

Identification of Quorum Sensing Molecules of N-acyl-Homoserine Lactone in *Gluconacetobacter* Strains by Liquid Chromatography-Tandem Mass Spectrometry

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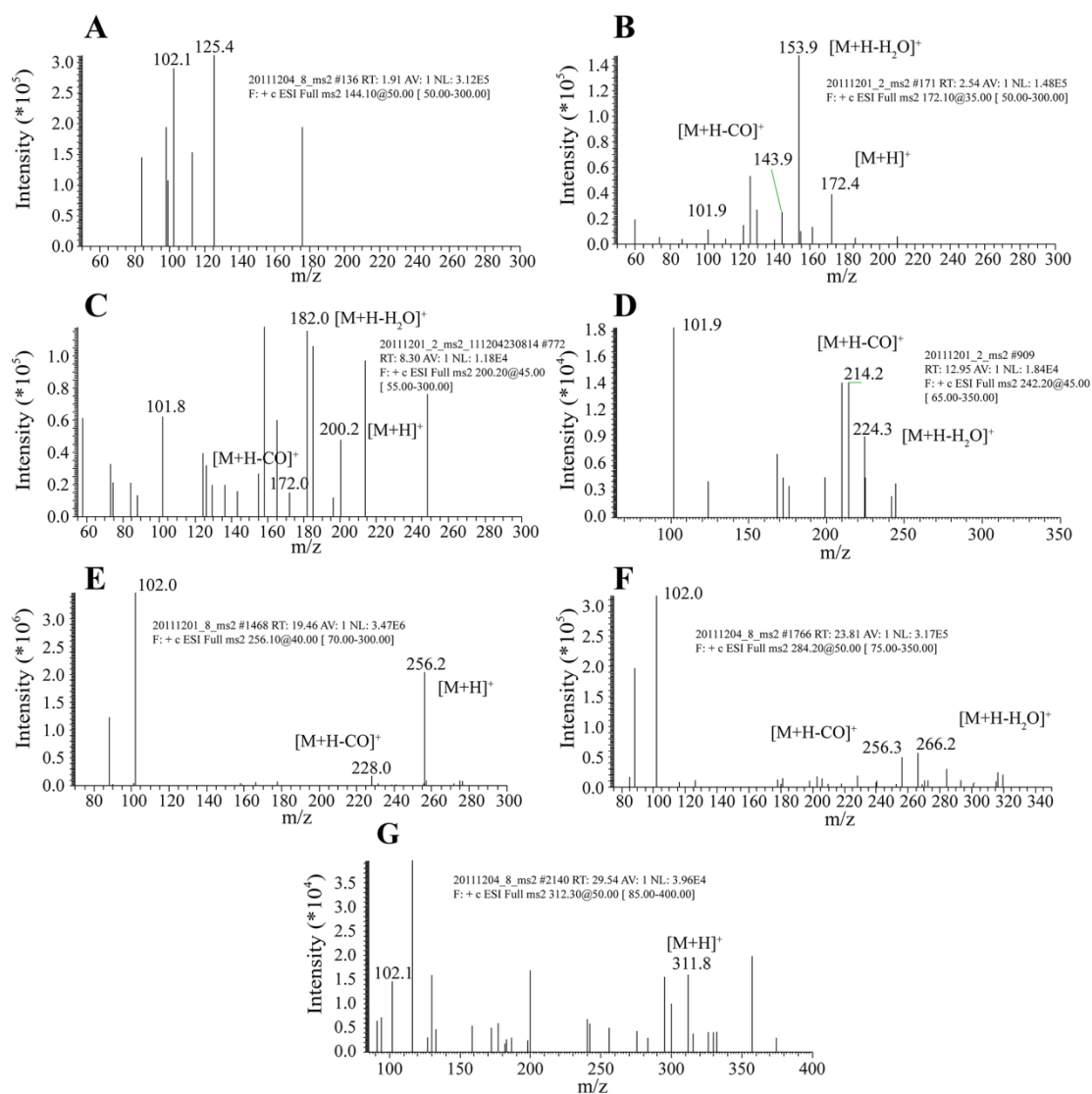


