SUPPLEMENTAL DATA_1

Gene name	Prot size	Chr	Start	Stop	Strand	Type	EST nb	Gene ID (V0 Genoscope, NCBI)	Gene ID (V1 CRIBI)
VvSTS1	392	10	14216112	14217677	plus	pseudo*	0	GSVIVG01026213001	VV10S0042G00840, 850, 860
VvSTS2	392	10	14246885	14248453	plus	pseudo*	3	not defined	VV10S0042G00870
VvSTS3	392	10	14264038	14265601	plus	pseudo*	4	not defined	VV10S0042G00880, 890
VvSTS4	392	10	14284187	14285750	plus	pseudo*	0	not defined	VV10S0042G00910
VvSTS5	392	10	14298957	14300520	plus	full	0	not defined	VV10S0042G00920
VvSTS6	392	10	14304787	14306350	plus	full	6	GSVIVG01026220001	VV10S0042G00930
VvSTS7	392	16	16239028	16240564	plus	full	17*	not defined	VV16S0100G00750
VvSTS8	nd	16	16252494	16254029	plus	pseudo	0	not defined	VV16S0100G00760
VvSTS9	392	16	16268816	16270352	plus	full	13*	GSVIVG01010590001	VV16S0100G00770
VvSTS10	392	16	16276570	16278105	plus	full	26*	GSVIVG01010589001	VV16S0100G00780
VvSTS11	nd	16	16284807	16285039	minus	pseudo	0	not defined	not defined
VvSTS12	nd	16	16286924	16287922	minus	partial	2	not defined	VV16S0100G00800
VvSTS13	nd	16	16289537	16290882	minus	partial	5	not defined	VV16S0100G00810
VvSTS14	nd	16	16323781	16324386	minus	partial	1	not defined	not defined
VvSTS15	392	16	16335697	16337233	plus	full	8*	not defined	VV16S0100G00830
VvSTS16	392	16	16343202	16344516	minus	full	3	GSVIVG01010585001	VV16S0100G00840
VvSTS17	392	16	16346580	16347949	minus	full	15*	GSVIVG01010584001	VV16S0100G00850
VvSTS18	392	16	16350059	16351428	minus	pseudo*	25*	GSVIVG01010583001	VV16S0100G00860
VvSTS19	392	16	16366907	16368410	minus	full	3	GSVIVG01010582001	VV16S0100G00880
VvSTS20	392	16	16386013	16387529	minus	full	18*	GSVIVG01010581001	VV16S0100G00900
VvSTS21	392	16	16398234	16399770	plus	full	8*	not defined	VV16S0100G00910
VvSTS22	392	16	16405205	16406519	minus	full	5	GSVIVG01010580001	VV16S0100G00920
VvSTS23	392	16	16408469	16409837	minus	full	19*	GSVIVG01010579001	VV16S0100G00930
VvSTS24	392	16	16411948	16413317	minus	full	26*	GSVIVG01010578001	VV16S0100G00940
VvSTS25	nd	16	16431088	16431720	minus	partial	32	not defined	VV16S0100G00950
VvSTS26	nd	16	16440517	16441617	minus	partial	3	not defined	VV16S0100G00960
VvSTS27	392	16	16467015	16468549	minus	full	13*	not defined	VV16S0100G00990
VvSTS28	392	16	16477097	16478613	minus	full	25	not defined	VV16S0100G01000
VvSTS29	392	16	16491597	16493131	minus	full	17*	not defined	VV16S0100G01010
VvSTS30	392	16	16503636	16505168	minus	full	2	GSVIVG01010574001	VV16S0100G01020
