# Modelamiento por homología *in silico* de la quinoproteína glucosa deshidrogenasa unida a membrana en *Pseudomonas fluorescens*

## Material suplementario

## Contenido

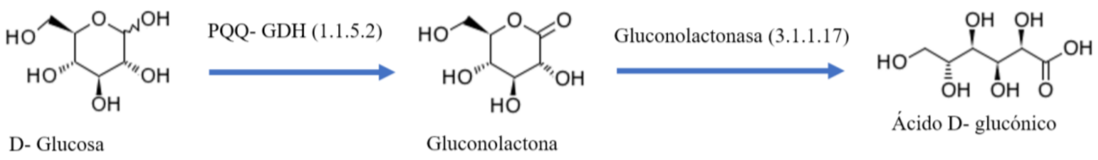


**Figura 1S.** Reacción general mediada por la Quinoproteina glucosa deshidrogenasa y gluconolactonasa para la producción de ácido glucónico (Ruta pentosa fosfato de la base de datos KEGG - https://www.genome.jp/kegg/).

**Tabla 1S:** Dominios más importantes identificados para la secuencia de PQQ- mGDH de *P. fluorescens.*

| Posicion (Puntaje, Valor=E) | Descripcion/NCBI-CDD |
|---|---|
| 34..803(1222, 0.0) | TIGR03074, PQQ_membr_DH, membrane-bound PQQ-dependent dehydrogenase, glucose/quinate/shikimate family. / 274418 |
| 12..804(1015, 0.0) | COG4993, Gcd, Glucose dehydrogenase [Carbohydrate transport and metabolism]./227326 |
| 173..802(901, 0.0) | cd10280, PQQ_mGDH, Membrane-bound PQQ-dependent glucose dehydrogenase./199838 |
| 163..784(240, 2e-69) | cd10277, PQQ_ADH_I, Ethanol dehydrogenase, a bacterial quinoprotein (PQQ-dependent type I alcohol dehydrogenase)./199835 |
| 170..784(235, 1e-67) | TIGR03075, PQQ_enz_alc_DH, PQQ-dependent dehydrogenase, methanol/ethanol family./274419 |
| 194..535(219, 9e-63) | cd00216, PQQ_DH_like, PQQ-dependent dehydrogenases and related proteins./199833 |
| 171..801(201, 1e-55) | cd10279, PQQ_ADH_II, PQQ_like domain of the quinohemoprotein alcohol dehydrogenase (type II)./199837 |
| 169..785(184, 5e-50) | TIGR04528, pyrrolo-quinoline_quinone, acido-empty-quinoprotein group A./275321 |
| 173..536(145, 1e-36) | cd10278, PQQ_MDH, Large subunit of methanol dehydrogenase (moxF)./199836 |
| 184..527(64.7, 6e-11) | cd10276, BamB_YfgL, Beta-barrel assembly machinery (Bam) complex component B and related proteins./199834 |
| 186..528(49.5, 5e-06) | TIGR03300, assembly_YfgL, outer membrane assembly lipoprotein YfgL./274511 |
| 186..397(46.8, 4e-05) | PRK11138, PRK11138, outer membrane biogenesis protein BamB; Provisional./236857 |
| 223..475(43.6, 2e-04) | pfam13360, PQQ_2, PQQ-like domain. This domain contains several repeats of the PQQ repeat./338699 |
| 22..143(42.4, 6e-04) | pfam02322, Cyt_bd_oxida_II, Cytochrome bd terminal oxidase subunit II./334894 |
| 12..77(41.3, 7e-04) | pfam04156, IncA, IncA protein./309330 |
| 1..110(41.7, 0.001) | COG1807, ArnT, 4-amino-4-deoxy-L-arabinose transferase and related glycosyltransferases of PMT family [Cell envelope biogenesis, outer membrane]./224720 |
| 3..142(40.7, 0.003) | pfam10101, DUF2339, Predicted membrane protein (DUF2339)./337627 |
| 4..140(39.5, 0.003) | pfam13398, Peptidase_M50B, Peptidase M50B-like./315961 |
| 680..712(37.2, 0.004) | pfam01011, PQQ, PQQ enzyme repeat./307240 |
| 16..134(39.5, 0.005) | COG4177, LivM, ABC-type branched-chain amino acid transport system, permease component [Amino acid transport and metabolism]./226645 |

