Supplementary material. It contains two Tables and two figures.

Table S1. List of ca. 200 alphaproteobacterial taxa and their aerobic functional traits as the basis for the distribution analysis of Supplementary Fig. S1 and Figs. 4 and 5 of the main text.

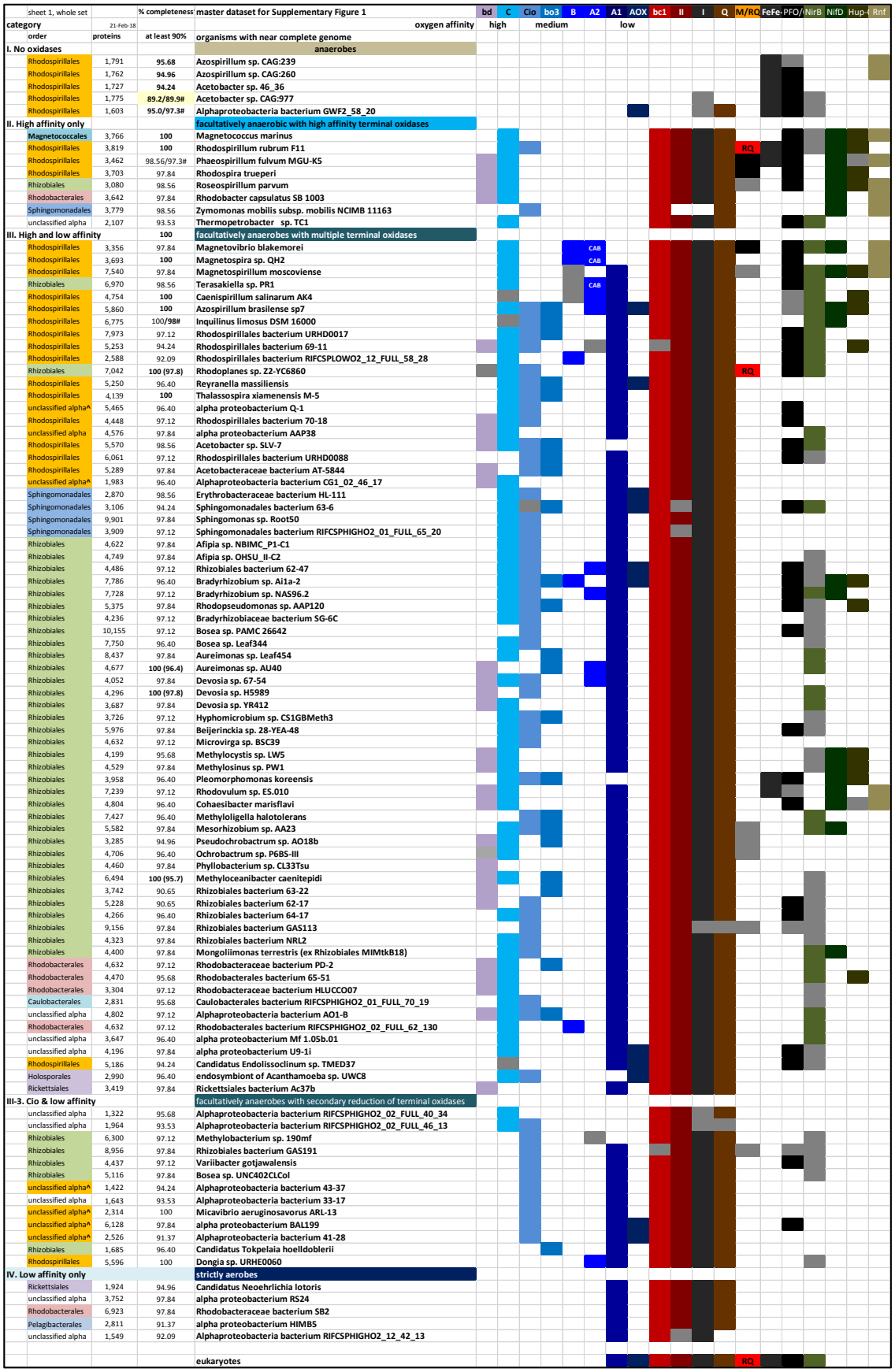
Table S2. Compilation of the accession numbers for all the key proteins of the metabolic traits listed in Fig. 4.

