

A3 - Material suplementario: Modelado molecular y predicción funcional de la proteína bli4781 de *Bradyrhizobium diazoefficiens* (USDA 110)

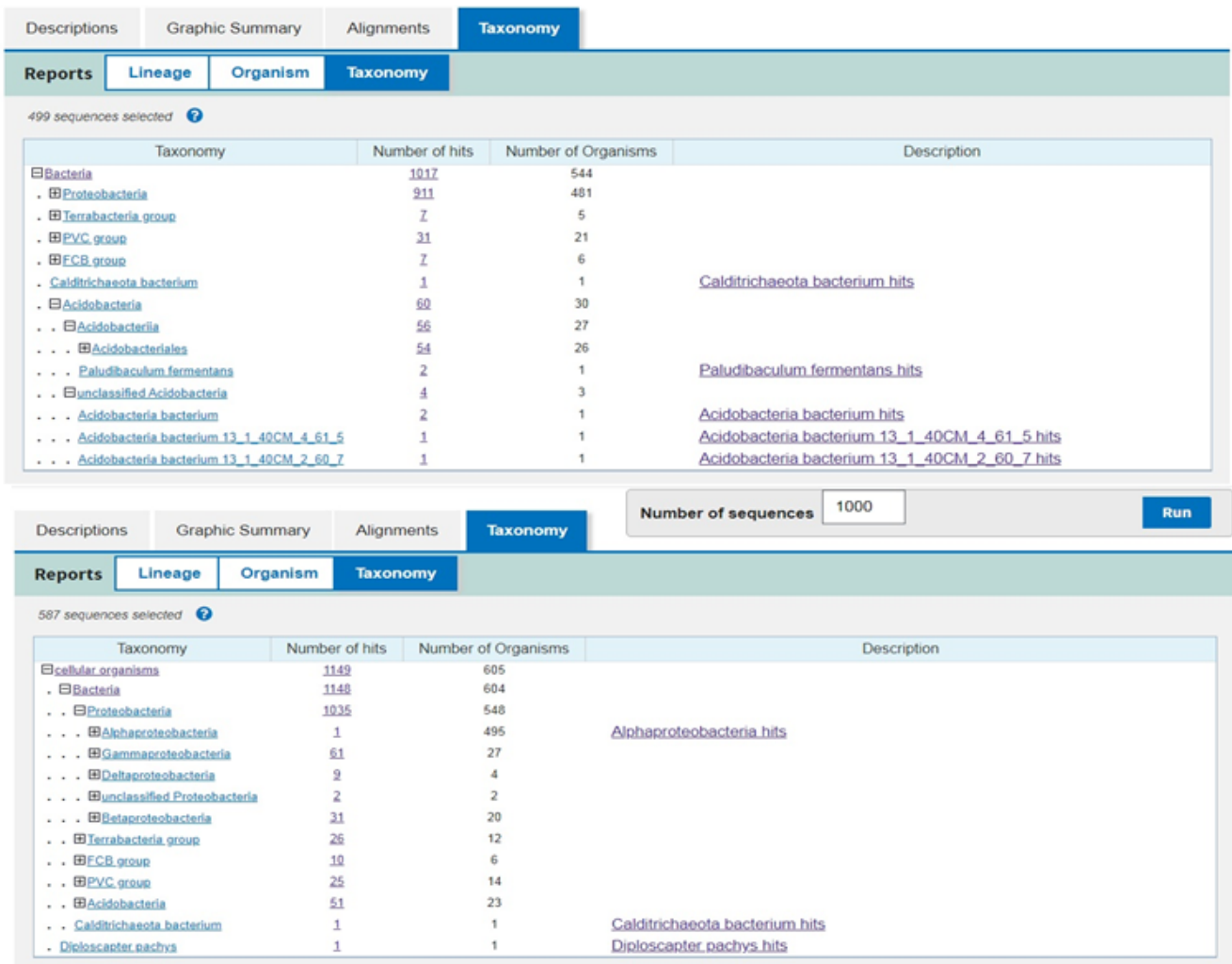


Figura S1. Distribución taxonómica en BLAST (arriba) y PSI-BLAST (abajo)

