

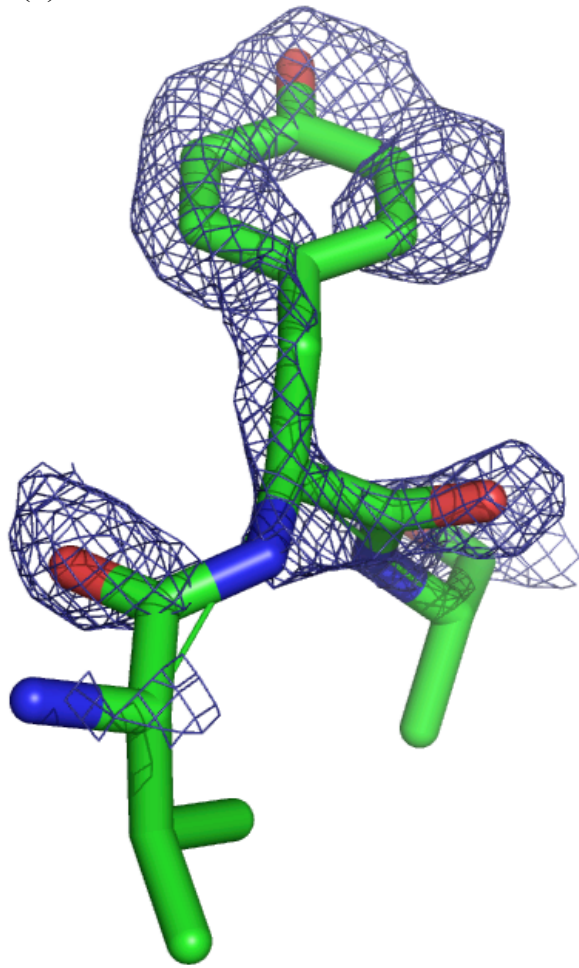
PatA-DUF	APSELANS . QFAYV LGT LGYDFGTEARRDTFKQLMPPFDFA G . NMVPA	462
TruA-DUF	APSELANS . QFAYV LGT LGYDFGTEARRDTFKQLMPPFDFA G . NMVPA	431
ArtA-DUF	APSELASS . QL VYALGT LGYDFGSEARRDTFKQLMPPFEI SEGVSVPA	404
LynA-DUF	APSELADMGQLVYALGT LGYDFGTEARRDSFKQLMPPFDLGGGVMVPA	424
MicA-DUF	APSQIADLGQI VYV LGT LGYDFGTEARRDSFKQLMPPFDLGGGIMVPA	417
TenA-DUF	APSELPLD LGPLVYS LGT LGYDFGTEARRDSFKQLMPPFDI GGGVMVPA	423
AcyA-DUF	APSDLAQV . NLVYALGT LGYDFGSEARRDSFKQLMPPGVQIDG . TAI PA	418
PagA-DUF	APSEL E GK . NLVYALGV LGYDFGSEARRDSFKQLMPPGVSI EG . TMI PA	415
PatA-DUF	NPYDARQMVDY LGNNISEARS LIWTVNIELTPVYAI DPTGPFASSTYH	510
TruA-DUF	NPYDARQMVDY LGNNISEARS LIWTVNIELTPVYAI DPTGPFASSTYH	479
ArtA-DUF	NPYDARQMVDY L ASDI SEARS LIWTVNIELTPVYAI EPKGGPFAREAYL	452
LynA-DUF	NPYDARQMVDY LG ENISESRS LIWTVNIELTPVYAI DPTGPFAAEA YR	472
MicA-DUF	NPYDARQMVDY LG ENISESRS LIWTVNIELTPVYAI APTGPFASDVYR	465
TenA-DUF	NPYDARQMVDY LD ANISEARS LIWTVNIELTPVYAI DPTGPFAAESYR	471
AcyA-DUF	NPYDARQMVDY LGDNLS EAKSLIWTVNLELTPVYAI EP TGGFAARDVYA	466
PagA-DUF	NPYDARQMVDY LG ENLP EAKALIWTVNLELTP IYAI EPVGGF SRDVYE	463
PatA-DUF	ALQELLSGQIQAE DNEEYVERVS IPGVLTNR SVKLFSGQVVPVVEPQS	558
TruA-DUF	ALQELLSGQIQAE DNEEYVERVS IPGVLTNR SVKLFSGQVVPVVEPQS	527
ArtA-DUF	ALQELLSGQIQAE DDDYIERVS IPGVLTGR TVKLFSGQVVP IIEPQS	500
LynA-DUF	ALQELLSGQIQAE DTEYVERVS IPGILTG RKVKLFSGQV IPVIEPQS	520
MicA-DUF	ALQELLSGQIQAE SDAEYMERVS IPGVLTG KVKLFSGQV IPVIEPLG	513
TenA-DUF	ALHELSSGQIQAE SDAEYMERVS IPGILTK RTVKLYSGQV IPVLEPQS	519
AcyA-DUF	ILQQLLSGQIQAE DSEN YVERVS IPGILS GR SVKLFSGQVVPVIEV PN	514
PagA-DUF	V LQGLLSGQIQAE ENSPE FVQRVS IPGVLTGR SVKLFSGQVVPVIE I NN	511
PatA-DUF	TRGLYGWKVNG LVNAALEAVR AEGGDAGEAR IRQTL DGF LNRIYD LR	606
TruA-DUF	TRGLYGWKVNG LVNAALEAVR AEGGDAGEAR IRQTL DGF LNRIYD LR	575
ArtA-DUF	TRGLYGWKVNS LVNAALF ETVQA AEGEADRDAM SR T LGS FLNRVYD LR	548
