Supplementary Information

The molecular evolution of the Qo motif

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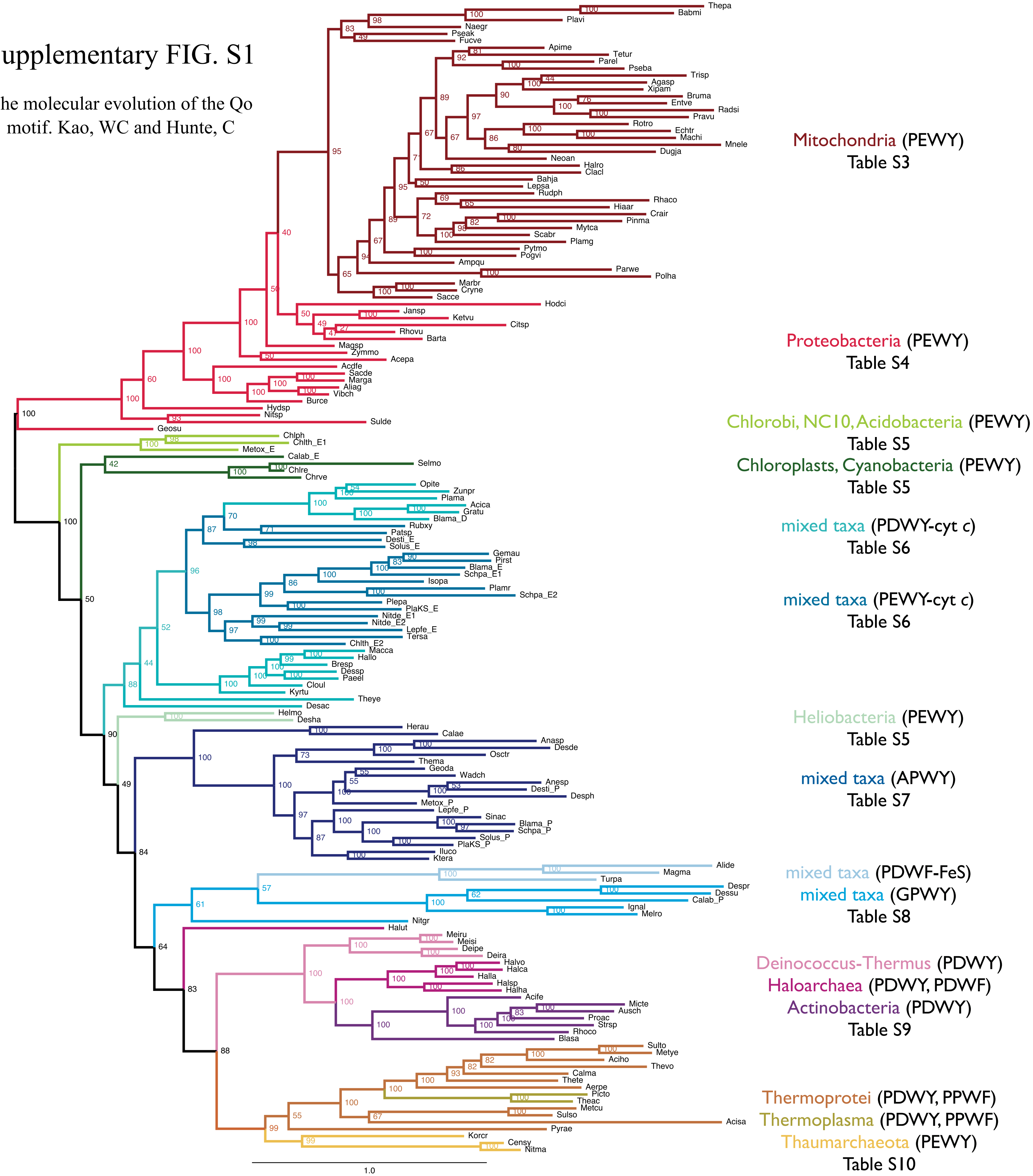
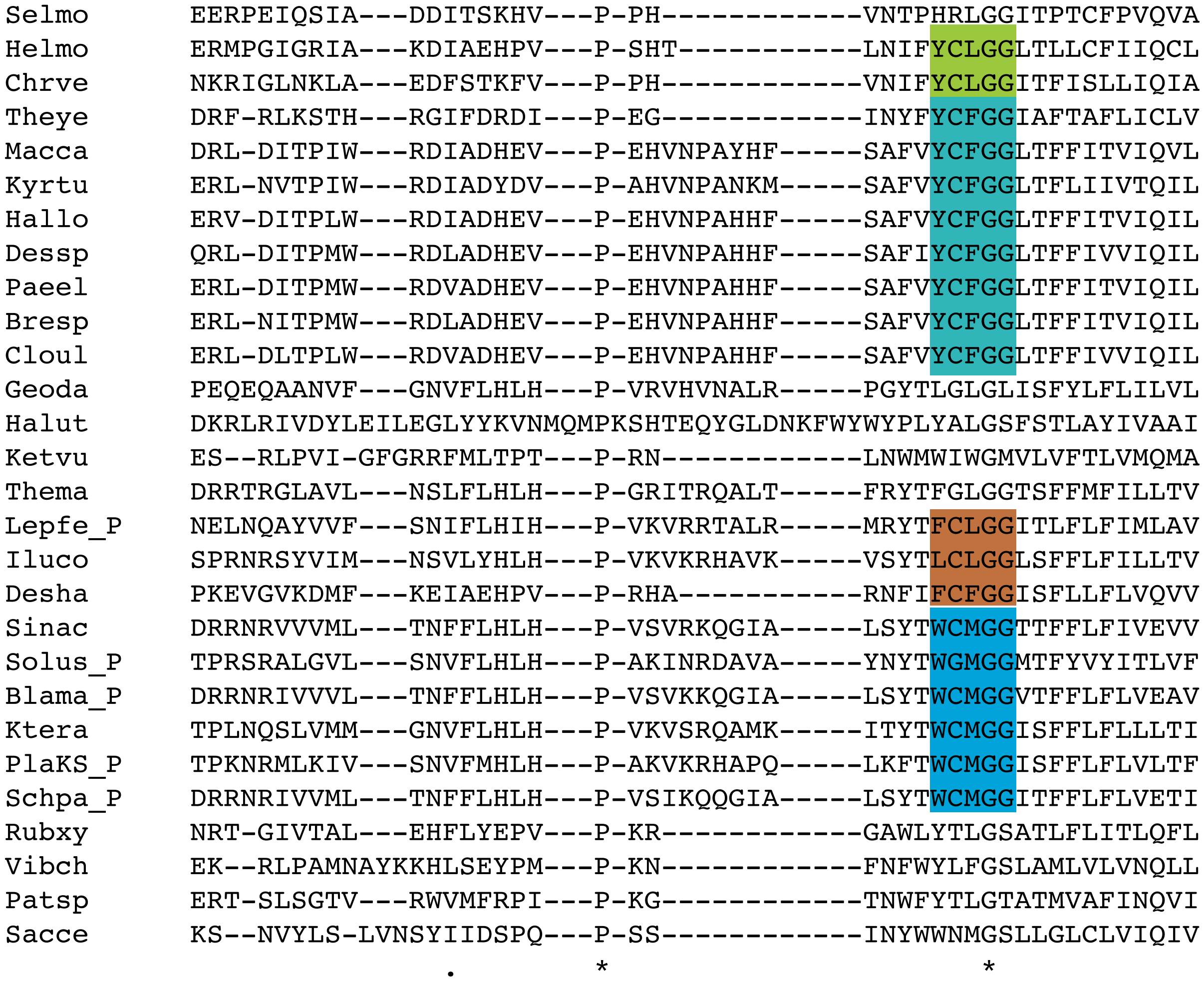
Supplementary FIG. S1

The molecular evolution of the Qo motif. Kao, WC and Hunte, C



Supplementary FIG. S 1: See previous page for the figure. The Bayesian inference tree of cyt *b*. The phylogenetic tree of **fig. 4** is represented in the midpoint-rooted, rectangular layout, showing all tip labels and branching probabilities (in percentage). The representative lineages and Qo motifs are noted next to each clade. Detailed descriptions of individual branches are described from **supplementary table S3** to **table S10**.



