimicacid; 3,4,5-Trihydroxy-1-cyclohexenecarboxylicacid;
5.36_287.0552m/z	49.95	NA	ko00941	C00974, C01378, C05631, C05906, C12127, C12136, C15525	Dihydrokaempferol; Aromadendrin; (+)-Dihydrokaempferol; (+)-Aromadendrin; Fustin; 2,3-Dihydrofisetin; Eriodictyol; Leucocyanidin; 2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,4,5,7-tetrol; 3,3',4,4',5,7-Flavanhexol; 3,4-Cyanidiol; Leucoanthocyanidol; Leucocianidol; Leucocyanidol; Leukocyanidine; Procyanidol; Resivit; 2,3-trans-3,4-cis-Leucocyanidin; (+)-Galocatechin; Gallocatechol; (-)-Epigallocatechin; Epigallocatechol; Eriodictyolchalcone; 2',3,4,4',6'-Pentahydroxychalcone; (2E)-3-(3,4-dihydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)prop-2-en-1-oneCatechin-4beta-ol3,4,2',4',6'-Pentahydroxychalcone

5.30_178.0626n	71.49	NA	ko00400, ko00940	C02666, C20327	Coniferylaldehyde; Coniferaldehyde; 4-Hydroxy-3-methoxycinnamaldehyde; Ferulaldehyde; 2-Oxo-4-phenylbutyricacid; 2-Oxo-4-phenylbutanoicacid; 2-Oxo-4-phenylbutanoate; (2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal
0.65_242.0189n	22.44	20.69	ko00400	C16848	6-Deoxy-5-ketofructose1-phosphate; 1-Deoxy-D-threo-hexo-2,5-diulose6-phosphate;
0.68_210.0532n	26.62	25.55	ko00940	C05619	5-Hydroxyferulicacidmethylester; 3-(3,4-Dihydroxy-5-methoxy)-2-propenoicacid
7.43_135.0803m/z	18.03	18.67	ko00940	C16930, C20464	Chavicol; Isochavicol; t-Anol; trans-Anol; (E)-4-Propenylphenol; (E)-4-Hydroxypropenylbenzene;
5.06_312.1195n	26.15	23.97	ko00940	C05855	4-Hydroxycinnamylalcohol4-D-glucoside; p-Coumarylalcohol4-O-glucoside;
4.66_449.1076m/z	79.85	NA	ko00941	C16408	2',3,4,4',6'-Peptahydroxychalcone4'-O-glucoside; PHC4'-O-glucoside; 2',3,4,4',6'-Pentahydroxychalcone4'-O-beta-D-glucoside;
9.10_477.3186m/z	21.33	NA	ko00950	C11817	Deoxytubulosine;
8.20_195.0654m/z	18.10	16.42	ko00940	C01494, C12204	Ferulate; Ferulicacid; 4-Hydroxy-3-methoxycinnamicacid; 3-Methoxy-4-hydroxy-trans-cinnamate; 4-Hydroxy-3-methoxycinnamate; 5-Hydroxyconiferaldehyde; trans-Ferulicacid
0.61_132.0299m/z	64.28	NA	ko00460	C00049	L-Aspartate; L-Asparticacid; 2-Aminosuccinicacid; L-Asp;
4.40_163.0389m/z	20.23	20.34	ko00400, ko00940, ko00950	C01179, C01197	3-(4-Hydroxyphenyl)pyruvate; 4-Hydroxyphenylpyruvate; p-Hydroxyphenylpyruvicacid; Caffeate; Caffeicacid; 3,4-Dihydroxy-trans-cinnamate; trans-Caffeate; (2E)-3-(3,4-Dihydroxyphenyl)prop-2-enoate; 4-Hydroxyphenylpyruvicacid
0.68_237.0607m/z	20.26	16.34	ko00400	C00296	Quinate; Quinicacid; Kinicacid; Chinicacid; L-Quinicacid; L-Quinate; (-)-Quinicacid;

