**Table S1.** List of extant nitrogenase and outgroup protein sequences used for phylogenetic reconstruction and ancestral sequence inference.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Species** | **Accession/Locus Tag** | | | **Phylum** | **Class** |
| **NifH** | **NifD** | **NifK** |
| Acetobacterium woodii | WP\_014355191 | WP\_014355188 | WP\_014355187 | Firmicutes | Clostridia |
| Acidiferrobacter thiooxydans | WP\_065969940 | WP\_065969942 | WP\_065969944 | Proteobacteria | Gammaproteobacteria |
| Acidihalobacter prosperus | WP\_070071968 | WP\_070073945 | WP\_070071969 | Proteobacteria | Gammaproteobacteria |
| Acidithiobacillus ferrooxidans | WP\_113525799 | WP\_113525798 | WP\_113525797 | Proteobacteria | Acidithiobacillia |
| Actinobacteria bacterium HGW-Actinobacteria-10 | PKQ29728 | PKQ29729 | PKQ29730 | Actinobacteria | - |
| Afifella marina | WP\_092811147 | WP\_092811149 | WP\_092811151 | Proteobacteria | Alphaproteobacteria |
| Agarivorans albus | WP\_016403298 | WP\_016403297 | WP\_016403296 | Proteobacteria | Gammaproteobacteria |
| Alkalibacter saccharofermentans | WP\_073269025 | WP\_073269336 | WP\_073269028 | Firmicutes | Clostridia |
| Anaerobacillus alkalilacustris | WP\_071308028 | WP\_071308027 | WP\_071308026 | Firmicutes | Bacilli |
| Anaeromyxobacter sp. K | WP\_012527198 | WP\_012527199 | WP\_012527200 | Proteobacteria | Deltaproteobacteria |
| Anaerovirgula multivorans | WP\_089285040 | WP\_089282036 | WP\_089282035 | Firmicutes | Clostridia |
| Aneurinibacillus terranovensis | WP\_027417121 | WP\_027417120 | WP\_027417119 | Firmicutes | Bacilli |
| Arcticibacter svalbardensis | WP\_016195754 | WP\_016195751 | WP\_040299905 | Bacteroidetes | Sphingobacteriia |
| Azohydromonas australica | WP\_029001236 | WP\_029001237 | WP\_029001238 | Proteobacteria | Betaproteobacteria |
| Azomonas agilis DSM 375 | LX59DRAFT\_00350 | LX59DRAFT\_00351 | LX59DRAFT\_00352 | Proteobacteria | Gammaproteobacteria |
| Azospira sp. I13 | WP\_109041643 | WP\_109041644 | WP\_109041645 | Proteobacteria | Betaproteobacteria |
| Azospirillum halopraeferens | WP\_029011025 | WP\_029011024 | WP\_029011023 | Proteobacteria | Alphaproteobacteria |
| Azotobacter vinelandii DJ, ATCC BAA-1303 | Avin\_01380 | Avin\_01390 | Avin\_01400 | Proteobacteria | Gammaproteobacteria |
| Azovibrio restrictus | WP\_026687661 | WP\_026687660 | WP\_026687659 | Proteobacteria | Betaproteobacteria |
| Bacillus caseinilyticus | WP\_090885364 | WP\_090885366 | WP\_090885368 | Firmicutes | Bacilli |
| Beijerinckia indica | WP\_012383484 | WP\_012383485 | WP\_012383486 | Proteobacteria | Alphaproteobacteria |
| Betaproteobacteria bacterium HGW-Betaproteobacteria-11 | PKO84828 | PKO84829 | PKO84997 | Proteobacteria | Betaproteobacteria |
| Blastopirellula marina | WP\_105335631 | WP\_105335632 | WP\_105335633 | Planctomycetes | Planctomycetia |
| Bradyrhizobium diazoefficiens USDA 110 | blr1769 | blr1743 | blr1744 | Proteobacteria | Alphaproteobacteria |
| Brenneria salicis ATCC 15712 | Bresa\_01966 | Bresa\_01965 | Bresa\_01964 | Proteobacteria | Gammaproteobacteria |
| Caenispirillum bisanense | WP\_097278677 | WP\_097278676 | WP\_097278675 | Proteobacteria | Alphaproteobacteria |
| Caldicellulosiruptor saccharolyticus | WP\_011917964 | WP\_011917961 | WP\_011917960 | Firmicutes | Clostridia |
| Calditerrivibrio nitroreducens | WP\_013450808 | WP\_013450809 | WP\_013450810 | Deferribacteres | Deferribacteres |
| Candidatus Atelocyanobacterium thalassa isolate ALOHA | WP\_012954002 | WP\_012954003 | WP\_012954004 | Cyanobacteria | - |
| Candidatus Lambdaproteobacteria bacterium RIFOXYC1\_FULL\_56\_13 | OGH03497 | OGH03496 | OGH03495 | Proteobacteria | Candidatus Lambdaproteobacteria |
| Candidatus Lambdaproteobacteria bacterium RIFOXYD2\_FULL\_50\_16 | OGG94501 | OGG94500 | OGG94499 | Proteobacteria | Candidatus Lambdaproteobacteria |
| Candidatus Magnetoovum chiemensis | KJR40986 | KJR40987 | KJR40988 | Nitrospirae | Nitrospira |
| Candidatus Margulisbacteria bacterium GWD2\_39\_127 | OGH94801 | OGH94911 | OGH94798 | Candidatus Margulisbacteria | - |
| Candidatus Marispirochaeta associata | WP\_069897282 | WP\_069897284 | WP\_069897285 | Spirochaetes | Spirochaetia |