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Selmo      EERPEIQSIA---DDITSKHV---P-PH------------VNTPHRLGGITPTCFPVQVA
Helmo      ERMPGIGRIA---KDIAEHPV---P-SHT-----------LNIFYCLGGLTLLCFIIQCL
Chrve      NKRIGLNKLA---EDFSTKFV---P-PH------------VNIFYCLGGITFISLLIQIA
Theye      DRF-RLKSTH---RGIFDRDI---P-EG------------INYFYCFGGIAFTAFLICLV
Macca      DRL-DITPIW---RDIADHEV---P-EHVNPAYHF-----SAFVYCFGGLTFFITVIQVL
Kyrtu      ERL-NVTPIW---RDIADYDV---P-AHVNPANKM-----SAFVYCFGGLTFLIIVTQIL
Hallo      ERV-DITPLW---RDIADHEV---P-EHVNPAHHF-----SAFVYCFGGLTFFITVIQIL
Dessp      QRL-DITPMW---RDLADHEV---P-EHVNPAHHF-----SAFIYCFGGLTFFIVVIQIL
Paeel      ERL-DITPMW---RDVADHEV---P-EHVNPAHHF-----SAFVYCFGGLTFFITVIQIL
Bresp      ERL-NITPMW---RDLADHEV---P-EHVNPAHHF-----SAFVYCFGGLTFFITVIQIL
Cloul      ERL-DLTPLW---RDVADHEV---P-EHVNPAHHF-----SAFVYCFGGLTFFIVVIQIL
Geoda      PEQEQAANVF---GNVFLHLH---P-VRVHVNALR-----PGYTLGLGLISFYLFLILVL
Halut      DKRLRIVDYLEILEGLYYKVNMQMPKSHTEQYGLDNKFWYWYPLYALGSFSTLAYIVAAI
Ketvu      ES--RLPVI-GFGRRFMLTPT---P-RN------------LNWMWIWGMVLVFTLVMQMA
Thema      DRRTRGLAVL---NSLFLHLH---P-GRITRQALT-----FRYTFGLGGTSFFMFILLTV
Lepfe_P    NELNQAYVVF---SNIFLHIH---P-VKVRRTALR-----MRYTFCLGGITLFLFIMLAV
Iluco      SPRNRSYVIM---NSVLYHLH---P-VKVKRHAVK-----VSYTLCLGGLSFFLFILLTV
Desha      PKEVGVKDMF---KEIAEHPV---P-RHA-----------RNFIFCFGGISFLLFLVQVV
Sinac      DRRNRVVVML---TNFFLHLH---P-VSVRKQGIA-----LSYTWCMGGTTFFLFIVEVV
Solus_P    TPRSRALGVL---SNVFLHLH---P-AKINRDAVA-----YNYTWGMGGMTFYVYITLVF
Blama_P    DRRNRIVVVL---TNFFLHLH---P-VSVKKQGIA-----LSYTWCMGGVTFFLFLVEAV
Ktera      TPLNQSLVMM---GNVFLHLH---P-VKVSRQAMK-----ITYTWCMGGISFFLFLLLTI
PlaKS_P    TPKNRMLKIV---SNVFMHLH---P-AKVKRHAPQ-----LKFTWCMGGISFFLFLVLTF
Schpa_P    DRRNRIVVML---TNFFLHLH---P-VSIKQQGIA-----LSYTWCMGGITFFLFLVETI
Rubxy      NRT-GIVTAL---EHFLYEPV---P-KR------------GAWLYTLGSATLFLITLQFL
Vibch      EK--RLPAMNAYKKHLSEYPM---P-KN------------FNFWYLFGSLAMLVLVNQLL
Patsp      ERT-SLSGTV---RWVMFRPI---P-KG------------TNWFYTLGTATMVAFINQVI
Sacce      KS--NVYLS-LVNSYIIDSPQ---P-SS------------INYWWNMGSLLGLCLVIQIV
                          .        *                      *
```

Supplementary FIG. S 2: Multiple sequence alignment of all cyt *b* N-terminal proteins from COB_50, with cyt *b* of *S. cereviseae*. The column containing the potential heme c_i binding motif (CxGG) and its upstream amino acid are highlighted according to their specific patterns. Cyt *b* from photosynthetic organisms: green (**supplementary table S** 5); cyt *b* clustered PEWY-cyt *c* and PDWY-cyt *c* clades: blue-green (**supplementary table S** 6); Cyt *b* from Planctomycetes and Chloroflexi in the APWY clade: blue (**supplementary table S** 7); others: brown (**supplementary table S** 7, S 5).

```
NP_559242         PGMQVIEIPTSALMPWDKLYLYGEEVPPTLKATQSYVSVYTITYLTPFGFVLRQFHLWAA
YP_001056794      PSLDVRQIPASAIMKWDQLYGVE---GGEVSATGSYLSVYKIVYLTPFGFILRQFHLWAA
YP_005260411      PGMAVKEVPTSALMPWDVLHPK---KTETVQATQSYLSVYTITYLTPFGFILRQFHLWAA
YP_005084460      PGVSTTVKTPPDI-------LSGHAAAESYVATQSYGSVYRIVYLTPLGFIVREIHLWAA
YP_004337861      PGVTPTYTIQT--------------LGGSAEVSQSYYSVYKIAYLTPLGFILREIHLWAA
NP_009315         SNIELAFS-----------------------------SVEHIMRDVHNGYILRYLHANGA
                    :                                  **  *   .  *:::* :*  .*

NP_559242         YLMIFAALVHFFAKFVLGSYKRKGGGALWLIGVLLGFLTISQAVLGYILPLHLDGILALM
YP_001056794      YLMIMAALVHFFAKFVLGAYKRRGGGALWFLGVLLGVLTINQAVLGYILPLHLDGILALM
YP_005260411      YMMIMAAFVHFFAKFVLGSYKRKGGGALWFLGVLLGFLTVNQAVLGYILPLHLDGILALL
YP_005084460      YMMIFATLAHFFAKFILGSYKRRGGGALWLLGVLLGFLTINQAVLGYILPLHLDGILALQ
YP_004337861      YMMVFAAITHFFAKFVLGSYKRRGGGALWLLGVLLGVLTVTQAVLGYILPLHLDGALALQ
NP_009315         SFFFMVMFMHMAKGLYYGSYRS-PRVTLWNVGVIIFILTIATAFLGYCCVYGQMSHWGAT
                   ::.:. : *:   :  *:*:     :** :**:: .**:  *.***       .  .

NP_559242         IGLNLFRYFDYIGIPVGGAIIALMGSNYPTDAVVKIIYVAHIL----IVPAIILILLVLK
YP_001056794      IGLNLFRYFDYLGIPVGGTIIALLGSNYPTNEVVKMVYVLHIL----IVPAVILILLGLK
YP_005260411      IGLNLFRYFDYIGIPVGGLIIALLGSNYPTDAVIKMIYVAHIL----VVPAIILILLGLK
YP_005084460      IGLNIFRYFDYLGIPVGQLILALLGSNFVTDQVIKIIYSLHIL----IVPAVILVLLGLK
YP_004337861      IGLNIFRYLEYFGVPVGQVVVSVLGSTFITSGIMKDIYTLHVL----VVPAIILVLLGLK
NP_009315         VITNLFSAIPFVGNDIVS---WLWGGFSVSNPTIQRFFALHYLVPFIIAAMVIMHLMALH
                  : *:*  : :.*  :      : *.   :.  :: .:  * *    :.  :*: *: *:

NP_559242         IQGILYGGVSPPPVKNEEIRRKMVEDKEPFYPHRFALM--VGQVFLQISLLLLLVAFFPL
YP_001056794      IQGILYGGVSPPPVKNEALRQKMVEDKEPFYPHRFALM--VGQVFLQISFLLLLVAFFPQ
YP_005260411      IQGILYGGVSPPPVRDQELAKKMVDDKEPFYPHRFALM--TGQVFLQISLLLLLVAFFPQ
YP_005084460      INGILYGGVSPPPVKDPAVREKALQEKEPFYPHRFALT--VGQLFLQLSVLLLLVAVFPL
YP_004337861      INGILYGGVSPPPTKNNAARERALAETEPFYPHRFALT--VGQLLLQLSVLLLLVAVFPQ
NP_009315         IHG-----SSNPLGITGNLDR------IPM--HSYFIFKDLVTVFLFMLILALFVFYSPN
                  *.*      * *        .       *:  * : :      ::* : .* *:*   *

NP_559242         PL--LEPWAPGEPV--PPGVRPPWPVMWYYTYVKMIDPF-ISVGLPIVLVLFALVVPLLD
YP_001056794      PL--LEPWAPGQGV--PTGVRPPWPVMWYYTYVKMIDPF-ISVGLPFLLVLFALVVPLLD
YP_005260411      PL--LEPWAPGEIV--PAGVRPPWPVMWYYTYVKMIDPF-ISVGIPIIMVLFALVVPLLD
YP_005084460      PL--LEPWLPGQPV--PAGVRPPWPVMWYYTYVKMIDPF-ISVGLPFVLVLFALVVPLLD
YP_004337861      PL--LEPWLPGQPV--PSGVRPPWPVEWYYTYVKAINPF-ISVGIPIFMVLFALIVPLID
NP_009315         TLGHPDNYIPGNPLVTPASIVPEWYLLPFYAILRSIPDKLLGVITMFAAILVLLVLPFTD
                   *   : : **: :  * .: * * :  :*: :: *    :.*   :  :*. *::*: *
```

Supplementary FIG. S 3: Multiple sequence alignment of Pyrobaculum cyt *b* homologs, with cyt *b* of *S. cereviseae*. The column containing the conserved three axial ligands of heme *b* are highlighted in blue, and the amino acids aligned to the fourth axial ligand of *S. cereviseae* are highlighted in pink. The Qo motif is colored in brown. List of organisms: NP_559242: *Pyrobaculum aerophilum* str. IM2; YP_001056794: *Pyrobaculum calidifontis* JCM 11548; YP_005260411: *Pyrobaculum oguniense* TE7; YP_005084460: *Pyrobaculum* sp. 1860; YP_004337861: *Thermoproteus uzoniensis* 768-20; NP_009315: *S. cerevisiae*.