VvSTS31	392	16	16507942	16509479	minus	full	13*	not defined	VV16S0100G01030
VvSTS32	392	16	16511216	16512602	plus	full	4	GSVIVG01010572001	VV16S0100G01040
VvSTS33	nd	16	16520734	16521936	minus	pseudo	0	GSVIVG01010570001	VV16S0100G01060
VvSTS34	nd	16	16523409	16523861	minus	pseudo	0	not defined	not defined
VvSTS35	392	16	16526326	16527862	minus	full	38*	GSVIVG01010568001	VV16S0100G01070
VvSTS36	392	16	16555945	16557435	minus	full	28*	GSVIVG01010565001	VV16S0100G01100
VvSTS37	392	16	16587447	16588984	minus	full	5	not defined	VV16S0100G01110
VvSTS38	392	16	16607176	16608730	minus	full	9*	GSVIVG01010563001	VV16S0100G01110
VvSTS39	392	16	16615702	16617258	minus	full	6	not defined	VV16S0100G01120
VvSTS40	nd	16	16618991	16620545	minus	pseudo	0	not defined	VV16S0100G01130
VvSTS41	392	16	16623086	16624624	minus	full	15*	not defined	VV16S0100G01130
VvSTS42	392	16	16627536	16629091	minus	full	8	GSVIVG01010561001	VV16S0100G01140
VvSTS43	392	16	16644190	16645747	minus	full	5*	not defined	VV16S0100G01150
VvSTS44	nd	16	16647473	16649027	minus	pseudo	0	not defined	not defined
VvSTS45	392	16	16673986	16675524	minus	full	25	GSVIVG01010557001	VV16S0100G01160
VvSTS46	392	16	16682709	16684264	minus	full	17	GSVIVG01010556001	VV16S0100G01170
VvSTS47	392	16	16698303	16699842	minus	full	23*	GSVIVG01010554001	VV16S0100G01190
VvSTS48	392	16	16710281	16711818	minus	full	81*	not defined	VV16S0100G01200
VvCHS1	393	14	24673534	24674845	plus	full	>200*	GSVIVG01032968001	VV14S0068G00920
VvCHS2	393	14	24687036	24688374	plus	full	>200*	not defined	VV14S0068G00930
VvCHS3	389	5	13597483	13599348	plus	full	>200*	GSVIVG01000521001	VV05S0136G00260
VvCHSL1	392	3	1006320	1007936	plus	full	0	GSVIVG01024107001	VV03S0038G01460
VvCHSL2	389	15	13099195	13100654	minus	full	4*	GSVIVG01018219001	VV15S0021G02170
VvCHSL3	nd	nd	39310453	39311279	minus	partial	0	not defined	not defined
VvCHSL4	381	16	12591519	12592910	plus	pseudo*	0	not defined	VV16S0022G01000
VvCHSL5	384	16	12636904	12638528	plus	full	0	not defined	VV16S0022G01020
VvCHSL6	nd	16	12709873	12710073	plus	pseudo	0	not defined	not defined
VvCHSL7	nd	16	12725807	12727082	plus	pseudo	0	not defined	not defined
VvCHSL8	343	16	12763168	12764673	plus	full	0	not defined	VV16S0022G01020
VvCHSL9	nd	16	12826871	12827452	plus	partial	0	not defined	not defined
VvCHSL10	386	16	12946634	12949378	plus	full	0	not defined	VV16S0022G01140
VvCHSL11	386	16	13045635	13047296	plus	full	0	not defined	VV16S0022G01190

