Supporting Information for

The archaeal transcription termination factor aCPSF1 is a robust phylogenetic marker for archaeal taxonomy

This file contains:

Supplementary Figures. S1 to S4;

Caption for Supplementary Dataset S1 Information of the investigated archaeal genomes downloaded from NCBI database

Caption for Supplementary Dataset S2 Information of the 779 archaeal genomes used for taxonomy ranking based on aCPSF1

Caption for Supplementary Dataset S3 Identified 144 unclassified archaeal genomes in

NCBI database based on aCPSF1 taxonomy system

Caption for Supplementary Dataset S4 Sequence similarities of the duplicated aCPSF1

orthologs in 56 out of 366 haloarchaeal genomes

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MTH_MTH_1203		$TT \xrightarrow{\beta2} \alpha2 \alpha3 \xrightarrow{\beta3} \eta^1$
MTH_MTH_1203 TAG_Tagg_1253 DMU_Desum_1273 SNR_Smar_0337 HBU_Hbut_1568 FFO_FFONT_1081 IAC_Iqa_0046 SAI_Saci_0639 MSE_Msed_2254 HBO_GM_0009 ASC_ASAC_0309 MSE_Msed_2254 HBO_GM_0009 ASC_ASAC_0309 MSC_NEQ076 VDI_Vdis_1675 CMA_Cmac_0455 PCL_Pcal_0030 Kcr_Kcr_1411 NNR_Nmar_1727 CSY_CENSYa_1545 nga_Ngar_c32500 CSU_CSUB_C1103 PFO_PAB_07900 MMF_MMP0694 MOK_Metck_0979 MCG_Metig_0294 MCG_Metig_0294 MCG_Msiz27 TVO_TVG0658611 FAI_FAD_473 MCA_M3_374 MAM_MM_0695 MBU_MFU_0375 HAL_VNG_0401G NFM_P0210A_ncsA MEM_MSIS	MV SEMLEETKRIT MORLEESHOV AKVEF MKID KSVINKN LALLGSTVOBIEPELLEISNIE MKID RILLEKN KLELLKNIME I PALLEISNIE MKID RILLEKN KLELLKNIME I PALLEISNIE MKID RILLEKN KLELLKNIME I PALLEISNIE MKID RILLEKN KLELLKNIME MKID RILLEKN KLELLKNIME MKID RILLEKN KLELLKNIME MKID RILLEKN KLEIT KELLKNIME MKID RILLEKN KLEN MSFRIDINYIR KVIFKLIPPIA MSFRIDINYIR VIFKLIPPIA MSFRIDISSIYN MSFRIDISSIYN MSFRIDISSIYN MSFRIDISSIYN MSSRIDISSIYN MSSRIDISSIYN MSSRIDISSIYN MSSRIDISSIYN MSSRIDISSIYN MSSRIDISSIYN MSSRIDISSIYN MSSRIDISSIYN MSSRITERI MSSCA MSSRA MSSR MSSRA	30 40 50 60 70 60 EVVYVRNEKAISEHL. DLAQNIAKVVRKEVVIEVSTESEL 60 EVVYVRNEKAISEHL. DLAQNIAKVVRKEVVIEVSTESEL 61 EVVYVRNEKAISEHL. DLAQNIAKVVRKEVVIEVSTESEL 62 EISTVYVRNEKAISEHL. DLAQNIAKVVRKEVVIEVSTESEL 64 EISTVYVRNEKAISEHL. DLAQNIAKVVRERVVIEVSTESEL 65 EISTVYVRNEKAISEHL. DLAQNIAKVVRERVVIEVSTESEL 66 EISTVYVRNEKAISEHL. DLAQNIAKVVRERVVIEVSTESEL 66 EISTYVRNEKAISEHL. DLAQNIAKVVRERVVIEVSTESEL 60 EISTYVRNEKAISEHL. DLAQNIAKVVRERVVIEVSTESEL 60 EISTYVRNEKAISEHL. DLAQNIAKVVRERVVIEVSTESEL 60 EISTYVRNEKAISEN 60 EISTYNKNEKAISEN 60 EISTYNKNESEN 60