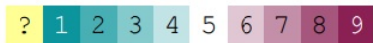
Tabla S1. Secuencias elegidas para realizar el alineamiento múltiple

DUF5076 (Especies)	Accession number	Secuencia
<i>Bradyrhizobium erythrophlei</i>	WP_079603347.1	MSGPKQQLPPDVIGRDDATEVLRAFVVDGGLSIAFTRAFEEPPDMWGLLVLDARHAARAYARESFAFTEDEALTRIVDMFEAEIARPTDPGTTTPRSQQGH
<i>Bradyrhizobium elkani</i>	GEC52187.1	MAGPKQQLPPDVIMGRDDAIEVLRAFVVDGGLSIAFQRAFEPPDMWGLMLVDIARHAARAYARESEYTEDEALARIVEMFEAEIARPTDMGQTKPRSQQGH
<i>Bradyrhizobium yuanmingense</i>	TGN80551.1	MAGPKQQLPPDVIMTRDDAVEILRVFVLDGGLSMAFQRAFEPPDMWGLLVVDLARHAARAYARESEYTEEDALNRILDMFQAEIERPTDTGTTTPRGKGH
<i>Bradyrhizobium</i> sp. Tv2a-2	WP_024518800.1	MAGPKQQLPPDVIGREDATEVLRAFVLDGGLSIAFTRAFEEPPDMWGLLVLDIARHAARAYSRESYSEEEALDRILEMFSAEIERPTDMGTTTPRSQKGH
<i>Rhodopseudomonas palustris</i>	WP_119857868.1	MAGPKQQLPPDVVEGREDATEVLRAFVLDGGLSIAFMRAFEPPDMWGLLVDIARHAARAYSRESNYTEDEALERIVEMFEAEIARPSDLGSTTERPQ
unclassified <i>Tardiphaga</i>	WP_143573479.1	MAGPKQQLPPDVVGREEAVEVLRAFVVDGGLSIAFTRAFEEPPDMWGMLLVDIARHAARAYARESDYSEDEALARIVDMFQAEIARPTDVGNTTTPRSQQGH
<i>Microvirga aerophila</i>	WP_114188594.1	MTEKKEALNVPPDVLEKGGVEILRASVVDGAVSIALRRAFDDPFTWGVLLVLDLARHAARVYAMETDFSEEEALAEISAGIQAEIADDPDPGPTQAIN
DUF5076 (Especies)	Accession number	Secuencia
<i>Methylobacterium</i> sp. YIM 132548	WP_150964006.1	MPKAFQPLSVPDALEKGGVEVLRASVVDGAVSVALRRSFDPPFTWGVLLIDLARHAARVYAEITDLSEEEAFAQIRAGLEAETDPPDGPDSLLN

<i>Mesorhizobium sp.</i> WSM4312	PBB66311.1	MFGKLSSELSPPPNAKNARAVEVLRVWAEPGAQQVLKTTWKEPGAWGLL LADVARHAARAYVAEGISEAQALDRILMLFKAEEFAAPT DAPS
<i>Sphingomonas sp.</i> Leaf230	WP_056057410.1	MADHPANHPNAIALDKGALQTESVEVARIWITNGAGSNVLIDAGILEDPTVF GYLLADTIRHAARAYAGTWGLDEDAALQAIVDGVTGLREQFTTITTIQEGMH
<i>Dechloromonas sp.</i> CZR5	WP_150427584.1	MFGRKGIELEPPLSRDAGAFEILRVWGGDNLPPQQYSLKTVRDDPGAWGLM LVDIARHVAKAYGNTGDFSEEAALKRIKELFDAEWASPTDTPQLVK
<i>Ralstonia sp.</i>	WP_048934697.1	MKSELPIPPAALQDVDSKELLRVWAAAGNQHSIATGVWENPTIWGIMLVDL LRHIARSYKVGNSVSYEESMRLIKAGFDAEWESPT E
<i>Lactobacillus crispatus</i>	WP_133467175.1	MAGPKQLPPDVMGRDDAVEVLRVVDGGLSIAFQRAFEEDPMWGLM LVDIARHAARAYSRESEYTEDEALARIVEMFEAEIARPTD
<i>Granulicella sp.</i> S156	WP_158821490.1	MSGNKYLDPPAAVRDKASFELLRVWVAEQGQHVSLRPGTWDDPFWAGIV LADLARHIVNAESIHRKNFDEDAFLERMLEGFRAIESPTDDPEGEIMQ
<i>Calditrichaeota bacterium</i>	RMI08682.1	MAAENPDAFEVLRWITAPGAYQQVILRTSWEDPGAWGILLVDIARHAARAYE REGWDRREALDRIFLDAEWDPTDEPLDITRDS



