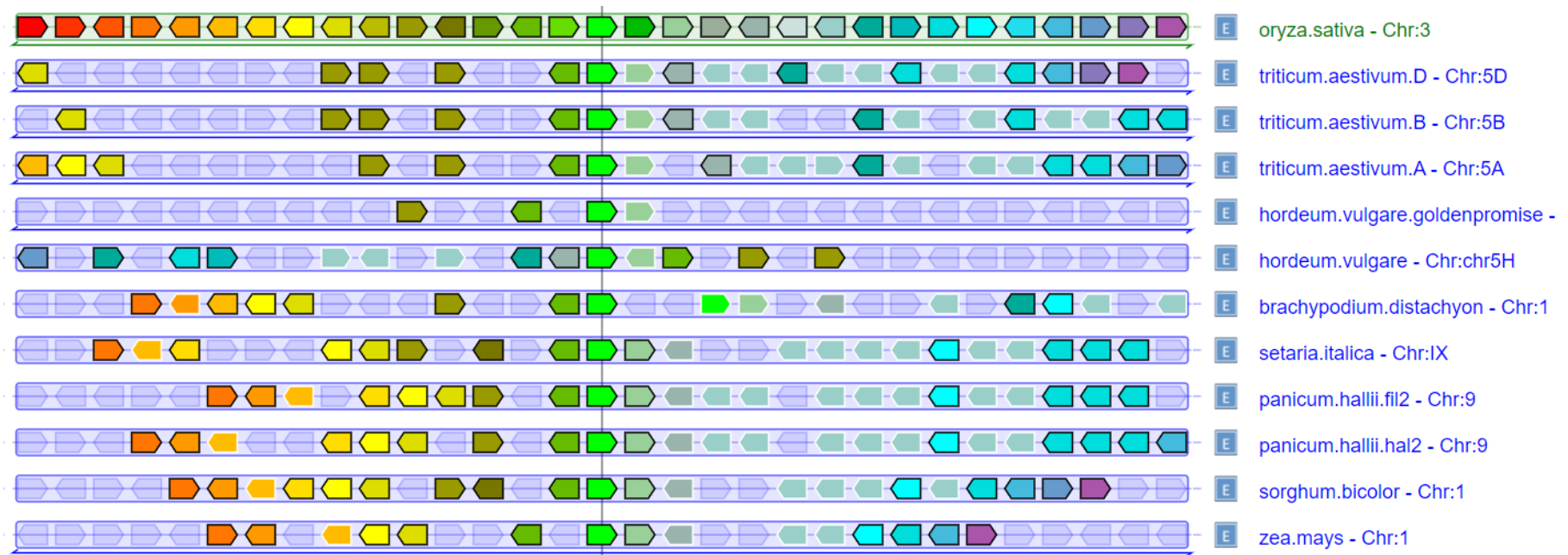


Supplementary Material



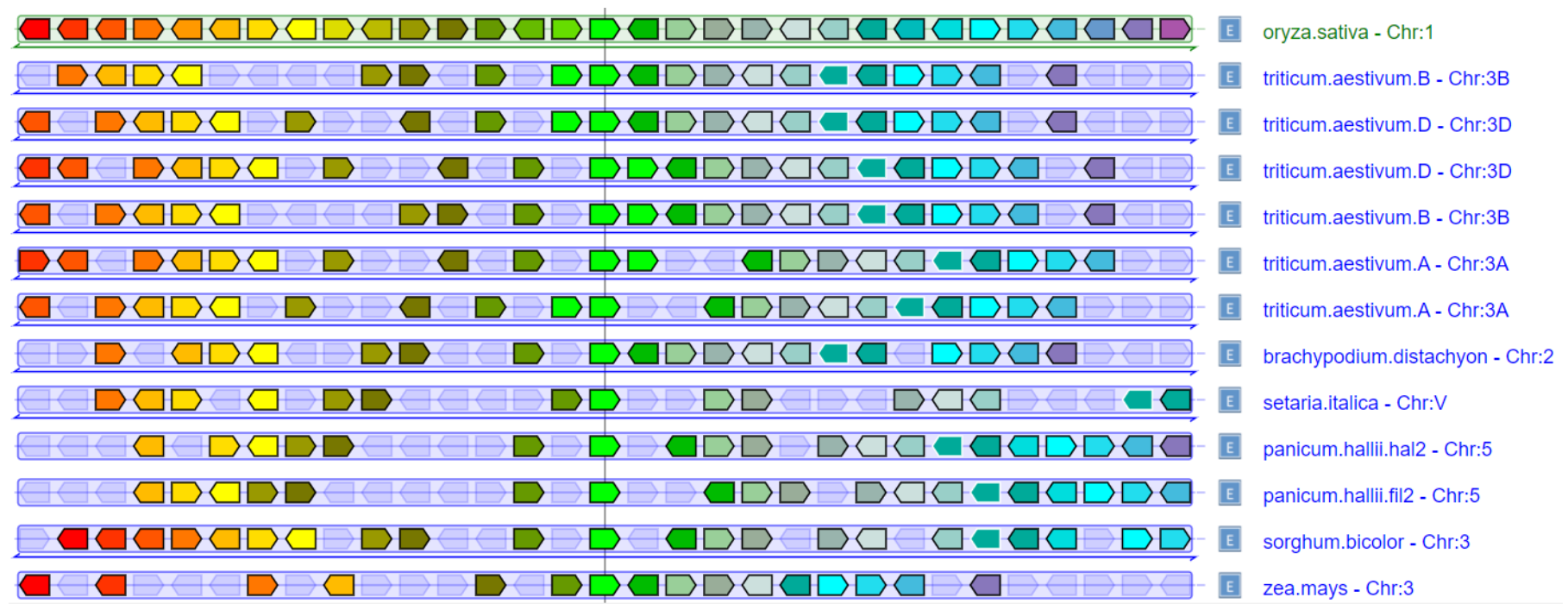


Figure S2. Synteny conservation of PHO2.



Transit Peptide



L80 Insertion

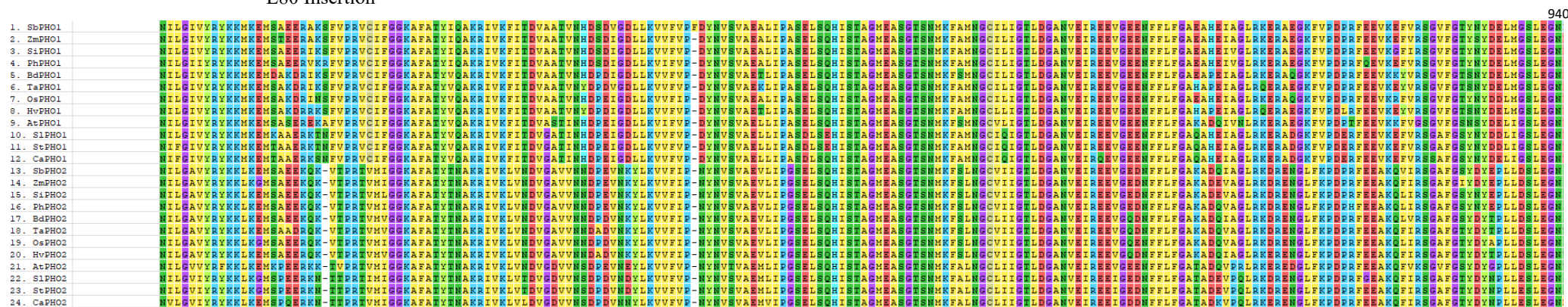