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MTH_MTH_1203	$\begin{array}{ccc} \alpha 4 & & & & \beta 4 & & \beta 5 \\ \alpha 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0$	$\begin{array}{cccc} \alpha 5 & \alpha 6 & \beta 6 \\ \underline{\rho} & $
MTH_MTH_1203 TAG_Tagg_1253 DMU_Desum_1273 SMR_Smar_0397 HBU_Hbut_1568 FFO_FFONT_1081 IAG_Iqag_0046 SAI_Saci_0639 MSE_Maed_2254 H00 Igni_0009 ASC_ASAC_0317 APE_APE_0522.1 TPE_Tpen_0309 NEQ_NEQ076 VDI_Vdis_1675 CCM_Cmac_0455 PCL_Pcal_0030 kcr_Kcr_1411 NNR_Nmar_1727 CSY_CENSYa_1545 nga_Ngar_c23500 CSU_CSUB_C1103 PFU_PF1405 PFAC_PAP_07900 MMP_MMP0694 M07_Mcbc_0979 MIG_Mcig20294 M07_MJ_1236 MND_ML27 TVO_TVG0658611 FAI_FAD_1473 MAC_MA_3874 MMA_MM_0595 MBU_MPU_04016	D P EKAI T RK THE T V PED. A AT I TN I S T D V T C E VI T E A RK P P V D E AKK T LE I A P RD. A G LD P NG I Y P D T S C V V V K V V K V K P P G E AKK T LE I A P RD. A G LD P NG I Y P D T S C V V V K V V K V K P P G E AKK T LE LI V P K A G LD P NG I Y P D T S C V V V K V K V K V P S E KAT K K I LE I V P K A G V D P NG I Y P D T S C V V K K V K V K V K V P E E KAK K I LE I V P K A G V D NG I V P D T T R C V V L K A K K V P E E AK K I LE V V K V P P A G K K A K I K K P V V L C V V I K K K K K K K L K K V P P P T G C C G C V V C K V V C V C K K K K K K K K K K	ŪLVIGKYGSTËR. ETVKNTG APKTLR. TPPTSSE. IT GLVIGKYGSTËR. ETVKNTG APKTLR. TPPTSSE. IT GLVIGKGCN.YMHKILAETG RAVVPMR. APLESK. VI GLVIGKGGSTMRHLILAKTGGRVIVG QR. APLESK. AL GLVGKGGSTMRHLILAKTGGRVIVG QR. APLESK. AL GLVGKGGSTINNKVLAETGGRMVVR. APPTSK. AL GLVIGKGGSTINNKVLAETGGRMVVR. APPTSK. IL HILEEKS. NOILVYTGGRPTVIR. APPMSK. VV GLVIGKGGSSLQCKIFAETYR PILVR. APPHSK. VV GLVIGKGG.SLQCKIFAETYR PILVR. APPLKSR. TV GLVIGKGG.LIQQKIMPTYR VR GLVIGKGSSLQCKIFAETYR PILVR. APPLKSR. TV GLVIGKGG.SLQCKIFAETYR PILVR. APPLKSR. TV GLVIGKGG.SLQCKIFAETYR PILVR. APPLKSR. TV GLVIGKGG.SLQCKIFAETYR PILVR. APPLKSR. TV GLVIGKGG.SLQCKIFAETYR PILVR. APPLKSR. TV GLVIGKGG.HRLKIITATGKPVVMR. NPLKSR. TV GLVIGKGG.HRLKIITATGKPVVMR. NPLKSR. TV GKLIGGGR.VRRNUVLAATGRLEVQR. KPPLVSK. TL EKIPP.FUNNRVFFETLTFRVIR. KPPVHSS. TU VR. ARS.KIEKEILAETGKVVVVN. NPLKSR. TV VR. ARS.KIEKEILAETGKVVVN. NPLKSR. TV VR. ARS.KIEKEILAETGKVVVN. NPLKSR. TV VR. ARS.KIEKEILAETGKVVISTALANSKGLPRD. DI GVVGKGG.ANTVEIKETGKVVVR. ATTVPSR. TI WLQRNAKEFNHAEVTEKTGKVVISTALATSSS. TM WLQRNASEFSHADVEKIGGVINGKVSR. TPPLQSQ. TI GLVIGKNGETIR.LITEKVR APKVVR. TPPLQSQ. TI GLVIGKNGETIR.LITEKVR APKVVR. TPPLQSQ. TI GLVIGKNGETIR.LITEKKAIKAPKVR. TPPISS. TI GLVIGKNGETIR.LITEKKAIKAPKVR. TPPLQSQ. TI GLVIGKNGETIR.LITEKKAIKAPKVR. TPPISS. TI GLVIGKNGETIR.LITEKKAIKAPKVR.TPPISS. TI TANDEFFNIKSKIFKAFTNGOSPRIVS.APFNYSE. TI GLVIGKNGETIR.SETTNTTONT