4.36_576.1263m/z	NA	68.83	ko00942	C12095, C16297	Cyanidin3-O-(6-O-p-coumaroyl)glucoside; Pelargonidin3-O-(6-caffeoyl-beta-D-glucoside);
6.71_163.0389m/z	20.80	25.97	ko00400, ko00940, ko00950	C01179, C01197	3-(4-Hydroxyphenyl)pyruvate; 4-Hydroxyphenylpyruvate; p-Hydroxyphenylpyruvicacid; Caffeate; Caffeicacid; 3,4-Dihydroxy-trans-cinnamate; trans-Caffeate; (2E)-3-(3,4-Dihydroxyphenyl)prop-2-enoate; 4-Hydroxyphenylpyruvicacid
0.71_289.0293m/z	20.78	15.72	ko00941	C10028, C12123	Chrysin; 5,7-Dihydroxyflavone; 7,4'-Dihydroxyflavone;
7.43_295.1178m/z	16.55	14.72	ko00940	C05855	4-Hydroxycinnamylalcohol4-D-glucoside; p-Coumarylalcohol4-O-glucoside;
5.31_303.0501m/z	31.58	NA	ko00941, ko00944	C00389, C02906, C10192	Quercetin; 3,3',4,5,7-Pentahydroxyflavone; 3,5,7,3',4'-Pentahydroxyflavone; Dihydromyricetin; Ampelopsin; (+)-Dihydromyricetin; (+)-Ampelopsin; Tricetin; 5,7,3',4',5'-Pentahydroxyflavone;
4.29_385.0766m/z	33.26	38.17	ko00940	C02887	Sinapoylmalate; Sinapoyl-(S)-malate;
3.78_289.0705m/z	16.38	13.30	ko00941	C00974, C01378, C05631, C05906, C12127, C12136, C15525	Dihydrokaempferol; Aromadendrin; (+)-Dihydrokaempferol; (+)-Aromadendrin; Fustin; 2,3-Dihydrofisetin; Eriodictyol; Leucocyanidin; 2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,4,5,7-tetrol; 3,3',4,4',5,7-Flavanhexol; 3,4-Cyanidiol; Leucoanthocyanidol; Leucocianidol; Leucocyanidol; Leukocyanidine; Procyanidol; Resivit; 2,3-trans-3,4-cis-Leucocyanidin; (+)-Gallocatechin; Gallocatechol; (-)-Epigallocatechin; Epigallocatechol; Eriodictyolchalcone; 2',3,4,4',6'-Pentahydroxychalcone; (2E)-3-(3,4-dihydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)prop-2-en-1-oneCatechin-4beta-ol3,4,2',4',6'-Pentahydroxychalcone

5.24_465.1011m/z	77.10	NA	ko00941, ko00944	C05623, C16410	Quercetin3-O-glucoside; Isoquercitrin; 2-(3,4-Dihydroxyphenyl)-3-(beta-D-glucofuranosyloxy)-5,7-dihydroxy-4H-1-benzopyran-4-one; Isotrifoliin; Bracteatin6-O-glucoside; Bracteatin6-O-beta-D-glucoside;
5.07_320.0891n	20.73	19.37	ko00940, ko00941	C02947	4-Coumaroylshikimate; trans-5-O-(4-Coumaroyl)shikimate;
8.24_241.0718m/z	33.77	NA	ko00940	C12205	5-Hydroxyconiferylalcohol;
3.61_135.0801m/z	NA	81.46	ko00940	C16930, C20464	Chavicol; Isochavicol; t-Anol; trans-Anol; (E)-4-Propenylphenol; (E)-4-Hydroxypropenylbenzene;
3.45_152.0469n	35.22	34.19	ko00950	C04043	3,4-Dihydroxyphenylacetaldehyde; Protocatechuatealdehyde;
3.73_761.2331m/z	45.30	NA	ko00942	C20493	Cyanidin5-O-beta-D-glucoside3-O-beta-D-sambubioside;
4.30_177.0545m/z	32.38	32.38	ko00940	C01494, C12204	Ferulate; Ferulicacid; 4-Hydroxy-3-methoxycinnamicacid; 3-Methoxy-4-hydroxy-trans-cinnamate; 4-Hydroxy-3-methoxycinnamate; 5-Hydroxyconiferaldehyde; trans-Ferulicacid
8.41_335.1514m/z	NA	182.00	ko00950	C05315	Palmatine; 5,6-Dihydro-2,3,9,10-tetramethoxydibenzo[a,g]quinolizinium;
8.73_353.1641m/z	NA	81.93	ko00950	C05315, C21586	Palmatine; 5,6-Dihydro-2,3,9,10-tetramethoxydibenzo[a,g]quinolizinium; (S)-1-Hydroxy-N-methylcanadine;
6.91_225.0751m/z	86.07	NA	ko00400, ko00940	C00482, C20653, C20654	Sinapate; Sinapicacid; 3,5-Dimethoxy-4-hydroxycinnamicacid; 2-Benzylmalicacid; 2-Benzylmalate; 3-Benzylmalicacid; 3-Benzylmalate; 2-benzyl-3-hydroxybutanedioicacid
6.75_370.1632n	76.37	NA	ko00950	C21586	(S)-1-Hydroxy-N-methylcanadine;
4.54_207.0648m/z	40.00	NA	ko00400, ko00940	C00482, C20653, C20654	Sinapate; Sinapicacid; 3,5-Dimethoxy-4-hydroxycinnamicacid; 2-Benzylmalicacid; 2-Benzylmalate; 3-Benzylmalicacid; 3-Benzylmalate; 2-benzyl-3-hydroxybutanedioicacid