LynA-DUF	TRGLYGWKVNS LVSAAMDAVQA EDGAADEET IRKTL DGF LNRIYD LR	568
MicA-DUF	TRGIYGWKVNS LVNAAMEAVQA EDGT ADEEDR IRKTL DGF LNRIYD LR	561
TenA-DUF	TRGIYGWKVNS LVSAAMAAVQA EA GA ADEET IRKTL DGF LNRIYD LR	567
AcyA-DUF	TRGLYGWKVNT LVQAAI QT VQA QATEAQEES IRRT LGS FL SR IYD LR	562
PagA-DUF	TRGLYGWKVNS LVSAAI ES VQSEAGDA QEDA IRRT LSS FLNR IYD LR	559
PatA-DUF	NLGTTSQDRALNF AVTNAFQAAQTFSQSVA A GMELDSVTVEKSPFCRL	654
TruA-DUF	NLGTTSQDRALNF AVTNAFQAAQTFSQSVA A GMELDSVTVEKSPFCRL	623
ArtA-DUF	NLGTTSQDRALNF SVTNAFQAAQTFSQAVAVQ GMELDSITVEKSPFCRM	596
LynA-DUF	NLGTTSQDRALNFS VTNAFQAAQTFSQAVAV GMELDSVTVEKSPFCRM	616
MicA-DUF	NLGTTSQDRALNF AVTNAFQAAQTFSQAVAV GMELDSVTVEKSPFCRI	609
TenA-DUF	NLGM T SQDRALNF AVTNAFQAAQTFS EAVAV GMELDSVTVEKSPFCRM	615
AcyA-DUF	NLGTTSQDRALNF ASTNAFQAAQT FAEAVAT GMELDSITVEKSPFCRL	610
PagA-DUF	NLGTTSQDRALNF AS TNAFQAAQT F AQAVGA GY ELDSITVEKSPFCRL	607
PatA-DUF	DSDCWDIKLKFFDPEN N RRAKKIYRFT IDVSD LVPVTMGEVRSWSS .	700
TruA-DUF	DSDCWDIKLKFFDPEN N RRAKKIYRFT IDVSD LVPVTMGEVRSWSS SY	671
ArtA-DUF	DSDCWDV K L K F F D P E N S R R A K K I F R F T I D V S D L I P V T L G E V R S W S S P Y	644
LynA-DUF	DSDCWDV K L K F F D P E N S R R A K K I Y R F T I D V S D L I P V T L G E V R S W S S P Y	664
MicA-DUF	DSDCWDV K L K F F D P E N S R R A K K I F R F T I D V S D L I P V T L G E V R S W S S P Y	657
TenA-DUF	DSDCWDV K L K F F D P E N N R R A K K I F R F T I D V S D L I P V T L G E V R S W S S P Y	663
AcyA-DUF	DSDCWDV K L K F F D P E N S R R A K K L F R F T I D V S D I I P V T L G E V R S W S T P Y	658
PagA-DUF	DSDCWDV K L K F F D P E N S R R A K K I Y R F T I D V S D T I P V T L G E V R S W S S A Y	655

**Fig. S1A** Sequence alignment between PatA-DUF and homologues from related cyanobactin biosynthetic pathways. Residues involved in  $Zn^{2+}$  coordination (as identified in the PatG-DUF<sub>sp.</sub> structure) are highlighted with red triangles.