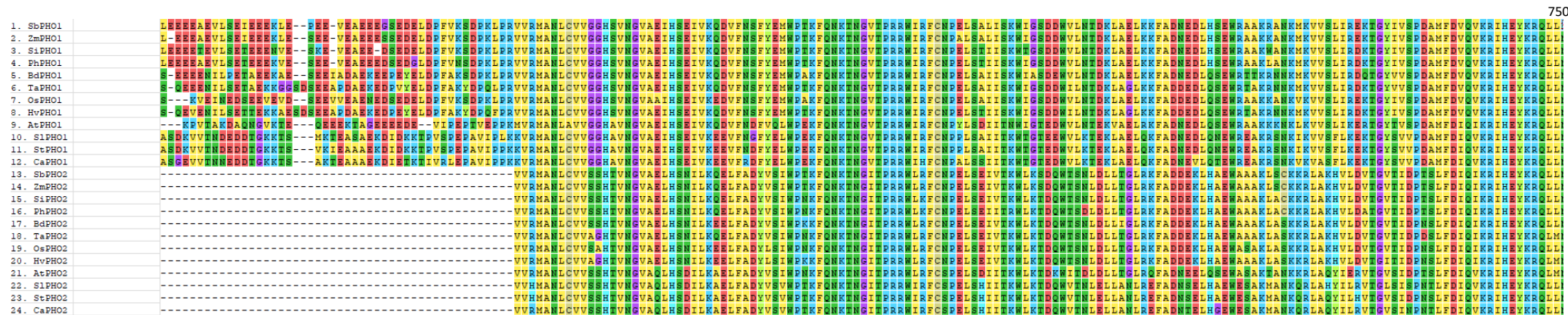




Figure S3. Multiple alignment of PHO sequences in range of species. The sequences of PHO1 include the transit peptide and L80 insertion. Full alignment parts is shown.