Figure S1: MS-MS fragmentation of AHLs extracted from supernatants of *Gluconacetobacter sp.* strain SX-1. (A) C2-HSL; (B) C4-HSL; (C) C6-HSL; (D) 3-oxo-C8-HSL; (E) C10-HSL; (F) C12-HSL; (G) C14-HSL

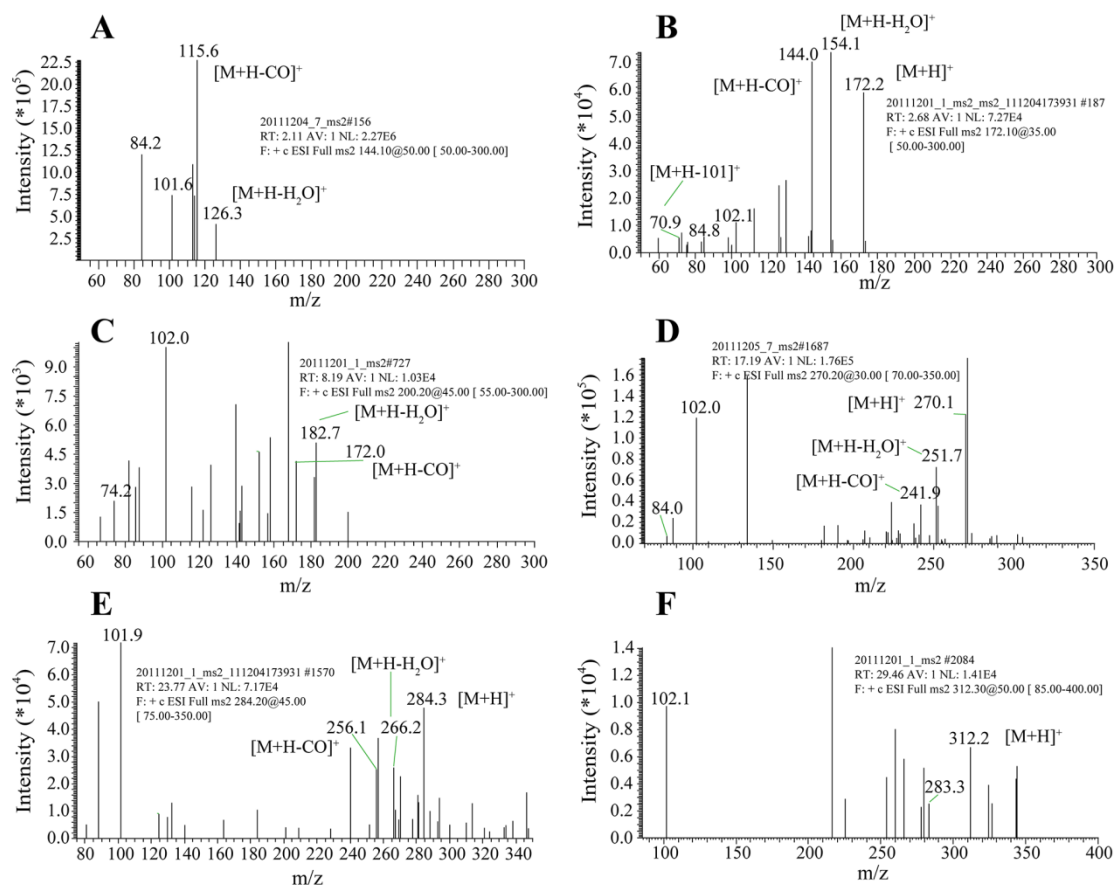


Figure S2. MS-MS fragmentation of AHLs extracted from supernatants of *G. xylinus* CGMCC no. 2955. (A) C2-HSL; (B) C4-HSL; (C) C6-HSL; (D) 3-oxo-C10-HSL; (E) C12-HSL; (F) C14-HSL.