```
YP_002512829        YYSVKDIVGVGVFLILFFAVVFFAPEAGGYFLKAANFVKSDPLVTPDFIPPVWYYGAFYT
YP_003461444        YYTVKDIVGVGVFLMVFAVIMFFFPMGGGLFLKPDNMIPADPLVTPELIPPVWYFTSMYS
YP_007217743        YYTVKDLVGVGVFFIAFFAVVFFAPEMGGLFLKPANMIPADPLVTPDLIPPVWYFTSFYS
YP_743042           YYTVKDLFGVGVFLIVFSVVVFFIPEVGGYFIKYDNFIPADPLTTPSHIPPVWYFAPHYA
ZP_08929533         YYTVKDLVGVGVFLIAFFAVVFFAPEMGGLFLKPANMIPADPLVTPDLIPPVWYFTSFYS
NP_230225           YGTVKDLIGVAGFLFLFCYVLFFNPEMGGYFLEPPNFEAANPLKTPEHIAPVWYFTPFYA
NP_253120           YYTVKDIVGVVVFLFIFCTVIFFFPEMGGYFLEKPNFEMANQFKTPEHIAPVWYFTPFYA
NP_275042           YYVVHDILAVTIFLIVFCAVMFFAPEGGGYFLEAPNFDAANALKTPPHIAPVWYFTPFYA
NP_298199           YYTLKEMVAVCVLLLLAAFVIFFAPEFGGLFLEYGNFVEANPLMTPEDMKPVWYFAPYYA
NP_521049           YYSVHDIVGVAVFLFLFSAILFFAPEMGGYFLEANNFIPADSLKTPPHIAPVWYFTPFYS
NP_637677           YYTVKDLVGVGFLLVIAAFIIFFAPAFGGLFLEHDNFTEANRLVTPEHIKPVWYYTPYYA
NP_009315           YFIFKDLVTVFLFMLILALFVFYSPNTLG---HPDNYIPGNPLVTPASIVPEWYLLPFYA
                    *  .:::. *  ::.    .:*: *   *   .  *   .: : **  : * **    *:
```

Supplementary FIG. S 4: Multiple sequence alignment of selected β- and γ-proteobacteria and *S. cerevisiae* cyt *b* showing the Qo motif (highlighted in brown) and amino acids aligned to His253 of the yeast enzyme (highlighted in blue). 342 out of 350 β-proteobacterial cyt *b*, and 590 out of 629 γ-proteobacterial cyt *b* employ Glu253 (**supplementary table S** 1). Interestingly, five alkaliphilic strains use a lysine residue at the Glu253 equivalent position, which may facilitate proton transfer at high pH. List of organisms: YP_002512829: *Thioalkalivibrio sulfidophilus* HL-EbGr7; YP_003461444 : *Thioalkalivibrio* sp. K90mix; YP_007217743: *Thioalkalivibrio nitratireducens* DSM 14787; YP_743042: *Alkalilimnicola ehrlichii* MLHE-1; ZP_08929533: *Thioalkalivibrio thiocyanoxidans* ARh 4; NP_230225: *Vibrio cholerae* O1 biovar El Tor str. N16961; NP_253120: *Pseudomonas aeruginosa* PAO1; NP_275042: *Neisseria meningitidis* MC58; NP_298199: *Xylella fastidiosa* 9a5c; NP_521049: *Ralstonia solanacearum* GMI1000; NP_637677: *Xanthomonas campestris* pv. campestris str. ATCC 33913; NP_009315: *S. cerevisiae*.

```
BLASTP 2.2.27+

Query= gi|121591043|ref|ZP_01678359.1| ubiquinol--Cytochrome c reductase,
cytochrome B [Vibrio cholerae 2740-80]

Length=235

>ref|ZP_23822384.1| cytochrome b family protein [Vibrio cholerae O1 str. 116063]
Length=421

 Score =  465 bits (1196),  Expect = 5e-165, Method: Compositional matrix adjust.
 Identities = 229/229 (100%), Positives = 229/229 (100%), Gaps = 0/229 (0%)

Query  1    MQALLDWVEKRLPAMNAYKKHLSEYPMPKNFNFWYLFGSLAMLVLVNQLLTGIWLTMNYV  60
            MQALLDWVEKRLPAMNAYKKHLSEYPMPKNFNFWYLFGSLAMLVLVNQLLTGIWLTMNYV
Sbjct  1    MQALLDWVEKRLPAMNAYKKHLSEYPMPKNFNFWYLFGSLAMLVLVNQLLTGIWLTMNYV  60

Query  61   PSGEGAFASIEYIMRDVEYGWLLRYMHSTGASAFFVVVYLHMFRGLIYGSYQKPRELLWI  120
            PSGEGAFASIEYIMRDVEYGWLLRYMHSTGASAFFVVVYLHMFRGLIYGSYQKPRELLWI
Sbjct  61   PSGEGAFASIEYIMRDVEYGWLLRYMHSTGASAFFVVVYLHMFRGLIYGSYQKPRELLWI  120

Query  121  FGMLIFLVLMAEAFMGYLLPWGQMSYWGAQVIISLFGAIPVIGDDLTLWIRGDYVISGAT  180
            FGMLIFLVLMAEAFMGYLLPWGQMSYWGAQVIISLFGAIPVIGDDLTLWIRGDYVISGAT
Sbjct  121  FGMLIFLVLMAEAFMGYLLPWGQMSYWGAQVIISLFGAIPVIGDDLTLWIRGDYVISGAT  180

Query  181  LNRFFALHVIALPIVLLLLIVLHILALHEVGSNNPDGIETKLPKGSMGE  229
            LNRFFALHVIALPIVLLLLIVLHILALHEVGSNNPDGIETKLPKGSMGE
Sbjct  181  LNRFFALHVIALPIVLLLLIVLHILALHEVGSNNPDGIETKLPKGSMGE  229


Query= gi|121591034|ref|ZP_01678350.1| ubiquinol--cytochrome c reductase,
cytochrome B [Vibrio cholerae 2740-80]

Length=147

>ref|ZP_21092526.1| cytochrome b family protein [Vibrio cholerae HC-78A1]
Length=421

 Score =  299 bits (765),  Expect = 2e-101, Method: Compositional matrix adjust.
 Identities = 146/147 (99%), Positives = 147/147 (100%), Gaps = 0/147 (0%)

Query  1    MLFFNPEMGGYFLEPPNFEAANPLKTPEHIAPVWYFTPFYAILRAVPDKLLGVIAMGASI  60
            +LFFNPEMGGYFLEPPNFEAANPLKTPEHIAPVWYFTPFYAILRAVPDKLLGVIAMGASI
Sbjct  275  VLFFNPEMGGYFLEPPNFEAANPLKTPEHIAPVWYFTPFYAILRAVPDKLLGVIAMGASI  334

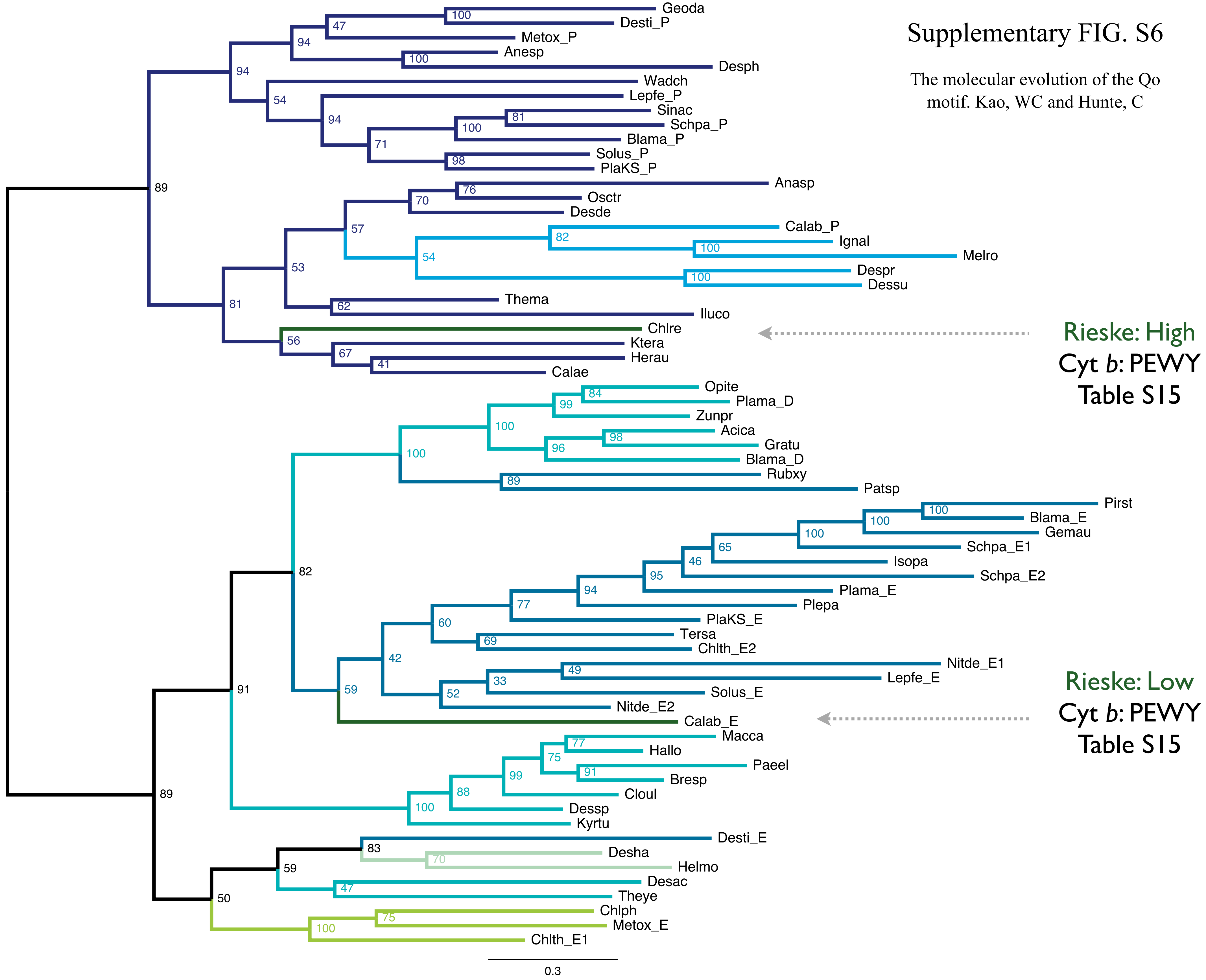
Query  61   VVLFLLPWLDRCKVRSYRYRSKFHLFNIAQFTVSFIALGILGALPATPTYTLLAQIFSLC  120
            VVLFLLPWLDRCKVRSYRYRSKFHLFNIAQFTVSFIALGILGALPATPTYTLLAQIFSLC
Sbjct  335  VVLFLLPWLDRCKVRSYRYRSKFHLFNIAQFTVSFIALGILGALPATPTYTLLAQIFSLC  394