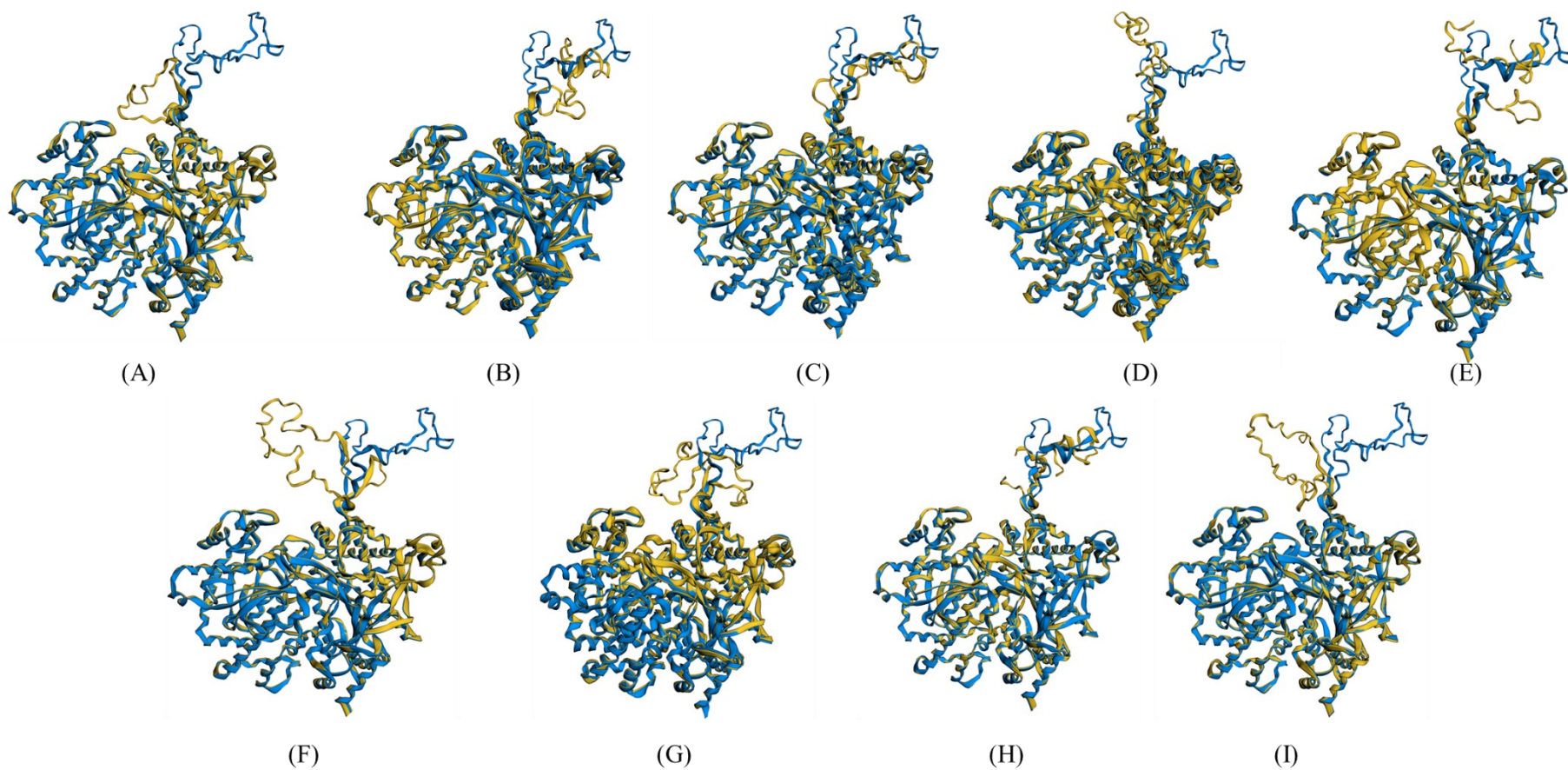


Figure S4. Superimposed structures of the predicted PHO1 (yellow colored) over the *H. vulgare* PHO1 (blue colored) in range of species. (A) AtPHO1. (B) SbPHO1. (C) CaPHO1. (D) OsPHO1. (E) PhPHO1. (F) SiPHO1. (G) SlPHO1. (H) StPHO1. (I) TaPHO1.

