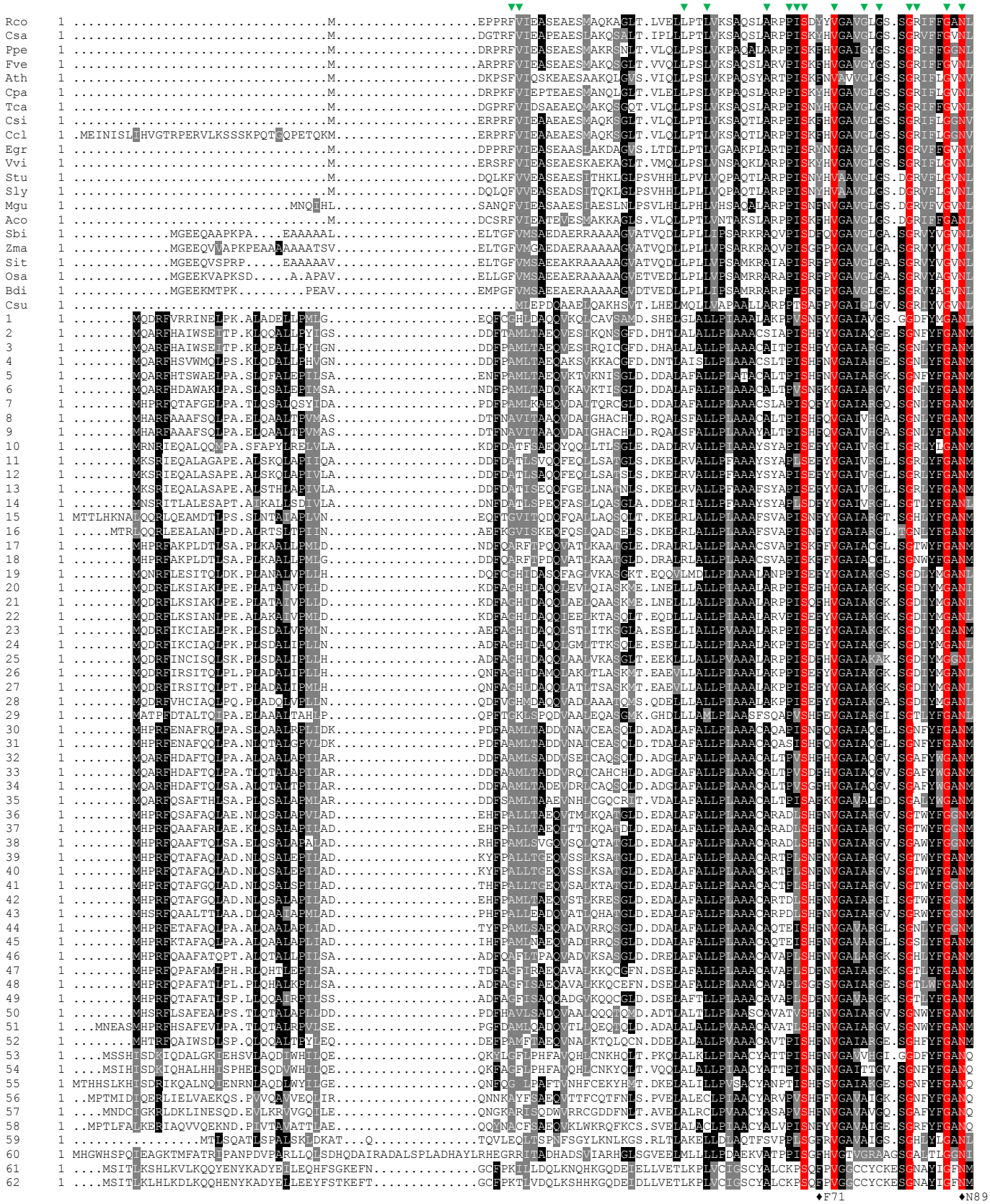
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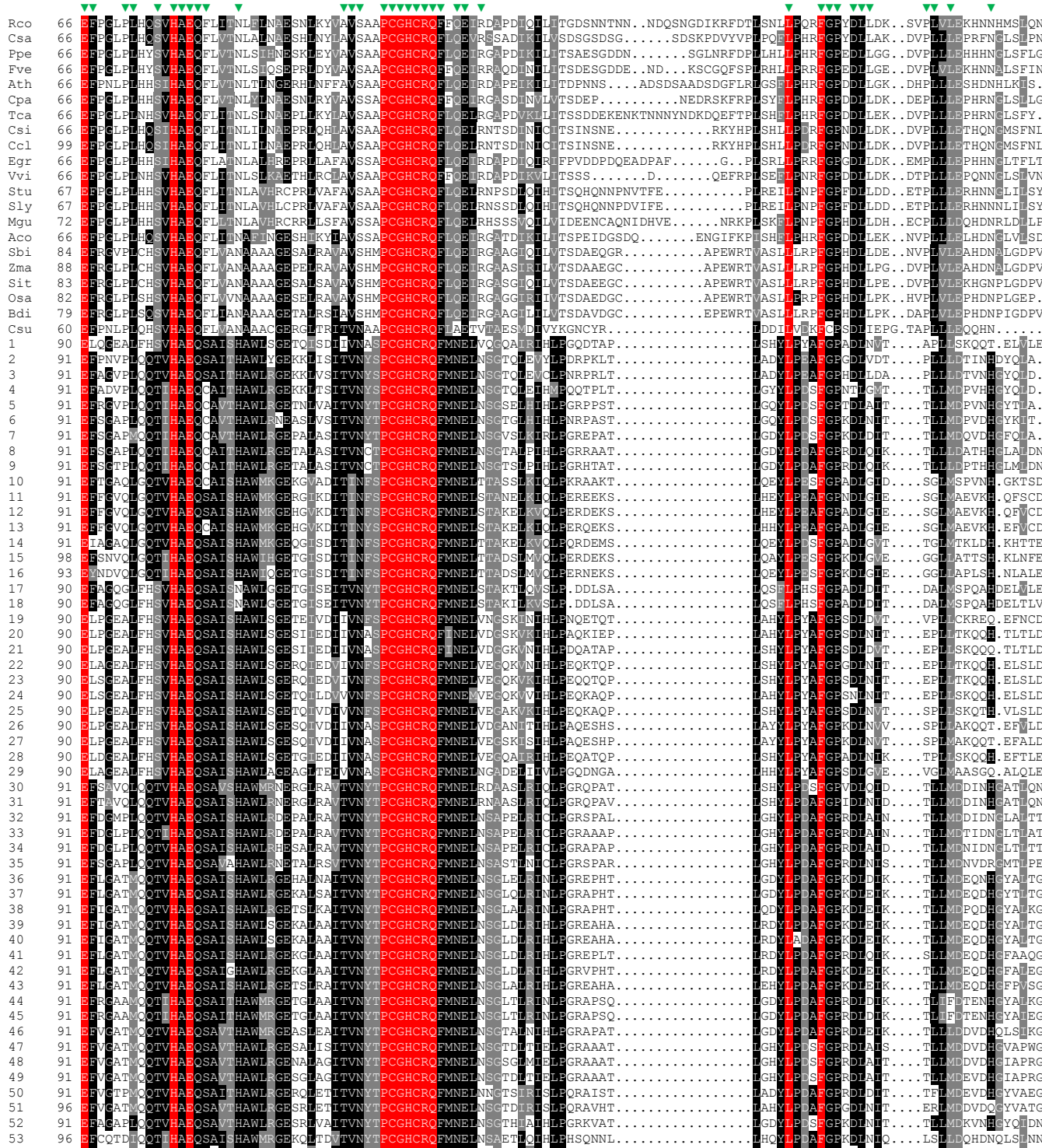
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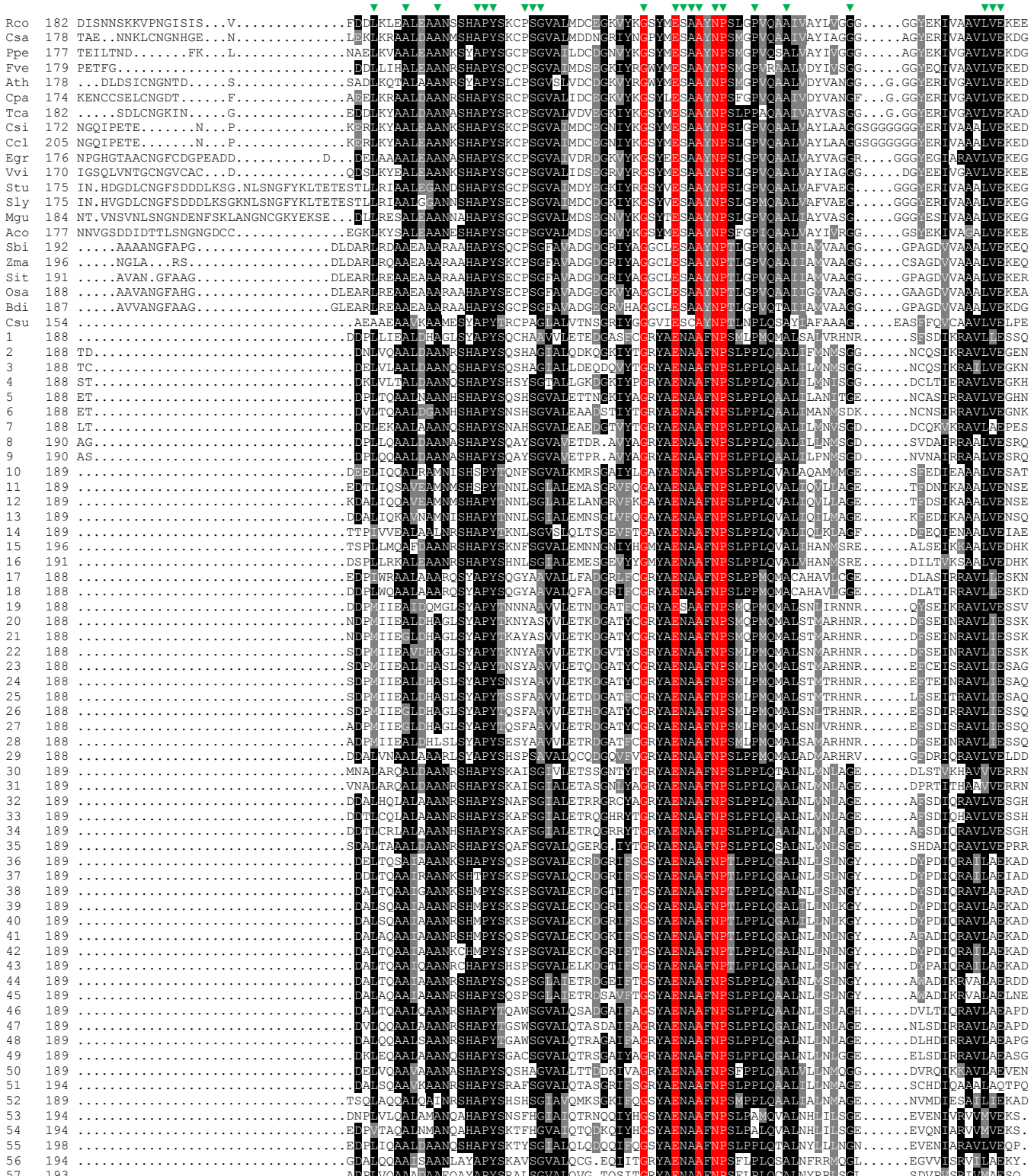
♦F165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52   269 SLLTQWDATQATLTALGCRQIQRVTI............
53   273 NTIHYKAMAEELLSTISDVKLDYFAV............
54   273 ASISYKAMAEELLGTLANVKLEYIAI............
55   277 FRISYRGMTEELLAYLGDIPLDYIQVS...........
56   272 AVISHRAMTESLVKNLLNLPLEYVKI............
57   271 GGISHRSITEQLAHSYLGLELEYFAI............
58   272 GTTSHRQMSEALAESFLGLNLEYIEV............