Query  121  YFMFFVLLFFYSKNEATKPLPTRVTYK  147
            YFMFFVLLFFYSKNEATKPLPTRVTYK
Sbjct  395  YFMFFVLLFFYSKNEATKPLPTRVTYK  421
```

Supplementary FIG. S 5: BLAST result of the sequence of the N-terminal region (ZP_01678359) and C-terminal region of cyt *b* (ZP_01678350) of *Vibrio cholerae* 2740-80, showing the high identities to the full-length homologs from other strains of the same species.

Supplementary FIG. S6

The molecular evolution of the Qo motif. Kao, WC and Hunte, C



Rieske: High
Cyt *b*: PEWY
Table S15

Rieske: Low
Cyt *b*: PEWY
Table S15

Rieske: Mid$^+$, High
Cyt *b*: APWY
Table S13

Rieske: Mid$^+$, High
Cyt *b*: GPWF
Table S13

Rieske: Low, Mid$^-$
Cyt *b*: PDWY-cyt *c*
Table S14

Rieske: Low, Mid$^-$, Mid$^+$,High
Cyt *b*: PEWY-cyt *c*
Table S15

Rieske: Low
Cyt *b*: PDWY, PEWY
Table S15

Rieske: Low
Cyt *b*: PEWY
Table S15

Supplementary FIG. S 6: See previous page for the figure. The Bayesian inference tree of Rieske iron-sulfur proteins. The phylogenetic tree in **fig. 6** is represented in the midpoint-rooted, rectangular layout, showing all tip labels and branching probabilities (in percentage). The predicted midpoint potential of Rieske ISP and the type of corresponding cyt *b* are annotated next to each clades. Low: 150 mV; Mid^{-}: around 200 mV; Mid^{+}: around 260 mV; High: above 260 mV. Detailed descriptions of individual branches are found from **supplementary table S13** to **S15**.

Supplementary Table S 1: Lineage-specific occurrence of amino acid residues identified on His253 and Glu272 equivalent positions in all cyt *b* homologs identified: Organisms that encode full-length or split cyt *b*, but without cyt b_6f complexes.

	Full length cyt *b*									Split cyt *b*				
253 Equivalent residue ►	Asp	His	Glu	Glu	Glu	all	all	all	all	all	all	all	all	TOTAL
272 Equivalent residue ►	Glu	Glu	Glu	Val	all†	Glu	Asp	Pro	all	Glu	Asp	Pro	Val	
Metazoa	**3231**	2	32	2	–	29	2	–	3	–	–	–	–	3301
Fungi	**42**	**74**	4	–	–	–	–	–	–	–	–	–	–	120
Amoebozoa	1	5	–	–	–	–	–	–	–	–	–	–	–	6
α-Proteobacteria	**28**	**343**	**56**	–	–	18	2	–	2	1	–	–	–	450
ε-Proteobacteria	**395**	–	–	–	–	–	–	–	–	–	–	–	–	395
Aquificae	4	–	–	–	–	7	–	–	–	–	–	–	–	11
β-Proteobacteria	–	–	1	**342**	5	–	2	–	–	–	–	–	–	350
γ-Proteobacteria	–	–	–	**590**	26	5	–	–	6	–	–	–	2	629
δ-Proteobacteria	–	–	–	–	–	**12**	–	**12**	–	–	–	3	–	27
Chlorobi	–	–	–	–	–	**12**	–	–	–	–	–	–	–	12
Acidobacteria	–	–	–	–	–	**4**	**5**	1	–	–	–	1	–	11
Planctomycetes	–	–	–	–	–	**8**	2	–	–	–	–	5	–	15
Nitrospirae	–	–	–	–	–	2	–	1	2	1	–	3	–	9
Chloroflexi	–	–	–	–	–	–	1	2	1	–	–	1	–	5
Actinobacteria	–	–	–	–	–	–	**613**	–	–	4	–	1	–	618
Deinococcus-Thermus	–	–	–	–	–	–	**21**	–	–	–	–	–	–	21
Verrucomicrobia	–	–	–	–	–	–	**3**	–	–	–	–	–	–	3
Thaumarchaeota	–	–	–	–	–	**9**	–	–	–	–	–	–	–	9
Halobacteria	–	–	–	–	–	–	**41**	–	2	–	**62**	–	–	105
Crenarchaeota	–	–	–	–	–	–	**20**	**52**	1	–	–	–	–	67
Thermoplasma	–	–	–	–	–	–	**3**	**2**	–	–	–	–	–	5
Other Organisms	–	11	–	1	–	4	2	9	–	9	–	–	–	36

Supplementary Table S 2: Lineage-specific occurrence of amino acid residues identified on His253 and Glu272 equivalent positions in all cyt *b* homologs identified: Organisms which encode cyt b_6f complexes and/ or cyt bc_1 complexes.

	Cyt bc_1 complexes									Cyt b_6f complexes				
253 Equivalent residue ▶ 272 Equivalent residue ▶	Asp Glu	His Glu	Glu Glu	Glu Val	Glu all[†]	all Glu	all Asp	all Pro	all all	all Glu	all Asp	all Pro	all Val	TOTAL
Firmicutes	–	–	–	–	–	–	–	–	2	2	**297**	3	–	304
Cyanobacteria	–	–	–	–	–	–	–	–	–	**123**	–	–	–	123
Alveolata	5	**20**	–	–	8	–	–	–	–	**4**	–	–	–	37
Stramenopiles	10	**20**	1	–	–	–	–	–	–	**15**	–	–	–	46
Rhodophyta	–	**8**	–	–	–	–	–	–	–	**6**	–	–	–	14
Viridiplantae	–	**80**	–	–	–	2	–	–	–	**276**	–	–	–	358

– represents zero. [†] Other amino acid residues than what is denoted in either the 253rd or the 272nd position.

Note: the number of cyt bc_1 and cyt b_6f complexes has no strict correspondence, since not all the organelle genomes of the same species were subjected to sequencing.

Supplementary Table S 3: Cyt *b* from the mitochondrial clades

Abbreviation	Qo-motif	253rd equiv. residue	Accession Number	Kingdom (Superphylum)	Organism
Pseak	PEWY	H	YP_025795	Viridiplantae	*Pseudendoclonium akinetum*
Fucve	PEWY	E	YP_448625	Stramenopiles	*Fucus vesiculosus*
Naegr	PEWY	H	NP_066512	Heterolobosea[a]	*Naegleria gruberi*
Plavi	PEWY	H	YP_272128	Alveolata	*Plasmodium vivax* Sal-1
Thepa	PEWY	D	YP_001994287	Alveolata	*Theileria parva*
Babmi	PEWY	D	YP_007024786	Alveolata	*Babesia microti*
Sacce	PEWY	H	NP_009315	Fungi	*Saccharomyces cerevisiae* S288c
Marbr	PEWY	D	YP_004842018	Fungi	*Marssonina brunnea* f. sp. 'multigermtubi'
Cryne	PEWY	H	YP_006883709	Fungi	*Cryptococcus neoformans* var. grubii H99
Agasp	PEWY	D	YP_665494	Metazoa	*Agamermis sp.* BH-2006 (nematode)
Ampqu	PEWY	D	YP_001031207	Metazoa	*Amphimedon queenslandica* (desmosponge)
Apime	PEWY	D	NP_008093	Metazoa	*Apis mellifera* ligustica (common honey bee)
Bahja	PEWY	D	YP_007026918	Metazoa	*Bahadzia jaraguensis* (amphipod)
Bruma	PEWY	D	NP_694907	Metazoa	*Brugia malayi* (agent of lymphatic filariasis)
Clacl	PEWY	D	YP_007890326	Metazoa	*Clathrina clathrus*
Crair	PEWY	D	YP_003541100	Metazoa	*Crassostrea iredalei* (tropical oyster)
Dugja	PEWY	D	YP_004936148	Metazoa	*Dugesia japonica*
Echtr	PEWY	D	YP_007183134	Metazoa	*Echinorhynchus truttae* (thorny-headed worm)
Entve	PEWY	D	YP_002261318	Metazoa	*Enterobius vermicularis* (human pinworm)
Halro	PEWY	D	NP_038246	Metazoa	*Halocynthia roretzi* (sea squirt)
Hiaar	PEWY	D	YP_784020	Metazoa	*Hiatella arctica* (arctic hiatella)
Lepsa	PEWY	D	YP_271856	Metazoa	*Lepeophtheirus salmonis* (salmon louse)

[a] Class.

Abbreviation	Qo-motif	253rd equiv. residue	Accession Number	Kingdom (Superphylum)	Organism
Machi	PEWY	D	YP_007183167	Metazoa	*Macracanthorhynchus hirudinaceus* (giant thorny-headed worm)
Mnele	PDWF	E	YP_004927442	Metazoa	*Mnemiopsis leidyi* (sea walnut)
Mytca	PEWY	N	YP_004842037	Metazoa	*Mytilus californianus* (California mussel)
Neoan	PEWY	D	YP_073318	Metazoa	*Neomaskellia andropogonis* (sugarcane whitefly)
Parwe	PEWY	D	NP_059460	Metazoa	*Paragonimus westermani* (lung fluke)