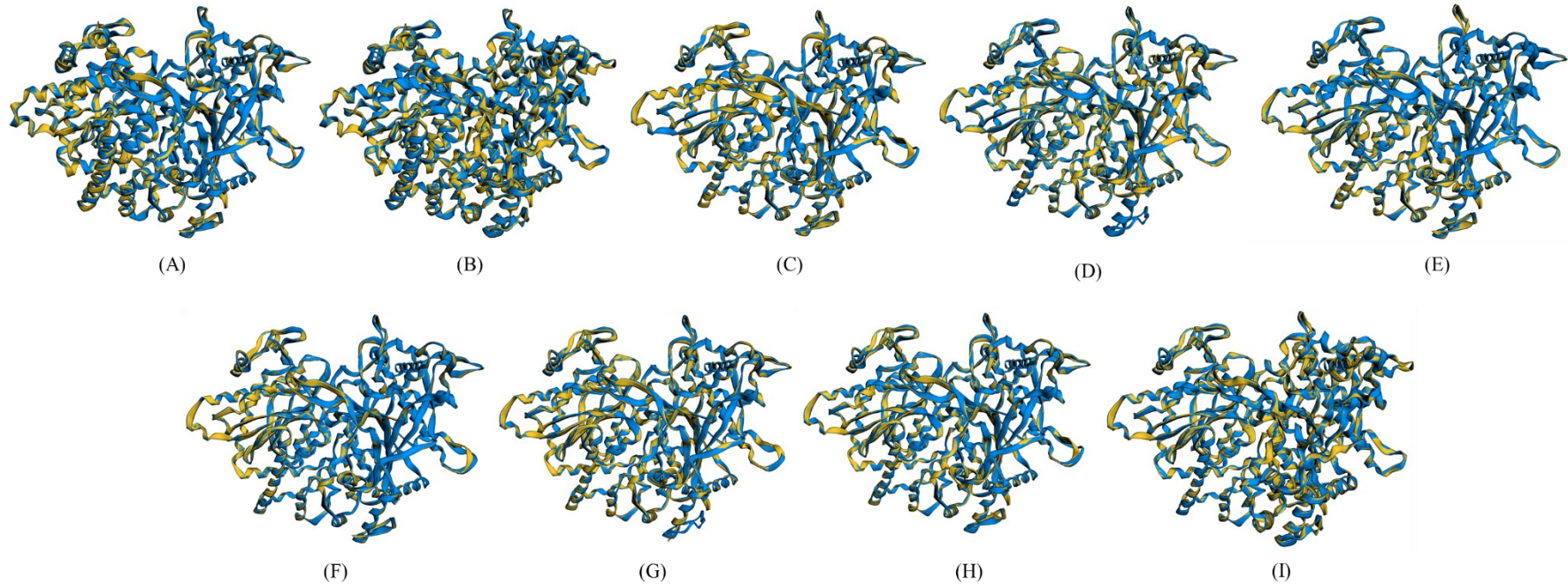


Figure S5. Superimposed structures of the predicted PHO2 (yellow colored) over the *A. thaliana* PHO2 (blue colored) in range of species. (A) AtPHO2. (B) SbPHO2. (C) CaPHO2. (D) OsPHO2. (E) PhPHO2. (F) SiPHO2. (G) SlPHO2. (H) StPHO2. (I) TaPHO2.

Table S1. Percent similarity of exons (upper row) and introns (lower row) of *PHO1* in different species with respect to exons of *PHO1* of *O. sativa*.

Species	Exon/Intron number														
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
<i>Z. mays</i>	52.2	85.0	80.4	86.2	89.1	90.1	89.0	78.3	85.0	89.1	89.0	92.2	93.0	87.1	56.9
	39.6	62.6	47.8	60.0	36.1	56.3	65.2	51.8	52.2	23.8	9.7	36.6	52.5	32.7	-
<i>S. italica</i>	67.5	86.7	86.3	85.4	90.9	88.6	89.0	79.1	85.0	86.8	90.7	90.9	90.9	88.6	59.3
	39.3	41.7	40.3	40.0	44.4	42.8	41.7	38.5	39.7	22.9	39.8	30.0	34.3	44.6	-
<i>P. hallii</i>	67.3	85.4	86.3	86.0	88.8	89.3	90.7	78.3	86.3	83.7	90.3	92.2	91.4	89.1	59.2
	41.1	38.1	40.2	37.2	44.4	44.9	33.7	42.1	40.1	22.8	38.0	37.6	49.6	41.9	-
<i>B. distachyon</i>	65.8	88.4	85.3	88.2	88.4	89.3	90.7	80.3	90.2	86.0	90.3	93.5	92.5	89.6	61.2