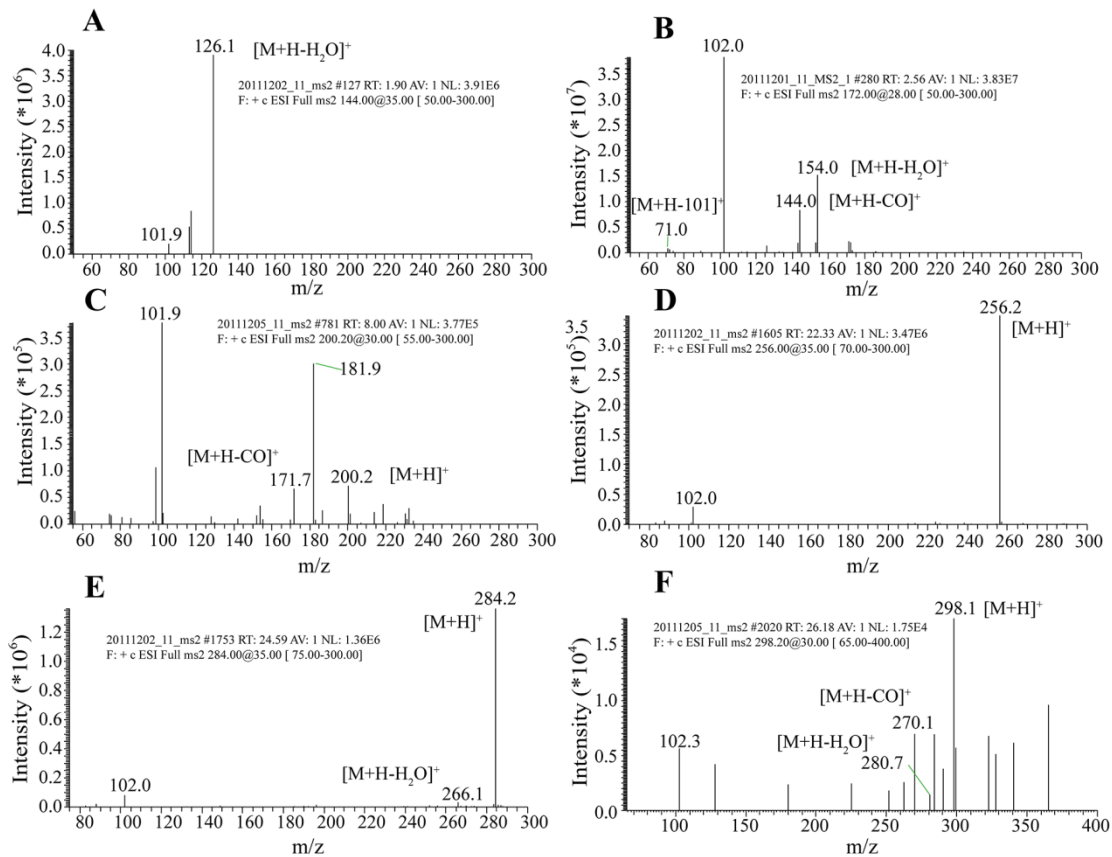


Figure S3: MS-MS fragmentation of AHLs extracted from supernatants of *Pseudomonas aeruginosa* PAK. (A) C2-HSL; (B) C4-HSL; (C) C6-HSL; (D) C10-HSL; (E) C12-HSL; (F) 3-oxo-C12-HSL.