Parel	PEWY	D	YP_006234167	Metazoa	*Paratemnoides elongatus* (pseudoscorpion)
Pinma	PEWY	E	YP_006883014	Metazoa	*Pinctada maxima* (silver-lipped pearl oyster)
Plamg	PEWY	D	YP_272043	Metazoa	*Placopecten magellanicus* (sea scallop)
Pogvi	PEWY	E	YP_220666	Metazoa	*Pogona vitticeps* (central bearded dragon)
Polha	PEWY	L	YP_004891181	Metazoa	*Polylabris halichoeres* (parasitic flatworm)
Pravu	PEWY	D	YP_007507205	Metazoa	*Pratylenchus vulnus* (walnut meadow nematode)
Pseba	PEWY	D	YP_006234176	Metazoa	*Pseudogarypus banksi* (pseudoscorpion)
Pytmo	PEWY	E	YP_004733497	Metazoa	*Python molurus* molurus (Indian python)
Radsi	PEWY	D	YP_003204886	Metazoa	*Radopholus similis* (banana-root nematode)
Rhaco	PEWY	D	YP_004581444	Metazoa	*Rhabdopleura compacta* (hemichordate)
Rotro	PEWY	D	YP_003331189	Metazoa	*Rotaria rotatoria* (rotifer)
Rudph	PEWY	D	NP_543037	Metazoa	*Ruditapes philippinarum* (Japanese littleneck clam)
Scabr	PEWY	D	YP_007627191	Metazoa	*Scapharca broughtonii*
Tetur	PEWY	A	YP_001795379	Metazoa	*Tetranychus urticae* (two-spotted spider mite)
Trisp	PEWY	D	NP_077260	Metazoa	*Trichinella spiralis* (trichinosis nematode)
Xipam	PEWY	D	YP_025922	Metazoa	*Xiphinema americanum* (American dagger nematode)

Supplementary Table S 4: Cyt *b* from the proteobacterial clades.

Abbreviation	Qo-motif	253^{rd} equiv. residue	Fused cyt *c*?	Accession Number	Class	Organism
Hydsp	PEWY	P		ZP_02177717	Aquificae	*Hydrogenivirga sp.* 128-5-R1-1
Acepa	PEWY	E		ZP_16286000	α-Proteobacteria	*Acetobacter pasteurianus* subsp. pasteurianus LMG 1262
Barta	PEWY	H		ZP_10466437	α-Proteobacteria	*Bartonella tamiae* Th239
Hodci	PEWY	N		YP_003038798	α-Proteobacteria	*Candidatus* Hodgkinia cicadicola Dsem
Jansp	PEWY	H		YP_508268	α-Proteobacteria	*Jannaschia sp.* CCS1
Ketvu	PEWY	H		YP_003965199+200	α-Proteobacteria	*Ketogulonicigenium vulgare* Y25
Magsp	PEWY	E	true	ZP_23004544	α-Proteobacteria	*Magnetospirillum sp.* SO-1
Rhovu	PEWY	H	true	ZP_10898046	α-Proteobacteria	*Rhodovulum sp.* PH10
Zymmo	PEWY	D		YP_004661509	α-Proteobacteria	*Zymomonas mobilis* subsp. pomaceae ATCC 29192
Burce	PVWY	E		ZP_04939832	β-Proteobacteria	*Burkholderia cenocepacia* PC184
Acdfe	PPWY	E		YP_002220760	γ-Proteobacteria	*Acidithiobacillus ferrooxidans* ATCC 53993
Aliag	PVWY	E		ZP_10351680	γ-Proteobacteria	*Alishewanella agri* BL06
Citsp	PEWY	S		ZP_04561410	γ-Proteobacteria	*Citrobacter sp.* 30_2
Sacde	PVWY	E	true	YP_528630	γ-Proteobacteria	*Saccharophagus degradans* 2-40
Vibch	PVWY	E		ZP_01678359+50	γ-Proteobacteria	*Vibrio cholerae* 2740-80
Marga	PVWY	E	true	ZP_01617541	γ-Proteobacteria	marine gamma proteobacterium HTCC2143
Geosu	PEWY	F		NP_952700	δ-Proteobacteria	*Geobacter sulfurreducens* PCA
Nitsp	PEWY	D		YP_001357048	ε-Proteobacteria	*Nitratiruptor sp.* SB155-2
Sulde	PEWY	F		YP_003303190	ε-Proteobacteria	*Sulfurospirillum deleyianum* DSM 6946

NOTE.–The “+” sign within the accession number of NCBI RefSeq database indicates that the cyt *b* homolog was concatenated from the two accession numbers of sequences of the N- and C-terminal regions.

Supplementary Table S 5: Cyt *b* from clades comprinsing of photosynthetic organisms.

Abbreviation	Qo-motif	heme c_i motif	Accession Number	Phylum/ Class	Organism
Desha	PDWY	FCFGG	ZP_17060832+33	Firmicutes/ Clostridia	*Desulfitobacterium hafniense* DP7
Helmo	PEWY	YCLGG	YP_001679865+66	Firmicutes/ Clostridia	*Heliobacterium modesticaldum* Ice1

Abbreviation	Qo-motif	heme c_i motif	Accession Number	Phylum	Organism
Calab_E	PEWY		ZP_09551543	(unclassified)	*Caldithrix abyssi* DSM 13497
Selmo	PERH		XP_002993891+92	Streptophyta	*Selaginella moellendorffii*
Chlre	PEWY	YCIGG	NP_958365+59	Chlorophyta	chloroplast *Chlamydomonas reinhardtii*
Chrve	PEWY	YCLGG	YP_003795329+5262	Alveolata/ Chromerida	chloroplast *Chromera velia*

Abbreviation	Qo-motif	heme c_i motif	Accession Number	Phylum	Organism
Chlph	PEWY		YP_001960378	Chlorobi	*Chlorobium phaeobacteroides* BS1
Chlth_E1	PEWY		YP_004862186	Acidobacteria	*Candidatus* Chloracidobacterium thermophilum B
Metox_E	PEWY		YP_003205722	candidate division NC10	*Candidatus* Methylomirabilis oxyfera

NOTE.–The “+” sign within the accession number of NCBI RefSeq database indicates that the cyt *b* homolog was concatenated from the two accession numbers of sequences of the N- and C-terminal regions.

Supplementary Table S 6: Cyt *b* from the PEWY-cyt *c* clade and PDWY-cyt *c* clade.

Abbreviation	Qo-motif	heme c_i motif	Fused cyt *c*?	Accession Number	Phylum/ Class	Organism
Bresp	PDWY	YCFGG	true	ZP_10742446+45	Firmicutes/ Bacilli	*Brevibacillus sp.* CF112
Dessp	PDWY	YCFGG	true	ZP_08462740+41	Firmicutes/ Bacilli	*Desmospora sp.* 8437
Hallo	PDWY	YCFGG	true	YP_006180888+87	Firmicutes/ Bacilli	*Halobacillus halophilus* DSM 2266
Kyrtu	PDWY	YCFGG	true	YP_003589550+49	Firmicutes/ Bacilli	*Kyrpidia tusciae* DSM 2912
Macca	PDWY	YCFGG	true	YP_002560515+14	Firmicutes/ Bacilli	*Macrococcus caseolyticus* JCSC5402
Paeel	PDWY	YCFGG	true	ZP_09079292+93	Firmicutes/ Bacilli	*Paenibacillus elgii* B69
Cloul	PDWY	YCFGG	true	ZP_23165745+44	Firmicutes/ Clostridia	*Clostridium ultunense* Esp
Desac	PAWY			YP_006465273	Firmicutes/ Clostridia	*Desulfosporosinus acidiphilus* SJ4
Theye	PEWY	YCFGG		YP_002248983+84	Nitrospirae	*Thermodesulfovibrio yellowstonii* DSM 11347
Acica	PDFF		true	YP_002755480	Acidobacteria	*Acidobacterium capsulatum* ATCC 51196
Gratu	PDFA		true	YP_004217982	Acidobacteria	*Granulicella tundricola* MP5ACTX9
Zunpr	PDWY		true	YP_003583939	Bacteroidetes	*Zunongwangia profunda* SM-A87
Blama_D	PDWY		true	ZP_01094311	Planctomycetes	*Blastopirellula marina* DSM 3645
Plama_D	PDWY		true	ZP_01854221	Planctomycetes	*Planctomyces maris* DSM 8797
Opite	PDWY		true	YP_001820421	Verrucomicrobia	*Opitutus terrae* PB90-1
Tersa	PEWY		true	YP_004182035	Acidobacteria	*Terriglobus saanensis* SP1PR4
Chlth_E2	PEWY		true	YP_004862044	Acidobacteria	Candidatus *Chloracidobacterium thermophilum* B
Solus_E	PEWY		true	YP_827419	Acidobacteria	Candidatus *Solibacter usitatus* Ellin6076
Patsp	PEWY		true	ZP_09470202+03	Actinobacteria/ Rubrobacteridae	*Patulibacter sp.* I11