The table lists all the accession numbers (sometimes more than one per protein) for the proteins, either subunits or single protein enzymes, presented in Fig. 4. Besides the terminal oxidases and metabolic traits presented in Supplementary Fig. S1 with the same colour code, additional anaerobic traits were considered as they are shared by some alphaproteobacteria and eukaryotes (cf. Atteia et al., 2013). The acronyms for these anaerobic traits are as folows: FDR, fumarate reductase, membrane bound and reacting with Q or RQ; FeFe-Hyd., [FeFe]-hydrogenase HydA; HydEFG, maturases for [FeFe]-hyrogenase; PFO/OAFO/PNO, pyruvate:ferredoxin (flavodoxin) oxidoreductase PFO, 2-oxoacid:acceptor oxidoreductase (OAFO) or the eukaryotic variant PNO; PFL, pyruvate formate lyase; PFL_AE, pyruvate formate lyase activating enzyme (sets the glycyl radical); ACK1/ACK2, acetate kinase; PTA1/PTA2, phosphate acetyltransferase isoform 1 and 2; ADH, phosphotransacetylase bifunctional alcohol/ aldehyde dehydrogenase; ACS_ADP, acetyl-CoA synthase ADP forming; ASCTI, Acetate succinate CoA transferase (any of three types); malic enzyme; fumarase, fumarate lyase; P450_NOR, P450-related nitrate reductase of fungi; NirK, soluble nitrate reductase also present in some mitochondria. ASCTI, malic enzyme and fumarase are not shown in Fig. 4, also to simplify its graphical layout.

Fig. S1. List of 100 alphaproteobacterial taxa and their terminal oxidases as well other functional traits. 100 taxa were selected from those initially analysed and reported in Supplementary Table S1 so as to represent all major families of alphaproteobacteria and various unclassified taxa that had genome estimated to have at least 90% completeness, coding for more than 1000 proteins and at least 16 tRNA - therefore to be considered nearly complete (Bowers et al., 2017). The taxa were organized according to the presence and oxygen affinity of terminal oxidases in their genomes, as discussed in the text. The terminal oxidases are colour coded as in Fig. 2 while other metabolic traits are colour coded as reported previously (Degli Esposti and Martinez-Romero, 2017). Taxa labelled in orange on the left column of taxonomy were found to cluster within the family of Rhodospirillaceae by multiple phylogenetic trees (cf. Degli Esposti, 2017).

Fig. S2. Phylogenetic analysis of various COX1 proteins of A and B family terminal oxidases of the HCO superfamily. A) Maximum-likelihood phylogeny of the catalytic subunit I of selected HCOs. Alignment was performed in Clustal and the phylogenetic reconstruction in IQ-Tree (LG+I+G4, 1000 bootstraps). The tree is rooted between A and B family. B) **Representative NJ tree of COX1 proteins of A and B family terminal oxidases.** Representative COX1 proteins indicated by the accession number were first aligned by ClustalW and then the alignment was manually refined taking into account also the 3D structure of bacterial COX1 (Iwata et al., 1995). The phylogenetic analysis of the resulting alignment was undertaken following the ML approach with 500 bootstraps using the program MEGA5 as described previously (Degli Esposti, 2017).