5.21_149.0963m/z	33.18	NA	ko00940	C10428, C10452	Anethole; t-Anethole; trans-Anethole; Estragole; 1-Methoxy-4-(2-propenyl)benzene; Methylchavicol;
4.00_474.1735m/z	NA	60.40	ko00950	C11813, C11814	Demethylalangiside; Demethylisoalangiside;
4.53_386.1201n	18.90	17.05	ko00940	C01175	1-O-Sinapoyl-beta-D-glucose; 1-O-Sinapoyl-beta-D-glucoside;
5.15_177.0544m/z	NA	29.83	ko00940	C01494, C12204	Ferulate; Ferulicacid; 4-Hydroxy-3-methoxycinnamicacid; 3-Methoxy-4-hydroxy-trans-cinnamate; 4-Hydroxy-3-methoxycinnamate; 5-Hydroxyconiferaldehyde; trans-Ferulicacid
8.45_333.1805m/z	NA	40.86	ko00950	C05202, C06516, C06518, C06520	3'-Hydroxy-N-methyl-(S)-coclaurine; (S)-3'-Hydroxy-N-methylcoclaurine; (R)-Norreticuline; N-Norreticuline; (S)-Nororientaline; (S)-Norreticuline; (S)-3-Hydroxy-N-methylcoclaurine
4.63_753.1810m/z	NA	47.72	ko00944	C12635	Kaempferol3-sophorotrioside; Kaempferol3-O-beta-D-glucosyl-(1->2)-beta-D-glucosyl-(1->2)-beta-D-glucoside;
8.88_428.1708n	NA	35.28	ko00950	C21588	(13S,14R)-1-Hydroxy-13-O-acetyl-N-methylcanadine;
8.37_369.1562m/z	NA	52.35	ko00950	C21587	(13S,14R)-1,13-Dihydroxy-N-methylcanadine;
8.45_372.1384n	NA	41.27	ko00940	C01533	Syringin; EleutherosideB;
4.65_323.0549m/z	NA	38.72	ko00944	C04293, C10098	Chrysoeriol; 5,7,4'-Trihydroxy-3'-methoxyflavone; 3'-O-Methyl-luteolin; Kaempferide; Kempferide; Kaempferol4'-methylether;
4.18_596.1714m/z	NA	36.43	ko00942	C08620, C08725, C16305, C20495	Cyanidin3-O-rutinoside; Cyanidin3-O-rhamnosylglucoside; Keracyanin; Pelargonin; Pelargonidin3,5-di-beta-D-glucoside; Pelargonidin3-O-sophoroside; Pelargonidin3,7-di-O-beta-D-glucoside; Cyanidin3-rutinoside
5.21_135.0802m/z	NA	32.38	ko00940	C16930, C20464	Chavicol; Isochavicol; t-Anol; trans-Anol; (E)-4-Propenylphenol; (E)-4-Hydroxypropenylbenzene;