Rubxy	PEWF			YP_645679+78	Actinobacteria/ Rubrobacteridae	*Rubrobacter xylanophilus* DSM 9941
Desti_E	PEWY		true	YP_006446863	δ-Proteobacteria	*Desulfomonile tiedjei* DSM 6799
Plepa	PEWY		true	ZP_01912028	δ-Proteobacteria	*Plesiocystis pacifica* SIR-1
Gemau	PEWY		true	YP_002760208	Gemmatimonadetes	*Gemmatimonas aurantiaca* T-27
Nitde_E1	PEWY			YP_003796589	Nitrospirae	*Candidatus Nitrospira* defluvii
Nitde_E2	PEWY		true	YP_003799486	Nitrospirae	*Candidatus Nitrospira* defluvii
Lepfe_E	PAWY		true	YP_005469368	Nitrospirae	*Leptospirillum ferrooxidans* C2-3
Blama_E	PEWY		true	ZP_01090199	Planctomycetes	*Blastopirellula marina* DSM 3645
Isopa	PEWY		true	YP_004179079	Planctomycetes	*Isosphaera pallida* ATCC 43644
Pirst	PEWY		true	YP_003372364	Planctomycetes	*Pirellula staleyi* DSM 6068
Plama_E	PEWF		true	ZP_01856609	Planctomycetes	*Planctomyces maris* DSM 8797
Schpa_E1	PEWY		true	ZP_11092181	Planctomycetes	*Schlesneria paludicola* DSM 18645
Schpa_E2	PEWY		true	ZP_11091336	Planctomycetes	*Schlesneria paludicola* DSM 18645
PlaKS_E	PEWY		true	ZP_10101269	Planctomycetes	*planctomycete KSU-1*

NOTE.–The “+” sign within the accession number of NCBI RefSeq database indicates that the cyt *b* homolog was concatenated from the two accession numbers of sequences of the N- and C-terminal regions.

Supplementary Table S 7: Cyt *b* from the APWY clade.

Abbreviation	Qo-motif	heme c_i motif	Accession Number	Phylum/ Class	Organism
Solus_P	APWY		YP_825633+32	Acidobacteria	*Candidatus* Solibacter usitatus Ellin6076
Iluco	APWY	LCLGG	YP_007562653+54	Actinobacteria/ Acidimicrobidae	*Ilumatobacter coccineum* YM16-304
Anasp	APWY		ZP_09484367	Bacteroidetes	*Anaerophaga sp.* HS1
Wadch	APWY		YP_003710306	Chlamydiae	*Waddlia chondrophila* WSU 86-1044
Calae	APWY		YP_005441946	Chloroflexi	*Caldilinea aerophila* DSM 14535 = NBRC 104270
Herau	APWY		YP_001547012	Chloroflexi	*Herpetosiphon aurantiacus* DSM 785
Ktera	APWY	WCMGG	ZP_06967906+05	Chloroflexi	*Ktedonobacter racemifer* DSM 44963
Osctr	AAWY		ZP_07687042	Chloroflexi	*Oscillochloris trichoides* DG-6
Anesp	APWY		YP_002133819	δ-Proteobacteria	*Anaeromyxobacter sp.* K
Desti_P	APWY		YP_006445645	δ-Proteobacteria	*Desulfomonile tiedjei* DSM 6799
Desph	APWF		ZP_24025636	δ-Proteobacteria	*Desulfotignum phosphitoxidans* DSM 13687
Desde	APWY		YP_005166714	δ-Proteobacteria	*Desulfovibrio desulfuricans* ND132
Geoda	APWY		YP_002535600+599	δ-Proteobacteria	*Geobacter daltonii* FRC-32
Thema	APWY		YP_004101177+176	Firmicutes/ Clostridia	*Thermaerobacter marianensis* DSM 12885
Metox_P	APWY		YP_003205672	candidate division NC10	*Candidatus* Methylomirabilis oxyfera
Lepfe_P	APWY	FCLGG	YP_005468543+44	Nitrospirae	*Leptospirillum ferrooxidans* C2-3
Blama_P	APWY	WCMGG	ZP_01091114+15	Planctomycetes	*Blastopirellula marina* DSM 3645
Schpa_P	APWY	WCMGG	ZP_11096294+93	Planctomycetes	*Schlesneria paludicola* DSM 18645
Sinac	APWY	WCMGG	YP_007201890+91	Planctomycetes	*Singulisphaera acidiphila* DSM 18658
PlaKS_P	APWY	WCMGG	ZP_10098673+70	Planctomycetes	*planctomycete KSU-1*

NOTE.–The "+" sign within the accession number of NCBI RefSeq database indicates that the cyt *b* homolog was concatenated from the two accession numbers of sequences of the N- and C-terminal regions.

Supplementary Table S 8: Cyt *b* from the GPWY clade and PDWF-FeS clade.

Abbreviation	Qo-motif	Accession	Phylum/ Class	Organism
Magma	PDWY	YP_421588	α-Proteobacteria	*Magnetospirillum magneticum* AMB-1
Alide	PDWF	YP_004128218	β-Proteobacteria	*Alicycliphilus denitrificans* BC
Turpa	PDWF	YP_006440259	Spirochaetes	*Turneriella parva* DSM 21527
Calab_P	GPWY	ZP_09550388	(unclassified)	*Caldithrix abyssi* DSM 13497
Despr	GPWF	YP_004195969	δ-Proteobacteria	*Desulfobulbus propionicus* DSM 2032
Dessu	GPWF	YP_007468775	δ-Proteobacteria	*Desulfocapsa sulfexigens* DSM 10523
Ignal	GPWY	YP_005846642	Ignavibacteria	*Ignavibacterium album* JCM 16511
Melro	GPWY	YP_006528019	Ignavibacteria	*Melioribacter roseus* P3M
Nitgr	PPWQ	ZP_21929800	Nitrospinae	*Nitrospina gracilis* 3/211

Supplementary Table S 9: Cyt *b* from the Halobacteria, Actinobacteria and Deinococcus-Thermus clades.

Abbreviation	Qo-motif	Accession Number	Phylum/ Class	Organism
Acife	PDWY	YP_003110412	Actinobacteria/ Acidimicrobidae	*Acidimicrobium ferrooxidans* DSM 10331
Ausch	PDWY	ZP_10950869	Actinobacteria/ Actinobacteridae	*Austwickia chelonae* NBRC 105200
Blasa	PDWY	YP_005329981	Actinobacteria/ Actinobacteridae	*Blastococcus saxobsidens* DD2
Micte	PDWY	YP_004222922	Actinobacteria/ Actinobacteridae	*Microbacterium testaceum* StLB037
Proac	PDWY	YP_006980403	Actinobacteria/ Actinobacteridae	*Propionibacterium acidipropionici* ATCC 4875
Rhoco	PDFY	ZP_21137794	Actinobacteria/ Actinobacteridae	*Rhodococcus sp.* AW25M09
Strsp	PDWY	ZP_06712394	Actinobacteria/ Actinobacteridae	*Streptomyces sp.* e14
Deipe	PDWY	YP_007180097	Deinococcus-Thermus/ Deinococci	*Deinococcus peraridilitoris* DSM 19664
Deira	PDWY	NP_294159	Deinococcus-Thermus/ Deinococci	*Deinococcus radiodurans* R1
Meiru	PDWY	YP_003506041	Deinococcus-Thermus/ Deinococci	*Meiothermus ruber* DSM 1279
Meisi	PDWY	YP_003683913	Deinococcus-Thermus/ Deinococci	*Meiothermus silvanus* DSM 9946
Halha	PAWF	ZP_11270956	Euryarchaeota/ Halobacteria	*Halococcus hamelinensis* 100A6
Halsp	PDWF	ZP_21626402	Euryarchaeota/ Halobacteria	*Haloferax sp.* ATCC BAA-646
Halvo	PDWF	YP_003533243	Euryarchaeota/ Halobacteria	*Haloferax volcanii* DS2
Halut	PDWY	YP_003129498+97	Euryarchaeota/ Halobacteria	*Halorhabdus utahensis* DSM 12940
Halla	PDWF	YP_002565995	Euryarchaeota/ Halobacteria	*Halorubrum lacusprofundi* ATCC 49239
Halca	PDWF	ZP_21576115	Euryarchaeota/ Halobacteria	*Halosimplex carlsbadense* 2-9-1

NOTE.–The "+" sign within the accession number of NCBI RefSeq database indicates that the cyt *b* homolog was concatenated from the two accession numbers of sequences of the N- and C-terminal regions.

Supplementary Table S 10: Cyt *b* from the archaeal clades.

Abbreviation	Qo-motif	Accession Number	Phylum/Class (Order)	Organism
Censy	PEWY	YP_874958	Thaumarchaeota/ Cenarchaeales	*Cenarchaeum symbiosum* A
Nitma	PEWY	YP_001582877	Thaumarchaeota/ Nitrosopumilales	*Nitrosopumilus maritimus* SCM1
