

## **Supplementary Information**

### **Protein Dynamics in F-like Bacterial Conjugation**

Nicholas Bragagnolo, Christina Rodriguez, Naveed Samari-Kermani, Alice Fours, Mahboubeh Korouzhdehi, Rachel Lysenko  
and Gerald F. Audette<sup>†</sup>

Department of Chemistry & Centre for Research on Biomolecular Interactions

York University, 4700 Keele St., Toronto, ON M3J 1P3 Canada

**Supplementary Table 1: Details Regarding Predicted Disordered Regions of Transfer Proteins from the F Plasmid\***

Protein	Size (aa)	Disorder (%)	GenBank	UniProtKB	AA Sequence
FinO	186	42%	M38047	P22707	MTEQKRPVLTLLKRRKTEGETLVRSRKTIIINVTPPKWKVKKQKLAEKAAREAEAAKKAQARQALS IYLNLP TLDDAVNTLKPWWPGLFDGDTPRLLACGIRDV LLEDVAQRNIP LSHKKLRRALKAITRSES YLCAMKAGACRYDTEGYVTEHISQEEEEAYAAERLDKIRRQNRRIKAE LQAVLDEK
TraJ	229	21%	BAA97942	P06626	MYPMDRIQQKHARQIDLLENLTA VIQDY PNPACIRD ETGKFIFCN TLFHESFL TQDQSAEKWLLSQR DFCELISVTEMEA YRNEHTHLNL VEDVFIQNRFWTISVQSFLNGHRN IILWQFYDAAHV RHKDSYN QKTIVSDDIRNI IRRMSDDSSVSSYVNDVFYL YSTGISHNAIARIL NISISTSKKHASLICDYFSVSNKD ELIILLYNKKFIYYLYEKAMCIINTR
TraA	70	20%	BAA97944	P04737	AGSSGQDLMASGNTTVKATFGKDSSVVKWVVLAEVLVGAVMYMMTKNVKFLAGFAIISVFI AVG MAVVGL
TraR	73	19%	BAA97953	P41065	MSDEADEAYSVTEQLTMTGINRIRQKINAHGIPVYLCEACGNPIPEARRKIFPGVTLCVECQAYQER QRKHYA
TraQ	94	22%	BAA97964	P18033	MISKRRFSLPRLDITGMWVFSLGVWFHIVARLVYSKPWMAFFLAELIAAILV LFGAYQVLD AWIAR VSREEREAL EARQQAMMEGQQEGGHVSH
TraX	248	13%	BAA97975	P22709	MTTDNTNTRND SLVARTDTWLQSLLVWSPGQRDIKTVALVLMVLDHANRILHLDQSWMFLAG RGAFPLFALVWGLNLSRHAHIRQLAINRLWGWA VFSQFWYFAGFPWYEGNILFAFAVAAQVLT WCETRSGWR TAAA ILMMALWG PLSGTSYGIAGLLMLA VSHRLYRAEDR MERLVLVACLLA VIPA LNLATSDAAA VAGLVMTVLT VGLVSCAGKLLSRFPWPGDFPFTFYACHLAVLGV LAL
TraB	475	44%	BAA97948	P41067	MASINTIVKRKQYLWLGIVVVG TASAIGGALYLSDVDMSGNGETVAEQEPVDMTG VVDTTFDDK VRQHATTEMQV TAAQMOKQYEEIRRELDV LNKQRGDDQRRIEKLGDNAALAEQVKALGANPV TATGEPVPQMPASPPGPEGEPQPGNTPVSFPPQGSVAVPPPTAFYPGNGVTPPPQV TYQSVV PNRIQ RKVFTRNEGKQGPSLPYIPSGSFAKAMLIEGADANASVTGNESTVPMQLRITGLVEMPNSKTYDAT GCFVGLEAWGDVSSERAIVRTRNISCLKDGKTIDMPIKGHVSRFGKNGIKGEVVMRNGKILGWAW GAGFVDGIGQG MERASQPAVGLGATAAYGAGDVLKMGIGGGASKAAQTLSDY YIKRAEQYHPVI PIGAGNEVT VVFQDGFQLKTVEEMALERTQSRAEEDNPESPVPVPPSAESHLNGFN TDQMLKQLGN LNPQQFMSGSQGGGNDGK
TraK	242	34%	BAA97947	P41066	MRKNNTAIIFGSLFFSCSVMAANGTLAPT VVPMVNGGQASIAISNTSPNLFTVPGDR IIAVNSLDGAL TNNEQTASGGVVVATV NKKPFTFILETERGLNLSIQAVPREGAGRTIQLVSDLRGTGEEAGAWETS TPYESLLVTISQAVRGGKLPAGWYQVPVTKETLQAPAGLSSVADAVWTGNHLK MVRFAVENKTL SALNIRESDFWQPGTRAVMFSQPASQLLAGARMDVYVIR DGEGN
TraV	171	61%	BAA97952	P41069	MKQTSFFIPLLGTLLLYGCAGTSTEFECNATTS DTCMTMEQANEKAKK LERSSEAKPVAASL PRLA EGNFRTMPVQTVTATTPSGSRPAVTAHPEQKLLAPRPLFTAAREVKTVVPVSSVTPVTPPRPLRTGE QTAALWIAPYIDNQDVYHQPSVFFVIKPSAWGKPRIN