2.34_307.0830m/z	NA	81.81	ko00941	C05906, C12127, C12136	Leucocyanidin; 2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,4,5,7-tetrol; 3,3',4,4',5,7-Flavanhexol; 3,4-Cyanidiol; Leucoanthocyanidol; Leucocianidol; Leucocyanidol; Leukocyanidine; Procyanidol; Resivit; 2,3-trans-3,4-cis-Leucocyanidin; (+)-Gallocatechin; Gallocatechol; (-)-Epigallocatechin; Epigallocatechol; Catechin-4beta-ol
4.22_290.0788n	NA	60.20	ko00941	C03648, C05907, C06562, C09727, C09736	cis-3,4-Leucopelargonidin; Luteoforol; 3-Deoxyleucocyanidin; (+)-Catechin; D-Catechin; Cyanidanol; (2R-trans)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol; (2R,3S)-Catechin; (2R,3S)-(+)-Catechin; Cianidanol; (-)-Epicatechin; Fisetinidol-4beta-ol; (-)-Mollisacacidin; Fisetinin-3,4-diol; 5-Deoxyleucocyanidin; (-)-Catechin

Terpenoids

Compound.ID	Average ion intensity (TIC × 100,000)		Pathway	KEGG.ID	Description
	Ostiolear tissues	Female florets			
5.94_219.1744m/z	106.84	80.10	ko00909	C09627, C09737, C17954, C19939	Capsidiol; Solavetivone; Albaflavenone; Pentalen-13-al; capsidiol
2.43_241.1543m/z	46.23	75.06	ko00909	C09737, C17954, C19939	Solavetivone; Albaflavenone; Pentalen-13-al;
7.89_235.1688m/z	20.37	17.16	ko00909	C19678	GermacreneAacid; Germacra-1(10),4,11(13)-trien-12-oate;
5.06_312.1195n	26.15	20.17	ko00909	C06080	Nivalenol;
7.43_295.1178m/z	15.21	13.77	ko00909	C06080	Nivalenol;

4.38_417.1025m/z	19.42	19.40	ko00909, ko00900, ko00906, ko00100	C00448	trans,trans-Farnesyldiphosphate; Farnesyldiphosphate; Farnesylpyrophosphate; 2-trans,6-trans-Farnesyldiphosphate; (2E,6E)-Farnesyldiphosphate;
11.18_409.3798m/z	13.48	NA	ko00909, ko00100	C01054, C08615, C08616, C08628, C08637, C19801, C19819, C19820, C19832, C19833, C19835, C19918, C20187, C20191, C20192, C20193, C20195, C20200	(S)-2,3-Epoxy-squalene; Squalene2,3-epoxide; Squalene2,3-oxide; (S)-Squalene-2,3-epoxide; 2,3-Oxidosqualene; (3S)-2,3-Epoxy-2,3- dihydrosqualene; alpha-Amyrin; beta-Amyrin; beta-Amyrenol; Lupeol; Taraxerol; Isomultiflorenol; Cucurbitadienol; Protostadienol; (17Z)-Protosta-17(20),24-dien-3beta-ol; Thalianol; Germanicol; (3beta)-Olean-18-en-3-ol; CamelliolC; Parkeol; Lanost-9(11)-en-3beta-ol; AchilleolB; alpha-seco-Amyrin; 8,14- Secoursa-7,13-diene-3beta-ol; Marneral; beta-seco-Amyrin; 8,14- Secooleana-7,13-diene-3beta-ol; Tirucalla-7,24-dien-3beta-ol; Baruol; (3S)-2,3-epoxy-2,3-dihydrosqualene3S-squalene-2,3- epoxide
9.77_426.3858n	10.03	NA	ko00909, ko00100	C01054, C08615, C08616, C08628, C08637, C19801, C19819, C19820, C19832, C19833, C19835, C19918, C20187, C20191, C20192, C20193, C20195, C20200	(S)-2,3-Epoxy-squalene; Squalene2,3-epoxide; Squalene2,3-oxide; (S)-Squalene-2,3-epoxide; 2,3-Oxidosqualene; (3S)-2,3-Epoxy-2,3- dihydrosqualene; alpha-Amyrin; beta-Amyrin; beta-Amyrenol; Lupeol; Taraxerol; Isomultiflorenol; Cucurbitadienol; Protostadienol; (17Z)-Protosta-17(20),24-dien-3beta-ol; Thalianol; Germanicol; (3beta)-Olean-18-en-3-ol; CamelliolC; Parkeol; Lanost-9(11)-en-3beta-ol; AchilleolB; alpha-seco-Amyrin; 8,14- Secoursa-7,13-diene-3beta-ol; Marneral; beta-seco-Amyrin; 8,14- Secooleana-7,13-diene-3beta-ol; Tirucalla-7,24-dien-3beta-ol; Baruol; (3S)-2,3-epoxy-2,3-dihydrosqualene3S-squalene-2,3- epoxide
6.74_234.1612n	11.52	14.69	ko00909	C19678	GermacreneAacid; Germacra-1(10),4,11(13)-trien-12-oate;