	43.0	33.6	43.9	32.9	40.5	34.9	34.3	40.0	37.4	41.8	44.8	44.9	33.6	37.6	-
<i>H. vulgare</i>	64.2	86.4	83.2	86.6	87.4	88.4	90.1	79.2	89.7	85.2	89.1	92.9	91.5	89.2	60.5
	42.3	32.5	41.4	31.6	39.4	33.8	33.2	40.2	38.3	40.5	44.4	43.3	32.5	36.3	-
<i>T. aestivum</i>	63.2	85.4	83.5	85.7	86.3	89.0	90.2	78.4	88.9	85.6	88.2	90.2	89.4	88.6	58.2
	41.3	33.5	40.3	32.3	39.6	34.2	33.5	39.2	39.5	40.1	42.5	42.7	32.8	35.9	-
<i>S. bicolor</i>	60.8	85.8	84.3	86.0	87.7	89.3	90.7	78.4	85.6	87.6	89.9	92.2	92.5	89.1	61.9
	41.0	38.8	41.9	39.3	31.8	43.9	42.0	42.7	38.1	25.0	34.3	35.5	43.5	42.0	-
<i>A. thaliana</i>	45.4	66.7	57.8	76.3	71.4	74.6	80.5	52.4	73.9	77.5	79.8	77.9	77.5	72.6	45.3
	7.3	29.5	28.0	42.7	31.5	42.6	44.0	43.8	31.6	34.8	24.8	28.9	35.3	10.9	-
<i>S. lycopersi-</i> <i>cum</i>	37.5	65.4	67.6	79.9	71.0	79.0	77.1	56.9	74.5	71.3	78.9	75.3	82.9	79.1	46.2
	41.1	27.7	37.6	32.2	25.1	42.0	43.6	48.2	11.8	35.5	35.4	8.3	37.9	12.5	-
<i>S. tuberosum</i>	34.9	32.1	14.8	44.6	29.9	43.8	32.2	X	X	X	X	X	X	X	X
	16.9	41.2	20.3	9.3	16.1	35.6	-	-	-	-	-	-	-	-	-
<i>C. annuum</i>	33.7	65.7	69.6	79.2	69.6	78.3	77.1	56.1	71.9	71.3	79.7	81.8	82.4	56.8	47.5
	43.0	31.1	38.1	36.0	29.7	30.7	45.3	50.8	13.7	35.8	34.3	20.7	43.4	16.0	-

x indicates absence of exons, - indicates absence of introns

Table S2. Percent similarity of exons (upper row) and introns (lower row) of *PHO2* in different species with respect to exons of *PHO2* in *O. sativa*.

Species	Exon/Intron number														
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
<i>Z. mays</i>	66.8	96.1	88.7	82.6	90.0	92.5	87.0	89.0	82.6	87.2	90.2	85.5	86.7	90.6	52.0
	46.0	13.5	42.0	45.2	27.2	4.9	42.6	36.3	41.1	41.1	35.1	36.7	31.6	44.5	-
<i>S. italica</i>	72.9	92.8	88.7	82.6	90.0	91.4	87.0	89.0	84.8	88.6	91.2	87.4	86.7	90.1	58.1
	62.5	29.4	59.1	50.6	29.5	53.7	59.9	34.9	48.9	70.1	51.0	53.1	32.5	48.8	-
<i>P. hallii</i>	73.1	95.6	91.0	81.4	87.4	90.3	89.7	88.1	82.6	87.7	90.2	87.4	87.9	88.5	55.2
	45.2	29.3	40.6	43.5	21.0	43.4	46.4	35.6	41.5	41.3	39.6	43.6	34.2	19.5	-
<i>B. distachyon</i>	66.9	92.2	86.4	87.2	88.4	91.4	88.6	89.0	89.4	90.4	92.6	87.4	90.5	89.5	62.7
	58.6	32.9	59.1	53.6	57.9	54.1	48.0	39.9	23.5	70.9	55.9	55.6	60.3	45.9	-
<i>H. vulgare</i>	65.4	91.4	86.3	88.2	87.6	90.7	87.2	88.6	88.1	89.7	91.2	86.3	89.7	89.2	61.6
	46.2	33.2	58.2	50.2	56.2	53.8	47.2	38.8	24.2	70.4	53.2	53.7	58.9	52.0	-
<i>T. aestivum</i>	62.8	90.5	87.5	81.2	89.1	89.4	85.2	82.1	80.6	86.7	90.1	84.2	86.2	89.0	52.3
	43.0	14.2	45.6	42.3	26.7	52.4	46.3	37.2	40.5	67.5	49.1	45.6	34.9	41.6	-
<i>S. bicolor</i>	73.8	96.1	88.1	80.2	87.9	92.5	88.1	91.5	84.1	87.2	89.7	86.8	85.6	91.1	53.9