46 **Fig. S1.**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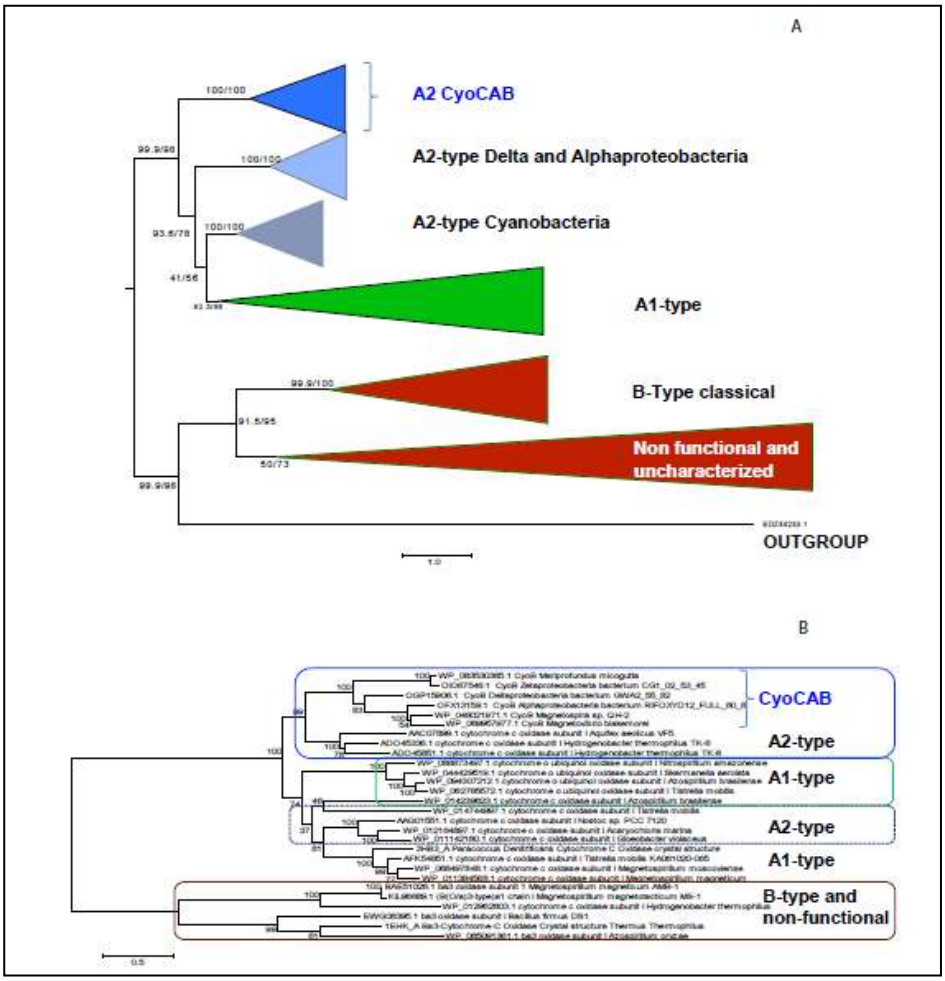
category
21-Feb-18
oxygen affinity
high
medium
low
order
proteins
at least 90%
organisms with near complete genome
I. No oxidases
anaerobes
Rhodospirillales 1,791 95.68 Azospirillum sp. CAG:239
Rhodospirillales 1,762 94.96 Azospirillum sp. CAG:260
Rhodospirillales 1,727 94.24 Acetobacter sp. 46_36
Rhodospirillales 1,775 89.2/89.9# Acetobacter sp. CAG:977
Rhodospirillales 1,603 95.0/97.3# Alphaproteobacteria bacterium GWF2_58_20
II. High affinity only
facultatively anaerobic with high affinity terminal oxidases
Magnetococcales 3,766 100 Magnetococcus marinus
Rhodospirillales 3,819 100 Rhodospirillum rubrum F11
Rhodospirillales 3,462 98.56/97.3# Phaeospirillum fulvum MGU-K5
Rhodospirillales 3,703 97.84 Rhodospira trueperi
Rhizobiales 3,080 98.56 Roseospirillum parvum
Rhodobacterales 3,642 97.84 Rhodobacter capsulatus SB 1003
Sphingomonadales 3,779 98.56 Zymomonas mobilis subsp. mobilis NCIMB 11163
unclassified alpha 2,107 93.53 Thermopetrobacter sp. TC1
III. High and low affinity
100
facultatively anaerobes with multiple terminal oxidases
Rhodospirillales 3,356 97.84 Magnetovibrio blakemorei
Rhodospirillales 3,693 100 Magnetospira sp. QH2
Rhodospirillales 7,540 97.84 Magnetospirillum moscoviense
Rhizobiales 6,970 98.56 Terasakiella sp. PR1
Rhodospirillales 4,754 100 Caenispirillum salinarum AK4
Rhodospirillales 5,860 100 Azospirillum brasilense sp7
Rhodospirillales 6,775 100/98# Inquilinus limosus DSM 16000
Rhodospirillales 7,973 97.12 Rhodospirillales bacterium URHD0017
Rhodospirillales 5,253 94.24 Rhodospirillales bacterium 69-11
Rhodospirillales 2,588 92.09 Rhodospirillales bacterium RIFCSPLOWO2_12_FULL_58_28
Rhizobiales 7,042 100 (97.8) Rhodoplanes sp. Z2-YC6860
Rhodospirillales 5,250 96.40 Reyranella massiliensis
Rhodospirillales 4,139 100 Thalassospira xiamenensis M-5
unclassified alpha^ 5,465 96.40 alpha proteobacterium Q-1
Rhodospirillales 4,448 97.12 Rhodospirillales bacterium 70-18
unclassified alpha 4,576 97.84 alpha proteobacterium AAP38
Rhodospirillales 5,570 98.56 Acetobacter sp. SLV-7
Rhodospirillales 6,061 97.12 Rhodospirillales bacterium URHD0088