4.57_245.1859m/z	NA	37.02	ko00909, ko00900	C01126, C03220, C09704, C16143, C18245, C19746, C19755, C19974, C20181	(2E,6E)-Farnesol; 2-trans,6-trans-Farnesol; trans-Farnesol; (2Z,6E)-Farnesol; 2-cis,6-trans-Farnesol; Nerolidol; (3S,6E)-Nerolidol; (1E,4S,5E,7R)-Germacra-1(10),5-dien-11-ol; Germacradienol; 8-epi-Cedrol; (3R,6E)-Nerolidol; Patchoulol; (+)-Caryolan-1-ol; Avermitilol; (Z)-Farnesol(2-cis,6-trans)-farnesol
5.47_220.1825n	15.08	NA	ko00909, ko00900	C03461, C17953, C17955, C19676, C19711	2-trans,6-trans-Farnesal; trans,trans-Farnesal; Farnesal; (2E,6E)-3,7,11-Trimethyl-2,6,10-dodecatrienal; (2E,6E)-Farnesal; (5S)-Albaflavenol; (5R)-Albaflavenol; Germacra-1(10),4,11(13)-trien-12-ol; Solavetivol; (2-trans,6-trans)-farnesal
6.14_203.1792m/z	13.50	NA	ko00909, ko00900	C03461, C17953, C17955, C19676, C19711	2-trans,6-trans-Farnesal; trans,trans-Farnesal; Farnesal; (2E,6E)-3,7,11-Trimethyl-2,6,10-dodecatrienal; (2E,6E)-Farnesal; (5S)-Albaflavenol; (5R)-Albaflavenol; Germacra-1(10),4,11(13)-trien-12-ol; Solavetivol; (2-trans,6-trans)-farnesal
8.10_235.1688m/z	NA	16.19	ko00909	C19678	GermacreneAacid; Germacra-1(10),4,11(13)-trien-12-oate;
7.25_234.1614n	NA	24.08	ko00909	C19678	GermacreneAacid; Germacra-1(10),4,11(13)-trien-12-oate;
4.68_245.1858m/z	NA	16.60	ko00909, ko00900	C01126, C03220, C09704, C16143, C18245, C19746, C19755, C19974, C20181	(2E,6E)-Farnesol; 2-trans,6-trans-Farnesol; trans-Farnesol; (2Z,6E)-Farnesol; 2-cis,6-trans-Farnesol; Nerolidol; (3S,6E)-Nerolidol; (1E,4S,5E,7R)-Germacra-1(10),5-dien-11-ol; Germacradienol; 8-epi-Cedrol; (3R,6E)-Nerolidol; Patchoulol; (+)-Caryolan-1-ol; Avermitilol; (Z)-Farnesol(2-cis,6-trans)-farnesol

Footnote:

NA: secondary metabolites that were not listed in the top 10% SMCDs.

Supplementary Table 16. Comparisons of gene expression in CYP450, GST and CCE gene families between adults and larvae of *W. pumilae* using DEseq2 in transcriptomes. Bold rows represent genes that significant upregulated at the larval stage with high expression (read counts > 200).