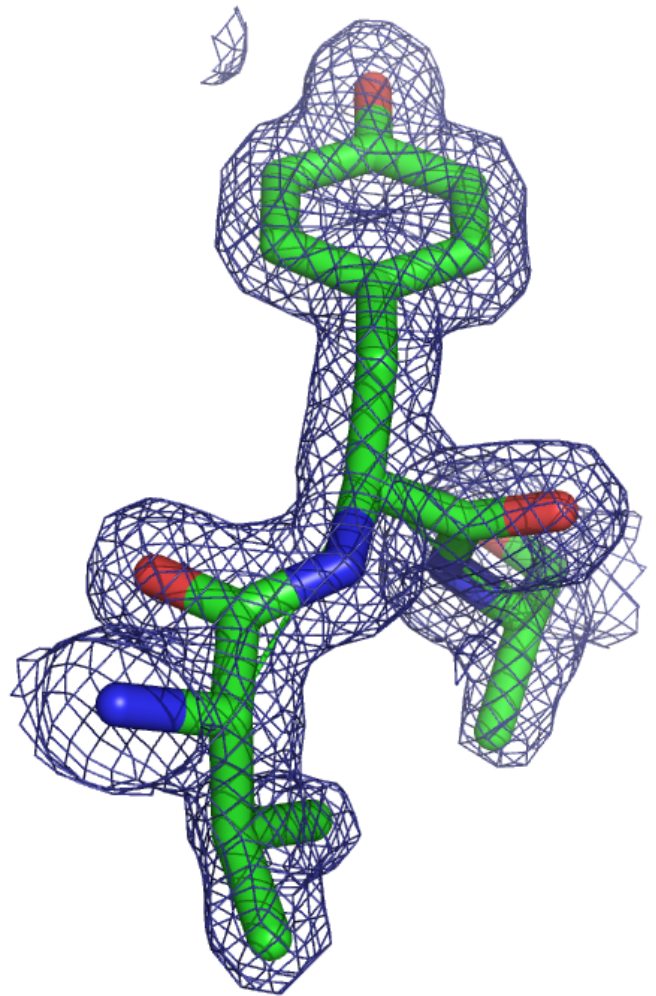
PatG-DUF <sub>sp.</sub>	VEASTAFSGNVYALGTIGYDFGDEARRDRTFKERMA.....DPP	950
TruG-DUF	VEASTAFSGNVYALGTIGYDFGDEARRLNTFKERTMAPVNLHGVMVPPDPP	761
ArtG-DUF	VQPSKAGSGHVYALGTIGYDFGDEARRDRTFKERTMAPVNLHGVMVPPDPP	1051
LynG-DUF	VEASTAFSGHVYALGTIGYDFGDETRVDTFKERMAPVEMDSSLVLPDPP	1053
MicG-DUF	VEASTAFSGHVYALGTLSYDFGDETCVDTFKERMAPVEMDSSLVLPDPP	1108
TenG-DUF	VEASTAYDGNVYALGTIGYDFGDETRRRDSFKELMPPTQVNGIMVSPDPP	1059
AcyG-DUF	.....SAAASKLVYALGTIGYDFGSEARRDSFKQLMPAVNEIDGITIPANP	471
PagG-DUF	.....ASAAASKLVYVYVLTIGYDFGSEARRDSFKQLMPAVNEIDGITIPANP	452
PatG-DUF <sub>sp.</sub>	YDARQMVERLDRNPDEARS LIWT LNLEGDVIYALDLPKGP FATNVYEIF	998
TruG-DUF	YDARQMVEHLDRNPDEARS LIWT LNLEGDVIYALDLPKGP FATNVYEIF	809
ArtG-DUF	YDARQMVEHLDRNH PDAAYS LIWT LNLDQNTIYALDLPKGP FADDIYEMF	1099
LynG-DUF	YDPRQMVEHLDRNPDES RSLIWT LSLDGGDTIYVLEPTGAFSDQIYEMF	1101