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ATU74371.1      1  ----- MPELPAMV*ARLYTDI*FDLAADI*RGAPDHQALAEAFGAL*VSRLGPHAYSMG
SAY48253.1     1  ---- MPSPESMPELPAMV*ARLYTDI*FDLAADI*RGAPDHQALAEAFGAL*VSRLGPHAYSMG
WP_014104176.1 1  ----- M IYL FENVI DLA AANRQASEI DELNQS FRTLVARL GPF*FAHAAG
WP_039734006.1 1  ----- M IYL FENVI DLA AANRQASEI DELNQS FRTLVARL GPF*FAHAVG
WP_129551332.1 1  ----- M DLF KNI I DLTAE*NRACDADSLNNAFRAL*LACL GPF*FAHAAG
WP_003616525.1 1  ----- M LHL F EDALNSVENM*QNSENI NOLNAE*FRSLTKL*KHFVHTAG
WP_012227016.1 1  ----- MTKTVSFDKAF*DLI EPL*RRSTTASEL*RAAFV*RATKSI*SDCYI*ASG
BAK82671.1     1  ----- ----- FGA*LI*ARL*GPHAYSI*G
NC_006841.2    1  ----- MNI KNI NANEKI I DKIKT*CNNKDI*NQCLSEI*AKI*IHCEY*LFA
WP_096765104.1 1  MSDSFSLVPSV*PFVKVATEAF*AVEFCR*FLDQT*DAVARSD*QLFDLLSGFALN*DCPWI*AYG
NP_250121.1    1  ----- MALV*DGFL*ELE*RSSG*LEWSAI*LQK*MASD*LGF*SKI*LF*G
ATU72277.1     1  ----- ----- MRNESFSTNDLI*NKI*Y*YLNKI*IGTDI*TYVSG
consensus      1  m l y i d l i r l n f l v r l g p a g

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ATU74371.1     51  T I HKTD --- PLQ- RHLI*ATTYPD*H*MAHY*VARNY*H*HI*DPVI*DPLR*HG*- LHPY*DWKDI*H
SAY48253.1     57  T I HKTD --- PLQ- RHLI*ATTYPD*H*MAHY*VARNY*H*HI*DPVI*DPLR*HG*- LHPY*DWKDI*H
WP_014104176.1 44  T I HKTR --- LGD- RYLI*DTTYP*QWLE*HYV*QNNY*QKI*DPVI*DPVN*HG*- LTPY*DW*NQVY
WP_039734006.1 44  I I HKTR --- LGE- RYLV*DTTYP*KWLE*HYV*RNNY*QKI*DPVI*DPVN*HG*- LTPY*DW*KQVY
WP_129551332.1 44  T VHKTR --- RDE- RYLI*DTTYP*AH*WME*HYTRNNY*QNI*DPVI*DPVN*HG*- LTPY*NW*DQAY
WP_003616525.1 44  L VHKTR --- VTE- CYLI*DSTYP*DDW*QHYI*DNCY*QNI*DPVI*ATAR*HE- FL*YP*GW*SVG
WP_012227016.1 46  R VKGGA --- PVN- AETALV*TPDAWL*KHY*HERK*YLDI*DP*TI*VNAGR*S- YVP*YRWEALQ
BAK82671.1     17  T I HRTD --- LVQ- RHLI*GTTPD*- AM*THY*VT*QHY*H*HI*DPVI*DPVR*HG*CL*LHPY*DW*KDAR
NC_006841.2    45  I I YPHS --- I I KPDV*SI*DNY*PE*KWR*KY*Y*DDAG*L*EY*DPV*VDYS*KSH- HS*PI*NW*NVFE
WP_096765104.1 61  P LRPNQKVL*PLARC*DPE*VM*NY*PE*W*LK*RYS*EM*GY*DRI*DP*TI*NKS*RKR- VCAF*R*MEVY
NP_250121.1    39  L L P KDS --- QDYENAF*I*VGN*Y*PA*ARE*HY*DRAGY*ARV*DP*TVSH*CT*QS- VL*PI*F*W*EPSI
ATU72277.1     32  C I L SVD --- LDVP*FCL*TF*FK*EWL*DY*HQ*Q*EYI*HYD*PV*V*SYGL*GS- L*K*PAL*FSDI*S
consensus      61  i hkt l r l i t t y p d w r h y v n y h i d p v i d p l r h g l p y w i