TraF	247	17%	BAA97961	P14497	MNKALLPLLLCCFIFPASGKDAGWQWYNEKINPKEKENKPVPAAPRQEPDIMQKLAALQTATKRALYEAILYPGVDNFVKYFRLQNYWAQQAGLFTMSARKAMLAHPELDYNLQYSHYNGTVRNQLAADQAQQRQAIAKLAEHYGIMFFYRGQDPIDGQLAQVINGFRDITYGLSVIPVSDGVINPLLPDSRTDQGGQAQRLGVKYFPAMMLVDPKQGSVRPLSYGFISQDDLAKQFLNVSEDFKPNF
TrbB	181	31%	BAA97965	P18035	MSLTKSLLFTLLSAAA VQASTRDEIERLWNPQGMATQPAQPAAGTSARTAKPAPRWFRSLNGRQVNLADWKVVLFMQGHCPYCHQFDPVLKQLAQYGFVSFYSYTLDGQGDATFPEALPVPDVMQTFPNIPTVATPTTFLVNVNTLEALPLLQGATDAAGFMARVDTVLQMYGGKKGAK
TraC	875	15%	BAA97954	P18004	MNNPLEAVTQAVNSLV TALKLPDESAKANEVLGEMSFQFSRLLPYRDYNQESGLFMNDTTMGFMLEAIPINGANESIVEALDHMLR TKLPRGIPLCIHLMSSQLVGDRIEYGLREFSWSGEQAERFNAITRAYYMKAAATQFPLPEGMNLPLTLRH YRVFISYCSPSKKKSRADILEMENLVKIIRASLQGASITQT VDAQAFIDIVGEMINHPDSL YPKRRQLDPYSDLNYQCVEDSFDLKV RADYLTGLRENGRNSTARILNFHLARNPEIAFLWNMADNYSNLLNPELSISCPFILTLTLVVEDQVKTHSEANLKYMDLEKKS KTSYAKWFPSVEKEAKEW GELRQLR LGSQSSVVS YFLNITAFCKDNNETALEVEQDILNSFRKNGFELISPRFNHMRNFLTCLPFMAGKGLFKQLKEAGVVQRAESFNVANLMPLVADNPLTPAGLLAPTYRNQLAFIDIFFRGMNNTNYNMAVCGTSGAGKTGLIQPLIRSVLDSGGFAVVFDMDGDYKSLCENMGGVYLDGETLRFNPFANITDIDQSAERVRDQLSVMASPNGNLDEVHEGLLQAVRASWLAKENRARIDDVVDLKNASDSEQYAESPTIRSR LDEMIVLLDQY TANGTYGQYFNSDEPSLRDDAKMVVLELGGLED RPSLLVAVMFSLIYIENRMYRTPRNLKKNVIDEGWRLDFKNHKVGEFIEKGYRTARRHTGAYITITQNI VDFDSDKASSAARAAWGNSSYKIILKQSAKEFAKYNQLYPDQFLPQRDMIGKFGAAKDQWFSSFLQVENHSSWHRLFVDPLSRAMYSSDGPDFEFVQQKRKEGLSHEAVWQLA WKKSGPEMASLEAWLEEHEKYRSVA
TraW	210	16%	BAA97956 (cont.)	P18472	MRCRGLIALLIWGQSVAAADLGTWGDLPVKEPDMMLTVIMQRLTALEQSGEMGRKMDAFKERVIRNSLRPPAVPGIGRTEKYGSR LFDPSVRLAADIRDNEGRV FARQGEVMNPLQYVFPNQTL YFINGDDPAQVAWMKRQTPPTLESKIILVQGSIPEMQKSLDSRVYFDQNGVLCQRLGIDQV PARVSAVPGDRFLKVEFIPAEGRK
TrbC	212	29%	BAA97958	P18473	MKLSMKSLAALLMMLNGAVMASENVNTPENRQFLKQQENLSRQLREKPDHQLKAWAEKQVLENPLQRS DNHF LDELVRKQQASQDGKPRQGALYFVSFSIPEEGLKRMLGETRHF GIPATLRGMVNNDLKTAEAVLSLVKDGATDGVQIDPTLFSQYGIRTVPALVVFCSQGYDIIRGNLRV GQALEKVAATGDCRQVAHDLLAGKGD SGK
TraP	196	24%	BAA97949	P41068	MANNMSSRQACHAARYVVARVLRGLFWCLKYTVILPLATMALMALFVLWKDNTTPGKLLVKEINFVRQTAPAGQFPVSECFWSSSDSSGRSEIQGICHYRAADAADYVRETDRSLMQLVTALWATLALMYVSLAAITGKYVPRPGMKCIRVVTADEHLKEVYTEDASLPGKIRKCPVYLPDDR TNRNNGDKN EHA
TraE	188	11%	BAA97946	P08322	MEHGARLSTSRVMAIAFIMSVLIVLSLSVNVIQGVNNYRLQNEQRTAVTPMAFNAPFAV SQNSADASYLQQMALSFIALRLNVSSETVDASHQALLQYIRPGAQNQMKVILAEAEAKRIKNDNVNSAFFQTSVRVWPQYGRVEIRGV LK TWIGDSKPFTDIKH YILILKRENGVTWLDNFGETDDEKK
TraL	91	13%	BAA97945	P08321	MSGDENKLLKYRFPETLTNQSRWFLPLDELIPAAICIGWGITTSKYLFGIGA AVL VYFGIKK LKKG RGSSWLRDLIYWYMP TALLRGIFS