The conservation scale:



Variable Average Conserved

- e** - An exposed residue according to the neural-network algorithm.
- b** - A buried residue according to the neural-network algorithm.
- f** - A predicted functional residue (highly conserved and exposed).
- s** - A predicted structural residue (highly conserved and buried).

Figura S2. En escala de colores, posiciones menos y más conservadas según el programa ConSurf.

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MSA
The multiple sequence alignment result as produced by T-coffee.

T-COFFEE, Version_11.00 (Version_11.00)
Cedric Notredame
SCORE=98
*
  BAD AVG GOOD
*
tr|O89KW9|O89KW      : 98
3IC3_1|Chains       : 98
cons                 : 9

tr|O89KW9|O89KW      1 ---MAGPKEOPLPPDVTREDAVEILRVFVLDGGLSMAFORAFEEDPMWGLLLVLDLARHAARAYARESEYTEEDALSRILEMFO 81
3IC3_1|Chains       1 SNAMTGPQQPLPPDVEGREDAIEVLRVFLDGGLSIAFMRAFEDPEMMWGLLLVDIARHAARSYARESEYTEDEALERIVEMFE 84
cons                 1  *:.***:*****  *****:.*  *****:.*  *****:.*  *****:*****:*****:*****:.*  *:.***: 84

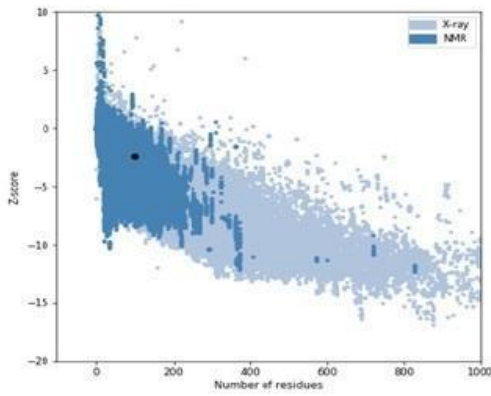
tr|O89KW9|O89KW      82 AEIERPTDTGTTTPRGKGH 100
3IC3_1|Chains       85 AELSRPTDTGATTERTQ-- 101
cons                 85 **:.*****:**  * : 103

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Figura S3. Alineamiento entre la query sequence y la template generado por T-Coffee.

Overall model quality

Z-Score: -2.43



Local model quality

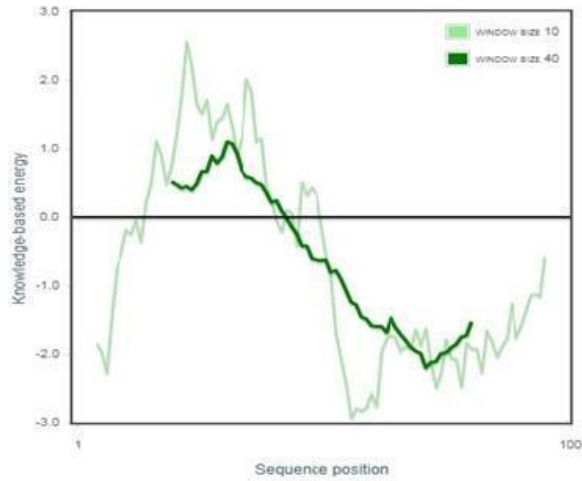


Figura S4. Resultados gráficos de evaluación y perfil energético obtenido por ProSa.