Table S1: Detailed annotation and nomenclature of the *STS* and *CHS* gene families of *V. vinifera* PN40024.

Column legend:

- Gene name: Stilbene Synthase (*STS*), Chalcone Synthase (*CHS*) and Chalcone Synthase-like (*CHSL*).
- Prot. size: Number of amino acid encoded by the predicted CDS. The protein size is not defined (nd) for pseudogenes and partial genes.
- Chr: Chromosome number. Note that the *VvCHSL3* gene is localized on an unmapped scaffold.
- Start and Stop: Positions of predicted CDS relative to the 12x PN40024 pseudochromosomes. Complete curated intron-exon structures are available in the FLAGdb^{++} database (http://urgv.evry.inra.fr/FLAGdb). Final CDS are also available as a multifasta file (Supplemental Data 2).
- Strand: chromosome strand.
- Type: Full (complete perfect CDS), partial (suspended by an unsequenced region) and pseudo (probable pseudogene disrupted by numerous stop codons, frameshifts and/or small deletions). * means that there is only one fatal position in the predicted CDS (*i.e.* one frameshift or one stop codon) which can be the result of a sequencing error.
- EST nb: Number of cognate EST/cDNA in the available transcript resources. * means that the whole CDS is covered by the EST/cDNA contig.

Gene ID: Corresponding name in the official automatic annotation (v0) of the 12x PN40024 genome obtained with GAZE (http://www.genoscope.cns.fr/externe/GenomeBrowser/Vitis/). Note that the structure of the genes predicted by GAZE can be different of the curated ones described in this paper. Not defined means that the gene have not been predicted by GAZE. Cross-links with the gene IDs from the v1 annotation of the 12x PN40024 genome (CRIBI, http://genomes.cribi.unipd.it/) are provided.

Compound	**RT**	**structure**	**ESIMS(-)**	**formula**	**MS/MS**	**formula**	**MS/MS**	**formula**
A	1,68	resveratrol-O-hexoside	389,1245	$C_{20}H_{21}O_8$	227,0709	$C_{14}H_{11}O_3$	161,0444	$C_6H_9O_5$
B	2,56	trans-piceid	389,1248	$C_{20}H_{21}O_8$	227,0710	$C_{14}H_{11}O_3$	161,0439	$C_6H_9O_5$
C	2,94	cis-piceid	389,1248	$C_{20}H_{21}O_8$	227,0710	$C_{14}H_{11}O_3$	161,0445	$C_6H_9O_5$
D	3,17	piceid methyl ether	403,1403	$C_{21}H_{23}O_8$	241,0868	$C_{15}H_{13}O_3$	161,0440	$C_6H_9O_5$
E	3,33	piceid methyl ether	403,1404	$C_{21}H_{23}O_8$	241,0869	$C_{15}H_{13}O_3$	161,0444	$C_6H_9O_5$
F	3,41	resveratrol methyl ether - O-hexoside	445,1510	$C_{23}H_{25}O_9$	241,0860	$C_{15}H_{13}O_3$	203,0558	$C_8H_{11}O_6$
G	3,53	resveratrol methyl ether - O-hexoside	445,1508	$C_{23}H_{25}O_9$	241,0867	$C_{15}H_{13}O_3$	203,0556	$C_8H_{11}O_6$
H	4,82	pterostilbene	255,1025	$C_{16}H_{15}O_3$				

Table S2 : MS/MS characterization of resveratrol derivatives produced in *N. benthamiana* leaves following transient *STS* expression

RT: retention time in min,
ESIMS(-): Compound mass in negative ion mode electrospray ionization mass spectrometry ($[M-H]^-$)
MS/MS: fragment mass

Gene	Piceid (*cis* and *trans*) µg/gFW	Pterostilbene µg/gFW
VvSTS5	13,79 ±1,82	1,22 ±0,14
VvSTS10	14,42 ±1,07	1,70 ±0,20
VvSTS16	8,59 ±1,77	1,34 ±0,33
VvSTS28	13,88 ±1,34	1,22 ±0,14
VvSTS29	12,60 ±2,90	1,83 ±0,51
VvSTS36	10,67 ±0,99	1,34 ±0,20
VvSTS38	12,66 ±2,04	2,11 ±0,32
VvSTS46	6,26 ±1,65	1,24 ±0,17
VvSTS48	11,75 ±1,80	1,19 ±0,24

Table S3: Quantification of stilbenes in *N. benthamiana* leaves following transient *STS* expression

Only cis-piceid, trans-piceid and trans-pterostilbene were quantified, as these compounds were available as authentic standards. Traces amounts of resveratrol were detected in some samples. Results correspond to the mean (± SD) of 6 experiments, expressed as µg per g (fresh weight) of leaf.