TraH	458	25%	BAA97968	P15069	<p> MMPRIKPLLVLCAALLT VTPAASADVNSDMNQFFNKLGFASNTTQPGVWQGOAAGYAYGGSLYA  RTQVKNVQLISM TLPDINAGCGGIDAYLGSFSFINQEQLQRFVKQIMSNAAGYFFDLALQTTVPEIK  TAKDFLQKMASDINSMNLSSCQAAQGIIGGLFPRTQVSQQKVCQDIAGESNIFADWAASRQGCTVG  GKSDSVRDKASDKDKERVTKNINIMWNALSKNRMFDGNKELKEFVMTLTGSLVFGPNGEITPLSA  RTTDRSIIRAMMEGGTAKISHCNDSDKCLKVVADTPVTISRDNALKSQITKLLASIQNKA VSDTPLD  DKEKGFISSTTIPVFKYL VDPQMLGVSNSMIYQLTDYIGYDILLQYIQELIQQARAMVATGNIDEAV  IGHINDNMNDATRQIAAFQSQVQVQQDALLVVDQRMSYMRQQLSARMLSRYQNNYHFGGSTL </p>
TrbI	128	23%	BAA97955	P18006	<p> MSSTQKPADVTAERRSHWWVTPVPGCLAMVLLNAAVSYGIVRLNAPVTVAFNMKQTVDAFFDSA  SQKQLSEAQSKALSARFNTALEASLQAWQQKHHAVILVSPA VVQGAPDITREIQQDIARRMRAEP </p>
TraN	602	25%	BAA97959	P24082	<p> MKRILPLILALVAGMAQADSNSDYRAGSDFAHQIKGGQSSSIQGFKPQESIPGYNANPDETKYYGG  VTAGGDGGLKNDGTTEWATGETGKTITESFMNKPKDILSPDAPFIQTGRDVVNRADSIVGNTGQQC  SAQEISRSEYTNYT CERDLQVEQYCTR TARMELQGSTTWETRTLEYEMS QLPAREVNGQYVVSITS  PVTGEIVDAHYSWSR TYLQKSVPMITITVLGTPLSWNAKYSADASFTPVQKTLTAGVAFTSSHPVRV  GNTKFKRHTAMKRLRVVRVKKASYTPYVWVWSESCPFSEKELGKLTKECTEAGGNRTL VKDGQSY  SMYQSCWAYRDTYVTQSADKGTCTYTDNPACTLVSHQCAFYSEEACLHEYATYSCESKTS GK  VMVCGGDVFLDGEDKAQSGKSNDFAEAVSQAALAAAGKDVAALNGVDVRAFTGQAKFKCK  AAAGYSNCCKDSGWGQDIGLAKCSDEKALAKAKSNKLTVSVGEFCSK KVLGVCLEKKRSYCF  DSKLAQIVQQQRNGQLRISFGSAKHPDCRGITVDELQKIQFNRLDFTNFYEDLMNNQKIPDSGVLT  QKVKEQIADQLKQAGQ </p>