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ATU74371.1     104  I E*NRROD --- TML*REF*GEM*GFRS*G*HAV*PLAL*AP*GT*LLL*VS*I*ASYDP*HI*DTR*---- QOMA
SAY48253.1     110  I E*NRROD --- TML*REF*GEM*GFRS*G*HAV*PLAL*AP*GT*LLL*VS*I*ASYDP*HI*DTR*---- QOMA
WP_014104176.1 97  I RNADOR --- KI MNE*FRDI*GF*QSG*HAI*PLYL*TPS*M*LL*VSV*ASPE*KEI*DFR*---- TQAL
WP_039734006.1 97  I RNADOR --- KI MNE*FRDI*GF*QSG*HAI*PLYL*TPS*M*LL*VSV*ASPE*KEI*DFR*---- TQAL
WP_129551332.1 97  I CNADQK --- KI MNE*FRDV*GF*QAG*HAI*PLHL*TPG*M*LL*VSV*ASPE*KEI*DFR*---- TQAL
WP_003616525.1 97  V RNKSOK --- NMQE*F*QDI*GF*RS*GY*AV*PL*V*SV*SM*LL*VGM*ASND*KEI*NFR*---- DRTI
WP_012227016.1 99  D I SVKOR --- QMFL*DI*AET*GI*KGGI*TMSL*HT*PDR*AAF*V*TS*FA*FT*KAV*SEDR*---- DLVA
BAK82671.1     71  I TTPQQO --- TLL*HE*F*GMS*GAAT*PC*PS*RS*RE*QC*VS*ASH*R- P*NSR*STPA*---- SRWP
NC_006841.2    99  K KTI KKES*P- NVI*KEA*QES*G*LI*T*GF*SF*PI*HT*AS*NG*F*GML*SFA*HS*D*KDI*Y*TD*SL*F*HASTN
WP_096765104.1 119  S DASTTEI*ERRV*DE*AAM*FL*RS*GI*F*SVP*MHG*P*DSS*FAI*MS*FA*QP*SE*CF*DN- RTI*TY
NP_250121.1    93  Y QTRKQH --- EFFE*E*ASA*AG*LV*Y*GL*T*M*PL*H*GARGE*L*GAL*S*L*SVE*AEN*RAE*AN*RF*ME*SVL*P
ATU72277.1     84  S P YAKSRE --- LRL*HAA*ERGI*F*RS*GF*VV*PL*R*GPL*VN*RAM*V*CF*SS*LER*PE*QWKS*--- TCVSL
consensus      121  i n r q r m l e f e m g f r s g a v p h l p l l l v s i a s d k i d r t

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ATU74371.1     156  I Q*L AAS*Q*F*H*YR*- H*Q*LGR*KHAGI*TGT*GL*TR*RE*RE*CL*T*WA*OQ*GK*DT*ADI*G*HI*LALS*- DNT
SAY48253.1     162  I Q*L AAS*Q*F*H*YR*- H*Q*LGR*KHAGI*TGT*GL*TR*RE*RE*CL*T*WA*OQ*GK*DT*ADI*G*HI*LALS*- DNT
WP_014104176.1 149  L Q*VI*VG*OY*H*TR*- C*Q*LAK*LL*SH*DD*Q*PL*V*T*ERE*Q*ECL*L*WA*OQ*GK*DT*I*E*LSI*LSI*- DNT
WP_039734006.1 149  L Q*LI*VG*OY*H*TR*- C*Q*LAK*LL*RH*DD*R*LL*V*T*ERE*Q*ECL*L*WA*OQ*GK*DT*I*E*LSI*LSI*- DNT
WP_129551332.1 149  I Q*LI*VG*OY*H*TR*- C*Q*LAML*I*TY*DE*K*PL*M*T*ERE*RE*CL*L*WA*OQ*GK*DT*I*E*GAI*LSI*LSI*- DNT
WP_003616525.1 149  L Q*TAI*NOY*HACY*- M*Q*T*NG*TS*KE*DCS*L*S*DRE*RE*CL*L*WA*OQ*GK*NT*LE*SSI*LNI*LSI*- DNT
WP_012227016.1 151  L G*FI*NS*OY*YETL*- S*K*L*SE*AE*L*PG*V*PT*FS*RRE*RE*CL*L*W*SR*GK*T*W*DS*V*I*GL*LSI*- ENT
BAK82671.1     122  S S L P P A S S I T V T - A S L G W T G H R V P G Q Y A H G N G N A C H G R H R A G I R R K S V I S L P S A T T P N S T
NC_006841.2    158  V P L M L P S L V D N Y - Q K I N T T R K K S D - S I L T K R E K E C L A W A S E G K S T W D I S K I L G C S - E R T
WP_096765104.1 175  L Q*LAAA*H*F*HL*KI*- ARL*ANS*SGI*AS*APN*L*SP*RE*KE*CI*F*W*ARG*K*SS*WDI*GI*I*LG*S- DNT
NP_250121.1    150  T L W M L K D Y A L Q S G A G L A F E H P V S K P V V L T S R E K E V L Q W C A I G K T S W E I S V I C N C S - E A N
ATU72277.1     139  Q A Q F I Q L A R E L H E N V L A I G H F P Q A E V A L T A R Q K C L K W A S L G K T A S E T A M I G L T - E R A
consensus      181  i q l i v q y h r y q l a l t r e r e c l w a q g k t e i g i l a i s d n t