	Sequence Name	**CDS AN**	**Protein AN**
Arachis hypogaea	AhCHS	AY735111	AAU43217
	AhCHS1	AY192572	AAO32821
	AhSTS	AB027606	BAA78617
	AhSTS1	A00769	CAA00091
	AhSTS3	L00952	AAA96434
Arabidopsis thaliana	AtCHS	AY044331	AAK73272
Psilotum nudum	PnCHS	AB022682	BAA87922
	PnCHSSF	AB040027	BAA92742
	PnSTS	AB022684	BAA87924
	PnSTSb	AB022685	BAA87925
Pinus strobus	PstrCHS	AJ004800	CAA06077
	PstrCHSL	AJ002156	CAA05214
	PstrSTS1	Z46914	CAA87012
	PstrSTS2	Z46915	CAA87013
Pinus sylvestris	PsylCHS	X60754	CAA43166
	PsylSTS	X60753	CAA43165
Populus trichocarpa	PtCHS1	DQ371804	EEE99396
	PtCHS2	CM000337	EEE84086
	PtCHS3	CM000337	EEE84087
	PtCHS4	CM000339	EEE78798
	PtCHS5	CM000339	EEE78799
	PtCHS6	CM000339	EEE78800
	PtCHS7	EQ140118	EEF06787
	PtCHSL1	CM000337	EEE84002
	PtCHSL2	DS017597	EEE73513
Sorghum bicolor	SbCHS1	AF152548	AAD41873
	SbCHS2	AF152549	AAD41874
	SbCHS3	AF152550	AAD41875
	SbCHS4	AF152551	AAD41876
	SbCHS5	AF152552	AAD41877
	SbCHS6	AF152553	AAD41878
	SbCHS7	AF152554	AAD41879
	SbSTS1	AY069951	AAL49965

Table S4 : Species, sequence names, CDS and proteins accession numbers (AN) of the sequences used in the multispecies analysis.

Model	**Proportion of sites**			**dN/dS ratios**			**Likelihood**	
							InL	**P-value**
Multispecies								
BModel w2				wb=0.077 CHS	wf1=0.084 STS Vv	wf2=0.179 STS o	-28279.42215	0 (<e-308) (BM w0) 0.331103 (BM w1o)
BModel w1v				wb=0.095 CHS+STS o	wf=0.084 STS Vv		-28318.90344	0.159322
BModel w1o				wb=0.079 CHS+STS Vv	wf=0.178 STS o		-28279.89444	0 (<e-308)
BModel w1vo				wb=0.078 CHS	wf=0.120 STS Vv + STS o		-28302.34656	3.14 E-09
BM w0 control				w0= 0.093			-28319.89376	
CModel	p0=0.438	p1=0.047	p2=0.516	w0b=0.021 CHS w0f1=0.021 STS Vv w0f2=0.021 STS o	w1b=1 CHS w1f1=1 STS Vv w1f2=1 STS o	w2b=0.1183 CHS w2f1=0.1179 STS Vv w2f2=0.2891 STS o	-27715.85062	0 (<e-308)
CM control							-28114.09939	
FM2a	p1=0.511	p2=0.059	p3=0.091	w1= 0.00001	w2=0.153	w3=1	-27592.35651	0 (<e-308)
FMX	p0=0.866	p1=0.132	p2=0.002	w0= 0.024421	w1=1.000017	w2=9.99985	-27699.07975	0 (<e-308)
FM control							-27752.59095	
Vitis vinifera								
BModel				wb=0.089 CHS	wf=0.083 STS		-11840.90213	0.554592
BM control				w0= 0.085			-11841.07671	
BSite	p0=0.923	p1=0.061	p2a=0.015 p2b=0.001	w0b=0.059 CHS w0f=0.059 STS	w1b=1 CHS w1f=1 STS	w2ba=0.059 CHS w2fa,2bb,2fb =1 STS,CHS,STS	-11702.85446	1
BS control							-11702.85446	
CModel	p0=0.421	p1=0.050	p2=0.529	w0b=0.017 CHS w0f=0.017 STS	w1b=1 CHS w1f=1 STS	w2b=0.148 CHS w2f=0.082 STS	-11634.15808	0 (<e-308)
CM							-11706.64354	