TraG	938	43%	BAA97969	P33790	<p> MNEVYVIAGGEWLRNNLNAIAAFMGTWTWDSIEKIALTSLVLA VAVMVVQRHNVMDDL GWVA  VFVLISLLVNRVTSVQIHDNSDLVKVHRVDNVPVGLAMPLSLTTRIGHAMVASYEMIFTQPDSVTYS  KTGMLFGANLIVKSTDFLSRNPEIINLFQDYVQNCVLGDIYLNHKYTLEDLMASADPYTLIFSRPSPL  RGVYDNNNNFITCKDASVTLKDRNLNLDTKTGGKTWHYVYVQQIFGGRPD PDLFRQLVSDSYSYFY  GSSQSASQIMRQNVMTNALKEGITSNAARNGDTASLVSLATTSSMEKQRLAHVSIGHVTMRNLPM  VQILTGIAIGIFPLLILAAVFNKLTLSVLKGYVFALMWLQTWPLLYAILNSAMTFYAKQNGAPVVL  SELSQIQLKYSNLASTAGYLSAMIPPLSWMMVKGLGAGFSSVYSHFASSSISPTASAAGSVVDGNYS  YGNMQTENVNGFSWSTNSTTSFGQMMYQTGSGATATQTRDGNMVMMDASGAMSRLPVGINATRQ  IAAAQQEMAREASNRAESALHGFSSSIA SAWNTLSQFGSNRGSSDSVTGGADSTMSAQDSMMASR  MRSAVESYAKAHNISNEQATRELASRSTNASLGLYGDAYAKGHLGISVLGNGGGVGLQAGAKASI  DGSDLDSHEASSGSRASHDARHDIDARATQDFKEASDYFTSRKVSESGSHTDNNADSRVDQLSAAL  NSAKQSYDQYTTNMTRSHEYAEMASRTESMSGQMSDLSQQFAQYVMKNAPQDVEAILTNTSSP  EIAERRAMAWSFVQEQVQPGVDNTWRESRRDIGKGMESVPSGGGSQDIADHQGHQAIIERTQD  SNIRNDVKHQVDNMVTEYRGNIGDTQNSIRGEENIVKGQYSELQNHKTEAL TQNNKYNEEKLAQ  ERIPGADSPKELLEKAKSYQHKE </p>
TraU	330	26%	BAA97957	P18471	<p> MKRRLWLLMLFLFAGHVPAAASADSACEGRFVN PITDICWSCIFPLSLGSIKVSQGV PDTANPSMPI  QICPAPPPLFRRI GLAIGYWEPMALTDVTRSPGCMVNLGFSLPAFGKTAQGTAKKDEKQVNGAFYH  VHWYKYPLTYWLNITSLGCL EGGDMEDIAYLSEIDPTWTDSSLTTILNPEAVIFANPIAQGACAADAI  ASAFNMPLDVLFWCAGSQGSMYPFNGWVSNESPLQSSLLVSERMAFKLHRQGMIMETIGKNNAV  CNEYPSILPKERWRYQMVMNMYPDSGQCHPFGRSVTRWETGKNPENTKKNFGYLMWRKRNCVFL </p>