	53.5	29.3	56.7	47.5	29.2	52.0	56.1	34.9	47.9	67.8	48.9	49.0	34.0	42.6	-
<i>A. thaliana</i>	38.0	42.3	42.7	29.3	28.4	34.4	30.6	37.6	42.7	35.3	44.7	39.9	35.3	40.4	23.7
	35.4	32.3	44.8	10.8	23.3	22.5	39.0	24.4	19.7	38.1	43.2	44.1	40.7	26.2	=
<i>S. lycopersi-</i> <i>cum</i>	26.8	43.2	43.8	29.0	27.3	31.6	30.6	34.0	44.1	35.1	41.9	40.8	32.5	39.2	23.7
	33.5	17.7	20.4	11.3	23.3	27.7	16.8	47.8	24.0	11.7	46.8	45.4	1.8	26.4	=
<i>S. tuberosum</i>	16.9	40.3	46.2	29.2	27.3	32.3	33.4	36.0	43.4	34.5	42.3	40.8	34.0	39.6	23.3
	38.1	31.2	5.2	11.4	24.6	28.7	6.5	43.8	23.6	10.0	42.4	45.1	3.3	25.4	=
<i>C. annuum</i>	31.1	35.4	46.1	28.8	29.7	34.6	29.6	33.5	42.7	37.9	43.9	42.7	32.2	39.3	23.8
	28.8	16.8	1.0	10.8	17.3	27.9	9.6	45.2	23.4	9.7	5.8	45.8	1.0	25.9	=

x indicates absence of exons, - indicates absence of introns, = have intron but did not analyze

Table S3. Simple sequence repeats (SSRs) and retro-elements identified in *PHO1*.

Species	Position in bp	Type	Repeat	Size(bp)
<i>S. bicolor</i>	147-199	SSR	(CGC)n	50
	1665-1739	SSR	(TTCTATT)n	45
<i>Z. mays</i>	183-239	SSR	(CGC)n	52
	4442-4480	SSR	(AAGAGCA)n	41
	6512-6558	SSR	(ATCTT)n	48
<i>S. italica</i>	8-49	SSR	(CATCG)n	46
	90-138	SSR	(CGC)n	45
<i>P.hallii</i>	77-136	SSR	(CGCCTC)n	60
	138-162	SSR	(GGGGGC)n	25
	2633-2719	SSR	(ATGTTT)n	89
<i>B. distachyon</i>	104-163	SSR	(CCG)n	60
<i>O. sativa</i>	26-63	SSR	(CT)n	38
	150-171	SSR	(CGGCGG)n	122
	407-436	SSR	(CG)n	30
	5138-5171	SSR	(TCTTCA)n	33
<i>A. thaliana</i>	2621-2667	Low-complexity	GA-rich	47
<i>C. annuum</i>	3128-3197	SSR	(TTCTT)n	64
	7350-7407	SSR	(TTTTCT)n	57

Table S4. Simple sequence repeats (SSRs) and retro-elements identified in *PHO2*.

Species	Position in bp	Type	Repeat	Size(bp)
<i>S. bicolor</i>	5917-5940	SSR	(T)n	24
<i>S. italica</i>	1-33	SSR	(TCC)	30
<i>P.hallii</i>	45-77	SSR	(CTCCCA)	33
<i>B. distachyon</i>	3812-3836	SSR	(TTTA)n	26
<i>O. sativa</i>	31-62	SSR	(CCGTT)n	32
<i>A. thaliana</i>	225-256	Low-complexity	A-rich	31
	849-887	SSR	(TG)n	
<i>S. lycopersicum</i>	5122-5168	SSR	(AATTAC)n	45
	8035-8068	SSR	(TATTCT)n	34
	11669-11703	SSR	(CTATTC)n	35
<i>S. tuberosum</i>	141-169	SSR	(TCTTT)n	28
	2048-2082	SSR	(TTATTT)n	33
	5826-5846	SSR	(TG)n	21
	6987-7033	SSR	(AATTAC)n	45
<i>C. annuum</i>	3543-3597	SSR	(CAA)n	54
	1849418541	Low-complexity	G-rich	47
	18620-18670	SSR	(ATTCA)n	49
	31248-31296	SSR	(CAA)n	45
	31355-31402	Low-complexity	A-rich	50
	32006-32087	Low-complexity	GA-rich	77