Gene ID	Gene name	Average expression (read counts)*		Log ₂ (fold change)	Adjusted p-value
		Adults	Larvae		
WPUM_100104-RA	<i>WpumCYP2_1</i>	7.45	0.07	-6.80 ± 2.07	0.009
WPUM_100105-RA	<i>WpumCYP2_2</i>	4.54	25.43	2.49 ± 0.73	< 0.001
WPUM_100106-RA	<i>WpumCYP2_3</i>	353.20	5.24	-6.07 ± 0.48	< 0.001
WPUM_100107-RA	<i>WpumCYP2_4</i>	20.16	9.59	-1.07 ± 0.94	0.330
WPUM_100108-RA	<i>WpumCYP2_5</i>	254.45	892.10	1.81 ± 0.23	< 0.001
WPUM_100109-RA	<i>WpumCYP2_6</i>	794.82	373.87	-1.09 ± 0.37	0.011
WPUM_100110-RA	<i>WpumCYP2_7</i>	8.09	28.02	1.79 ± 1.36	0.235
WPUM_100111-RA	<i>WpumCYP3_1</i>	1160.36	0.58	-10.96 ± 0.93	< 0.001
WPUM_100120-RA	<i>WpumCYP3_10</i>	775.90	1.14	-9.41 ± 0.71	< 0.001
WPUM_100121-RA	<i>WpumCYP3_11</i>	76.33	0.07	-10.12 ± 0.95	< 0.001
WPUM_100122-RA	<i>WpumCYP3_12</i>	4.25	4.59	-0.11 ± 1.39	0.942
WPUM_100112-RA	<i>WpumCYP3_2</i>	16.78	337.36	4.33 ± 2.67	0.045
WPUM_100113-RA	<i>WpumCYP3_3</i>	0.02	0.45	4.56 ± 3.21	0.136
WPUM_100114-RA	<i>WpumCYP3_4</i>	1.27	0.30	-2.10 ± 2.04	0.271
WPUM_100115-RA	<i>WpumCYP3_5</i>	2368.85	55.64	-5.41 ± 0.49	< 0.001
WPUM_100116-RA	<i>WpumCYP3_6</i>	0.68	13.29	4.28 ± 1.75	0.015
WPUM_100117-RA	<i>WpumCYP3_7</i>	2782.10	288.59	-3.27 ± 0.97	0.004
WPUM_100118-RA	<i>WpumCYP3_8</i>	149.71	139.88	-0.10 ± 0.75	0.913
WPUM_100124-RA	<i>WpumCYP4_1</i>	24.84	4190.51	7.40 ± 0.39	< 0.001
WPUM_100125-RA	<i>WpumCYP4_2</i>	2.89	1.76	-0.72 ± 1.30	0.587
WPUM_100126-RA	<i>WpumCYP4_3</i>	0.03	11.87	8.84 ± 1.08	< 0.001
WPUM_100127-RA	<i>WpumCYP4_4</i>	858.80	0.95	-9.83 ± 0.73	< 0.001
WPUM_100128-RA	<i>WpumCYP4_5</i>	25.85	60.15	1.22 ± 0.42	0.016
WPUM_100129-RA	<i>WpumCYP4_6</i>	606.64	2818.24	2.22 ± 0.54	< 0.001
WPUM_100130-RA	<i>WpumCYP4_7</i>	12.23	4.25	-1.53 ± 1.32	0.294
WPUM_100131-RA	<i>WpumCYP4_8</i>	1.51	0.52	-1.54 ± 1.59	0.298
WPUM_100132-RA	<i>WpumCYP4_9</i>	98.63	616.52	2.64 ± 0.28	< 0.001
WPUM_100133-RA	<i>WpumCYPM_1</i>	0.03	24.86	9.73 ± 0.91	< 0.001
WPUM_100134-RA	<i>WpumCYPM_2</i>	0.61	0.11	-2.53 ± 3.25	0.466
WPUM_100135-RA	<i>WpumCYPM_3</i>	30.10	13.20	-1.19 ± 0.62	0.065
WPUM_100136-RA	<i>WpumCYPM_4</i>	16.81	69.72	2.05 ± 0.62	0.006
WPUM_100137-RA	<i>WpumCYPM_5</i>	35.57	257.59	2.86 ± 0.52	< 0.001
WPUM_100138-RA	<i>WpumCYPM_6</i>	113.44	18.45	-2.62 ± 0.89	0.012
WPUM_100139-RA	<i>WpumGSTδ_1</i>	4569.31	2420.29	-0.92 ± 0.34	0.054
WPUM_100140-RA	<i>WpumGSTδ_2</i>	3.97	6.33	0.67 ± 2.25	0.774
WPUM_100141-RA	<i>WpumGSTδ_3</i>	7.64	7.97	0.06 ± 0.55	0.908