TraI	1756	20%	BAA97974	P14565	MMSIAQVRSAGSAGNYITDKDNYVVLGSMGERWAGRGAEQLGLQGSVDKDVFTRLLEGRLPDG ADLSRMQDGSNRHRPGYDLTFSAPKSVSMAMLGDKRLIDAHNQAVIDFAVRQVEALASTRVM TDGQSETVLTGNLVMALFNHDTSRDQEPQLHTHAVVANVTQHNGEWKTLSSDKVGKTGFIENVY ANQIAFGRLYREKLKEQVEALGYETEYVVGKHGMWEMPGVPVEAFSGRSQTIREAVGEDASLKSRD VAALDTRKSKQHVDPEIKMAEWMQTLKETGFDIRAYRDAADQRADLRLTPGPASQDGPDVQQA VTQAIAGLSERKVQFTYTDVLRARTVGILPPENGVIERARAGIDEAISREQLIPLDREKGLFTSGIHVLD ELSVRALS RDIMKQNRVTVHPEKSVPRTAGYSDAVSVLAQDRPSLAIVSGQGGAGQRERVAELV MMAREQGREVQIIAADRRSQMNMKQDERLSGELITGRRQLLEGMAFTPGSTVIVDQGEKLSLKET LTLLDGAARHNVQVLITDSGQRTGTGSALMAMKDAGVNTYRWQGGEQRPATIISEPDRNVRYAR LAGDFAASVKAGEESVAQVSGVREQAILTQAIRSELKTQGVGLLPEVTMTALSPVWLDSSRSRYLRD MYRPGMVMEQWNPETRS HDRYVIDRVTAQSHSLTLRDAQGETQVVRISLSDSSWSLFRPEKMPVA DGERLRVTGKIPGLRVSGGDR LQVASVSEDAMTVVVPGRAEPATLPVSDSPFTALKLENGWVETP GHSVSDSATVFASVTQMAMDNATLNGLARSGRDVRLYSSLDETRTAEKLARHPSFTV VSEQIKTR AGETSLETAISHQKSALHTPAQQAIHLALPVVESKLA FMSVDLLTEAKSFAAEGTGFTLGGEINA QIKRGDLLYVDVAKGYGTGLLVS RASYEAEKSILRHILEGKEAVMPLMERVPELMKELTSGQRA ATRMILETS DRFTVVQGYAGVGKTTQFRVMSAVNMLPESERPRV VGLGPHTRAVGEMRSQVD AQT LASFLHDTQLQQRSGETPDFSNTLFLLD ESSMVGNTDMARAYALIAAGGGRAVASGDTDQLQ AIAPGQPFRLQQTRSAADVAIMKEIVRQTPELREAVYSLINRDVERALSGLESVKPSQVPRQEGAW APEHSVTEFSHSQEAKLAE AQKAMLKGEAFPDVPMTLYEAIVRDYTGRTPEAREQTLIVTHLNED RRVLNSMIHDVREKAGELGKEQVMVPVLNTANIRDGELRRLSTWETHRDALVLVDNVYHRIAGIS KDDGLITLQDAEGNTRLISP REVAEGVTL YTPDTIRVGTGDRMRFTKSDRERGYVANSVWTVTA VSGDSVTLSDGQQTREIRPGQEQA EQHIDLAYAITAHGAQGASETFAIALEGTEGNRKL MAGFESA YVALSRMKQHVVYTDNRQGWTDAINNAVQKGT AHDVFEPKPDREVMNAERLFSTARELRDVA AGRAVLRQAGLAGGDS PARFIAPGRKYPQYVALPAFDRNGKSAGIWLNPLTTDDGNGLRGFSGE GRVKGSGDAQFVALQGS RNGESLLADNMQDGVRIARDNPDSGVVVRIAGEGRPWNPGAITGGRV WGDIPDNSVQPGAGNGEPVTA EVLAQRQAEEAIRRETERRADEIVRKM AENKPDLPDGKTEQAVR EIAGQERDRAAITEREAALPEGV LREPQRVREAVREIARENLLQERLQQMERDMVRDLQKEKTLG GD
TraY	131	25%	BAA97943	P06627	MKRFGTRSATGKMVKLKL PVDVESLLIEASNRSGRSRSFEAVIRLKDHLHRYPKFN RAGNIYGKSL VKYLTMRLDDETNQLLIAAKNRSGWCKTDEAADRVIDHLIKFPDFYNSEIFREADKEEDITFNTL
TraM	127	33%	BAA97941	P10026	MAKVNLYISNDAYEKINAIEKRRQEGAREKDV SFSATASMLLELGLRVHEAQMERKESAFNQTEF NKLLLECVVKTQSSVAKILGIESLSPHVS GNSKFEYANMVEDIREKVSSEMERFFPKNDDE