Rhodospirillales 5,289 97.84 Acetobacteraceae bacterium AT-5844
unclassified alpha^ 1,983 96.40 Alphaproteobacteria bacterium CG1_02_46_17
Sphingomonadales 2,870 98.56 Erythrobacteraceae bacterium HL-111
Sphingomonadales 3,106 94.24 Sphingomonadales bacterium 63-6
Sphingomonadales 9,901 97.84 Sphingomonas sp. Root50
Sphingomonadales 3,909 97.12 Sphingomonadales bacterium RIFCSPHIGHO2_01_FULL_65_20
Rhizobiales 4,622 97.84 Afipia sp. NBIMC_P1-C1
Rhizobiales 4,749 97.84 Afipia sp. OHSU_II-C2
Rhizobiales 4,486 97.12 Rhizobiales bacterium 62-47
Rhizobiales 7,786 96.40 Bradyrhizobium sp. Ai1a-2
Rhizobiales 7,728 97.12 Bradyrhizobium sp. NAS96.2
Rhizobiales 5,375 97.84 Rhodopseudomonas sp. AAP120
Rhizobiales 4,236 97.12 Bradyrhizobiaceae bacterium SG-6C
Rhizobiales 10,155 97.12 Bosea sp. PAMC 26642
Rhizobiales 7,750 96.40 Bosea sp. Leaf344
Rhizobiales 8,437 97.84 Aureimonas sp. Leaf454
Rhizobiales 4,677 100 (96.4) Aureimonas sp. AU40
Rhizobiales 4,052 97.84 Devosia sp. 67-54
Rhizobiales 4,296 100 (97.8) Devosia sp. H5989
Rhizobiales 3,687 97.84 Devosia sp. YR412
Rhizobiales 3,726 97.12 Hyphomicrobium sp. CS1GBMeth3
Rhizobiales 5,976 97.84 Beijerinckia sp. 28-YEA-48
Rhizobiales 4,632 97.12 Microvirga sp. BSC39
Rhizobiales 4,199 95.68 Methylocystis sp. LW5
Rhizobiales 4,529 97.84 Methylosinus sp. PW1
Rhizobiales 3,958 96.40 Pleomorphomonas koreensis
Rhizobiales 7,239 97.12 Rhodovulum sp. ES.010
Rhizobiales 4,804 96.40 Cohaesibacter marisflavi
Rhizobiales 7,427 96.40 Methyloligella halotolerans
Rhizobiales 5,582 97.84 Mesorhizobium sp. AA23
Rhizobiales 3,285 94.96 Pseudochrobactrum sp. AO18b
Rhizobiales 4,706 96.40 Ochrobactrum sp. P6BS-III
Rhizobiales 4,460 97.84 Phyllobacterium sp. CL33Tsu
Rhizobiales 6,494 100 (95.7) Methyloceanibacter caenitepidi
Rhizobiales 3,742 90.65 Rhizobiales bacterium 63-22
Rhizobiales 5,228 90.65 Rhizobiales bacterium 62-17
Rhizobiales 4,266 96.40 Rhizobiales bacterium 64-17
Rhizobiales 9,156 97.84 Rhizobiales bacterium GAS113
Rhizobiales 4,323 97.84 Rhizobiales bacterium NRL2
Rhizobiales 4,400 97.84 Mongoliimonas terrestris (ex Rhizobiales MIMtkB18)
Rhodobacterales 4,632 97.12 Rhodobacteraceae bacterium PD-2