| | |
|---|---|
| 7..108(39.3, 0.008) | TIGR03920, T7SS_EccD, type VII secretion integral membrane protein EccD./274855 |
| 22..99(38.2, 0.014) | TIGR00896, Inner_membrane_transport_protein_YeaN, cyanate transporter./129974 |
| 22..144(38.0, 0.016) | cd17409, MFS_NIMT_like, 2-nitroimidazole transporter and similar proteins of the Major Facilitator Superfamily of transporters./340967 |
| 19..141(37.9, 0.019) | cd13125, MATE_like_10, Uncharacterized subfamily of the multidrug and toxic compound extrusion (MATE) proteins./240530 |
| 18..139(37.2, 0.021) | pfam02654, CobS, Cobalamin-5-phosphate synthase./335026 |
| 224..256(35.2, 0.021) | smart00564, PQQ, beta-propeller repeat./128836 |
| 21..140(37.5, 0.031) | PRK10577, PRK10577, iron-hydroxamate transporter permease subunit; Provisional./236720 |
| 18..107(37.2, 0.032) | pfam06772, LtrA, Bacterial low temperature requirement A protein (LtrA)./336501 |
| 7..78(36.8, 0.045) | PRK15402, PRK15402, multidrug efflux system translocase MdfA; Provisional./185300 |
| 26..140(36.1, 0.059) | pfam09594, GT87, Glycosyltransferase family 87./337450 |
| 19..78(36.2, 0.065) | PRK13375, pimE, mannosyltransferase; Provisional./172015 |
| 13..135(35.8, 0.070) | cd13956, PT_UbiA, UbiA family of prenyltransferases (PTases)./260119 |
| 5..146(35.7, 0.079) | pfam09930, DUF2162, Predicted transporter (DUF2162)./313202 |
| 47..107(34.0, 0.080) | pfam07332, Phage_holin_3_6, Putative Actinobacterial Holin-X, holin superfamily III./336675 |
| 18..90(36.0, 0.086) | PRK11021, PRK11021, putative transporter; Provisional./236823 |
| 21..140(35.2, 0.12) | cd13962, PT_UbiA_UBIAD1, 1,4-Dihydroxy-2-naphthoate octaprenyltransferase./260125 |
| 40..139(34.8, 0.18) | COG0559, LivH, Branched-chain amino acid ABC-type transport system, permease components [Amino acid transport and metabolism]./313202 |
| 25..128(34.3, 0.29) | cd17410, MFS_CynX_like, Cyanate transport protein CynX and similar proteins of the Major Facilitator Superfamily of transporters./340968 |
| 41..146(34.1, 0.29) | cd17316, MFS_SV2_like, Metazoan Synaptic vesicle glycoprotein 2 (SV2) and related small molecule transporters of the Major Facilitator Superfamily./340874 |
| 45..136(33.6, 0.31) | COG2391, COG2391, Predicted transporter component [General function prediction only]./225264 |
| 38..141(34.3, 0.34) | COG4232, COG4232, Thiol:disulfide interchange protein [Posttranslational modification, protein turnover, chaperones / Energy production and conversion]./226685 |
| 6..110(33.4, 0.36) | pfam02366, PMT, Dolichyl-phosphate-mannose-protein mannosyltransferase./280519 |
| 21..125(33.8, 0.42) | COG2807, CynX, Cyanate permease [Inorganic ion transport and metabolism]./225365 |