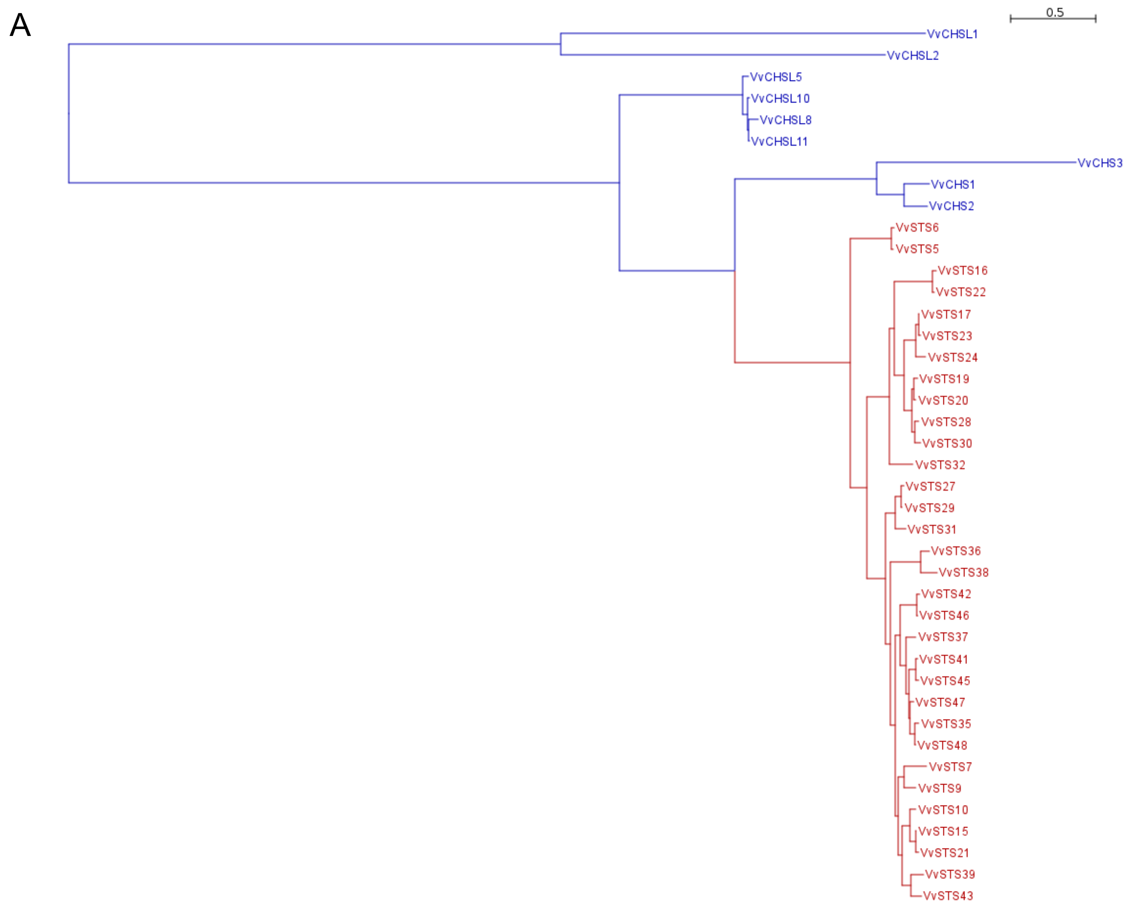
control								
FM2a	p1=0.909	p2=0.054	p3=0.038	w1=0.024	w2=1	w3=1.660	-11611.94129	1.03 E-14
FMX	p0=0.608	p1=0.314	p2=0.078	w0=0 (<0.000001)	w1=0.107	w2=1.316	-11608.49082	3.33 E-16
FM control							-11641.17816	

Table S5 : Main results of the dN/dS analyses of the “multispecies” and “*Vitis vinifera”* sets of sequences.

BModel or BM = branch model; CModel or CM = clade model; FM = fit model (M2a model and MX model, see M&M section); BSite or BS = branch site model; control = null model; w = dN/dS; b = background; f = foreground; p0, p1, p2, p3 = proportion of sites with dN/dS ratios = w0, w1, w2 and w3, respectively (same colour for corresponding p and w); STS Vv = STS from *Vitis vinifera*; STS o = STS from other species than *Vitis vinifera* (see Table S1); lnL = ln of the likelihood; P-value = p-value of the likelihood ratio test.