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MTH MTH 1203	α7 α8	β7	β8 β9	
	000000000 00000000000000000 150 160 170	180 190	200	210 220 T
MTH_MTH_1203 TAG_Tagg_1253	E R I R R T L R K N S K E R K K I L Q Q L G N R I H Q K P K Y D N R E V V A G T L K Q S E Y R L E F L R R L G D R I H R D V I F K N	NYVRITALGGFREV	GRSSILVETRESRLL	LDC <mark>GV</mark> N.VAGGDD.KNSYPYL LDM <mark>GI</mark> NT.GVMDDPFKAFPYI
DMU_Desmu_1273 SMR_Smar_0937	YEVLNNVLKQSSYRVEFLRRLGERIHRDVVFKN KVIMSNLLKESDYRLRFLRKLGERIHRDVIFKN	NYVKVTGL <mark>G</mark> GFRE <mark>V</mark>	GRSSILVETRESKVL GRSAILVETRESRVL	L <mark>DLGI</mark> NT.GAIDDPGKAYPLL LDL <mark>GI</mark> NV.GAGTDYDRAYPFI
HBU_Hbut_1568 FFO_FFONT_1081	NKIIDYMLSQSSYRLEFLRSSGERIHRGVIFEN DSILGQLIAESNYRKTFLRNIGERIHRDLLFKT	RYVRITAL <mark>G</mark> GFME <mark>V</mark>	GRSAILIETSESKIL	LDVGINP.SGI.GYN.LYPRL LDAGVNP.GSS.SFPSIAPRF
IAG_Igag_0046	E E VMHGYLSQSEYRLNFLRELGETIHRDVLLAK	NGSNYVRVTFL <mark>G</mark> GAQE <mark>V</mark>	GRSAILVETAESRVL	LDF <mark>GL</mark> NP.GRS.LSPNAF <mark>P</mark> RI
SAI_Saci_0639 MSE_Msed_2254	D G V L T H I Y N E T E Y R A K A L R V F G E R I H R D I L F K D E G V L T H I Y N E T E Y R A K M L K T F G E R I H R E I L F K D	RYVRVTAL <mark>G</mark> AFQE <mark>V</mark>	GRSAVLVETPESRVL	LDV <mark>GL</mark> NP.SVS.YGEKLFPRI MDV <mark>GV</mark> NP.SVN.FGERMFPKL
IHO_Igni_0009 ASC_ASAC_0317	STIRAFYRENTKRRLEALLEIGNRIHRPLLFKT ASLNTLYLMASGERRHALREIGERIYRDMISGP	NYVRITAL <mark>G</mark> AFKE <mark>V</mark>	GRSCILIDTSESKIL	LDF <mark>G</mark> ANVGSYDPQKHFP LDV <mark>G</mark> FAQ.SGFGPDAYPMF
APE_APE_0522.1 TPE_Tpen_0309	DSVLRHLQRHAEERRRALRDIGERIFRDTLIGT SEIRELYRASKQERIDFLRKLGYKVYRKPIFP.	RHVRVVGL <mark>G</mark> SFGE <mark>V</mark>	GRSAILVDTGESKVL	LDAGLSP.SGYGPDSYPYY LDAGLKP.TGNGDELPLF
NEQ_NEQ076	DMVRAYMFOHSNERIKLLHEIGKNISEKWSIOK	G.OTWVRVSFL <mark>G</mark> GASOV	GRSALLLQTKESRIL	L <mark>D</mark> F <mark>G</mark> VDL.SLPPNNKNAY <mark>P</mark> IV
VDI_Vdis_1675 CMA_Cmaq_0455	DAVKQIQIATAKDRLEFLRRLGMRIHREPVYK. DAVNNVDMLMSKERAEFLKSIGLRIHRLPVYK.	NEYVKVTCLGACFEV	GRSALLIETSESRVL	L <mark>D</mark> C <mark>GV</mark> KP.SSSGDEAP LDAGVKP.SGGMDEAP
PCL_Pcal_0030 kcr_Kcr_1411	LAVRQIFHGAYEQRRELMERLARFIHQEPVVK. DIFYNVIISGAPERKKVMKKLSERIFREPLNL.	EGPITVTFLGGAMEV SRGLYATFLGAAREV	GRSAVLVSTGESNVL GRSSVLITTDESNVL	L <mark>D</mark> C <mark>GL</mark> KP.VQDDEDFP LDC <mark>GI</mark> SL.SSRSAFP