Korcr	PEWY	YP_001737595	Korarchaeota	*Candidatus Korarchaeum* cryptofilum OPF8
Pyrae	PPWP	NP_559242	Crenarchaeota/ Thermoprotei	*Pyrobaculum aerophilum* str. IM2
Picto	PDWY	YP_023912	Euryarchaeota/ Thermoplasmata	*Picrophilus torridus* DSM 9790
Theac	PDWY	NP_394678	Euryarchaeota/ Thermoplasmata	*Thermoplasma acidophilum* DSM 1728
Thevo	PPWF	NP_110886	Euryarchaeota/ Thermoplasmata	*Thermoplasma volcanium* GSS1
Aciho	PPWF	YP_004458829	Crenarchaeota/ Thermoprotei	*Acidianus hospitalis* W1
Acisa	PDLF	YP_003816924	Crenarchaeota/ Thermoprotei	*Acidilobus saccharovorans* 345-15
Aerpe	PPWF	NP_148127	Crenarchaeota/ Thermoprotei	*Aeropyrum pernix* K1
Calma	PLWF	YP_001541746	Crenarchaeota/ Thermoprotei	*Caldivirga maquilingensis* IC-167
Metcu	PDWY	YP_004410337	Crenarchaeota/ Thermoprotei	*Metallosphaera cuprina* Ar-4
Metye	PPWF	ZP_09705161	Crenarchaeota/ Thermoprotei	*Metallosphaera yellowstonensis* MK1
Sulso	PDWY	NP_344285	Crenarchaeota/ Thermoprotei	*Sulfolobus solfataricus* P2
Sulto	PPWF	NP_375984	Crenarchaeota/ Thermoprotei	*Sulfolobus tokodaii* str. 7
Thete	PPWF	YP_004892075	Crenarchaeota/ Thermoprotei	*Thermoproteus tenax* Kra 1

Supplementary Table S 11: Cyt *b* encoded as separate N- and C-terminal proteins in Proteobacteria

N-terminal	C-terminal	Qo-motif	Clade	Class	Organism
YP_003965199	YP_003965200	PEWY	Proteobacteria	α-Proteobacteria	*Ketogulonicigenium vulgare* Y25
ZP_01678359	ZP_01678350	PVWY	Proteobacteria	γ-Proteobacteria	*Vibrio cholerae* 2740-80
–[a]	ZP_01957767	PVWY	Proteobacteria	γ-Proteobacteria	*Vibrio cholerae* MZO-3
–[a]	ZP_01976654	PVWY	Proteobacteria	γ-Proteobacteria	*Vibrio cholerae* B33
–[a]	ZP_01972814	PVWY	Proteobacteria	γ-Proteobacteria	*Vibrio cholerae* NCTC 8457
ZP_09225811	ZP_09225812	PVWY	Proteobacteria	γ-Proteobacteria	*Pseudoalteromonas sp.* BSi20652
YP_006721080	YP_006721081	APWY	Bacterial P272	δ-Proteobacteria	*Geobacter metallireducens* GS-15
ZP_12703809	ZP_12703808	APWY	Bacterial P272	δ-Proteobacteria	*Geobacter metallireducens* RCH3
YP_002535600	YP_002535599	APWY	Bacterial P272	δ-Proteobacteria	*Geobacter sp.* sp. FRC-32

[a] The N-terminal polypeptide is absent in the genome.

Supplementary Table S 12: Rieske ISP and cyt *b* of the organisms which encode multiple copies of cyt bc_1 complexes.

Abbreviation	Rieske Signature	Rieske Accession Number	Qo-motif	Cyt *b* Accession Number	Phylum/ Class	Organism
Blama_D	G-Y	ZP_01094312	PDWY	ZP_01094311	Planctomycetes	*Blastopirellula marina* DSM 3645
Blama_E	S-F	ZP_01090200	PEWY	ZP_01090199	Planctomycetes	*Blastopirellula marina* DSM 3645
Blama_P	S-F	ZP_01091113	APWY	ZP_01091114+15	Planctomycetes	*Blastopirellula marina* DSM 3645
Calab_E	G-F	ZP_09551544	PEWY	ZP_09551543	(unclassified)	*Caldithrix abyssi* DSM 13497
Calab_P	S-F	ZP_09550387	GPWY	ZP_09550388	(unclassified)	*Caldithrix abyssi* DSM 13497
Chlth_E1	G-Y	YP_004862187	PEWY	YP_004862186	Acidobacteria	*Candidatus* Chloracidobacterium thermophilum B
Chlth_E2	S-F	YP_004862045	PEWY	YP_004862044	Acidobacteria	*Candidatus* Chloracidobacterium thermophilum B
Desti_E	G-F	YP_006446862	PEWY	YP_006446863	δ-Proteobacteria	*Desulfomonile tiedjei* DSM 6799
Desti_P	S-F	YP_006445644	APWY	YP_006445645	δ-Proteobacteria	*Desulfomonile tiedjei* DSM 6799
Lepfe_E	S-Y	YP_005469369	PAWY	YP_005469368	Nitrospirae	*Leptospirillum ferrooxidans* C2-3
Lepfe_P	S-Y	YP_005468542	APWY	YP_005468543+44	Nitrospirae	*Leptospirillum ferrooxidans* C2-3
Metox_E	G-Y	YP_003205721	PEWY	YP_003205722	candidate division NC10	*Candidatus* Methylomirabilis oxyfera
Metox_P	S-F	YP_003205671	APWY	YP_003205672	candidate division NC10	*Candidatus* Methylomirabilis oxyfera
Nitde_E1	S-Y	YP_003796588	PEWY	YP_003796589	Nitrospirae	*Candidatus* Nitrospira defluvii
Nitde_E2	S-F	YP_003799487	PEWY	YP_003799486	Nitrospirae	*Candidatus* Nitrospira defluvii
PlaKS_E	G-F	ZP_10101268	PEWY	ZP_10101269	Planctomycetes	*planctomycete* KSU-1
PlaKS_P	S-F	ZP_10098674	APWY	ZP_10098673+70	Planctomycetes	*planctomycete* KSU-1
Plama_D	G-Y	ZP_01854220	PDWY	ZP_01854221	Planctomycetes	*Planctomyces maris* DSM 8797
Plama_E	A-F	ZP_01856608	PEWF	ZP_01856609	Planctomycetes	*Planctomyces maris* DSM 8797
Schpa_E1	S-F	ZP_11092182	PEWY	ZP_11092181	Planctomycetes	*Schlesneria paludicola* DSM 18645
Schpa_E2	A-F	ZP_11091337	PEWY	ZP_11091336	Planctomycetes	*Schlesneria paludicola* DSM 18645
Schpa_P	S-F	ZP_11096295	APWY	ZP_11096294+93	Planctomycetes	*Schlesneria paludicola* DSM 18645
Solus_E	S-F	YP_827420	PEWY	YP_827419	Acidobacteria	*Candidatus* Solibacter usitatus Ellin6076
Solus_P	S-Y	YP_825634	APWY	YP_825633+32	Acidobacteria	*Candidatus* Solibacter usitatus Ellin6076

NOTE.–The "+" sign within the accession number of NCBI RefSeq database indicates that the cyt *b* homolog was concatenated from the two accession numbers of sequences of the N- and C-terminal regions.

Supplementary Table S 13: Rieske and cyt *b* from the APWY clade and the GPWY clade. Sequences were sorted according to the “Rieske Signature”.

Abbreviation	Rieske Signature	Rieske Accession Number	Qo-motif	Cyt *b* Accession Number	Phylum/ Class	Organism
Anasp	S-F	ZP_09484366	APWY	ZP_09484367	Bacteroidetes	*Anaerophaga sp.* HS1
Calae	S-F	YP_005441947	APWY	YP_005441946	Chloroflexi	*Caldilinea aerophila* DSM 14535 = NBRC 104270
Herau	S-F	YP_001547013	APWY	YP_001547012	Chloroflexi	*Herpetosiphon aurantiacus* DSM 785
Osctr	S-F	ZP_07687041	AAWY	ZP_07687042	Chloroflexi	*Oscillochloris trichoides* DG-6
Metox_P	S-F	YP_003205671	APWY	YP_003205672	candidate division NC10	*Candidatus* Methylomirabilis oxyfera
Geoda	S-F	YP_002535598	APWY	YP_002535600+599	δ-Proteobacteria	*Geobacter daltonii* FRC-32
Desde	S-F	YP_005166713	APWY	YP_005166714	δ-Proteobacteria	*Desulfovibrio desulfuricans* ND132
Desph	S-F	ZP_24025637	APWF	ZP_24025636	δ-Proteobacteria	*Desulfotignum phosphitoxidans* DSM 13687
Desti_P	S-F	YP_006445644	APWY	YP_006445645	δ-Proteobacteria	*Desulfomonile tiedjei* DSM 6799
Thema	S-F	YP_004101175	APWY	YP_004101177+176	Firmicutes/ Clostridia	*Thermaerobacter marianensis* DSM 12885
Sinac	S-F	YP_007201889	APWY	YP_007201890+91	Planctomycetes	*Singulisphaera acidiphila* DSM 18658
