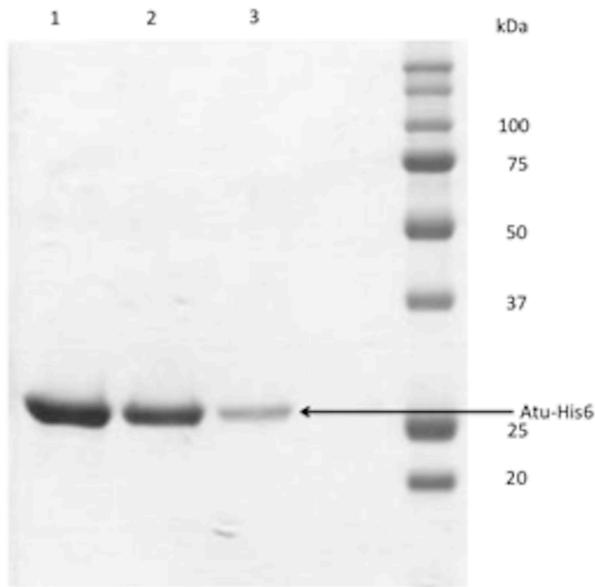
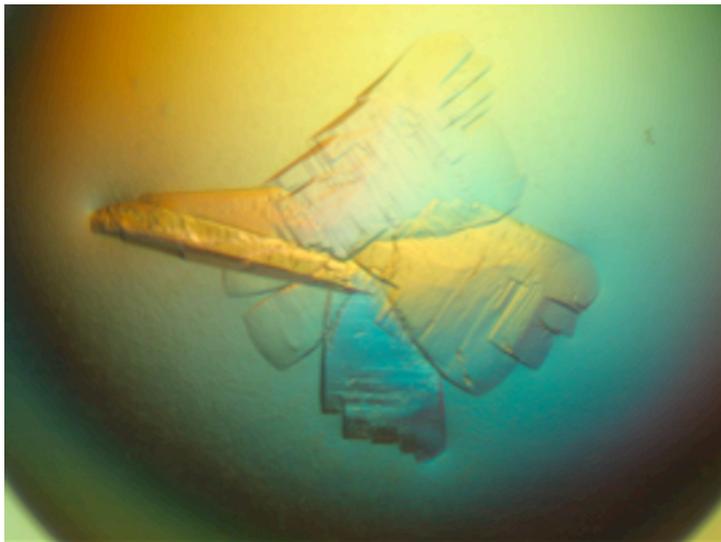


1 **Supplementary data set S1**



2

3 **A**



4

5 **B**

6 Supplementary Figure S1. (A) Purification of AtuE-His6. Lanes 1-3 show different
7 amounts of purified AtuE-His6 on a 12% SDS-PAGE and subsequent staining with
8 Coomassie brilliant blue. Note the absence of any visible impurities even at higher
9 protein concentrations (35) (B) Cluster of AtuE crystals.

10

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1      10      20      30      40      50      60
PA2890/1-264 . . . . .MSLPHCETLLLEFIEGVITRTINRQSRNAMSLAMVGE[RAV]A AVRDRDSV[RA]LVIR[Q]ADGH[F]
PA4330/1-257 . . . . .MSELIRVERETGLITLIRIDRQDKK[NA]LTRAMYSRMAE[AL]LEAQADTA[V]VVLIT[Q]GDAC[F]
PA0745/1-272 MNTAVEPYKASSFDLTHK[LV]EKHGH[TAL]TINHP[PA]NTWDRDSLIG[RL]LEHLNRDD[IV]YLVV[TV]QGGK[F]
PA1021/1-253 . . . . .MSGLLQETRGTVRL[LR]FDNPAR[NA]LSPALRME[LR]LEAAEC[DP]IR[SV]LLT[Q]GEEV[F]
PA1240/1-265 . . . . .MSEANSGPGRVTRFQRGH[LFL]IGTRAGKR[NA]FDSAMLAD[AL]AMGEYERSE[ER]CAVIT[AH]GCH[F]
PA1629/1-261 . . . . .MSADPPSPVVLEFFAAD[IAL]LRINRQAR[NA]LNDEVRQR[AS]HFTLGDADPA[RV]VVLV[TV]GDS[RC]F
PA1748/1-229 . . . . .MSELISYQFEDG[IAL]TLTINN[.GK]VNAISPAVIDAF[NO]LDQALQDKAV[.V]VIT[Q]GPGIL[F]
PA1821/1-270 . . . . .MTEYNARVVELADK[IA]HVQINR[PK]INAMNQDFWRE[IE]IFRWVDDTDE[V]VVLV[TV]GAG[KH]F
PA2767/1-322 . . . . .MTLAPRHLRIEQGRV[VL]QLDNP[PA]NFLTAVMQE[AD]LLEDLEQRQD[IG]AVL[SV]GAA[DV]F
PA2841/1-263 . . . . .MNDTLPGRITSRERRG[LL]GLDRVAKR[NA]FDLPMLDD[VA]AIGEYEA[DD]LRCALL[FA]HGE[.H]F
PA3426/1-256 . . . . .MSVIVERNR[GV]TTLVLA[PK]ERR[NA]VDRFTAQALAD[AL]REFEADD[TR]VAVL[TV]GSG[.GN]F
PA3591/1-265 . . . . .MSSPPGAVRPELV[LER]FEGV[AL]LRNP[AV]LNALNR[LR]EAL[AE]HVRALDECAD[RV]VVLV[TV]GTA[.F]
PA4980/1-263 . . . . .MTDLSTQTRVEAG[IA]WLV[IN]R[PK]R[NA]LDIPTLEA[HV]R[.D]ACERDPA[RV]VVLV[TV]GSGRS[.F]