|  |  |
|---|---|
| 16..143(33.3, 0.44) | pfam03772, Competence, Competence protein./309048 |
| 13..115(33.1, 0.45) | pfam05857, TraX, TraX protein./310445 |
| 24..104(33.4, 0.45) | pfam14362, DUF4407, Domain of unknown function (DUF4407)./316850 |
| 15..140(33.4, 0.50) | COG0475, KefB, Kef-type K+ transport systems, membrane components [Inorganic ion transport and metabolism]./223551 |
| 28..137(33.6, 0.56) | TIGR03434, ADOP, Acidobacterial duplicated orphan permease./274576 |
| 22..139(32.9, 0.57) | cd13964, PT_UbiA_1, UbiA family of prenyltransferases (PTases), Unknown subgroup./260127 |
| 15..117(33.3, 0.64) | cd10329, SLC5sbd_SGLT1-like, Na(+)/glucose cotransporter SGLT1 and related proteins./271363 |
| 10..104(33.0, 0.65) | COG0600, TauC, ABC-type nitrate/sulfonate/bicarbonate transport system, permease component [Inorganic ion transport and metabolism]./223673 |
| 15..81(32.3, 0.69) | pfam00335, Tetraspannin, Tetraspanin family./334016 |
| 10..107(31.9, 0.71) | pfam07331, TctB, Tripartite tricarboxylate transporter TctB family./336674 |
| 16..107(32.9, 0.74) | COG0697, RhaT, Permeases of the drug/metabolite transporter (DMT) superfamily [Carbohydrate transport and metabolism / Amino acid transport and metabolism / General function prediction only]./223769 |
| 42..141(32.8, 0.75) | COG1835, COG1835, Predicted acyltransferases [Lipid metabolism]./224748 |
| 17..110(31.8, 0.81) | pfam01694, Rhomboid, Rhomboid family./334640 |
| 10..112(31.5, 0.81) | pfam06271, RDD, RDD family./336359 |
| 14..146(32.6, 0.83) | pfam05940, NnrS, NnrS protein./336253 |
| 15..145(33.0, 0.83) | pfam09843, DUF2070, Predicted membrane protein (DUF2070)./313128 |
| 2..86(33.1, 0.83) | COG3264, COG3264, Small-conductance mechanosensitive channel [Cell envelope biogenesis, outer membrane]./225803 |
| 11..113(32.5, 0.85) | TIGR02210, Rod_shape-determining_protein_RodA, rod shape-determining protein RodA./274033 |

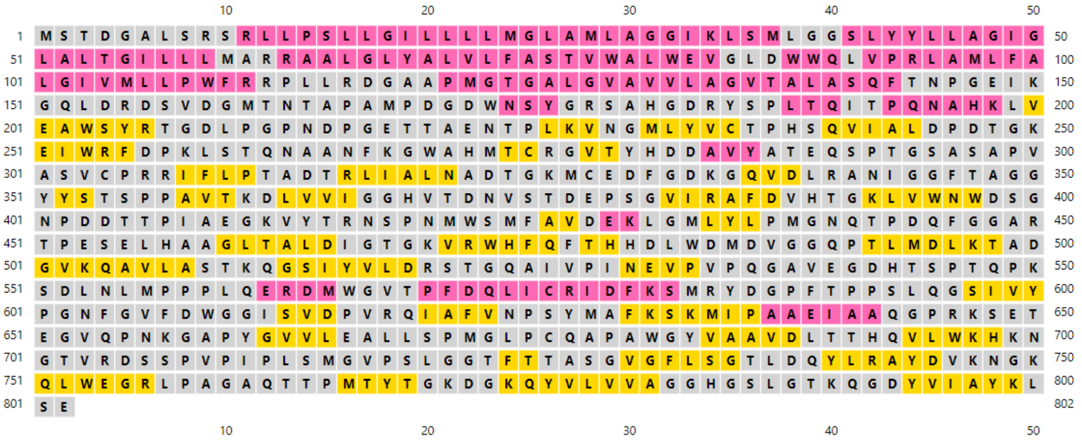


**Figura 2S.** Gráfico de secuencia y relación con la estructura secundaria para la enzima PQQ- mGDH de *P. fluorescens* utilizando la aplicación PSIPRED. En amarillo se identifican los residuos con tendencia a formar hojas beta, en rosa los residuos con tendencia a formar hélices alfa y en gris se muestran los residuos sin tendencia específica a formar una estructura secundaria.