NMR_Nmar_1727 CSY_CENSYa_1545	QTINATLKQASTERSKQLKQVGDEIFRPRLTQR QVINRTLRASSIERGKQLKQIGDDIFRPKLATR	TEVSLYTL <mark>G</mark> GFGQ <mark>V</mark> SEISLTALGGFGOV	GRSSLLLSTPESKIL GRSCMLLSTLDSKVL	IDCGINPGARSPMDAFPRL VDCGVNPGAAHPSESYPRL
nga_Ngar_c23500	EALYRTLGEAVGERTKFYREVGDKIFRDKLSES.	AEASLMTL <mark>G</mark> GFA <mark>E</mark> V	GRSCMLLTTSESKVL	LDCGLNIYAKDSLAAMPRF LDCGLSAGATSSLSFYPRF
CSU_CSUB_C1103 PFU_PF1405	ERVKRYLYWDTEEKLDILRRVGERVFRTMTFES YLIRQILQTESKDRRKFLRQVGRNIYRKPEYKS	RWIRITGL <mark>G</mark> GFREV	GRSALLVOTDESFVL	VDFGIN.VAALNDPYKAFPHF
PPAC_PAP_07900 MMP_MMP0694	YSIRQILQSESKDRRKFLRQVGRNIYRKPELKS KAIRATMYRERADVKDILRRIGRRIHRDVRLRD	DSWVRTSFL <mark>G</mark> GSREV	GRTCLYHQTPESRIL	V <mark>D</mark> F <mark>GI</mark> N.VAALHDPKKAVPHF VDC <mark>GI</mark> N.IAVEDEKAFPHF
MOK_Metok_0979 MIG_Metig_0294	KAIRATMYRERTDVKEILRRIGRRIHRDVKLRE KAIRATLYRERADVKEILRRIGRRIHRDIKIRE	DCWIRMSFL <mark>G</mark> GARE <mark>V</mark>	GRICNYLOTPESRIL	DCGIN, VAIDGD, KAFPHF
MJA_MJ_1236 MRU_mru_1978	KAIRATLYRERHEVKEILRRIGRRIHRDIVVRG DRIRNTLLNNSKERKKFLQTLGARIHQGGKYPS	DYWIRVSFL <mark>G</mark> GARE <mark>V</mark>	GRSCLYVQTPDTRVL GRSCMLLQTPNSRVL	IDCGIN.IAVEGDRAYPHF IDCGIN.VACEDKAFPHF LDCGVN.VAGQDD.KTSFPML
LOKI_Lokiarch_44440	QLIRGMLKKERQTQKDILLEIGKRIHR.PALFN	NLNIRMNAL <mark>G</mark> GFRE <mark>V</mark>	GRSCILMQTRDSNVL	LDVGLN.VGNPNDRFPYF
MKA_MK1227 TVO_TVG0658611	NTTRRLILSDDSRRKFLRNVSARIFCGRTRSRG KEIREYMRDIKQERKEFLHNLGVKLSGPPLVGE	TWVRLTAL <mark>G</mark> GHSE <mark>V</mark>	GRSSLFLHTEESRVL GRSATLVSTKNSKVL	L <mark>D</mark> C <mark>GV</mark> N.VAANGTDAYPHF IDC <mark>G</mark> MMNVGPDADPWDAAPYL
FAI_FAD_1473 MAC_MA_3874	KEVREYLRDVKKERKEFLHNLGIKLTTPLMPGE KNIREFMRNNLKERKEILKTVGRKIHRECTSKD	OWVRVTALCGCKEV	GRSATLISTNNSKVL GRSCFLLSTPESRIL	IDCGMMNVGPDADPWDAAPYL VDCGMININDPEHPWEEAPYL IDCGVNVGSDENMTPYL
MMA_MM_0695 MBU_Mbur_0375	KN IREFMRNNLKERKEILKT VGRKIHRECTSKD KNIREFMRTNHKDRKEILKA VGRNIHRECTSKD	QWVRVTALGGCKEV	GRSCFLLSTPESRIL	IDC <mark>GV</mark> NVGSDENMTPYL IDC <mark>GV</mark> NVGSDDNMTPYL
HAL_VNG_0401G	SNVRNFLKOERDERRDILETVGROIHREEMODD.	E YVRVTTLCCCREV	GRASFVLSTPETRIL	VDCGDKPGSEDEVPYL IDCGDKPGAEGEVPYL
NPH_NP_0210A_ncsA_ HWA_HQ_1716A	SNVRNFLKQEREERRDILERIGRQIHREEMSDD SNVRNFLKQERDERRDILERVGRQIHREELSDD	EWVRISTLGCCREV	GRASEVISTPETRIL	DCCDKPGS.DDVPYL