70      80      90      100
PA2890/1-264 CA[G]G[D]K[D]MAGARAA . . . . .GAEAYRTLNR . . . . .FGSLLEEAQ[AA]P[QL]LVA
PA4330/1-257 TS[G]N[D]L[L]D[F]LEQPPS . . . . .LRDS . . . . .PVGRF . . . . .MSALLE . . . . .FPK[FA]VIA
PA0745/1-272 SA[G]AD[L]N[F]ADGDKA . . . . .RA . . . . .REMAR . . . . .FGEAFALRDFR[GV]SIA
PA1021/1-253 CA[G]G[D]G[D]M[V]TELA . . . . .AGRARMQDN . . . . .ARLV[RV]QMVRM[K]FLIA
PA1240/1-265 TA[G]L[D]LME[L]APKLA . . . . .SGFRYPDGGVD . . . . .PWGVVQ[PR]S . . . . .KFL[V]V
PA1629/1-261 AA[G]A[D]R[D]L[ST]STA . . . . .GLY . . . . .GRH . . . . .GERYWEAT[AR]CPK[FA]VIA
PA1748/1-229 SG[V]Y[D]K[V]M[T] . . . . .GPNAVNLVAA . . . . .GSTLARRL[LS]H[FP]VIV
PA1821/1-270 AV[FG]K[V]G[AG]L[V]A[CG]T[V]CGAG . . . . .RFARAGFKVGLLAD[GL]H[L]P[RI]T[OW]G[AR]C[L]MFGOV[VE]EA
PA2767/1-322 LT[H]F[D]V[E]L[ER]AVAP[IT]SPMPAWL[R]LLESE[SL]LRHL[PK]ARKL[R]RTLAGVAD[M]NLFHEVTAHMRMD[KV]FIA
PA2841/1-263 TA[G]L[D]LANVGETFRQGWKLP[EG]AVDPWGT[FG]G . . . . .RRP[S]KEL[V]V
PA3426/1-256 CA[G]A[D]LAAVAEDGERRNLEAEG . . . . .DGPMPGSRMQLG[K]FLIA
PA3591/1-265 AA[G]A[D]LNE[L]AEASALEIQ[RG]V . . . . .ERHWQALAA[CR]K[FL]IA
PA4980/1-263 CA[G]A[D]LAEWAAAEARGELESYCWTEAA . . . . .HALMGR[L]HALD[K]FTVA