Blama_P	S-F	ZP_01091113	APWY	ZP_01091114+15	Planctomycetes	*Blastopirellula marina* DSM 3645
PlaKS_P	S-F	ZP_10098674	APWY	ZP_10098673+70	Planctomycetes	*planctomycete* KSU-1
Schpa_P	S-F	ZP_11096295	APWY	ZP_11096294+93	Planctomycetes	*Schlesneria paludicola* DSM 18645
Iluco	S-Y	YP_007562655	APWY	YP_007562653+54	Actinobacteria/ Acidimicrobidae	*Ilumatobacter coccineum* YM16-304
Solus_P	S-Y	YP_825634	APWY	YP_825633+32	Acidobacteria	*Candidatus* Solibacter usitatus Ellin6076
Wadch	S-Y	YP_003710307	APWY	YP_003710306	Chlamydiae	*Waddlia chondrophila* WSU 86-1044
Ktera	S-Y	ZP_06967904	APWY	ZP_06967906+05	Chloroflexi	*Ktedonobacter racemifer* DSM 44963
Anesp	S-Y	YP_002133818	APWY	YP_002133819	δ-Proteobacteria	*Anaeromyxobacter sp.* K
Lepfe_P	S-Y	YP_005468542	APWY	YP_005468543+44	Nitrospirae	*Leptospirillum ferrooxidans* C2-3
Calab_P	S-F	ZP_09550387	GPWY	ZP_09550388	(unclassified)	*Caldithrix abyssi* DSM 13497
Despr	S-F	YP_004195968	GPWF	YP_004195969	δ-Proteobacteria	*Desulfobulbus propionicus* DSM 2032
Dessu	S-F	YP_007468776	GPWF	YP_007468775	δ-Proteobacteria	*Desulfocapsa sulfexigens* DSM 10523
Ignal	S-F	YP_005846643	GPWY	YP_005846642	Ignavibacteria	*Ignavibacterium album* JCM 16511
Melro	S-Y	YP_006528018	GPWY	YP_006528019	Ignavibacteria	*Melioribacter roseus* P3M

NOTE.–The “+” sign within the accession number of NCBI RefSeq database indicates that the cyt *b* homolog was concatenated from the two accession numbers of sequences of the N- and C-terminal regions.

Supplementary Table S 14: Rieske ISP and cyt *b* from the PDWY-cyt *c* clade. Sequences were sorted according to the "Rieske Signature".

Abbreviation	Rieske Signature	Rieske Accession Number	Qo-motif	Cyt *b* Accession Number	Phylum/ Class	Organism
Paeel	A-Y	ZP_09079291	PDWY	ZP_09079292+93	Firmicutes/ Bacilli	*Paenibacillus elgii* B69
Bresp	G-Y	ZP_10742447	PDWY	ZP_10742446+45	Firmicutes/ Bacilli	*Brevibacillus sp.* CF112
Dessp	G-Y	ZP_08462739	PDWY	ZP_08462740+41	Firmicutes/ Bacilli	*Desmospora sp.* 8437
Hallo	G-Y	YP_006180889	PDWY	YP_006180888+87	Firmicutes/ Bacilli	*Halobacillus halophilus* DSM 2266
Kyrtu	G-Y	YP_003589551	PDWY	YP_003589550+49	Firmicutes/ Bacilli	*Kyrpidia tusciae* DSM 2912
Macca	G-Y	YP_002560516	PDWY	YP_002560515+14	Firmicutes/ Bacilli	*Macrococcus caseolyticus* JCSC5402
Cloul	G-Y	ZP_23165746	PDWY	ZP_23165745+44	Firmicutes/ Clostridia	*Clostridium ultunense* Esp
Desac	G-Y	YP_006465272	PAWY	YP_006465273	Firmicutes/ Clostridia	*Desulfosporosinus acidiphilus* SJ4
Theye	G-Y	YP_002248982	PEWY	YP_002248983+84	Nitrospirae	*Thermodesulfovibrio yellowstonii* DSM 11347
Acica	G-Y	YP_002755479	PDFF	YP_002755480	Acidobacteria	*Acidobacterium capsulatum* ATCC 51196
Gratu	G-Y	YP_004217983	PDFA	YP_004217982	Acidobacteria	*Granulicella tundricola* MP5ACTX9
Zunpr	G-Y	YP_003583938	PDWY	YP_003583939	Bacteroidetes	*Zunongwangia profunda* SM-A87
Blama_D	G-Y	ZP_01094312	PDWY	ZP_01094311	Planctomycetes	*Blastopirellula marina* DSM 3645
Plama_D	G-Y	ZP_01854220	PDWY	ZP_01854221	Planctomycetes	*Planctomyces maris* DSM 8797
Opite	G-Y	YP_001820420	PDWY	YP_001820421	Verrucomicrobia	*Opitutus terrae* PB90-1

NOTE.–The "+" sign within the accession number of NCBI RefSeq database indicates that the cyt *b* homolog was concatenated from the two accession numbers of sequences of the N- and C-terminal regions.

Supplementary Table S 15: Rieske ISP and cyt *b* from the Heliobacteria/ Desulfitobacteria clade, Cyanobacteria/ chloroplast clade, Chlorobi/ NC10/ Acidobacteria clade and the PEWY-cyt *c* clade. Sequences were sorted according to the "Rieske Signature".

Abbreviation	Rieske Signature	Rieske Accession Number	Qo-motif	Cyt *b* Accession Number	Phylum/ Class	Organism
Desha	G-F	ZP_17060831	PDWY	ZP_17060832+33	Firmicutes/ Clostridia	*Desulfitobacterium hafniense* DP7
Helmo	G-F	YP_001679864	PEWY	YP_001679865+66	Firmicutes/ Clostridia	*Heliobacterium modesticaldum* Ice1
Calab_E	G-F	ZP_09551544	PEWY	ZP_09551543	(unclassified)	*Caldithrix abyssi* DSM 13497
Chlre	S-Y	XP_001698786	PEWY	NP_958365+59	Chlorophyta	chloroplast *Chlamydomonas reinhardtii*
Chlph	A-Y	YP_001960379	PEWY	YP_001960378	Chlorobi	*Chlorobium phaeobacteroides* BS1
Chlth_E1	G-Y	YP_004862187	PEWY	YP_004862186	Acidobacteria	*Candidatus* Chloracidobacterium thermophilum B
Metox_E	G-Y	YP_003205721	PEWY	YP_003205722	candidate division NC10	*Candidatus* Methylomirabilis oxyfera
Tersa	G-F	YP_004182034	PEWY	YP_004182035	Acidobacteria	*Terriglobus saanensis* SP1PR4
Desti_E	G-F	YP_006446862	PEWY	YP_006446863	δ-Proteobacteria	*Desulfomonile tiedjei* DSM 6799
PlaKS_E	G-F	ZP_10101268	PEWY	ZP_10101269	Planctomycetes	*planctomycete* KSU-1
Rubxy	G-Y	YP_645680	PEWF	YP_645679+78	Rubrobacteridae	*Rubrobacter xylanophilus* DSM 9941
Patsp	G-Y	ZP_09470201	PEWY	ZP_09470202+03	Rubrobacteridae	*Patulibacter sp.* I11
Plama_E	A-F	ZP_01856608	PEWF	ZP_01856609	Planctomycetes	*Planctomyces maris* DSM 8797
Schpa_E2	A-F	ZP_11091337	PEWY	ZP_11091336	Planctomycetes	*Schlesneria paludicola* DSM 18645
Chlth_E2	S-F	YP_004862045	PEWY	YP_004862044	Acidobacteria	*Candidatus* Chloracidobacterium thermophilum B
Solus_E	S-F	YP_827420	PEWY	YP_827419	Acidobacteria	*Candidatus* Solibacter usitatus Ellin6076
Plepa	S-F	ZP_01912029	PEWY	ZP_01912028	δ-Proteobacteria	*Plesiocystis pacifica* SIR-1
Gemau	S-F	YP_002760209	PEWY	YP_002760208	Gemmatimonadetes	*Gemmatimonas aurantiaca* T-27
Pirst	S-F	YP_003372363	PEWY	YP_003372364	Planctomycetes	*Pirellula staleyi* DSM 6068
Blama_E	S-F	ZP_01090200	PEWY	ZP_01090199	Planctomycetes	*Blastopirellula marina* DSM 3645
Isopa	S-F	YP_004179080	PEWY	YP_004179079	Planctomycetes	*Isosphaera pallida* ATCC 43644
Schpa_E1	S-F	ZP_11092182	PEWY	ZP_11092181	Planctomycetes	*Schlesneria paludicola* DSM 18645
Nitde_E2	S-F	YP_003799487	PEWY	YP_003799486	Nitrospirae	*Candidatus* Nitrospira defluvii
Nitde_E1	S-Y	YP_003796588	PEWY	YP_003796589	Nitrospirae	*Candidatus* Nitrospira defluvii
Lepfe_E	S-Y	YP_005469369	PAWY	YP_005469368	Nitrospirae	*Leptospirillum ferrooxidans* C2-3

NOTE.–The "+" sign within the accession number of NCBI RefSeq database indicates that the cyt *b* homolog was concatenated from the two accession numbers of sequences of the N- and C-terminal regions.