Table S5. Details of 3D structure and quality assessment parameters of PHO1 (oligostate-homodimer) (upper row) and PHO2 (oligostate-homodimer; lower row) in all of the monocots and dicots obtained using Swiss-Model.

Species	Template used	% Identity	GMQE score	Quality assessment parameters	
				QMEAN 6 score	Dfire energy
<i>S. bicolor</i>	5lr8.1.A	86.98	0.78	0.88	-687.17
	4bqe.1.A	79.44	0.91	0.89	-2712.1
<i>Z. mays</i>	5lr8.1.A	87.51	0.79	0.89	-578.17
	4bqe.1.A	79.30	0.91	0.89	-2617.12
<i>S. italica</i>	5lr8.1.A	87.25	0.79	0.89	-581.25
	4bqe.1.A	79.18	0.91	0.89	-2812.12

<i>P. hallii</i>	5lr8.1.A	87.00	0.78	0.88	-612.21
	4bqe.1.A	79.20	0.83	0.90	-2632.12
<i>B. distachyon</i>	5lr8.1.A	91.96	0.80	0.90	-674.23
	4bqe.1.A	79.42	0.92	0.89	-2576.12
<i>T. aestivum</i>	5lr8.1.A	97.62	0.82	0.91	-643.12
	4bqe.1.A	80.24	0.92	0.90	-2721.15
<i>O. sativa</i>	5lr8.1.A	86.10	0.79	0.89	-674.12
	4bqe.1.A	80.92	0.93	0.90	-2671.32
<i>A. thaliana</i>	5lr8.1.A	76.43	0.77	0.88	-587.12
	4bqe.1.A	100	0.95	0.93	-2442.31
<i>S. lycopersicum</i>	5lr8.1.A	74.34	0.78	0.88	-567.43
	4bqe.1.A	81.33	0.90	0.90	-2521.45
<i>S. tuberosum</i>	5lr8.1.A	74.70	0.78	0.87	-589.32
	4bqe.1.A	81.43	0.91	0.90	-3489.52
<i>C. annuum</i>	5lr8.1.A	74.69	0.76	0.87	-598.23
	4bqe.1.A	80.36	0.91	0.90	-2563.27

Table S6. Model quality assessment scores of 3D structures of PHO1 (upper row) and PHO2 (lower row) in 11 species.

Species	PROCHEK				G-fac- tor	ERRAT	VERIFY3D	Status of 3D struc- ture from SAVES
	Favoured* region (%)	Allowed region (%)	Generously allowed re- gion (%)	Disallowed region (%)		Quality factor (%)	(3D-1D Pro- file) (%)	
<i>S. bicolor</i>	91.1	7.7	0.7	0.5	-0.11	95.19	0.2	PASS
	91.5	8.2	0.3	0.0	-0.04	95.88	0.2	PASS
<i>Z. mays</i>	90.4	8.3	0.8	0.6	-0.12	96.34	0.2	PASS
	91.5	8.2	0.3	0.0	0.00	96.62	0.2	PASS
<i>S. italica</i>	90.1	8.4	1.0	0.6	-0.11	97.70	0.2	PASS
	91.4	8.2	0.3	0.1	-0.03	96.19	0.2	PASS
<i>P. hallii</i>	90.4	7.7	1.1	0.7	-0.11	96.76	0.2	PASS
	91.5	8.2	0.3	0.0	0.00	96.62	0.2	PASS
<i>B. distachyon</i>	89.5	9.0	0.7	0.7	-0.07	96.20	0.2	PASS
	91.3	8.4	0.3	0.0	0.01s	95.34	0.2	PASS
<i>T. aestivum</i>	91.0	7.2	1.1	0.6	-0.12	96.82	0.2	PASS
	91.3	84	0.3	0.0	0.00	96.80	0.2	PASS