MHU_Mhun_0845	KQVRQYLRAAHQERKELLKRIGRRIHRDVIAKD DNIRNYLLSVREERSEILKRIGERIHRTSLIDE	QWIRVTTLGCCREV KWVRVTFLGGSREV	GRAAFLLSTPESRVL GRSCYLLQTPESRIL	IDCGEKPDSFEATPYL IDCGVNVSNLSSTPYL
AFU_AF_0482 FPL_Ferp_0914	ED <u>IRNFL</u> LSVRE <u>ER</u> KEI <u>LKKVGERI</u> HRGTIYKD	K <u>WVRIT</u> FL C GSRE <mark>V</mark>	<u>GR</u> SCYLLQ <mark>W</mark> PESKIM	IDCEVNVSNLNQT⊵YL ↑ I
	EDIRNFLLSVREEKKEILKKVGERIHRGTIYKD T TT TT $\beta_{0.000}$ $\alpha_{0.000}$	$M\beta L$ $\delta L \qquad $	α12 00000000000000000	α13 α13 α13 α000 α13
FPI_Ferp_0914 MTH_MTH_1203 MTH_MTH_1203	EDIRNFLLSVREERKEILKKVGERIHRGTIYKD T TT TT TT β_{10} α_{10} α_{11} z_{30} TTT 240 250 250 NMPEFTLDSUDAVITHAHLOHSGE/DYL	$M\beta L$ $260 \rightarrow 22$ $YHY, GYDG PVYCTAP$	α12 000000000000000 70 280 PRDLMTLLQLDHIDI	Impc@yNvsnlnqTPyL 1 000000000000000000000000000000000000
FPI_Ferp_0914 MTH_MTH_1203 MTH_MTH_1203 TAG_Tagg_1253 DMU_Desgu_1273	EDIRNFLLSVREERKEILKKVGERIHRGTIYKD T TT 0000 0010 230 TTT 240 0000 0000 240 250 NVPEFTDSLDAVITHAHLDBSGPPYL DVDSLKLBELDGVIVHSBDBVGLVEYL EVDSLRLDBLDGVIVHAB	<u>MβL</u> <u>β11</u> <u>Q2</u>	CI2 000000000000000000000000000000000000	Implement dl3 00000000 00000000 290 300 AHREDDEPLPFINVKHVKKSVKF SRSSRYLPFTEKDLTTMLL PRSGRYLPFTEKDLTTMLL PRSGRYLPFTEKDLTTMLL
FPL_Ferp_0914 MTH_MTH_1203 MTH_MTH_1203 TAG_Tagg_1253 DMU_Desmu_1273 SMR_Smar_0937 HBU_HBUL_1568	EDIRNFLLSVREERKEILKKVGERIHRGTIYKD TTT β10 α10 α11 230 TTT 240 2000 2000 NVPEFTLDSLDAVITHAHLDBSGPPYL DVDSLKL ELDGVIVHSHDBVGLVFIL EVDSLKL ELDGVIVHSHDBVGLVFIL DVGLVFIL DIDQLNL SELDAVIVHAHLDBIGFILVE DIGUVEN		C12 00000000000000 7000000000000 RCDLMTLLQLDHTDT RCLMVLKDLEV RCLMVLKDLEV RCLMVLKDLEV RCLMVLLLDLEV	Implement cl3 cl0 cl0
FFL_Ferp_0914 MTH_MTH_1203 MTH_MTH_1203 TAG_Tagg_1253 DMD_Desmu_1273 SMR_Smar_0937 HBU_Hbut_1568 FFO_FF0WT_1081	EDIRNFLLSVREERKEILKKVGERIHRGTIYKD T TT 230 , TTT 240 , 2000 , 2000 DVDSFTLDSLDAVITHAH DDRSGFLDYL DVDSLKLEELDGVIVTHAH DDRSGFLDYL DIDQLNLSELDAVVTHAH DDRIGLVPYL DIDQLNLEELDAVVTHAH DDRIGLVPHL DVDDFKIEELDAVVTHAH DDRIGLVPHL DVDDFKIEELDAVVTHAH DDRIGLVPHL DVDDFKIEELDAVVTHAH DDRIGLVPHL DVDFKIEELDAVVTHAH DDRIGLVPHL	MβL 260 260 $24HY, GYRG. PUYCTAP$ $YKY, GYRG. PUYVTKP$ $YKX, GYRG. PUYVTKP$ $YKX, GYRG. PUYVTKP$ $FXX, GYRG. PUYVTKP$ $FXX, GYRG. PUYVTKP$ $FXX, GYRG. PUYVTKP$ $FXX, GYRG. PUYVTKP$		CCC CI3 CCC CCCCCCCC CCC CCCCCCCCC CCC CCCCCCCCCC AREEDEPLPENVKHVKKSVKE SCR RRSGRYLPFTEKDLTTMILE RRSGRYLPFTEKDLTTMILE CRESKYPFSEKDLSTMLLW VGRSGKPYPTOQEVKKMULE VGRSGKPPTOQEVKKMULE VGRSGKPPTOQEVKKMULE