| Candidatus Thiodiazotropha endolucinida | WP\_069124654 | WP\_069124653 | WP\_069124652 | Proteobacteria | Gammaproteobacteria |
| Candidatus Viridilinea mediisalina | WP\_097642292 | WP\_097642294 | WP\_097642295 | Chloroflexi | Chloroflexia |
| Carboxydocella thermautotrophica | WP\_078665332 | WP\_078665331 | WP\_078665330 | Firmicutes | Clostridia |
| Cellulosilyticum lentocellum | WP\_013655494 | WP\_013655497 | WP\_013655498 | Firmicutes | Clostridia |
| Cereibacter changlensis | WP\_107662511 | WP\_107662510 | WP\_107662509 | Proteobacteria | Alphaproteobacteria |
| Chlorobium limicola | WP\_012465649 | WP\_012465646 | WP\_012465645 | Chlorobi | Chlorobia |
| Chloroherpeton thalassium ATCC 35110 | Ctha\_1035 | Ctha\_1032 | Ctha\_1031 | Chlorobi | Chlorobia |
| Chroococcidiopsis sp. TS-821 | WP\_104545041 | WP\_104545042 | WP\_104545043 | Cyanobacteria | - |
| Chrysiogenes arsenatis | WP\_027390771 | WP\_027390770 | WP\_027390769 | Chrysiogenetes | Chrysiogenetes |
| Clostridiales bacterium DRI-13 | WP\_034423366 | WP\_034423373 | WP\_034423375 | Firmicutes | Clostridia |
| Clostridium kluyveri DSM 555 | CKL\_3081 | CKL\_3078 | CKL\_3077 | Firmicutes | Clostridia |
| Cohaesibacter sp. ES.047 | WP\_096174773 | WP\_096174774 | WP\_096174775 | Proteobacteria | Alphaproteobacteria |
| Consotaella salsifontis | WP\_078709045 | WP\_078709046 | WP\_078709047 | Proteobacteria | Alphaproteobacteria |
| Coraliomargarita akajimensis | WP\_013044574 | WP\_013044573 | WP\_013044572 | Verrucomicrobia | Opitutae |
| Cupriavidus sp. amp6 | WP\_029049998 | WP\_029049999 | WP\_029050000 | Proteobacteria | Betaproteobacteria |
| Cylindrospermopsis raciborskii | WP\_061544850 | WP\_061544851 | WP\_061544852 | Cyanobacteria | - |
| Dechloromonas aromatica | WP\_011287173 | WP\_011287172 | WP\_011287171 | Proteobacteria | Betaproteobacteria |
| Defluviitalea phaphyphila | WP\_058485536 | WP\_058485595 | WP\_058485533 | Firmicutes | Clostridia |
| Dehalococcoides mccartyi | WP\_010936850 | WP\_010936847 | WP\_010936846 | Chloroflexi | Dehalococcoidia |
| Dehalogenimonas sp. WBC-2 | AKG53288 | AKG53285 | AKG53284 | Chloroflexi | Dehalococcoidia |
| Deltaproteobacteria bacterium HGW-Deltaproteobacteria-4 | PKN11897 | PKN11885 | PKN11884 | Proteobacteria | Deltaproteobacteria |
| Dendrosporobacter quercicolus | WP\_092073275 | WP\_092073284 | WP\_092073287 | Firmicutes | Negativicutes |
| Denitrovibrio acetiphilus | WP\_013010353 | WP\_013010354 | WP\_013010355 | Deferribacteres | Deferribacterales |
| Derxia gummosa | WP\_028310376 | WP\_028310375 | WP\_028310374 | Proteobacteria | Betaproteobacteria |
| Desertifilum sp. IPPAS B-1220 | WP\_069969273 | WP\_069969274 | WP\_069969275 | Cyanobacteria |  |
| Desulfarculus baarsii 2st14, DSM 2075 | Deba\_0443 | Deba\_0440 | Deba\_0439 | Proteobacteria | Deltaproteobacteria |
| Desulfatibacillum alkenivorans AK-01 | Dalk\_1522 | Dalk\_1519 | Dalk\_1518 | Proteobacteria | Deltaproteobacteria |
| Desulfitobacterium hafniense Y51 | WP\_005813529 | WP\_005813531 | WP\_011461720 | Firmicutes | Clostridia |
| Desulfobacca acetoxidans ASRB2, DSM 11109 | Desac\_0350 | Desac\_0353 | Desac\_0354 | Proteobacteria | Deltaproteobacteria |
| Desulfobacterium autotrophicum HRM2, DSM 3382 | HRM2\_09670 | HRM2\_09700 | HRM2\_09710 | Proteobacteria | Deltaproteobacteria |
| Desulfonatronum lacustre | WP\_028571559 | WP\_028571556 | WP\_028571555 | Proteobacteria | Deltaproteobacteria |
| Desulforegula conservatrix | WP\_027358827 | WP\_027358824 | WP\_027358823 | Proteobacteria | Deltaproteobacteria |
| Desulfosarcina cetonica | WP\_054697558 | WP\_054697549 | WP\_054697545 | Proteobacteria | Deltaproteobacteria |
| Desulfosporosinus sp. OT | DOT\_2734 | DOT\_2733 | DOT\_2732 | Firmicutes | Clostridia |
| Desulfotomaculum copahuensis | WP\_066665790 | WP\_066665786 | WP\_066665785 | Firmicutes | Clostridia |
| Desulfovibrio sp. 86-1 | Ga0302701\_112362 | Ga0302701\_112359 | Ga0302701\_112358 | Proteobacteria | Deltaproteobacteria |
| Desulfuribacillus alkaliarsenatis | WP\_069643779 | WP\_069643776 | WP\_069643775 | Firmicutes | Bacilli |