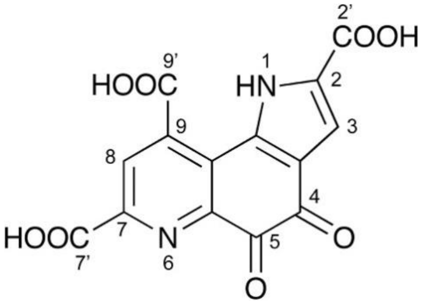


**Figura 3S.** Estructura química de Pirroloquinolina quinona (Takeda et al., 2019).

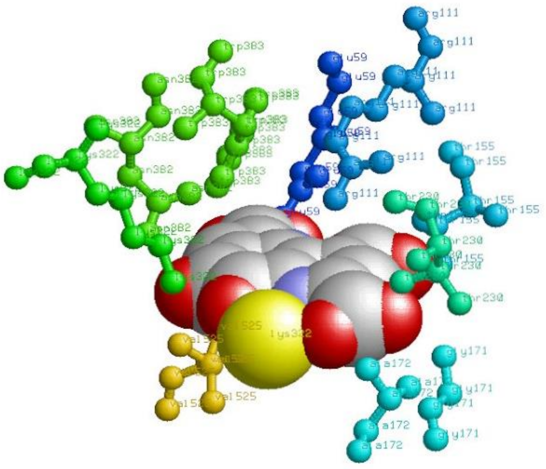
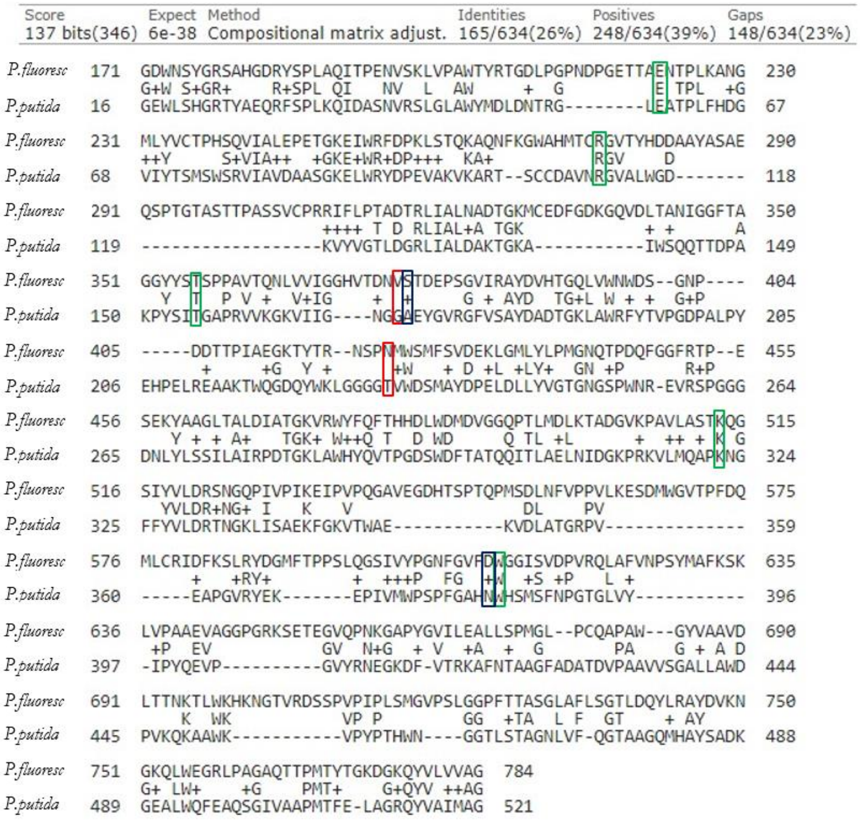


**Figura 4S.** Sitio activo de la enzima PQQ- mGDH formado por PQQ y los aminoácidos que interaccionan con el: Glu (59), Arg (111), Thr (155), Gly (171), Ala (172), Thr (230), Lys (322), Asn (382), Trp (383), Val (525) y un átomo de Ca (802) (amarillo).