MicG-DUF	YDPRQMVEHLDRNPDES RSLIWT LSLDGGDTIYVLEPTGAFSDQIYEMF	1156
TenG-DUF	YDVRQMVEHYLDRNPDES RSLIWT LSLDGGDTIYALDPTGAFSGQIYEIF	1107
AcyG-DUF	YDSQQMVNYLSENPAEAKPLIWT LNQE LTP IYALEP VSGFAAD IYETL	519
PagG-DUF	YDASQIVNYLAENSS ES KSLIWT INQE FNP VYALEV KGGFAAD VYEML	500
PatG-DUF <sub>sp.</sub>	LQMLAGQLEPETSADFIERLSVPARRRTTRTVELFSGGEVVPVNVVRDPRR	1046
TruG-DUF	LQMLAGQLEPETSADFIERLSVPARRRTTRTVELFSGGEVMPVNVVRDPRR	857
ArtG-DUF	LLMLNAGQLEPETSAEFMERVSIPGRQTNRTMVELFSGGEVVPVNVVRDPRR	1147
LynG-DUF	VLMLAGQLEPESSDEFVERISIPARRQTNRTVVELFSGGQVVPVVKVHDIRR	1149
MicG-DUF	VLMLVGGQLEQKSSDEFVERISIPARRQTNRTVVELFSGGQVVPVVKVHDIRR	1204
TenG-DUF	LLMLAGQLEPETSDEFVERISVPARRRTNRTVVELFSGGEVVPVNVVHDLRR	1155
AcyG-DUF	ILMLQGGIQPENSDDFVERVSIPARLTDRTVELFSGGQVVPVITLNTIR	567
PagG-DUF	NLMLAGQIEPESSDDYVERVSIPGQITDKTITL FSGGEVVPVITINNIR	548
PatG-DUF <sub>sp.</sub>	GMYGWNVNA LVDAALAT.V...EYEEADEEDSLRQGLTAF LN RVY HDLHN	1091