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Supplemental Figure S1. Multiple alignment of CDA sequences from plants, algae and bacteria.

To determine conserved amino acids in CDAs across kingdoms, a collection of genuine CDA sequences was obtained and aligned. Using the CDA from *A. thaliana* as query (locus At2g19570) in BLAST searches of Phytozome v9.1 (http://www.phytozome.net), CDAs from those plants were recovered which contained only a single copy *CDA* gene in their genome (in total 21 sequences, one from the algae *Coccomyxa subellipsoidea,* Csu). Assuming that CDA is an indispensable component of plant primary metabolism in every plant, this ensured that a functional CDA copy was chosen in each case. Additionally, the Concise

Protein Database at NCBI (http://www.ncbi.nlm.nih.gov/genomes/prokhits.cgi) was searched using CDA from *A. thaliana* as query excluding "Viridiplantae". Bacterial CDA sequences from completed genomes were obtained in this search (62 in total). Those sequences were selected which matched the query over the entire length representing CDAs of the dimeric type (*Escherichia coli*-type) whereas CDAs of the tetrameric type (*Bacillus subtilis*-type) were not selected (Faivre-Nitschke et al., 1999). A multiple alignment was generated with ClustalW and shaded with Boxshade. Amino acids absolutely conserved are marked with red background. Amino acids which are only conserved in the 20 single-copy plant CDAs were labeled with a green arrowhead above the alignment. Diamonds under the alignment mark residues of functional importance in the CDA of *E. coli* as revealed by crystal structure analysis (Betts et al., 1994; sequence numbering as in the original report). Involved in Zn binding: H102, C129, C132; involved in substrate binding via hydrogen bonds: N89, E91, A103 (backbone N), E104, Y126, T127 (backbone O); involved in substrate binding via hydrophobic interactions: F71, Y126, F165, F233; sterically important to generate the binding site for the transition state: P128, G130. The following sequences were used in this alignment:

label	organism	Uniprot accession	NCBI / EMBL accession	Gene locus identifier in Phytozome v9.1
Rco	*Ricinus communis*	B9RK96	XP_002514140	29912.m005381
Csa	*Cucumis sativus*		XP_004135706	Cucsa.397300
Ppe	*Prunus persica*	M5W9R1	EMJ03530	ppa009163m
Fve	*Fragaria vesca*		XP_004287542	mrna11427.1-v1.0-hybrid
Ath	*Arabidopsis thaliana*	O65896	NP_179547	At2g19570
Cpa	*Carica papaya*		none	evm.TU.contig_31168
Tca	*Theobroma cacao*		EOY30482	Thecc1EG037679t1
Csi	*Citrus sinensis*		none	orange1.1g022046m
Ccl	*Citrus clementina*		none	Ciclev10008864m
Egr	*Eucalyptus grandis*		none	Eucgr.C00902
Vvi	*Vitis vinifera*		XP_002282373	[1]
Stu	*Solanum tuberosum*	M1ACX7	none	PGSC0003DMP4000136
Sly	*Solanum lycopersicum*	K4CD31	XP_004242947	Solyc07g021750
Mgu	*Mimulus guttatus*		none	mgv1a026892m
Aco	*Aquilegia coerulea*		none	Aquca_001_00077
Sbi	*Sorghum bicolor*		XP_002458392	Sb03g032720
Zma	*Zea mays*		DAA57895	GRMZM2G380088_T01
Sit	*Setaria italica*		XP_004969732	Si002312m
Osa	*Oryza sativa*		NP_001044051	Os01g51540
Bdi	*Brachypodium distachyon*		XP_003569672	Bradi2g48040