| Desulfurispora thermophila | WP\_018085363 | WP\_018085366 | WP\_018085367 | Firmicutes | Clostridia |
| Desulfurivibrio alkaliphilus AHT2 | DaAHT2\_2455 | DaAHT2\_2458 | DaAHT2\_2459 | Proteobacteria | Deltaproteobacteria |
| Desulfurobacterium atlanticum | WP\_089322897 | WP\_089322840 | WP\_089322896 | Aquificae | Desulfurobacteriales |
| Desulfuromonas soudanensis | WP\_053552385 | WP\_053551332 | WP\_053551331 | Proteobacteria | Deltaproteobacteria |
| Desulfuromusa kysingii | WP\_092350255 | WP\_092350253 | WP\_092350324 | Proteobacteria | Deltaproteobacteria |
| Dethiobacter alkaliphilus | WP\_008518850 | WP\_008518845 | WP\_008518843 | Firmicutes | Clostridia |
| Dethiosulfatibacter aminovorans | WP\_073047220 | WP\_073047054 | WP\_073047056 | Firmicutes | Tissierellia |
| Dickeya dadantii Ech703 | Dd703\_0491 | Dd703\_0492 | Dd703\_0493 | Proteobacteria | Gammaproteobacteria |
| Dissulfuribacter thermophilus | WP\_067619323 | WP\_067619329 | WP\_067619330 | Proteobacteria | Deltaproteobacteria |
| Draconibacterium sediminis | WP\_045033459 | WP\_045033456 | WP\_045033455 | Bacteroidetes | Bacteroidia |
| Dysgonomonas capnocytophagoides | WP\_026626156 | WP\_051290673 | WP\_026626160 | Bacteroidetes | Bacteroidia |
| Ectothiorhodospira marina | WP\_090250046 | WP\_090250049 | WP\_090250051 | Proteobacteria | Gammaproteobacteria |
| Elusimicrobia RIFOXYB2\_FULL\_49\_7 | OGS33428 | OGS33426 | OGS33425 | Elusimicrobia | - |
| Ethanoligenens harbinense YUAN-3T, DSM 18485 | Ethha\_1567 | Ethha\_1564 | Ethha\_1563 | Firmicutes | Clostridia |
| Faecalicatena contorta | WP\_109714170 | WP\_109714176 | WP\_109714178 | Firmicutes | Clostridia |
| Firmicutes bacterium HGW-Firmicutes-14 | PKM81963 | PKM81966 | PKM81967 | Firmicutes | - |
| Firmicutes bacterium HGW-Firmicutes-2 | PKM68346 | PKM68349 | PKM68350 | Firmicutes | - |
| Fischerella sp. PCC 9605 | WP\_026731053 | WP\_026731054 | WP\_026731055 | Cyanobacteria | - |
| Fontibacillus panacisegetis DSM 28129 | Ga0074847\_109103 | Ga0074847\_109102 | Ga0074847\_109101 | Firmicutes | Bacilli |
| Frankia casuarinae | WP\_063578012 | WP\_063577989 | WP\_063577990 | Actinobacteria | Actinobacteria |
| Gallionellales GWA2\_59\_43 | OGS92466 | OGS92467 | OGS92468 | Proteobacteria | Betaproteobacteria |
| Gallionellales GWA2\_60\_18 | OGS90295 | OGS90408 | OGS90294 | Proteobacteria | Betaproteobacteria |
| Gammaproteobacteria bacterium 28-57-27 | OYY73708 | OYY73707 | OYY73706 | Proteobacteria | Gammaproteobacteria |
| Gammaproteobacteria bacterium HGW-Gammaproteobacteria-1 | PKM46060 | PKM46061 | PKM46062 | Proteobacteria | Gammaproteobacteria |
| Gammaproteobacteria bacterium RIFOXYD12\_FULL\_61\_37 | OGT91538 | OGT91539 | OGT91540 | Proteobacteria | Gammaproteobacteria |
| Geminisphaera colitermitum | WP\_043581909 | WP\_081721723 | WP\_043581908 | Verrucomicrobia | Opitutae |
| Geobacter metallireducens | WP\_004514270 | WP\_004514271 | WP\_004514272 | Proteobacteria | Deltaproteobacteria |
| Geobacteraceae bacterium GWC2\_53\_11 | OGU17931 | OGU17930 | OGU17929 | Proteobacteria | Deltaproteobacteria |
| Geofilum rubicundum | WP\_062122350 | WP\_062122347 | WP\_062122346 | Bacteroidetes | Bacteroidia |
| Geopsychrobacter electrodiphilus | WP\_020677891 | WP\_020677892 | WP\_020677893 | Proteobacteria | Deltaproteobacteria |
| Geothermobacter sp. EPR-M | WP\_085011015 | WP\_085010978 | WP\_085010979 | Proteobacteria | Deltaproteobacteria |
| Geovibrio sp. L21-Ace-BES | WP\_022850366 | WP\_022850365 | WP\_022850364 | Deferribacteres | Deferribacterales |
| Gorillibacterium timonense SN4 | Ga0112892\_17330 | Ga0112892\_17329 | Ga0112892\_17328 | Firmicutes | Bacilli |
| Gracilibacter sp. BRH\_c7a | KUO65809 | KUO65806 | KUO65805 | Firmicutes | Clostridia |
| Halanaerobium saccharolyticum | WP\_108140022 | WP\_108139986 | WP\_108139984 | Firmicutes | Clostridia |
| Halothece sp. PCC 7418 | WP\_015225829 | WP\_015225830 | WP\_015225831 | Cyanobacteria | - |
| Halothiobacillus sp. LS2 | WP\_066098062 | WP\_066098061 | WP\_066098060 | Proteobacteria | Gammaproteobacteria |
| Hartmannibacter diazotrophicus | WP\_099558078 | WP\_099558077 | WP\_099558076 | Proteobacteria | Alphaproteobacteria |