TruG-DUF	GMYGWNVNA LVDAALAT.V...EYEEADEEDSLRQGLTAF LN RVY HDLHN	902
ArtG-DUF	GMYGWNINL LVDAALGT.LN.NLEEGSEGLLREGLTAF LN RVY YELHN	1193
LynG-DUF	GMYGWKVNT LVNAAMAA.IARQVDEAQAPLVQQALTAFLN RVY ND LRN	1196
MicG-DUF	GMYGWKVNT LVNAAMVA.ISRQVDEAQAPLIQQALTSFLN RVY ND LRN	1251
TenG-DUF	GLYGWKVNA LVDAAMAA.ISRQVDEAQAPLVRQALITSFLN RVY ND LRN	1202
AcyG-DUF	GMYGWKVNS LVDAALQTV.ITGETAPAQEIAMRKALSSFLN RVY YDLQN	615
PagG-DUF	GMYGWKVNG LVDAALQTLSEELADANEIQMRRLSSFLKRVYFDLQN	595
PatG-DUF <sub>sp.</sub>	LGQTSRDRALNFTVTNTFQAASTFAQAIASGRQLDTEIENVNKSPYCRNLN	1139
TruG-DUF	LGQTSRDRALNFTVTNTFQAASTFAQAIASGRQLDTEIENVNKSPYCRNLN	950
ArtG-DUF	VGKTSRDRALNFVAVTNTFQAASATFAEAIADRRRLDTEI EVEKSPYCRNLN	1241
LynG-DUF	VGQTSRDRALNFVAATNIFQAASVFAKAI AERRQLDTEI KVEKSPFCRNLN	1244
MicG-DUF	VGQTSRDRALNFVAATNIFQAASVFAKAI AERRQLDTEI EVEKSPFCRNLN	1299