FFL_Ferp_0914 MTH_MTH_1203 TAG Tagg 1253 DMU_Desmu_1273 SMR_Smar_0937 HBU_Hbut_1568 FFO_FF0N_1081 IAG_Igag_0046 SAT_Saci_0639	EDIRNFLLSVREERKEILKKVGERIHRGTIYKD T TT 230 TTT 240 2000 210 NVPEFTLDSIDAVITHAHIOHSGFUYL DVDSLKLEELDGVIVTHAHIOHSGFUYL EVDSLRLBELDGVIVTHAHIDHVGLV9VL DIDQLNLEELDAVVTHAHIDHIGLVPLL DIDQLNLEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL DVDFKIEELDAVVTHAHIDHIGLVPLL	<u>MβL</u> <u>MβL</u> <u>β11</u> <u>Q260</u> <u>Q260</u> <u>Q27HY</u> , GYRG PUYCTAP <u>YKY</u> , GYRG PUYVTKP <u>YKY</u> , GYRG PUYVTKP <u>YKX</u> , GYRG PUYVTKP <u>FKX</u> , GYRG PUYVTKP <u>FKX</u> , GYRG PUYMTKP	CISCYLLOPPESKIM COCCOCCCCCCCC COCCCCCCCCCCC COCCCCCCCC	QCCQ QCCQ
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DMU_Desmu_1273	ELRARGRPEVLVPNILDTINLT
SMR_Smar_0937	RNPSTGYGANTMVYTPHLLDSIHLTARR
HBU_Hbut_1568	.ARHLGLPEDIRVYTPTILDTLHIAGVA
FFO_FFONT_1081	.KYANRALSDIRVIAPSILDAIALI
IAG_Igag_0046	SRKRLGDINVLTPKILESYTLAYNI
SAI_Saci_0639	KIKGIDNVYAPKILESIRTI
MSE_Msed_2254	RERERLGLRSANIYS <mark>P</mark> AILDSIRLDKTS
IHO_Igni_0009	VARGMKIYTPNIRDSIVFVENDI
ASC_ASAC_0317	.WDKLGFDASPEVVVPENLETIRVYPRSSKLHNALLYS
APE_APE_0522.1	.WSKLGFESPPIIEAPENLEGVRLYPRNLKMKLALQHS
TPE_Tpen_0309	.WFKKKTGLNLDVLTPKNAESIRIV
NEQ_NEQ076	KKLNVETNAPRNMD <mark>ALALRI</mark>
VDI_Vdis_1675	LQLKIPTVFMNNGETIRLV
CMA_Cmaq_0455	LKYKIDTVMLNHLESIRLV
PCL_Pcal_0030	LKYKITTVVPKVGERIRAL
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NMR_Nmar_1727	
CSY_CENSYa_1545	FRIPA.HYPQIQESIKL
nga_Ngar_c23500	FKIQT.QHPLVQEAIKLL
CSU_CSUB_C1103	TPASI.FTPHNLETIVPV
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MOK_Metok_0979	FKKET.RAPMNLDAIRMK
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LOKI_Lokiarch_44440	LRKST.KSPKNLEVVLLK
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TVO_TVG0658611	
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MMA MM 0695	LKIET.RALTNLETVRLL
MBU Mbur 0375	YRLET.RALTNLETIRLV
HAL VNG 0401G	
NPH NP 0210A ncsA	
HWA HQ 1716A	YNLRT.FAPKNLETFRFL
MHU Mhun 0845	LHIQT.TSPMNLETYRLI
AFU AF 0482	YRIËT.RAPMNLETIRFV
FPL Ferp 0914	FRIET.RAPMNLETVRLL