110     120     130     140     150     160     170
PA2890/1-264 LV[EG]AVLGGG[F]GLACV[S]DVA[.AA]AD . . . . .AQFGLPETS[LGI]LPAQ[.I]APFV[V]RR[IG]LTQ[ARR]LALTAARFDG[RE]A
PA4330/1-257 AV[NG]PAVGI[ST]LLH[CD]V[VF]VGRN . . . . .ARLKMFPV[N]LGLTPEF[.SS]LLI[PR]MLGHAKAAE[LL]MLGQDFSGE[QA]A
PA0745/1-272 AV[NG]YAMGG[LE]CALAC[.R]L[ER]EQ . . . . .QMALPEAR[VGL]LPCA[.GT]QLPWL[VE]GEGAKRM[IL]CNERVDA[RE]A
PA1021/1-253 AV[OG]T[CV]TAGI[EL]MLNAD[.I]AAVARG . . . . .T[RF]AHLEVL[RG]LPP[LG]STV[RF]PRA[.C]WTD[AM]NY[IL]TGDEFDA[DE]A
PA1240/1-265 AV[OG]YALGGG[C]ELAMH[CD]I[V]AGES . . . . .A[Q]FAQPE[IK]VGVMPGA[.GT]Q[RL]VRAV[CK]FQALRM[LF]TGC[V]KAF[PA]A
PA1629/1-261 A[C]GHAVAKS[AF]LLSAD[V]R[IG]VDC . . . . .PFQIGLNEVA[IG]MTHH[V]GIELAR[DR]LRKSAF[TR]SVNEMEMF[S]PAA
PA1748/1-229 AV[OC]Y[C]IGCAID[LV]SACD[.R]M[ST]AD . . . . .A[Q]FSKEID[IG]MADV[.C]TLQ[.I]P[RI]I[GD]GM[R]RE[LA]Y[.T]GRMVD[GEE]A
PA1821/1-270 AV[IG]LALGGG[C]ELALAC[.D]R[IM]MAEDDQ[VER]FLGQPEVL[IGLI]P[GG]GTQ[ML]ARS[LG]VARALE[LC]LEGLLEF[RO]A
PA2767/1-322 AV[OG]CYT[IG]I[EL]MLAAD[.I]NLCA[SN] . . . . .ARFAQLEV[QR]GILP[FG]AT[LR]M[HV]G[AG]WGNAMR[LL]TGDEFDA[DE]A
PA2841/1-263 AV[EG]YAVAGGLE[L]ALLAD[.R]MMAEDA[IC]GVFCR . . . . .RFVGLP[LD]GGSV[R]LPR[IV]GQGR[AL]DL[IL]TGRFVKA[DE]A
PA3426/1-256 AV[EG]HALGGG[C]ELAMH[CD]I[V]AGAS . . . . .ARFAQPE[IR]VGVMPGA[.GT]Q[RL]VRAV[CK]FQALRM[LF]TGC[V]R[AP]A
PA3591/1-265 AV[NG]S[V]AG[AM]D[L]ALCC[.D]E[R]LAAAS . . . . .ARFKAGY[.T]MAYCPDA[.S]ASWH[L]PRL[LG]SEA[KR]LFLDEAW[SA]E[RA]
PA4980/1-263