TenG-DUF	VGQTSRDRALNFVAATNIFQAASVFAKAI AERRQLDTEI KVEKSPFCRNLN	1250
AcyG-DUF	LGQLAKDRALNFSVTNAFQAASSFSQAISTGMQLDSIEVEKSPFCRNLN	663
PagG-DUF	LGKTSKDRALNFVAATNAFQAACSFAQAVS TGMELDTEIEI EKSPFCRVN	643
PatG-DUF <sub>sp.</sub>	SDCWDVLLTFYDPEHGRRSRRVFRFTLDVVYVLPVTVGSIKSWSLPG	1186
TruG-DUF	SDCWDVLLTFYDPEHGRRSRRVFRFTLDVVYVLPVTVGSIKSWSLPG	997
ArtG-DUF	SDCWDVLLTFFDPEDEGKRSRQVFRFTLDVADSMPTVTVGSIKRWAIPG	1288
LynG-DUF	SDCWDVKLEFFDPESSRRGRKVFRLFTLDVV LQMPVTLGSEVKSWSLP.	1290
MicG-DUF	SDCWDIKLEFFSDPERSSRRGRKVFRLFTLDVV LQMPVTLGKIKSWSMPL.	1345
TenG-DUF	SDCWDVKLEFYDPENSRGRKVFRLFTLDVRL LMPVTLGSEVKSWSLP.	1296
AcyG-DUF	SDCWDVKLKKFFDPERNGRRAKKVFLFTLDVSDRIPVTLGQVRSWSV.	708
PagG-DUF	SDCWDVKLKKFFDPERGLRAKKVYLFSDVSYMIPVTLGQVRSWSVP.	689

**Fig. S1B** Sequence alignment between PatAG-DUF<sub>sp.</sub> and homologues from related cyanobactin biosynthetic pathways. Residues involved in Zn<sup>2+</sup> coordination (as identified in the PatG-DUF<sub>sp.