Figure S1. Sequence alignment, secondary structure, and functional motifs of the aCPSF1 orthologs. Sequences were aligned using ClustalW program (1) and the diagram was prepared using ESPript program (2). Identical residues are highlighted as white type on a red background and similar residues are shown as red type. Species: MTH, *Methanothermobacter thermautotrophicus*; TAG, *Thermosphaera aggregans*; DMU, *Desulfurococcus mucosus*; SMR, *Staphylothermus marinus*; HBU, *Hyperthermus butylicus*; FFO, *Fervidicoccus fontis*; IAG, *Ignisphaera aggregans*; SAI, *Sulfolobus acidocaldarius* DSM 639; MSE, *Metallosphaera sedula*; IHO, *Ignicoccus hospitalis*; ASC, *Acidilobus saccharovorans*; APE, *Aeropyrum pernix*; TPE, *Thermofilum pendens*; NEQ, *Nanoarchaeum equitans*; VDI, *Vulcanisaeta distributa*; CMA, *Caldivirga maquilingensis*; PCL, *Pyrobaculum calidifontis*; Kcr, Ca. *Korarchaeum cryptofilum*; NMR, *Nitrosopumilus maritimus*; CSY, *Cenarchaeum symbiosum*; nga, Ca. *Nitrosophaera gargensis*; CSU, Ca. *Caldiarchaeum*