180     190     200     210     220     230     240     250
PA2890/1-264 LR[GL]LVHF[CE]ADADA[.E]QR[.E]ETL[E]Q[.R]RCAP[.N]NAAAT[.K]AL[.I]LASESGELGAL[.D]DAARQFAB[AV]G[AG]G[.S]R[GT]L
PA4330/1-257 AA[M]GLANAAL[ED]GATV[LE]HARD[.A]RRF[L]HLAF[S]AVVES[XRL]MKAPFEEFLRRV[IA]EEGDFSTR[LR]S[.P]FAI[.H]A[.S]
PA0745/1-272 LR[IG]LVEQ[V]VDSGEARGA[LL]AA[K]VARQSP[V]AI[RTI]K[PL]QGARERAPNT[L]PEERERFVD[LF]DAQ[.D]TR[.E]IGN
PA1021/1-253 LR[IG]LADR[.C]AAGGAL[AM]AL[.E]LAGRVEQQA[PL]LMTK[AL] . . . . .AEGDLL[.I]EREGLQSQ[.L]FLSDHAE[.G]KA
PA1240/1-265 LR[M]RLITE[V]VEPGE[L]ARAL[.E]Y[.A]ER[.A]RAAP[L]AVRALQ[S]AFQGRDEGDDA[AL]SRVNESLAA[LG]SEDDVRE[.G]VL
PA1629/1-261 LAMGLVSEVVADE[ST]LARAL[.E]LAME[.R]ARLPP[L]ALAQ[.I]K[V]VLAGADLP[LD]SAL[AL]ERKAFOL[.L]FD[.S]OQ[.K]E[.G]MH
PA1748/1-229 VDAGFLDT[V]SADQ[.U]ES[.A]RAAA[.Q]LKKLNMT[AHR]NT[.K]K[V]RKALET[LD]QAT[.E]LDKXHLG . . . . .
PA1821/1-270 RS[IG]LVNRYADQAA[LM]DGV[FE]LARQ[.I]AAKSP[.I]AIRGT[.K]EM[.I]RYMRDHRVDD[GL]EYVATWNA[ML]Q[SAD]LDRV[.A]MA
PA2767/1-322 LA[IG]LVNGL[.I]APAET[.L]EAADALAQ[.I]SRRSP[.Q]AVR[.I]KRS[.I]YQAASRDWTEG[.M]ASEKAGFLS[.A]ASQGNTR[.R]AMR
PA2841/1-263 YR[IG]LVQEV[T]AP[.E]DL[.D]H[.A]IALA[.E]RVAQA[PL]GVRAT[.L]GSARQALLEG[EA]VAAALPEAARR[.L]LDS[.E]D[.A]K[.E]L[.R]
PA3426/1-256 LQ[IG]LANR[V]VPSGAR[.E]A[.E]ELAE[.E]A[.A]FPQ[.T]CMLADR[.S]VYAQWELSF[DV]ALANEFQGGI[AV]IE[.S]G[.E]T[.L]L[.G]A[.Q]
PA3591/1-265 LA[IG]LVSEVVAADGQAL[DR]AL[.E]LARQ[.I]AGLPP[.L]ALAQ[.I]K[V]VLAGADLP[LD]QAL[AL]ERKAFOL[.L]FD[.S]OQ[.K]E[.G]MH
PA4980/1-263 LG[AG]LVGE[V]VAD[.E]R[.L]VEA[V]GAF[.A]R[.L]ASGP[.F]AFAQT[.R]L[RD]GAGRS[.L]AEQ[.L]RAEQAA[GL]C[GR]S[.E]LAA[.E]A[.R]

260
PA2890/1-264 AF[V]Q[KR]KPV[.W]AQ . . . . .
PA4330/1-257 AF[M]HR[.R]QPD[.F]SRFA . . . . .
PA0745/1-272 AF[L]E[KR]DPP[.K]WRNC . . . . .
PA1021/1-253 AF[L]AKRPP[.V]FRGN . . . . .
PA1240/1-265 AM[V]Q[KR]RAPAF[.K]GR . . . . .
PA1629/1-261 AF[L]E[KR]PPNY[.Q]GK . . . . .
PA1748/1-229 . . . . .
PA1821/1-270 AH[.M]AK[.K]QKPE[.F]AD . . . . .
PA2767/1-322 EV[.I]ERV[.R]T[.I]TR[.E]ERF[.R]RA[.D]E[.D]D[.L]TEGNAIDMAYR
PA2841/1-263 AL[.Q]ER[.R]P[.G]R[.E]O . . . . .
PA3426/1-256 RF[.R]D[.G]E[.G]R[.H]G[.R]F[.E] . . . . .
PA3591/1-265 AF[L]E[KR]TAE[V]L[.G]K . . . . .
PA4980/1-263 AV[.A]E[KR]SPQ[.E]SGR . . . . .

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13 Supplementary Figure S2. Sequence alignment of *P. aeruginosa* putative hydratases.

14

15 **Supplementary data set: *P. aeruginosa* proteins identified in the GeLC-MS/MS**
16 **approach.** Results from the GeLC-MS/MS experiment are shown on different Excel
17 sheets as indicated at the bottom: all identified proteins, proteins that showed a
18 significantly increased abundance in the presence of octanoate, proteins that showed a
19 significantly increased abundance in the presence of citronellate. Proteins exhibiting a
20 change in abundance ≥ 3 and a p-value ≤ 0.05 were considered as differentially
21 abundant.

22 The tables show the fold-change, p-value and the “number of peptides used for
23 quantification” as well as identifiers (Locus-Tag, NCBI accession number, gene
24 name) for each protein identified. In addition metadata like subcellular localization,
25 putative function, MW and pI as retrieved from the “Pseudomonas Genome
26 Database” are given for each protein. Only proteins with 80% peptide- and 99%
27 protein-probability (see materials and methods) and a minimum number of two
28 peptides per protein are listed.

29

30

31