	Gene	Forward primer	Reverse primer
A	VvSTS5	`CTTTGAAGCTCTGTGGGGGATTTTACTAGTCATCA`	`ATTTGATTTAATTAGAAATTGTCCCCTTCTGATTT`
	VvSTS10	`CCTCAATCTTCAGCTTCAATTTGAGTTCGTAGCTAGGAT`	`GTAGCACCTCCTCTGTAATACAATAAGACATGTCCCC`
	VvSTS16	`AACTTTTAAGCTTCGATTTCAGCAGTCATCCTACTAT`	`ATTTAAGGTCTCCAAGGAAATCCTCCAACAATTC`
	VvSTS28	`TTGAAGCTTCCATTTCAGTAGTCATCACACACTATCAATG`	`GATTTTGACTTGAGGTCTTTGAGGAGGTCCTCC`
	VvSTS29	`CCAAGCACTTGTGCACACTGAGTTCTCTTTCCTTCC`	`AGTTTCGGAGATAAATACCTTACTCCTATTCAAC`
	VvSTS36	`CTCAACCCAGCTCCAAGCACTCTTCTCTTTCCTTC`	`ACCGTAGAACATCAAAGGTACCATTCCCCTTCAC`
	VvSTS38	`GTTCTCTTTTCTTTCCAATTGGAGTAGCAGCAATG`	`CTTTGAACTGGAGGTCACTAAGGAAGCCCTCCAGC`
	VvSTS46	`CACTTGAGTTCTCTTTCCTTCCTCAACTTAATC`	`GATTACATTAAGACATTGAAGGGTCGAGC`
	VvSTS48	`GACAGGCTATAAAAGCCCGGCACCCACAACCAGCT`	`CCTATTTGATACATTACTGCATTGAAGGGTAAACC`
B	VvSTS5 Gateway	`GGGGACAAGTTTGTACAAAAAAGCAGGCTTGGTTCCGCGTGGATCAATGGCATCTGTGGAGGACATTAGA`	`GGGGACCACTTTGTACAAGAAAGCTGGGTTCATCAATTTGTAGCCCCAGCAACG`
	VvSTS10 Gateway	`GGGGACAAGTTTGTACAAAAAAGCAGGCTTGGTTCCGCGTGGATCAATGGCTTCAATTGAGGAAATTAGAAA`	`GGGGACCACTTTGTACAAGAAAGCTGGGTTCATCAATTTGTAACCATAGGAACGCTATG`
	VvSTS16 Gateway	`GGGGACAAGTTTGTACAAAAAAGCAGGCTTGGTTCCGCGTGGATCAATGGCTTCAGTCGAGGAAATTAGAA`	`GGGGACCACTTTGTACAAGAAAGCTGGGTTCATCAATTGGAATCCCTAGGAATACTGTG`
	VvSTS28 Gateway	`GGGGACAAGTTTGTACAAAAAAGCAGGCTTGGTTCCGCGTGGATCAATGGCTTCAGTCGAGGAAATTAGAA`	`GGGGACCACTTTGTACAAGAAAGCTGGGTTCACTAGTTTGAATCCGTACCAACGCTAT`
	VvSTS29 Gateway	`GGGGACAAGTTTGTACAAAAAAGCAGGCTTGGTTCCGCGTGGATCAATGGCTTCAGTCGAGGAAATTAGAA`	`GGGGACCACTTTGTACAAGAAAGCTGGGTTCATTAATTTGTCACCATAGGAATGCTATGC`