| Heliobacterium modesticaldum | WP\_012282218 | WP\_012282219 | WP\_012282220 | Firmicutes | Clostridia |
| Herbaspirillum seropedicae SmR1 | Hsero\_2853 | Hsero\_2852 | Hsero\_2851 | Proteobacteria | Betaproteobacteria |
| Holophaga foetida | WP\_005034263 | WP\_005034268 | WP\_005034270 | Acidobacteria | Holophagae |
| Hungateiclostridium cellulolyticum | WP\_010251784 | WP\_010251793 | WP\_010251796 | Firmicutes | Clostridia |
| Hydrococcus rivularis | WP\_073598931 | WP\_073599038 | WP\_073598932 | Cyanobacteria | - |
| Hydrogenophaga flava | WP\_066257627 | WP\_066257625 | WP\_066257623 | Proteobacteria | Betaproteobacteria |
| Hydrogenophilales bacterium 28-61-23 | OYY93902 | OYY93903 | OYY93904 | Proteobacteria | Hydrogenophilalia |
| Ilyobacter polytropus CuHBu1, DSM 2926 | Ilyop\_1410 | Ilyop\_1407 | Ilyop\_1406 | Fusobacteria | Fusobacteriia |
| Immundisolibacter cernigliae | WP\_068802292 | WP\_068802293 | WP\_068802294 | Proteobacteria | Gammaproteobacteria |
| Labilibaculum manganireducens | WP\_101310083 | WP\_101310080 | WP\_101310079 | Bacteroidetes | Bacteroidia |
| Lamprocystis purpurea | WP\_020505238 | WP\_020505237 | WP\_020505236 | Proteobacteria | Gammaproteobacteria |
| Lebetimonas sp. JS032 | WP\_024791553 | WP\_024791554 | WP\_024791555 | Proteobacteria | Epsilonproteobacteria |
| Lentisphaerae bacterium GWF2\_50\_93 | OGV59092 | OGV59114 | OGV59095 | Lentisphaerae | - |
| Lentisphaerae bacterium GWF2\_57\_35 | OGV45350 | OGV45347 | OGV45346 | Lentisphaerae | - |
| Leptolyngbya ohadii | WP\_088891457 | WP\_088891456 | WP\_088891455 | Cyanobacteria | - |
| Leptospirillum ferriphilum | WP\_099590653 | WP\_099590654 | WP\_099590466 | Nitrospirae | Nitrospira |
| Leptothrix cholodnii SP-6 | Lcho\_1430 | Lcho\_1431 | Lcho\_1432 | Proteobacteria | Betaproteobacteria |
| Lutibacter agarilyticus | WP\_089382364 | WP\_089382367 | WP\_089382368 | Bacteroidetes | Flavobacteriia |
| Lyngbya aestuarii | WP\_023065299 | WP\_023065312 | WP\_023065341 | Cyanobacteria | - |
| Magnetococcus marinus MC-1 | Mmc1\_1202 | Mmc1\_1201 | Mmc1\_1200 | Proteobacteria | Alphaproteobacteria |
| Magnetofaba australis | WP\_085442124 | WP\_085442125 | WP\_085442126 | Proteobacteria | Alphaproteobacteria |
| Magnetospirillum bellicus VDY | MagVDY\_03872 | MagVDY\_03871 | MagVDY\_03870 | Proteobacteria | Alphaproteobacteria |
| Magnetovibrio blakemorei | WP\_069958443 | WP\_069958444 | WP\_069958445 | Proteobacteria | Alphaproteobacteria |
| Mangrovibacter phragmitis | WP\_064601340 | WP\_064601339 | WP\_064601338 | Proteobacteria | Gammaproteobacteria |
| Marasmitruncus massiliensis | WP\_101909651 | WP\_101909654 | WP\_101909655 | Firmicutes | Clostridia |
| Marinilabilia sp. WTE | WP\_109262942 | WP\_109262939 | WP\_109262938 | Bacteroidetes | Bacteroidia |
| Marinobacter sp. ES-1 | WP\_022990315 | WP\_022990314 | WP\_036220149 | Proteobacteria | Gammaproteobacteria |
| Marinobacterium litorale | WP\_027854782 | WP\_027854783 | WP\_027854784 | Proteobacteria | Gammaproteobacteria |
| Mastigocoleus testarum | WP\_027846702 | WP\_058184423 | WP\_027846727 | Cyanobacteria | - |
| Megasphaera cerevisiae | WP\_074502485 | WP\_074502490 | WP\_074502493 | Firmicutes | Negativicutes |
| Methanobacteriales archaeon HGW-Methanobacteriales-1 | PKL66935 | PKL66932 | PKL66931 | Euryarchaeota | Methanobacteria |
| Methanobacterium paludis | WP\_013826522 | WP\_013826519 | WP\_013826518 | Euryarchaeota | Methanobacteria |
| Methanobrevibacter cuticularis | WP\_067259993 | WP\_067259996 | WP\_067259997 | Euryarchaeota | Methanobacteria |
| Methanocaldococcus infernus ME | WP\_013099459 | WP\_013099456 | WP\_013099455 | Euryarchaeota | Methanococci |
| Methanocella arvoryzae | WP\_012035713 | WP\_012035710 | WP\_012035709 | Euryarchaeota | Methanomicrobia |
| Methanococcus vannielii SB | WP\_011971883 | WP\_011971880 | WP\_011971879 | Euryarchaeota | Methanococci |
| Methanolacinia petrolearia DSM 11571 | Mpet\_0263 | Mpet\_0260 | Mpet\_0259 | Euryarchaeota | Methanomicrobia |
| Methanolobus psychrotolerans | WP\_094228266 | WP\_094228263 | WP\_094228262 | Euryarchaeota | Methanomicrobia |