</sub> structure) are highlighted with red triangles.

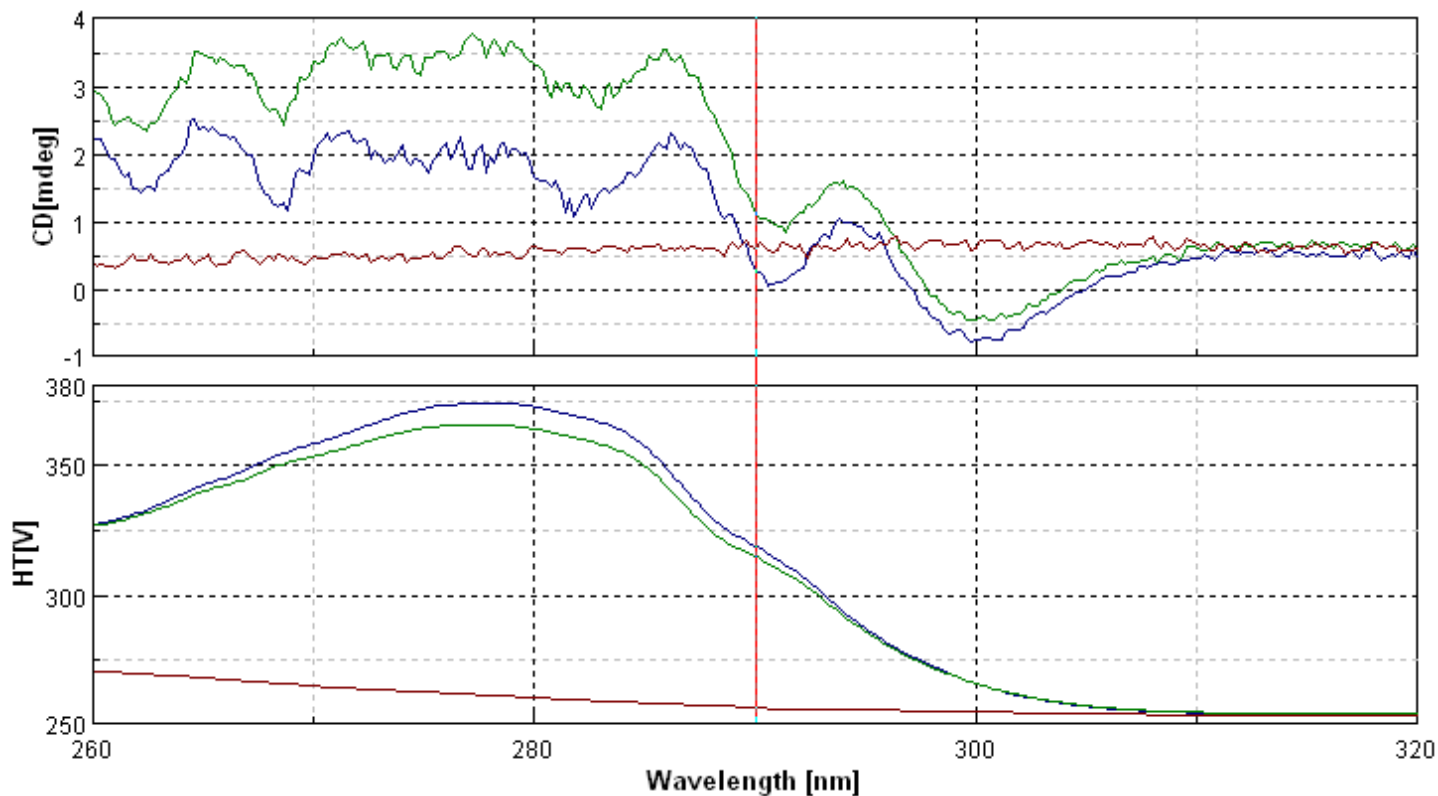
(a)



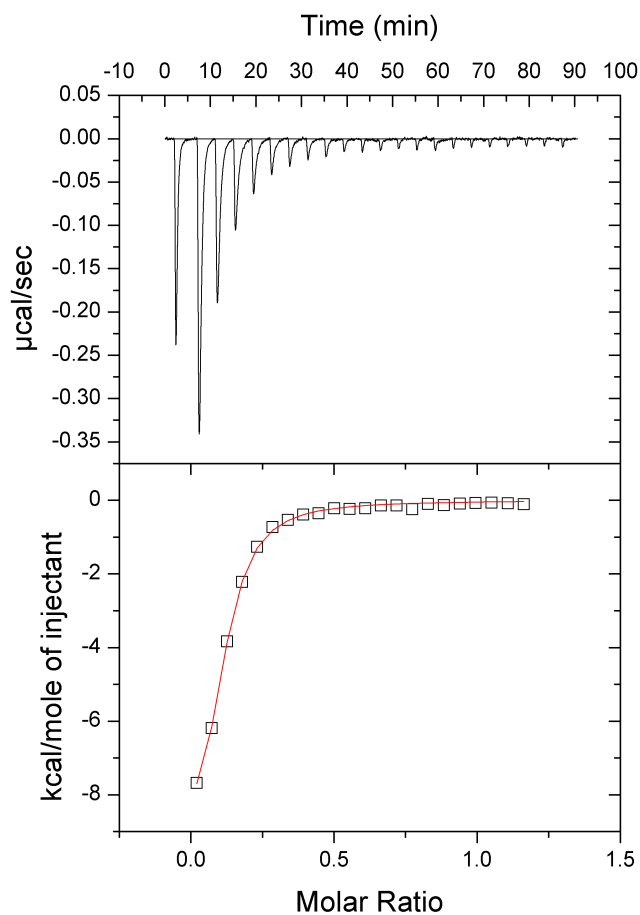
(b)



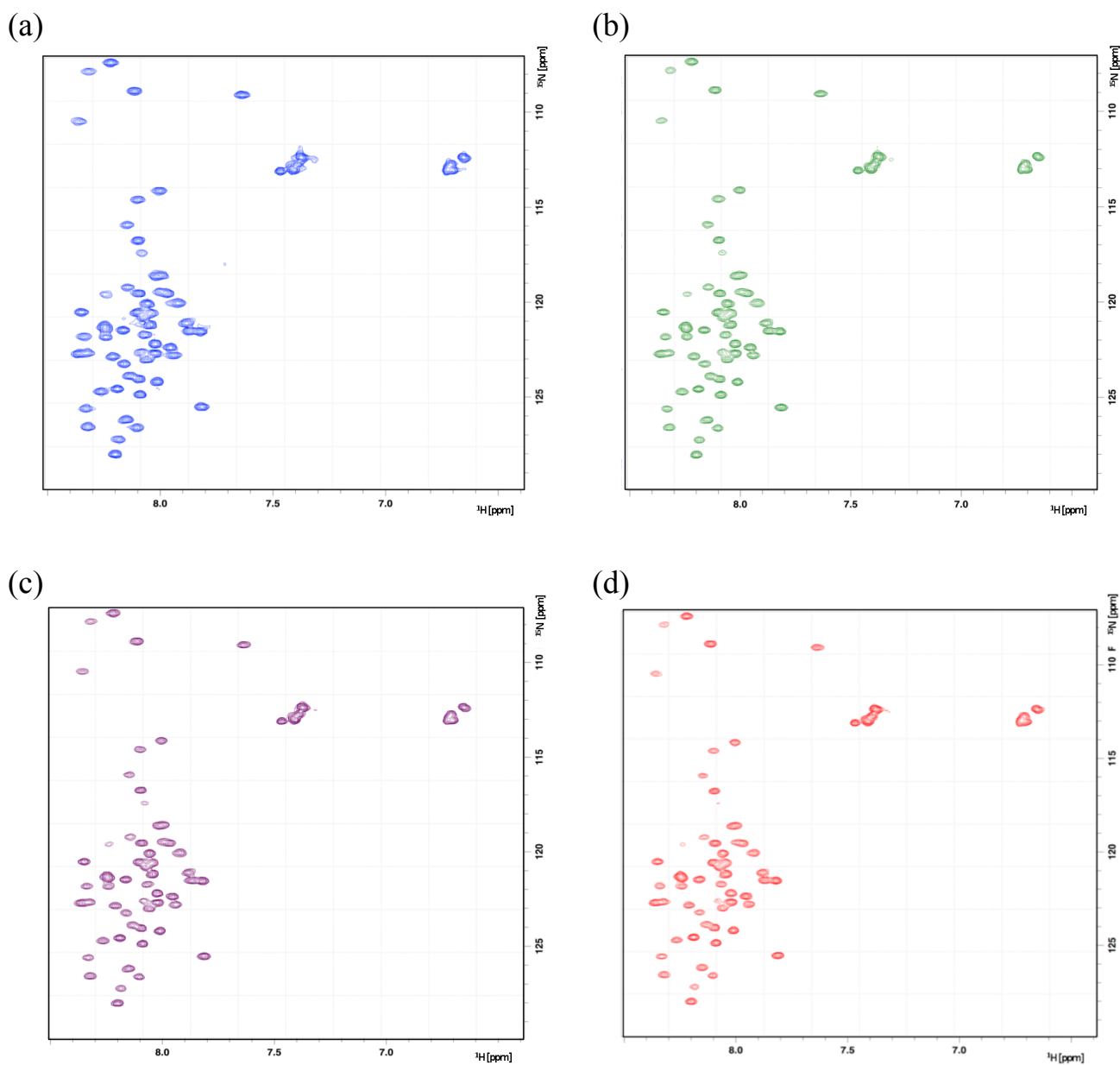
**Fig. S2** Final refined of PatG-DUF<sub>sp</sub> Y925 model with (a) Electron density map contoured at 1.2  $\sigma$  from PHENIX with experimental phases calculated from anomalous scattering atoms. (b) Electron density map calculated with phases after density PHENIX modification of experimental phases.



**Fig. S3** Near UV CD-spectra of PatG-DUF<sub>sp</sub> (green) and PatG-DUF<sub>di</sub> (blue). A blank containing only buffer is shown in red. The CD-spectra overlay well suggestion the sequence variations (three point mutations) do not alter the tertiary structure of the domain.