	VvSTS36 Gateway	`GGGGACAAGTTTGTACAAAAAAGCAGGCTTGGTTCCGCGTGGATCAATGGCTTCAGTCGAGGAAATTAGAA`	`GGGGACCACTTTGTACAAGAAAGCTGGGTTCATTAATTTATAACTGTAGGAATGCTACGCAG`
	VvSTS38 Gateway	`GGGGACAAGTTTGTACAAAAAAGCAGGCTTGGTTCCGCGTGGATCAATGGCTTCAGTCGAGGAAATTAGAA`	`GGGGACCACTTTGTACAAGAAAGCTGGGTTCATCAATTTGTACCCGTGGCAACG`
	VvSTS46 Gateway	`GGGGACAAGTTTGTACAAAAAAGCAGGCTTGGTTCCGCGTGGATCAATGGCATCTGTGGAGGACATTAGA`	`GGGGACCACTTTGTACAAGAAAGCTGGGTTCATTAATTTGTAACCGTAGGAATGCTATGC`
	VvSTS48 Gateway	`GGGGACAAGTTTGTACAAAAAAGCAGGCTTGGTTCCGCGTGGATCAATGGCTTCAGTTGAGGAATTTAGAAA`	`GGGGACCACTTTGTACAAGAAAGCTGGGTTCATTAATTTGTAACCGTAGGAATGCTATGC`
C	VvSTS5/6	`CTGAAACCCATTTAGACTCT`	`GAAATTGTCCCCTTGTGATT`
	VvSTS7	`GGGTCTTGAAACTTCAGTTAGA`	`GTCTCTACAATCTCCAACGAT`
	VvSTS9	`CCTCTTCCAGCTCGTCT`	`TCAATAAGATAGGGATCATATATCA`
	VvSTS10/15/21	`AAATAACGCAGGAGCACGA`	`GATTTAGGAGTACTATTATTAACT`
	VvSTS16/22	`CTGAAACTGCTTTGGACTCT`	`GTTGCGATAACTTCGTTATTGT`
	VvSTS17/23/24	`GTTTGATATCTGAAAACATAGAG`	`AGATGATTTCATGGTGATATATC`
	VvSTS19/20/28/30	`ACTCTTTCAACTTGTTTCAGCA`	`TCCAACAATCGTAAAATAACAATTCA`
	VvSTS27/29/31	`CAATGTGCCCACTTTAATTTCTG`	`CAGTCTGAACTTGAAACTCAAC`
	VvSTS32	`CTGAATCCGCTTTGGACTCT`	`CCATCTCTTCTATGGCTCACAA`
	VvSTS35/48	`AGGTACCTAGACTTGGTAG`	`AAGGGTCAACCATTCTCTTTTA`
	VvSTS36	`CTTGATAACTCAGTTAGAAGAGTT`	`ATCAAAGGTACCATTCCCCTT`
	VvSTS37	`TGCCATTGCCGGAAACTTAC`	`GAGTATTGAAAAGACCATTCTCC`
	VvSTS38	`CTTGATAACTCAGTTAGAAGAGTT`	`TGGAAAGCTTCTCCTTATGAC`
	VvSTS39/43	`TGCTGAGGTACCCAAACTC`	`ATTTCAGCTCACAAAGAAAGTCTA`
	VvSTS41/45	`AGGTACCTAGACTTGGTAG`	`AATCCAAATTTACCAATGTGATG`
	VvSTS42/46	`TTTCCAGCTCGTCTCAGCAG`	`ATTAAGACATTGAAGGGTCGAGC`