| Methanomassiliicoccus luminyensis | WP\_026069118 | WP\_019178611 | WP\_026069119 | Euryarchaeota | Thermoplasmata |
| Methanosarcina acetivorans C2A | MA3895 | MA3898 | MA3899 | Euryarchaeota | Methanomicrobia |
| Methanosphaerula palustris | WP\_012617253 | WP\_012617250 | WP\_012617249 | Euryarchaeota | Methanomicrobia |
| Methanospirillum stamsii | WP\_109942292 | WP\_109942295 | WP\_109942296 | Euryarchaeota | Methanomicrobia |
| Methanothermobacter marburgensis | WP\_013294983 | WP\_013294986 | WP\_013294987 | Euryarchaeota | Methanobacteria |
| Methanothermococcus thermolithotrophicus | WP\_018154785 | WP\_018154782 | WP\_018154781 | Euryarchaeota | Methanococci |
| Methanothrix soehngenii GP-6 | MCON\_0607 | MCON\_0610 | MCON\_0611 | Euryarchaeota | Methanomicrobia |
| Methanotorris igneus | WP\_013799857 | WP\_013799860 | WP\_013799861 | Euryarchaeota | Methanococci |
| Methylobacterium nodulans ORS 2060 | Mnod\_3996 | Mnod\_3995 | Mnod\_3994 | Proteobacteria | Alphaproteobacteria |
| Methylocaldum szegediense | WP\_026610013 | WP\_026610014 | WP\_026610015 | Proteobacteria | Gammaproteobacteria |
| Methylocystis parvus OBBP | O5ODRAFT\_01867 | O5ODRAFT\_01868 | O5ODRAFT\_01869 | Proteobacteria | Alphaproteobacteria |
| Methylomicrobium buryatense | WP\_017842415 | WP\_017842414 | WP\_017842413 | Proteobacteria | Gammaproteobacteria |
| Methyloversatilis sp. RAC08 | WP\_069038340 | WP\_069038341 | WP\_069038342 | Proteobacteria | Betaproteobacteria |
| Moorella thermoacetica | WP\_071521047 | WP\_071521044 | WP\_071521043 | Firmicutes | Clostridia |
| Myxosarcina sp. GI1 | WP\_036489259 | WP\_036489262 | WP\_081942974 | Cyanobacteria | - |
| Neiella marina | WP\_087506928 | WP\_087506927 | WP\_087506926 | Proteobacteria | Gammaproteobacteria |
| Nitrospirae bacterium GWA2\_46\_11 | OGW20163 | OGW20164 | OGW20165 | Nitrospirae | - |
| Nitrospirae bacterium GWC2\_57\_13 | OGW27708 | OGW27709 | OGW27710 | Nitrospirae | - |
| Nodosilinea nodulosa | WP\_017298849 | WP\_017298848 | WP\_017298847 | Cyanobacteria | - |
| Novosphingobium naphthalenivorans | WP\_067734406 | WP\_067734405 | WP\_067734404 | Proteobacteria | Alphaproteobacteria |
| Opitutaceae bacterium EW11 | WP\_107745278 | WP\_107745279 | WP\_107745280 | Verrucomicrobia | Opitutae |
| Opitutaceae bacterium TSB47 | AW736\_03595 | AW736\_03600 | AW736\_03605 | Verrucomicrobia | Verrucomicrobia |
| Orenia marismortui | WP\_018247481 | WP\_018247478 | WP\_018247477 | Firmicutes | Clostridia |
| Oscillatoria sp. PCC 10802 | WP\_017716686 | WP\_017716685 | WP\_017716684 | Cyanobacteria | - |
| Oscillochloris trichoides DG-6 | EFO82066 | EFO82064 | EFO82063 | Chloroflexi | Chloroflexia |
| Oxobacter pfennigii | WP\_054874024 | WP\_054874027 | WP\_054874028 | Firmicutes | Clostridia |
| Paenibacillus stellifer DSM 14472 | Ga0069362\_114164 | Ga0069362\_114163 | Ga0069362\_114162 | Firmicutes | Bacilli |
| Paludibacter propionicigenes | WP\_013444938 | WP\_013444941 | WP\_013444942 | Bacteroidetes | Bacteroidia |
| Paludibacterium yongneupense | WP\_028534981 | WP\_028534980 | WP\_028534979 | Proteobacteria | Betaproteobacteria |
| Pantoea cypripedii LMG 2657 | Ga0309980\_12282 | Ga0309980\_12281 | Ga0309980\_12280 | Proteobacteria | Gammaproteobacteria |
| Pararhodospirillum photometricum DSM 122 | RSPPHO\_02584 | RSPPHO\_02583 | RSPPHO\_02582 | Proteobacteria | Alphaproteobacteria |
| Pelobacter propionicus DSM 2379 | Ppro\_3467 | Ppro\_3468 | Ppro\_3469 | Proteobacteria | Deltaproteobacteria |
| Pelosinus propionicus DSM 13327 | Ga0074834\_1010107 | Ga0074834\_1010104 | Ga0074834\_1010103 | Firmicutes | Negativicutes |
| Peptococcaceae bacterium BRH\_c4a | KJR99751 | KJR99748 | KJR99747 | Firmicutes | Clostridia |
| Peptococcaceae bacterium BRH\_c8a | KJS11410 | KJS11413 | KJS11414 | Firmicutes | Clostridia |
| Peptococcaceae bacterium CEB3 | WP\_047829845 | WP\_047829846 | WP\_047829847 | Firmicutes | Clostridia |
| Petroclostridium xylanilyticum | WP\_094550765 | WP\_094550759 | WP\_094550757 | Firmicutes | Clostridia |
| Phaeospirillum fulvum DSM 114 | Ga0061132\_00876 | Ga0061132\_00875 | Ga0061132\_00874 | Proteobacteria | Alphaproteobacteria |