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ATU74371.1     213  I K F H L K N A L R K L G C H N R V Q A A V K A T C L G L I H P - - - - -
SAY48253.1     219  I K F H L K N A L R K L G C H N R V Q A A V K A T C L G L I H P - - - - -
WP_014104176.1 206  V K H H L K N V M Q K L G C H N R V Q A V V R A I Q L G L I H P - - - - -
WP_039734006.1 206  V K H H L K N V M Q K L G C H N R V Q A V V R A I Q L G L I H P - - - - -
WP_129551332.1 206  T K Y H L K N V M H K L G C H N R V Q A V V R A I Q L G L I Y P - - - - -
WP_003616525.1 206  V K Y H L K N I M Q K L G A H N R I Q A V V Q A I N L G L I H P - - - - -
WP_012227016.1 208  I N A Y L K N V I L K L G C S G R I Q A V L R A I D L N L I S P - - - - -
BAK82671.1     181  P R T S C T S W A A T T A C R R R R O P V M G S I P - - - - -
NC_006841.2    214  V T F H L T N T O M K L N T T N R C S I S K A I L T G A I N C P Y L K N
WP_096765104.1 232  V N F H V K N A N R K L D V T S R T V A A M K A V D F G I I Q L - - - - -
NP_250121.1    208  V N F H M G N I R R K F G V T S R T V A A I M A V N L G L I T L - - - - -
ATU72277.1     197  V R A H L V S A R S V L N A S N I T O A V A K A T A L H V I F - - - - -
consensus      241  v k f h l k n i l k l g c h n r v q a v v k a i l g l i p

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Figure S4. Multiple-amino-acid alignment of LuxR proteins from *G. xylinus* CGMCC no. 2955 and other bacterias. (ATU74371.1: *G. xylinus* CGMCC no. 2955; SAY48253.1: *Komagataeibacter rhaeticus* iGEM; WP_014104176.1: *Komagataeibacter medellinensis*; WP_039734006.1: *Komagataeibacter intermedius*; WP_129551332.1: *Komagataeibacter xylinus*; WP_003616525.1: *Komagataeibacter hansenii*; WP_012227016.1: *Gluconacetobacter diazotrophicus*; BAK82671.1: *Komagataeibacter medellinensis* NBRC 3288; NC_006841.2: *Vibrio fischeri* ES114; WP_096765104.1: *Rhizobium sophoriradicis*; NP_250121.1: *Pseudomonas aeruginosa* PAO1; ATU72277.1: *Gluconacetobacter xylinus* CGMCC no. 2955) Red asterisks indicate the nine conserved amino acids.