TraD	717	29%	BAA97972	P09130	MSFNAKDMTQGGQIASMRIRMFsqIANIMLYCLFIFFWILVGLVLWIKISWQTFVNGCIYWWCTTL EGMRDLIKSQPVYEIQYYGKTFRMNAAQVLHDKYMIWCSEQLWSAFVLAADVVALVICLITFFVVS WILGRQGGKQqSENEVTGGRQLTDNPKDVARMLKKDGKDSDIRIGDLPiIRDSEIQNFCLHGTVGAG KSEVIRRLANYARQGDMMVVIYDRSGEFVKSYYDPSIDKILNPLDARCAAWDLWKECLTQPDFDN TANTLIPMGTKEDPFwQGSgRTIFAEAAYLmRNDPNRSYSKLVDTLLSIKIEKLRTYLRNSPAANLV EEKIEKTAISIRAVLTNYVKAIrYLQqGIEHNGEpfTIRDWMRGVREDQKNGWLFISSNADTHASLKP VISMWLSIAIRGLLAMGENRNRrvWFFCDELPTLHKLpDLVEILPEARkFGGCYVFGIQSYAQLEDI YGEKAAASLFDVMNTRAFFRSPSHKIAEFAAGEIGEKEHLKASEQYSYGADPVRDGVSTGKDMER QTLVSYSDIQSLPDLTCYVTLPGPYPAVKLSLKYQTRPKVAPEFIPRDINPEMENRLSAVLAAREAE GRQMASLFEPDVPEVVSGEDVTQAEQPPQVSPAINDKKSDSGVNVpAGGIEQELKMKPEEEME QLPPGISESgeVVDMAAYEAwQqENHPDIQQMQRRREEVnINVHrERGEDVEPGDDF
TraT	244	34%	BAA97971	P13979	MMKTKKLMMVALVSSTLALSGCGAMSTAIKRNLEVKtQMSETIwLEPASERTVFLQIKNTSDKD MSGLQGKIADAVKAKGYQVVtSPDKAYYwIQANVLKADKMDLRESQGWLNrgYEGAAVGAAL GAGITGYNSNSAGATLGVGLAAGLVGMAADAMVEDVNYTMITDVQIAERTKATVTTDNVAALR QGTSGAKIQTSTETGNQHkyQTRVVSnANKVNLKFEEAKPVLEDQLAKSIANIL
TraS	173	8%	BAA97970	P09129	MITQqIISSEVLKkKHIDSGDIRIPSLWQGLKPLIIMGWMIFCPLLMSFLITQKTSETLTAVLAGGW LGLIILFIVARIRMLYFSLPEEFLKTSSVMRVISSKLKYFIVYMGVIFLWSFLGGGHIYFGGAILVTVI MAFLIQLDIGRYQFVGVIDAINSYVKNKkLSRVK

\*Disordered sequences of transfer proteins were predicted using the Phyre2 algorithm [1], using the amino acid sequences of the transfer proteins in FASTA format as input via the Phyre2 web interface. Results were manually collated from Phyre2 outputs, and regions of predicted disorder are shaded in grey in the amino acid sequences above.

## References

1. Kelley, L.A.; Sternberg, M.J.E. Protein structure prediction on the Web: a case study using the Phyre server. *Nat. Protoc.* **2009**, *4*, 363–371, doi:10.1038/nprot.2009.2.