subterraneum; PFU, Pyrococcus furiosus DSM 3638 ; PPAC, Palaeococcus pacificus; MMP, Methanococcus maripaludis S2; MOK, Methanothermococcus okinawensis; MIG, Methanotorris igneus; MJA, Methanocaldococcus jannaschii; MRU, Methanobrevibacter ruminantium; HAL, Halobacterium salinarum NRC-1; NPH, Natronomonas pharaonis; HWA, Haloquadratum walsbyi DSM 16790; MHU, Methanospirillum hungatei; AFU, Archaeoglobus fulgidus DSM 4304; FPL, Ferroglobus placidus. Secondary structural elements and the domains of the aCPSF1 ortholog (MTH1203) from *M. thermautotrophicus* are shown at the sequence top. The seven conserved motifs, Motifs I-IV and Motifs A–C, which are featured in the metalloβ-lactamase (MβL) superfamily proteins are labeled beneath the consensus residues.

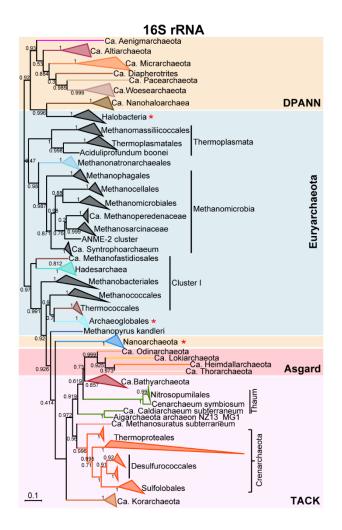


Figure S2. The 16S rRNA phylogeny of archaea in comparison of the aCPSF1 phylogeny shown in Figure 3A. 16S rRNA genes (>1200 bp) were retrieved from the same 143 representative archaeal genomes used in Figure 3A. Consensus 1200 bp-nucleotides of the 16S rRNA genes were used to construct a maximum likelihood phylogenetic trees using IQ-TREE (v.1.6.12) with "LG+I+G4" mode and 1000 times ultrafast. The phylogenetic tree was visualized with iTOL v5 (https://itol.embl.de/). Branch support values are indicated by percentages. Scale bar indicates the number of substitutions per site.

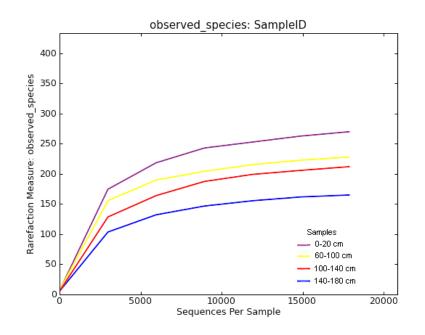


Figure S3. Rarefaction curves of the archaeal OTUs against 16S rRNA sequence reads in the four cold seep samples from the South China Sea. Duplicate 16S rRNA amplicon sequencings were performed for each sample and OTUs were clustered based on the threshold of 97% sequence similarity of 16S rRNA sequence.

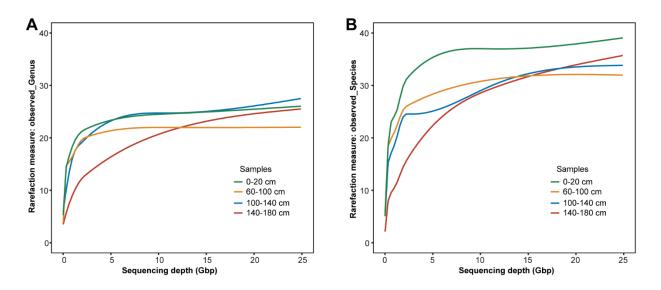


Figure S4. Rarefaction curves of archaeal richness at genus (A) and species (B) levels based on abundance of aCPSF1 genes in different sequencing depths. Rarefaction tool kit (RTK) (3) was used to rarefy a series of sequencing depths, *e.g.*, 5, 10 and 15Gb, and estimate the archaeal alpha-richness. aCPSF1 mapped reads were retrieved from the metagenomic sequences of each sample and the archaeal richness were merged based on the taxonomy of aCPSF1 genes listed in Supplementary Dataset S1.

SI References

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