Table S6: Primers
Primers used for PCR amplification of STS genes from *Vitis vinifera* PN40024 genomic DNA (A), for cloning into the Gateway-compatible entry vector pDONR207 (B) and for semi-quantitative RT-PCR (C).


A
0.5
VvCHSL1
VvCHSL2
VvCHSL5
VvCHSL10
VvCHSL8
VvCHSL11
VvCHS3
VvCHS1
VvCHS2
VvSTS6
VvSTS5
VvSTS16
VvSTS22
VvSTS17
VvSTS23
VvSTS24
VvSTS19
VvSTS20
VvSTS28
VvSTS30
VvSTS32
VvSTS27
VvSTS29
VvSTS31
VvSTS36
VvSTS38
VvSTS42
VvSTS46
VvSTS37
VvSTS41
VvSTS45
VvSTS47
VvSTS35
VvSTS48
VvSTS7
VvSTS9
VvSTS10
VvSTS15
VvSTS21
VvSTS39
VvSTS43

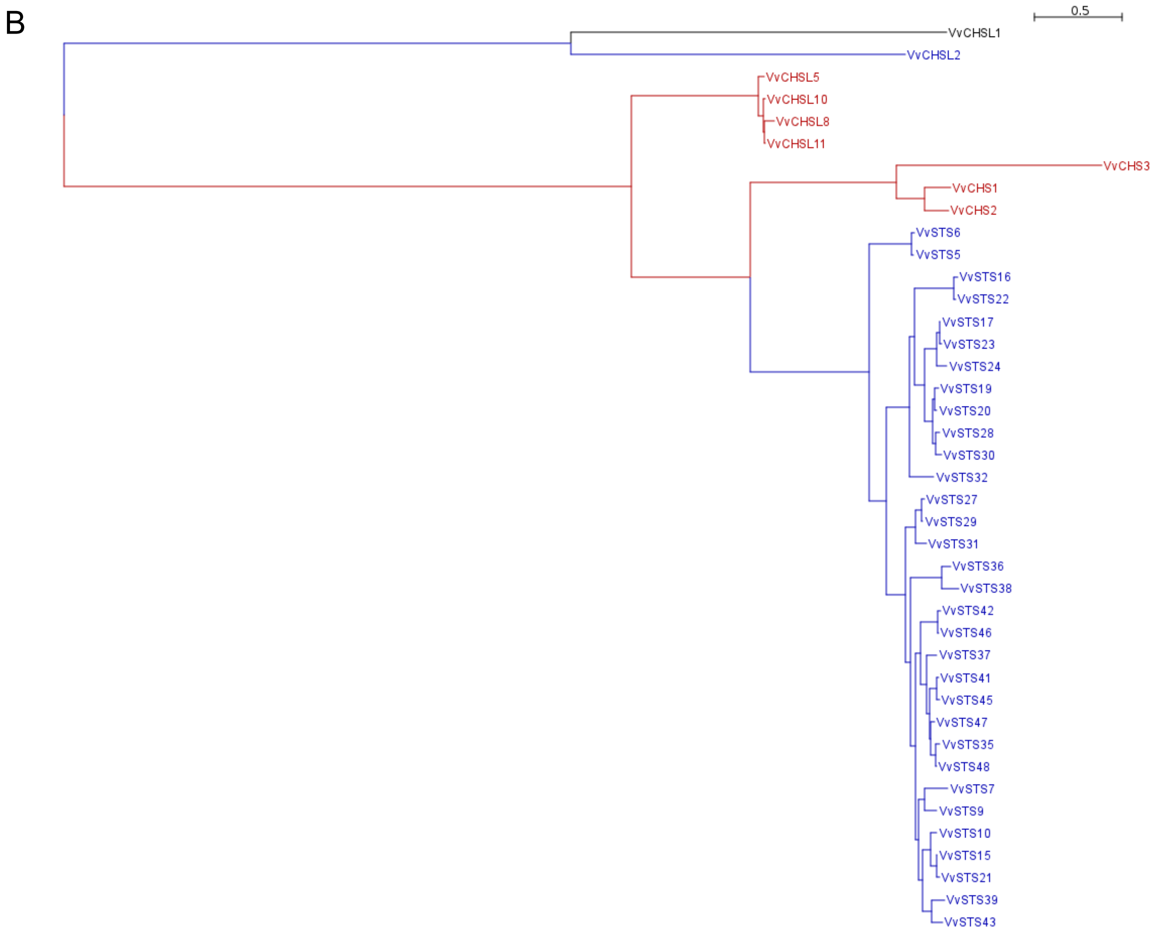


Figure S1:

Phylogenetic trees of the *Vitis vinifera* set of sequences showing the Fitmodel results for 2 contrasted sites evolving under A) positive selection (V_{230} in VvSTS10); B) purifying selection (S_{231} in VvSTS10) in *Vitis* STS proteins. Different colours indicate higher posterior probabilities of evolving under different selection regimes: red = positive selection; blue = purifying selection; black = neutral evolution.