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tr|Q89KW9| MAGPK--EQP L-----PPDV VTREDAVEIL RVFVLDGGL- SMAFQ-RAFE EPDMGMLLV DLARHAARAY A-RESEYTEE DALSRILEMF QAEIERPTDT GTTTPRGKG- H
WP_0796033| MSGPK--EQP L-----PPDV IGRDDATEVL RAFIVDGGGL- SIAFT-RAFE EPDMGMLLV DLARHAARAY A-RESAPTED EALTRIVDMF EAEIARPTDP GTTTPRSQQG H
GEC52187.1| MAGPK--EQP L-----PPDV MGRDDAIEVL RAFVVDGGL- SIAFQ-RAFE EPDMGMLLV DLARHAARAY A-RESEYTED EALARIVEMF EAEIARPTDM GQTKPRSQQG H
RMI08682.1| -----MA- AENPDAFEVL RIWTAPGAY- QQVILRTSWE DPGAWGILLV DIARHAARAY E-REG-WDRR EALDRIRELF DAEWDFPTDE PLDITR-DS- -
WP_0245188| MAGPK--EQP L-----PPDV IGRDDATEVL RAFVLDGGL- SIAFT-RAFE EPDMGMLLV DLARHAARAY S-RESDYSEE EALDRILEMF SAELERPTDM GTTTPRSQKG H
WP_1198578| MAGPK--QQP L-----PPDV EGREDATEVL RAFVLDGGL- SIAFM-RAFE EPDMGMLLV DLARHAARAY S-RESNYTED EALERIVEMF ESEIARPSDL GSTTER-P-- Q
WP_1435734| MAGPK--EQP L-----PPDV VGREEAPEVL RAFVVDGGL- SIAFT-RAFE EPDMGMLLV DLARHAARAY A-RESDYSED EALARIVDMF DAEIARPTDV GNTTTRSQQG H
WP_1141885| HTEKKFEALN V-----PPDV -LEKGGVEIL RASVVDGAV- SIALR-RAFD DPFTWGVLLV DLARHAARVY A-METDFSEE EALAEISAGI QAELODPSDP GTTQAI---- N
WP_1509640| MPKA-FQPLS V-----PPDA -LEKGGVEVL RASVVDGAV- SVALR-RSFD DPFTWGVLLI DLARHAARVY A-LETDLSEE EAFQIRAGL EAETDPPDG- PDSL-L---- N
PBB66311.1| MFGKLSSELS P-----PPN- AKNARAVEVL RVWAEPGAA- QQLVLKTTWK EPGAWGLLLA DVARHAARAY V-AEG-ISEA QALDRILMLF KAFAAPPTDA P-----S- -
WP_0560574| MADHP--ANH PNAIALDKGA QLTGESVEVA RIWITNGAGS NVLIDAGILE DPTVFGYLLA DDIRHAARAY A-GTWGLDED AALQAIVDGV GTELREQFTT ITTIQEGM-- H
WP_1504275| MFGKKGIELE E-----PPL- SRDAGAFEIL RVWGGDNLV- QQYSLKTVRD DPGAWGMLLV DIARHVAKAY G-NTGDFSEE AALKRIKELF DAENASPTDT PLQV----K- -
WP_0489346| MKS--ELP-- I-----PPAA LQDVDSKELL RVWAAAGNQ- HISIATGVWE NPTIMGIMLV DLLRHARSY E-KVGNVSYE ESMRLIKAGF DAEWESPTD- ----- -
WP_1334671| MAGPK--EQP L-----PPDV IGRDDAVEVL RAFVVDGGL- SIAFQ-RAFE EPDMGMLLV DLARHAARAY S-RESEYTED EALARIVEMF EAEIARPTD- ----- -
WP_1588214| MSGNK--VLD P-----PPAA VRDKASFELL RVWVAEQGQ- HVSLRPGTWD DPFAMGIVLA DLARHIVNAE SIHRKNFDED AFLERMLEGF RAEIESPTDD PEGEIM--Q- -
TGN80551.1| MAGPK--EQP L-----PPDV MTRDDAVEIL RVFVLDGGL- SMAFQ-RAFE EPDMGMLLV DLARHAARAY A-RESEYTEE DALNRILDMF QAEIERPTDT GTTTPRGKG- H
    
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Figura S5. Alineamiento múltiple en formato Phylip obtenido en T-Coffee.