Csu	*Coccomyxa subellipsoidea*		EIE20643	37578
1	*Shewanella amazonensis* SB2B		YP_927849	
2	*Xenorhabdus nematophila* ATCC 19061		YP_003711754	
3	*Xenorhabdus bovienii* SS-2004		YP_003466872	
4	*Photorhabdus asymbiotica*		YP_003041726	
5	*Yersinia pestis* KIM10+		NP_669958	
6	*Yersinia enterocolitica* subsp. enterocolitica 8081		YP_001006982	
7	*Serratia proteamaculans* 568		YP_001477800	
8	*Edwardsiella tarda* EIB202		YP_003295218	
9	*Edwardsiella ictaluri* 93-146		YP_002932714	
10	*Vibrio cholerae* O1 biovar El Tor str. N16961		NP_230876	
11	*Vibrio* sp. Ex25		YP_003286324	
12	*Vibrio parahaemolyticus* RIMD 2210633		NP_797677	
13	*Vibrio campbellii* ATCC BAA-1116		YP_001445308	
14	*Vibrio splendidus* LGP32		YP_002417326	
15	*Aliivibrio salmonicida* LFI1238		YP_002263107	

16	*Vibrio fischeri* MJ11	YP_002156297
17	*Aeromonas salmonicida* subsp. salmonicida A449	YP_001142202
18	*Aeromonas hydrophila* subsp. hydrophila ATCC 7966	YP_856425
19	*Shewanella frigidimarina* NCIMB 400	YP_750326
20	*Shewanella halifaxensis* HAW-EB4	YP_001674007
21	*Shewanella pealeana* ATCC 700345	YP_001502343
22	*Shewanella piezotolerans* WP3	YP_002312342
23	*Shewanella sediminis* HAW-EB3	YP_001474353
24	*Shewanella woodyi* ATCC 51908	YP_001760427
25	*Shewanella violacea* DSS12	YP_003557287
26	*Shewanella putrefaciens* CN-32	YP_001183092
27	*Shewanella baltica* OS155	YP_001050074
28	*Shewanella loihica* PV-4	YP_001093736
29	*Ferrimonas balearica* DSM 9799	YP_003912679
30	*Pectobacterium carotovorum* subsp. carotovorum PC1	YP_003017075
31	*Pectobacterium wasabiae* WPP163	YP_003260323
32	*Dickeya dadantii* 3937	YP_003882556
33	*Dickeya dadantii* Ech586	YP_003334050
34	*Dickeya zeae* Ech1591	YP_003004864
35	*Dickeya dadantii* Ech703	YP_002988053
36	*Enterobacter* sp. 638	YP_001177462
37	*Enterobacter cloacae* subsp. cloacae ATCC 13047	YP_003613937
38	*Enterobacter lignolyticus* SCF1	YP_003941104
39	*Shigella flexneri* 2a str. 301	NP_708043
40	*Escherichia coli* O157:H7 str. EDL933	NP_288726
41	*Citrobacter rodentium* ICC168	YP_003365817
42	*Citrobacter koseri* ATCC BAA-895	YP_001452236
43	*Klebsiella pneumoniae* subsp. pneumoniae MGH 78578	YP_001336232
44	*Cronobacter sakazakii* ATCC BAA-894	YP_001437196
45	*Cronobacter turicensis* z3032	YP_003211179
46	*Erwinia billingiae* Eb661	YP_003742355
47	*Erwinia pyrifoliae* Ep1/96	YP_002648374
48	*Erwinia amylovora* CFBP1430	YP_003531641
49	*Erwinia tasmaniensis* Et1/99	YP_001907235
50	*Pantoea vagans* C9-1	YP_003931651
51	*Pantoea ananatis* LMG 20103	YP_003520831
52	*Proteus mirabilis* HI4320	YP_002150412
53	*Aggregatibacter actinomycetemcomitans* D11S-1	YP_003256350
54	*Aggregatibacter aphrophilus* NJ8700	YP_003006930
55	*Haemophilus somnus* 2336	YP_001784141
56	*Haemophilus parasuis* SH0165	YP_002476019
57	*Actinobacillus succinogenes* 130Z	YP_001343737
58	*Actinobacillus pleuropneumoniae* serovar 5b str. L20	YP_001054032
59	*Coraliomargarita akajimensis* DSM 45221	YP_003548999
60	*Ketogulonicigenium vulgare* Y25	YP_003963506
61	*Entamoeba dispar* SAW760	XP_001737821
62	*Entamoeba histolytica* HM-1:IMSS	XP_656341

[1] gene structure wrongly annotated in Phytozome v9.1