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Score          Expect  Method                        Identities    Positives     Gaps
137 bits(346)  6e-38   Compositional matrix adjust.  165/634(26%)  248/634(39%)  148/634(23%)

P.fluoresc  171  GDWNSYGRSAHGDRYSPLAQITPENVSKLVPAWTYRTGDLPGPNDPGETTAENTPLKANG  230
                 G+W S+GR+    R+SPL QI   NV  L  AW     +  G         E TPL  +G
P.putida    16   GEWLSHGRTYAEQRFSPLKQIDASNVRSLGLAWYMDLDNTRG--------LEATPLFHDG  67

P.fluoresc  231  MLYVCTPHSQVIALEPETGKEIWRFDPKLSTQKAQNFKGWAHMTCRGVTYHDDAAYASAE  290
                 ++Y     S+VIA++  +GKE+WR+DP+++  KA+          RGV    D
P.putida    68   VIYTSMSWSRVIAVDAASGKELWRYDPEVAKVKART--SCCDAVNRGVALWGD-------  118

P.fluoresc  291  QSPTGTASTTPASSVCPRRIFLPTADTRLIALNADTGKMCEDFGDKGQVDLTANIGGFTA  350
                                   ++++ T D RLIAL+A TGK            + +      A
P.putida    119  ------------------KVYVGTLDGRLIALDAKTGKA-----------IWSQQTTDPA  149

P.fluoresc  351  GGYYSTSPPAVTQNLVVIGGHVTDNVSTDEPSGVIRAYDVHTGQLVWNWDS--GNP----  404
                   Y  T  P V +  V+IG    +  +     G + AYD  TG+L W + +  G+P
P.putida    150  KPYSITGAPRVVKGKVIIG----NGGAEYGVRGFVSAYDADTGKLAWRFYTVPGDPALPY  205

P.fluoresc  405  -----DDTTPIAEGKTYTR--NSPNMWSMFSVDEKLGMLYLPMGNQTPDQFGGFRTP--E  455
                       +     +G  Y +      +W   + D +L +LY+  GN +P      R+P
P.putida    206  EHPELREAAKTWQGDQYWKLGGGGTVWDSMAYDPELDLLYVGTGNGSPWNR-EVRSPGGG  264

P.fluoresc  456  SEKYAAGLTALDIATGKVRWYFQFTHHDLWDMDVGGQPTLMDLKTADGVKPAVLASTKQG  515
                    Y + + A+   TGK+ W++Q T  D WD     Q TL +L      +  ++ + K G
P.putida    265  DNLYLSSILAIRPDTGKLAWHYQVTPGDSWDFTATQQITLAELNIDGKPRKVLMQAPKNG  324

P.fluoresc  516  SIYVLDRSNGQPIVPIKEIPVPQGAVEGDHTSPTQPMSDLNFVPPVLKESDMWGVTPFDQ  575
                   YVLDR+NG+ I   K   V                 DL    PV
P.putida    325  FFYVLDRTNGKLISAEKFGKVTWAE-----------KVDLATGRPV--------------  359

P.fluoresc  576  MLCRIDFKSLRYDGMFTPPSLQGSIVYPGNFGVFDWGGISVDPVRQLAFVNPSYMAFKSK  635
                      +   +RY+        +  +++P  FG  +W  +S +P   L +
P.putida    360  -----EAPGVRYEK-------EPIVMWPSPFGAHNWHSMSFNPGTGLVY-----------  396

P.fluoresc  636  LVPAAEVAGGPGRKSETEGVQPNKGAPYGVILEALLSPMGL--PCQAPAW---GYVAAVD  690
                  +P  EV           GV  N+G  + V  +A  +  G       PA    G + A D
P.putida    397  -IPYQEVP----------GVYRNEGKDF-VTRKAFNTAAGFADATDVPAAVVSGALLAWD  444

P.fluoresc  691  LTTNKTLWKHKNGTVRDSSPVPIPLSMGVPSLGGPFTTASGLAFLSGTLDQYLRAYDVKN  750
                     K  WK           VP P        GG  +TA  L F  GT    + AY
P.putida    445  PVKQKAAWK-----------VPYPTHWN----GGTLSTAGNLVF-QGTAAGQMHAYSADK  488

P.fluoresc  751  GKQLWEGRLPAGAQTTPMTYTGKDGKQYVLVVAG  784
                 G+ LW+    +G    PMT+    G+QYV ++AG
P.putida    489  GEALWQFEAQSGIVAAPMTFE-LAGRQYVAIMAG  521
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**Figura 5S.** Alineamiento de secuencias Quinohemoproteina ADH de *P. putida* y PQQ- mGDH de *P. fluorescens.*