Rhodobacterales 4,470 95.68 Rhodobacterales bacterium 65-51
Rhodobacterales 3,304 97.12 Rhodobacteraceae bacterium HLUCCO07
Caulobacterales 2,831 95.68 Caulobacterales bacterium RIFCSPHIGHO2_01_FULL_70_19
unclassified alpha 4,802 97.12 Alphaproteobacteria bacterium AO1-B
Rhodobacterales 4,632 97.12 Rhodobacterales bacterium RIFCSPHIGHO2_02_FULL_62_130
unclassified alpha 3,647 96.40 alpha proteobacterium Mf 1.05b.01
unclassified alpha 4,196 97.84 alpha proteobacterium U9-1i
Rhodospirillales 5,186 94.24 Candidatus Endolissoclinum sp. TMED37
Holosporales 2,990 96.40 endosymbiont of Acanthamoeba sp. UWC8
Rickettsiales 3,419 97.84 Rickettsiales bacterium Ac37b
III-3. Cio & low affinity
facultatively anaerobes with secondary reduction of terminal oxidases
unclassified alpha 1,322 95.68 Alphaproteobacteria bacterium RIFCSPHIGHO2_02_FULL_40_34
unclassified alpha 1,964 93.53 Alphaproteobacteria bacterium RIFCSPHIGHO2_02_FULL_46_13
Rhizobiales 6,300 97.12 Methylobacterium sp. 190mf
Rhizobiales 8,956 97.84 Rhizobiales bacterium GAS191
Rhizobiales 4,437 97.12 Variibacter gotjawalensis
Rhizobiales 5,116 97.84 Bosea sp. UNC402CLCol
unclassified alpha^ 1,422 94.24 Alphaproteobacteria bacterium 43-37
unclassified alpha 1,643 93.53 Alphaproteobacteria bacterium 33-17
unclassified alpha^ 2,314 100 Micavibrio aeruginosavorus ARL-13
unclassified alpha^ 6,128 97.84 alpha proteobacterium BAL199
unclassified alpha^ 2,526 91.37 Alphaproteobacteria bacterium 41-28
Rhizobiales 1,685 96.40 Candidatus Tokpelaia hoelldoblerii
Rhodospirillales 5,596 100 Dongia sp. URHE0060
IV. Low affinity only
strictly aerobes
Rickettsiales 1,924 94.96 Candidatus Neoehrlichia lotoris
unclassified alpha 3,752 97.84 alpha proteobacterium RS24
Rhodobacterales 6,923 97.84 Rhodobacteraceae bacterium SB2
Pelagibacterales 2,811 91.37 alpha proteobacterium HIMB5
unclassified alpha 1,549 92.09 Alphaproteobacteria bacterium RIFCSPHIGHO2_12_42_13
eukaryotes
CAB
CAB
CAB
RQ
RQ
RQ
47

Fig. S2


A
A2 CyoCAB
A2-type Delta and Alphaproteobacteria
A2-type Cyanobacteria
A1-type
B-Type classical
Non functional and uncharacterized
OUTGROUP
B
CyoCAB
A2-type
A1-type
A2-type
A1-type
B-type and non-functional