<i>O. sativa</i>	90.8	7.8	0.9	0.5	-0.10	95.87	0.2	PASS
	91.8	7.9	0.3	0.0	-0.02	96.63	0.2	PASS
<i>A. thaliana</i>	91.5	7.4	0.6	0.4	-0.09	97.06	0.2	PASS
	91.3	8.4	0.3	0.0	0.01	97.61	0.2	PASS
<i>S. lycopersicum</i>	91.4	7.6	0.7	0.3	-0.08	94.71	0.2	PASS
	91.8	7.9	0.2	0.0	-0.04	96.63	0.2	PASS
<i>S. tuberosum</i>	91.2	7.5	0.9	0.4	-0.10	92.87	0.2	PASS
	91.8	7.9	0.3	0.0	0.00	95.77	0.2	PASS
<i>C. annuum</i>	90.9	7.4	1.1	0.6	-0.09	96.45	0.2	PASS
	92.2	7.6	0.2	0.0	-0.04	96.26	0.2	PASS

* Based on an analysis of 118 structures of resolution of at least 2.0 Å and R-factor no greater than 20%, a good quality model would be expected to have maximum number of amino acids in the most favoured regions.

Table S7. Predicted values of different parameters of superimposition of 3D protein structures of PHO1 and PHO2 of different plant species over 3D protein structure of *H. vulgare* PHO1 and *A. thaliana* PHO2 respectively.

Species	RMSD*		%Identity		%Similarity	
	PHO1	PHO2	PHO1	PHO2	PHO1	PHO2
<i>S. bicolor</i>	5.68	0.04	92.82	97.94	94.34	98.91
<i>Z. mays</i>	2.74	0.21	89.10	96.98	91.59	99.27
<i>S. italica</i>	2.04	0.06	86.29	95.53	88.95	98.55
<i>P. hallii</i>	2.42	1.63	86.65	56.56	91.68	70.45
<i>B. distachyon</i>	3.12	0.05	84.46	92.82	89.89	97.15
<i>T. aestivum</i>	3.62	0.07	83.14	90.55	88.83	95.88
<i>O. sativa</i>	2.20	0.25	73.73	79.32	85.54	90.33
<i>A. thaliana</i>	3.87	0.34	74.83	78.40	85.87	89.20
<i>S. lycopersicum</i>	2.10	0.26	74.70	78.67	86.41	89.21
<i>S. tuberosum</i>	2.41	0.37	74.09	77.27	85.23	89.12
<i>C. annuum</i>	5.68	0.04	92.82	97.94	94.34	98.91

*Root Mean Square Deviation.

Table S8. Ligand Binding amino acid residues and their positions in PHO1 and PHO2.

Species	Amino acids and their position															
	PHO1															
<i>S. bicolor</i>	L	G	G	R	W	V	K	Y	N	V	A	G	T	S	N	K
	149	193	194	197	637	714	715	799	800	801	804	826	827	828	829	831
<i>Z. mays</i>	L	G	G	R	W	V	K	Y	N	V	A	G	T	S	N	K
	149	193	194	197	636	713	714	798	799	800	803	825	826	827	828	830
<i>S. italica</i>	L	G	G	R	W	V	K	Y	N	V	A	G	T	S	N	K
	145	189	190	193	632	709	710	794	795	796	799	821	822	823	824	826
<i>P. hallii</i>	L	G	G	R	W	V	K	Y	N	V	A	G	T	S	N	K
	151	195	196	199	639	716	717	801	802	803	806	828	829	830	831	833
<i>T. aestivum</i>	L	G	G	R	W	V	K	Y	N	V	A	G	T	S	N	K
	140	184	185	188	623	700	701	785	786	787	790	812	813	814	815	817
<i>O. sativa</i>	L	G	G	R	W	V	K	Y	N	V	A	G	T	S	N	K
	144	188	189	192	630	707	708	792	793	794	797	819	820	821	822	824
<i>A. thaliana</i>	L	G	G	R	W	K	Y	N	V	A	G	T	S	N	K	
	159	203	204	207	614	692	776	777	778	781	803	804	805	806	808	
<i>H. vulgare</i>	L	G	G	R	W	V	K	Y	N	V	A	G	T	S	N	K
	137	181	182	185	620	697	698	782	783	784	787	809	810	811	812	814
<i>C. annuum</i>	PHO2															
	L	G	G	R	W	K	Y	N	V	A	G	T	S	N	K	L
	99	143	144	147	500	578	661	662	663	666	688	689	690	691	693	99

Note: Missing species are not identified to possess the ligand binding sites