WPUM_100142-RA	<i>WpumGSTδ_4</i>	9.44	5.48	-0.78 ± 0.71	0.231
WPUM_100143-RA	<i>WpumGSTω_1</i>	92.58	155.60	0.75 ± 0.18	< 0.001
WPUM_100144-RA	<i>WpumGSTω_2</i>	3.58	67.08	4.23 ± 0.56	< 0.001
WPUM_100145-RA	<i>WpumGSTσ_1</i>	0.02	0.40	4.19 ± 3.20	0.195
WPUM_100146-RA	<i>WpumGSTσ_2</i>	0.04	3.17	6.46 ± 3.14	0.024
WPUM_100147-RA	<i>WpumGSTσ_3</i>	93.25	374.78	2.01 ± 0.44	< 0.001
WPUM_100148-RA	<i>WpumGSTσ_4</i>	26.81	38.96	0.54 ± 0.66	0.472
WPUM_100149-RA	<i>WpumGSTζ_1</i>	131.83	352.39	1.42 ± 0.23	< 0.001
WPUM_008229-RA	<i>WpumCCEA_1</i>	46.76	49.43	0.08 ± 0.30	0.793
WPUM_100151-RA	<i>WpumCCEA_2</i>	20.76	14.95	-0.47 ± 0.91	0.631
WPUM_100152-RA	<i>WpumCCEA_3</i>	0.70	0.06	-3.66 ± 3.25	0.255
WPUM_005280-RA	<i>WpumCCED_1</i>	12.66	404.55	5.00 ± 0.32	< 0.001
WPUM_026029-RA	<i>WpumCCEE_1</i>	174.86	90.39	-0.95 ± 0.44	0.090
WPUM_100153-RA	<i>WpumCCEF_1</i>	1404.13	20.93	-6.07 ± 0.43	< 0.001
WPUM_100154-RA	<i>WpumCCEG_1</i>	387.26	259.86	-0.58 ± 0.25	0.006
WPUM_036964-RA	<i>WpumCCEI_1</i>	669.52	197.86	-1.76 ± 0.47	< 0.001
WPUM_036974-RA	<i>WpumCCEI_2</i>	392.49	2.25	-7.45 ± 0.64	< 0.001
WPUM_011514-RA	<i>WpumCCEJ_1</i>	57.33	32.88	-0.80 ± 0.39	0.042
WPUM_100150-RA	<i>WpumCCEJ_2</i>	216.65	448.22	1.05 ± 0.37	0.017
WPUM_036731-RA	<i>WpumCCEK_1</i>	9184.58	688.94	-3.74 ± 0.28	< 0.001

Footnote:

* The average expression (or average quantification) was calculated as the sum of gene expression in different samples divided by total sample size.

Full names of CCE families: CCEA: α-esterases; CCEB: Glutactin; CCEC: Lepidopteran JHEs and others; CCED: Uncharacterized; CCEE: Lepidopteran esterases; CCEF: Acetylcholinesterases; CCEG: Gliotactins; CCEH: Crustacean/AcariJhE; CCEI: Neuroligins; CCEJ: β-esterases; CCEK: Integument esterases; CCEL: Nonlepidopteran JHEs and like enzymes; CCEM: Neurotactins; CCEN: J'; CCEO: J''; CCEP: Undetermined.

Supplementary Table 17. Genes for *in vitro* functional assays with substrates and expected reaction products. There are two steps in the catalytic reaction of the two ACSLs with the intermediate product of hexadecanoyl-AMP and final product of Hexadecanoyl-CoA (Oba et al., 2005).

Species	Gene ID	Gene name	Substrate(s)	Expected product
<i>F. pumila</i> var. <i>pumila</i>	FPUM_021084-RA	<i>FpumACSL8</i>	Acetyl-CoA, ATP,	Hexadecanoyl-AMP
	FPUM_023966-RA	<i>FpumACSL10</i>	hexadecanoic acid	(intermediate product), Hexadecanoyl-CoA
	FPUM_016180-RA	<i>FpumADH4</i>	Decanal	Decanol
	FPUM_000863-RA	<i>FpumALDH1</i>	Decanoic acid	Decanal
<i>W. pumilae</i>	WPUM_100002-RA	<i>WpumOBP2</i>	Decanal, nonanal	--
	WPUM_100002-RA	<i>WpumOBP11</i>		--

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