| Phormidesmis priestleyi Ana | KPQ34319 | KPQ34320 | KPQ34321 | Cyanobacteria | - |
| Pleomorphomonas sp. 86 | Ga0302604\_11600 | Ga0302604\_11601 | Ga0302604\_11602 | Proteobacteria | Alphaproteobacteria |
| Prevotella oryzae | WP\_036881131 | WP\_036880219 | WP\_036880217 | Bacteroidetes | Bacteroidia |
| Propionispira arboris | WP\_091831461 | WP\_091831467 | WP\_091831469 | Firmicutes | Negativicutes |
| Propionispora vibrioides DSM 13305 | Ga0074833\_1194 | Ga0074833\_1197 | Ga0074833\_1198 | Firmicutes | Negativicutes |
| Pseudanabaena sp. SR411 | WP\_094531215 | WP\_094531213 | WP\_094531211 | Cyanobacteria | - |
| Pseudodesulfovibrio profundus | WP\_097013057 | WP\_097013060 | WP\_097013061 | Proteobacteria | Deltaproteobacteria |
| Pseudomonas stutzeri A1501 | PST\_1326 | PST\_1327 | PST\_1328 | Proteobacteria | Gammaproteobacteria |
| Rahnella sp. AA | WP\_101076633 | WP\_101076632 | WP\_101076631 | Proteobacteria | Gammaproteobacteria |
| Raoultella ornithinolytica JUb54 | Ga0304837\_101468 | Ga0304837\_101467 | Ga0304837\_101466 | Proteobacteria | Gammaproteobacteria |
| Rhodobacter capsulatus A52 | Ga0100862\_105159 | Ga0100862\_105160 | Ga0100862\_105161 | Proteobacteria | Alphaproteobacteria |
| Rhodoblastus acidophilus DSM 137 | Ga0170454\_10611 | Ga0170454\_10612 | Ga0170454\_10613 | Proteobacteria | Alphaproteobacteria |
| Rhodomicrobium vannielii ATCC 17100 | Rvan\_1953 | Rvan\_1954 | Rvan\_1955 | Proteobacteria | Alphaproteobacteria |
| Rhodopila globiformis | WP\_104518213 | WP\_104518212 | WP\_104518211 | Proteobacteria | Alphaproteobacteria |
| Rhodopseudomonas palustris CGA009 | RPA4620 | RPA4619 | RPA4618 | Proteobacteria | Alphaproteobacteria |
| Rhodospirillum rubrum ATCC 11170 | Rru\_A1010 | Rru\_A1011 | Rru\_A1012 | Proteobacteria | Alphaproteobacteria |
| Rhodovibrio salinarum | WP\_027289758 | WP\_027289759 | WP\_027289760 | Proteobacteria | Alphaproteobacteria |
| Rhodovulum sp. PH10 | A33M\_1296 | A33M\_1297 | A33M\_1298 | Proteobacteria | Alphaproteobacteria |
| Richelia intracellularis HH01 | CCH66462 | CCH66469 | CCH66470 | Cyanobacteria | - |
| Roseiflexus castenholzii | WP\_012122497 | WP\_012122495 | WP\_012122494 | Chloroflexi | Chloroflexia |
| Roseospirillum parvum | WP\_092620711 | WP\_092620709 | WP\_092620707 | Proteobacteria | Alphaproteobacteria |
| Saccharicrinis fermentans | WP\_027473409 | WP\_027473406 | WP\_027473405 | Bacteroidetes | Bacteroidia |
| Sediminispirochaeta smaragdinae | WP\_013255569 | WP\_013255566 | WP\_013255565 | Spirochaetes | Spirochaetia |
| Smithella sp. SCADC | KFO68400 | KFO68403 | KFO68404 | Proteobacteria | Deltaproteobacteria |
| Spirochaeta cellobiosiphila | WP\_028973004 | WP\_028973001 | WP\_028973000 | Spirochaetes | Spirochaetia |
| Spirochaeta thermophila | WP\_013313167 | WP\_013313164 | WP\_013313163 | Spirochaetes | Spirochaetia |
| Spirochaetes bacterium GWB1\_27\_13 | OHD05375 | OHD05378 | OHD05379 | Spirochaetes | - |
| Spirochaetes bacterium GWB1\_36\_13 | OHD11363 | OHD11360 | OHD11367 | Spirochaetes | - |
| Spirochaetes bacterium GWE1\_32\_154 | OHD39357 | OHD39354 | OHD39353 | Spirochaetes | - |
| Sporolactobacillus terrae | WP\_028984127 | WP\_028984128 | WP\_028984129 | Firmicutes | Bacilli |
| Sporomusa acidovorans | WP\_093792115 | WP\_093792109 | WP\_093792107 | Firmicutes | Negativicutes |
| Sulfuricurvum kujiense YK-1, DSM 16994 | Sulku\_1500 | Sulku\_1498 | Sulku\_1497 | Proteobacteria | Epsilonproteobacteria |
| Sulfuriferula sp. AH1 | WP\_087445781 | WP\_087445782 | WP\_087445783 | Proteobacteria | Betaproteobacteria |
| Sulfurimonas sp. | PNV83262 | PNV83260 | PNV83259 | Proteobacteria | Epsilonproteobacteria |
| Sulfurospirillum cavolei | WP\_060826056 | WP\_060826054 | WP\_082709164 | Proteobacteria | Epsilonproteobacteria |
| Sulfurovum sp. enrichment culture clone C5 | CUV65475 | CUV65477 | CUV65478 | Proteobacteria | Epsilonproteobacteria |
| Syntrophobacter fumaroxidans MPOB | WP\_011697884 | WP\_011697881 | WP\_011697880 | Proteobacteria | Deltaproteobacteria |
| Syntrophobotulus glycolicus FlGlyR, DSM 8271 | Sgly\_2841 | Sgly\_2840 | Sgly\_2839 | Firmicutes | Clostridia |