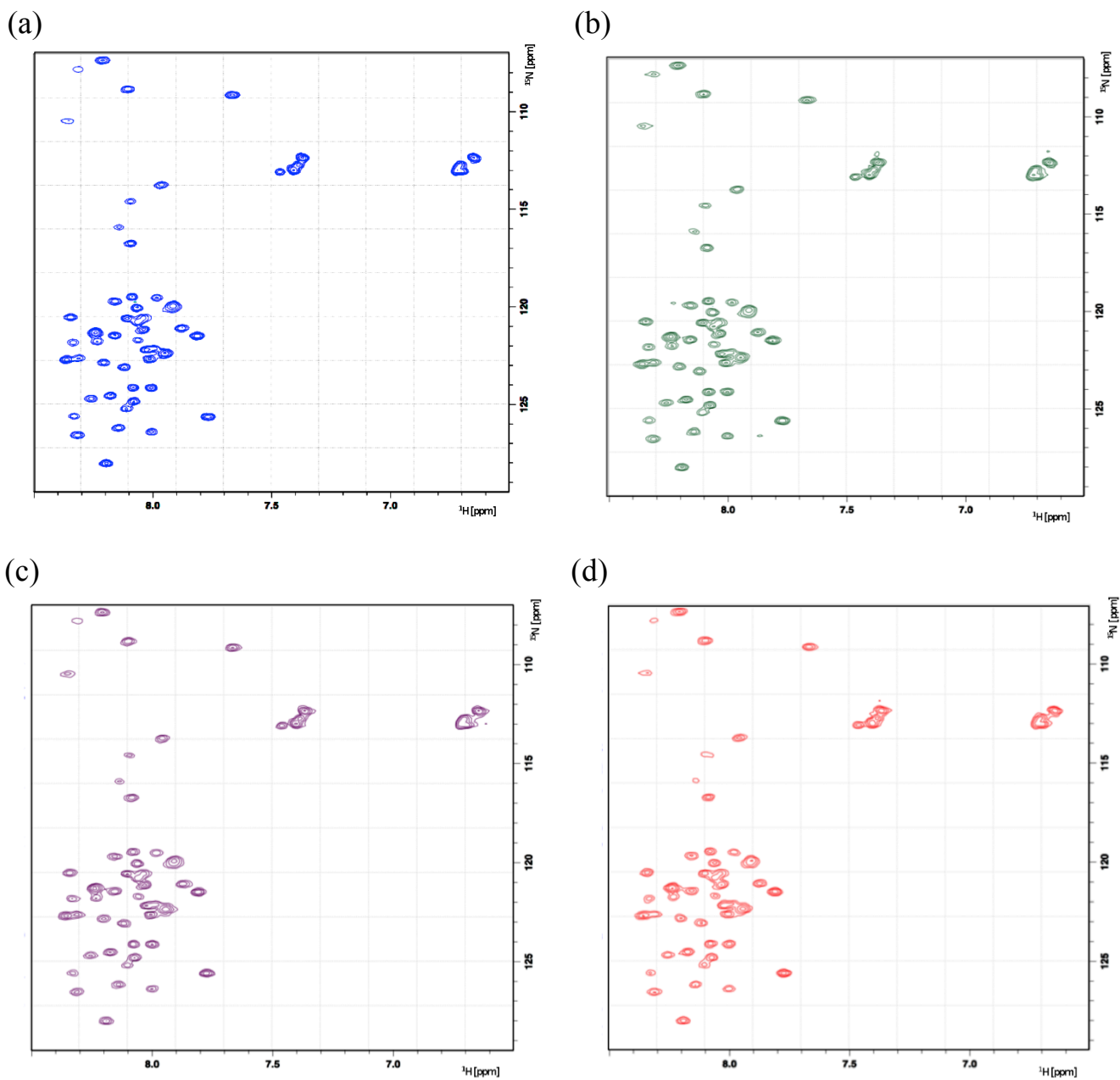


**Fig. S4** ITC data of PatE' titrated into PatG-DUF<sub>di</sub> solution. The top panel shows raw data representing the heat evolved in response to injections, the bottom panel shows the integrated heats of injections ( $\square$ ) and the best fit (-) to the one-site model (origin).



**Fig. S5A**  $^1\text{H}$ - $^{15}\text{N}$ -HSQC of  $\text{PatE}'$  (blue) with 0.5 (green), 1.0 (purple) and 2.0 (red) equivalence of  $\text{PatG-DUF}_{di}$ .





**Fig. S5B**  $^1\text{H}$ - $^{15}\text{N}$ -HSQC of heterocyclized-PatE' (blue) with 0.5 (green), 1.0 (purple) and 2.0 (red) equivalence of PatG-DUF $_{di}$ .