| Syntrophomonas zehnderi | WP\_046497554 | WP\_046497545 | WP\_046497542 | Firmicutes | Clostridia |
| Syntrophothermus lipocalidus DSM 12680 | WP\_013176275 | WP\_013176272 | WP\_013176271 | Firmicutes | Clostridia |
| Telmatospirillum siberiense | WP\_101250570 | WP\_101250571 | WP\_101250572 | Proteobacteria | Alphaproteobacteria |
| Teredinibacter turnerae | WP\_018277248 | WP\_018277247 | WP\_018277246 | Proteobacteria | Gammaproteobacteria |
| Terrimicrobium sacchariphilum | WP\_075078689 | WP\_084400275 | WP\_075078690 | Verrucomicrobia | Spartobacteria |
| Thauera sp. D20 | WP\_107492233 | WP\_107492234 | WP\_107492235 | Proteobacteria | Betaproteobacteria |
| Thermacetogenium phaeum | WP\_015049976 | WP\_015049979 | WP\_015049980 | Firmicutes | Clostridia |
| Thermicanus aegyptius | WP\_028986272 | WP\_028986273 | WP\_028986274 | Firmicutes | Bacilli |
| Thermincola potens JR | TherJR\_0688 | TherJR\_0691 | TherJR\_0692 | Firmicutes | Clostridia |
| Thermoanaerobacterium thermosaccharolyticum | WP\_013298321 | WP\_013298320 | WP\_013298319 | Firmicutes | Clostridia |
| Thermodesulfovibrio yellowstonii DSM 11347 | WP\_012546613 | WP\_012546033 | WP\_012545394 | Nitrospirae | Nitrospira |
| Thioflexothrix psekupsii | WP\_086487138 | WP\_086487137 | WP\_086487136 | Proteobacteria | Gammaproteobacteria |
| Thiohalocapsa sp. ML1 | WP\_058554369 | WP\_058554368 | WP\_058554367 | Proteobacteria | Gammaproteobacteria |
| Thiorhodococcus drewsii AZ1 | ThidrDRAFT\_2681 | ThidrDRAFT\_2682 | ThidrDRAFT\_2683 | Proteobacteria | Gammaproteobacteria |
| Thiothrix nivea DSM 5205 | EIJ36507 | EIJ36508 | EIJ36509 | Proteobacteria | Gammaproteobacteria |
| Tolumonas lignilytica BRL6-1 | H027DRAFT2334 | H027DRAFT2335 | H027DRAFT2336 | Proteobacteria | Gammaproteobacteria |
| Treponema primitia | WP\_010260142 | WP\_010260134 | WP\_010260131 | Spirochaetes | Spirochaetia |
| Trichodesmium erythraeum | WP\_011613474 | WP\_011613475 | WP\_011613476 | Cyanobacteria |  |
| Uliginosibacterium gangwonense | WP\_018607902 | WP\_018607903 | WP\_018607904 | Proteobacteria | Betaproteobacteria |
| uncultured Alphaproteobacteria bacterium | SBW06912 | SBW06906 | SBW06899 | Proteobacteria | Alphaproteobacteria |
| unicellular cyanobacterium SU2 | WP\_085434912 | WP\_085434911 | WP\_085434910 | Cyanobacteria | - |
| Verrucomicrobia bacterium LP2A | WP\_024807527 | WP\_024807526 | WP\_024807525 | Verrucomicrobia | - |
| Verrucomicrobia bacterium Tous-C9LFEB | PAW77340 | PAW77337 | PAW77336 | Verrucomicrobia | - |
| Verrucomicrobiae bacterium DG1235 | WP\_040901465 | WP\_008103118 | WP\_040899453 | Verrucomicrobia | Verrucomicrobiae |
| Vibrio diazotrophicus | WP\_102939852 | WP\_102939851 | WP\_102939850 | Proteobacteria | Gammaproteobacteria |
| Vulcanococcus limneticus | WP\_094591659 | WP\_094591660 | WP\_094591661 | Cyanobacteria |  |
| Xanthobacter autotrophicus Py2 | Xaut\_0088 | Xaut\_0089 | Xaut\_0090 | Proteobacteria | Alphaproteobacteria |
| Yangia sp. CCB-MM3 | WP\_066099558 | WP\_066099560 | WP\_066099562 | Proteobacteria | Alphaproteobacteria |
| Youngiibacter fragilis | WP\_023388904 | WP\_023388907 | WP\_023388908 | Firmicutes | Clostridia |
| Zavarzinia sp. HR-AS | WP\_109903383 | WP\_109903385 | WP\_109903387 | Proteobacteria | Alphaproteobacteria |
| Zetaproteobacteria bacterium CG17\_big\_fil\_post\_rev\_8\_21\_14\_2\_50\_50\_13 | PIQ34264 | PIQ34263 | PIQ34262 | Proteobacteria | Zetaproteobacteria |
| Zoogloea sp. LCSB751 | WP\_079432933 | WP\_079432932 | WP\_079432931 | Proteobacteria | Betaproteobacteria |
| Zymomonas mobilis | WP\_011241556 | WP\_011241557 | WP\_011241558 | Proteobacteria | Alphaproteobacteria |
|  |  |  |  |  |  |
| **Species** | **AnfH** | **AnfD** | **AnfK** | **Phylum** | **Class** |
| Azotobacter vinelandii DJ, ATCC BAA-1303 | Avin\_49000 | Avin\_48990 | Avin\_48970 | Proteobacteria | Gammaproteobacteria |
| Bacteroidales bacterium Barb6 | WP\_066182251 | WP\_066186490 | WP\_066182235 | Bacteroidetes | Bacteroidia |
| Brenneria salicis ATCC 15712 | Bresa\_00753 | Bresa\_00754 | Bresa\_00756 | Proteobacteria | Gammaproteobacteria |
| Chloroherpeton thalassium ATCC 35110 | Ctha\_1828 | Ctha\_1831 | Ctha\_1833 | Chlorobi | Chlorobia |
| Clostridium pasteurianum DSM 525, ATCC 6013 | Ga0069491\_113885 | Ga0069491\_113883 | Ga0069491\_113881 | Firmicutes | Clostridia |
| Dendrosporobacter quercicolus | WP\_092072016 | WP\_092072026 | WP\_092072032 | Firmicutes | Negativicutes |
| Desulfitobacterium chlororespirans | WP\_072772837 | WP\_072772834 | WP\_072772832 | Firmicutes | Clostridia |
| Desulfovibrio sp. 86-1 | Ga0302701\_111207 | Ga0302701\_111210 | Ga0302701\_111212 | Proteobacteria | Deltaproteobacteria |
| Dysgonomonas capnocytophagoides | WP\_026625686 | WP\_026625683 | WP\_026625681 | Bacteroidetes | Bacteroidia |
| Opitutaceae bacterium TSB47 | AW736\_03515 | AW736\_03520 | AW736\_03530 | Verrucomicrobia | Verrucomicrobia |
| Pantoea cypripedii LMG 2657 | Ga0309980\_12203 | Ga0309980\_12204 | Ga0309980\_12206 | Proteobacteria | Gammaproteobacteria |
| Pararhodospirillum photometricum DSM 122 | RSPPHO\_00490 | RSPPHO\_00489 | RSPPHO\_00487 | Proteobacteria | Alphaproteobacteria |
| Rhodobacter capsulatus A52 | Ga0100862\_105146 | Ga0100862\_105145 | Ga0100862\_105143 | Proteobacteria | Alphaproteobacteria |
| Rhodoblastus acidophilus DSM 137 | Ga0170454\_11380 | Ga0170454\_11381 | Ga0170454\_11383 | Proteobacteria | Alphaproteobacteria |
|  |  |  |  |  |  |
| **Species** | **VnfH** | **VnfD** | **VnfK** | **Phylum** | **Class** |
| Azomonas agilis DSM 375 | LX59DRAFT\_02210 | LX59DRAFT\_01075 | LX59DRAFT\_01073 | Proteobacteria | Gammaproteobacteria |
| Azotobacter vinelandii DJ, ATCC BAA-1303 | Avin\_02660 | Avin\_02610 | Avin\_02590 | Proteobacteria | Gammaproteobacteria |
| Chromatiales bacterium | PHBDraft\_25530 | PHBDraft\_25580 | PHBDraft\_25610 | Proteobacteria | Gammaproteobacteria |
| Clostridium kluyveri DSM 555 | CKL\_1748 | CKL\_1747 | CKL\_1745 | Firmicutes | Clostridia |
| Desulfobacter curvatus DSM 3379 | B147DRAFT\_02029 | B147DRAFT\_02028 | B147DRAFT\_02026 | Proteobacteria | Deltaproteobacteria |
| Ethanoligenens harbinense YUAN-3T, DSM 18485 | Ethha\_2309 | Ethha\_2312 | Ethha\_2314 | Firmicutes | Clostridia |
| Magnetospirillum bellicus VDY | MagVDY\_01910 | MagVDY\_01908 | MagVDY\_01906 | Proteobacteria | Alphaproteobacteria |
| Methanosarcina acetivorans C2A | MA1213 | MA1216 | MA1218 | Euryarchaeota | Methanomicrobia |
| Methylocystis parvus OBBP | O5ODRAFT\_02619 | O5ODRAFT\_02621 | O5ODRAFT\_02623 | Proteobacteria | Alphaproteobacteria |
| Paenibacillus durus P3L-5 | L664DRAFT\_00627 | L664DRAFT\_00626 | L664DRAFT\_00624 | Firmicutes | Bacilli |
| Phaeospirillum fulvum DSM 114 | Ga0061132\_02947 | Ga0061132\_02945 | Ga0061132\_02943 | Proteobacteria | Alphaproteobacteria |
| Rhodoblastus acidophilus DSM 137 | Ga0170454\_103245 | Ga0170454\_103247 | Ga0170454\_103249 | Proteobacteria | Alphaproteobacteria |
| Rhodopseudomonas palustris CGA009 | RPA1376 | RPA1378 | RPA1380 | Proteobacteria | Alphaproteobacteria |
| Tolumonas lignilytica BRL6-1 | H027DRAFT2934 | H027DRAFT2940 | H027DRAFT2942 | Proteobacteria | Gammaproteobacteria |
|  |  |  |  |  |  |
| **Species** | **Bch/ChlL** | **Bch/ChlN** | **Bch/ChlB** | **Phylum** | **Class** |
| Chlorobium phaeobacteroides DSM 266 | WP\_011746157 | WP\_011746159 | WP\_011746158 | Chlorobi | Chlorobia |
| Erythrobacter sp. NAP1 | WP\_007165005 | WP\_007165002 | WP\_007165003 | Proteobacteria | Alphaproteobacteria |
| Gloeobacter violaceus PCC 7421 | WP\_011142366 | WP\_011142365 | WP\_011140219 | Cyanobacteria | Gloeobacteria |
| Halorhodospira halophila | WP\_011814420 | WP\_011814423 | WP\_011814422 | Proteobacteria | Gammaproteobacteria |
| Heliobacterium modesticaldum | WP\_012282383 | WP\_012282384 | WP\_012282385 | Firmicutes | Clostridia |
| Hoeflea phototrophica DFL-43 | WP\_040449113 | WP\_007196612 | WP\_007196611 | Proteobacteria | Alphaproteobacteria |
| Roseiflexus castenholzii | WP\_012120059 | WP\_012120057 | WP\_012120058 | Chloroflexi | Chloroflexia |
| Synechococcus sp. CC9311 | WP\_011619890 | WP\_011619888 | WP\_011619889 | Cyanobacteria | - |
| Synechococcus sp. JA-2-3B'a(2-13) | WP\_011432649 | WP\_011432647 | WP\_011433773 | Cyanobacteria | - |
| Synechococcus sp. RCC307 | WP\_011935983 | WP\_011935981 | WP\_011935982 | Cyanobacteria | - |