

Supporting Information for the article:

**A Peptidomimetic Antibiotic Interacts with the Periplasmic Domain of LptD
from *Pseudomonas aeruginosa***

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- 1. PCR primers**
- 2. Homology modelling of *P. aeruginosa* LptD**
- 3. List of LptD/E peptides quantified by MS**

1. PCR primers

List of primers used to amplify *Pa* LptD and LptE from strain PAO1, with restriction sites underlined.

lptDfor atctacatatggcagtgaaatccctcg
lptDrev acaatggatccttacatagcttgatcttcacg
lptEfor ttacaccatgggcaaacgtatcctgaccagcgccgcgc
lptEhis6rev tacgtctcgagtc⁶aatggtgatgatggtgatgcggggtggggaactcgatcggcgactgc

2. Homology modelling of *P. aeruginosa* LptD

The full-length *P. aeruginosa* LptD (res. 34–924) comprises a C-terminal β -barrel domain (res. 324–924), a β jellyroll domain (res. 145–323), and an N-terminal insert domain (res. 45–144) characteristic of *Pseudomonas* spp. (Figure 2A). The recently solved X-ray structure of truncated *Pa* LptD/E (PDB 5IVA, residues 317–895) contains only the β -barrel domain.¹ A homology model of the conserved β jellyroll domain was generated after sequence alignment with the jellyroll domain in *Shigella flexneri* LptD (PDB 4Q35) (Figure S1).² The *Pa* jellyroll shows a sequence similarity of 47% (28% identity) with the aligned *Sf* LptD region (Table S1). An additional loop insertion between R165–K170 was adjusted manually and was energy minimized. The relative orientation of the β -jellyroll and the β -barrel domain in *Pa* LptD is likely to be very similar to that in the full-length *Sf* LptD structure based on a sequence alignment. In particular, the sequences of the region linking the β -jellyroll to the barrel in LptD from *P. aeruginosa* (I317–L326) and *Shigella flexneri* (V220–L229) contain highly conserved residues, indicating a similar fold in this region.

Attempts to identify secondary structure motifs or a protein homology template for the insert domain in *Pa* LptD using protein structure prediction methods (I-Tasser, MODELLER, PredictProtein, PSIPRED, JPRED, SwissModel) were unsuccessful. However, a sequence motif search in the PDB database with selected parts of the sequence provided similarities with a human V_H immunoglobulin (Ig) domain (PDB 1T2J) (Table S1 and Figure S2 and S3). After sequence alignment (25% sequence identity) a homology model was generated for the insert domain, with a truncated V_H-like fold. Interestingly, this model allows a disulfide to form between C49 and C134, which resembles an intra-domain disulfide commonly found in the Ig V_H fold, including bacterial Ig-like domains.³

Table S1. Sequence and structure comparisons of the jellyroll domain of *Pa* LptD with that of *Sf* LptD; and the N-terminal insert domain with the Ig-like domain (1T2J).

Alignment with <i>S. flexneri</i> LptD (PDB 4Q35)	Sequence identity	Sequence similarity	RMSD
jelly roll domain (G145–L326)	28 %	47 %	0.9 Å
Alignment with Ig-like domain PDB 1T2J			
Insert domain	25 %	34 %	1.1 Å

Figure S2. The sequence alignment of the insert domain (res. 45–146) of *P. aeruginosa* LptD and the Ig-like V_H domain (PDB file 1T2J). The β -strands (A1–G) in the V_H domain (1T2J) are indicated, with only the seven predicted β -strands B–F present in the model of the insert domain.

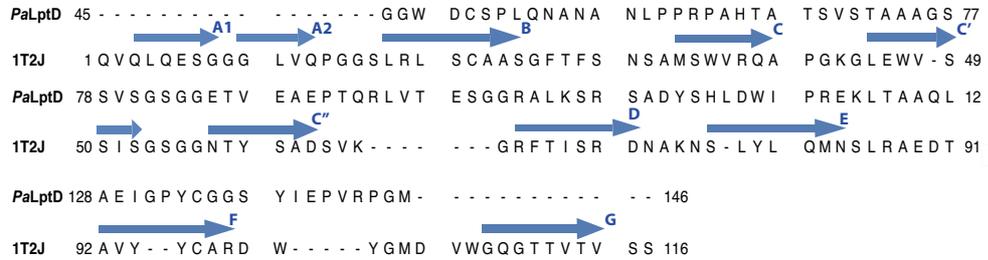
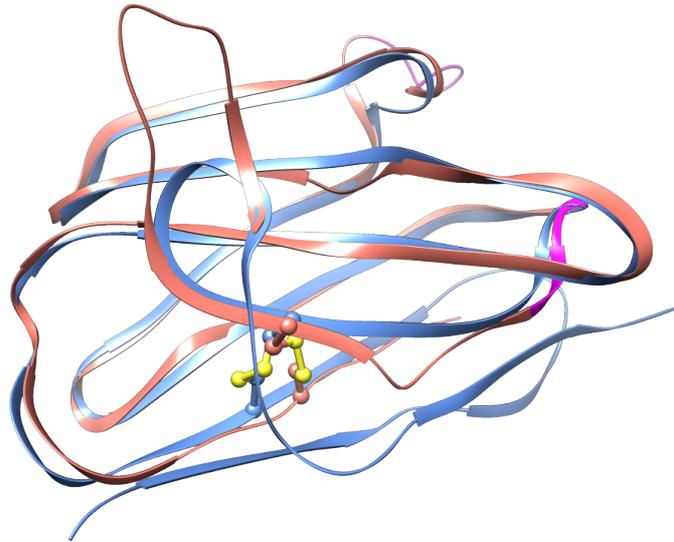


Figure S3. Superposition of a homology model of the N-terminal insert domain of *Pa* LptD (*red*, res. 45-144) with the Ig V_H domain (*blue*, 1T2J). The disulfide bridge in both proteins is displayed in ball-and-stick representation.



3. List of LptD/E peptides quantified by MS

Table S2. List of LptD/E peptides quantified by MS with measured abundance fold change upon photo-crosslinking with photoprobe **PAL6**. Peptides are sorted according to protein domain (insert orange; jellyroll purple; β -barrel green; LptE light blue), green and red arrows indicate biologically significant up- and downregulation (\log_2 fold change $> \pm 0.58$) and stars indicate statistically significant abundance changes (q -value < 0.05). The ETV (res. 85-87) and ENR (res. 199-201) sequence motifs of LptD insert and jellyroll domain, respectively, are highlighted in bold.

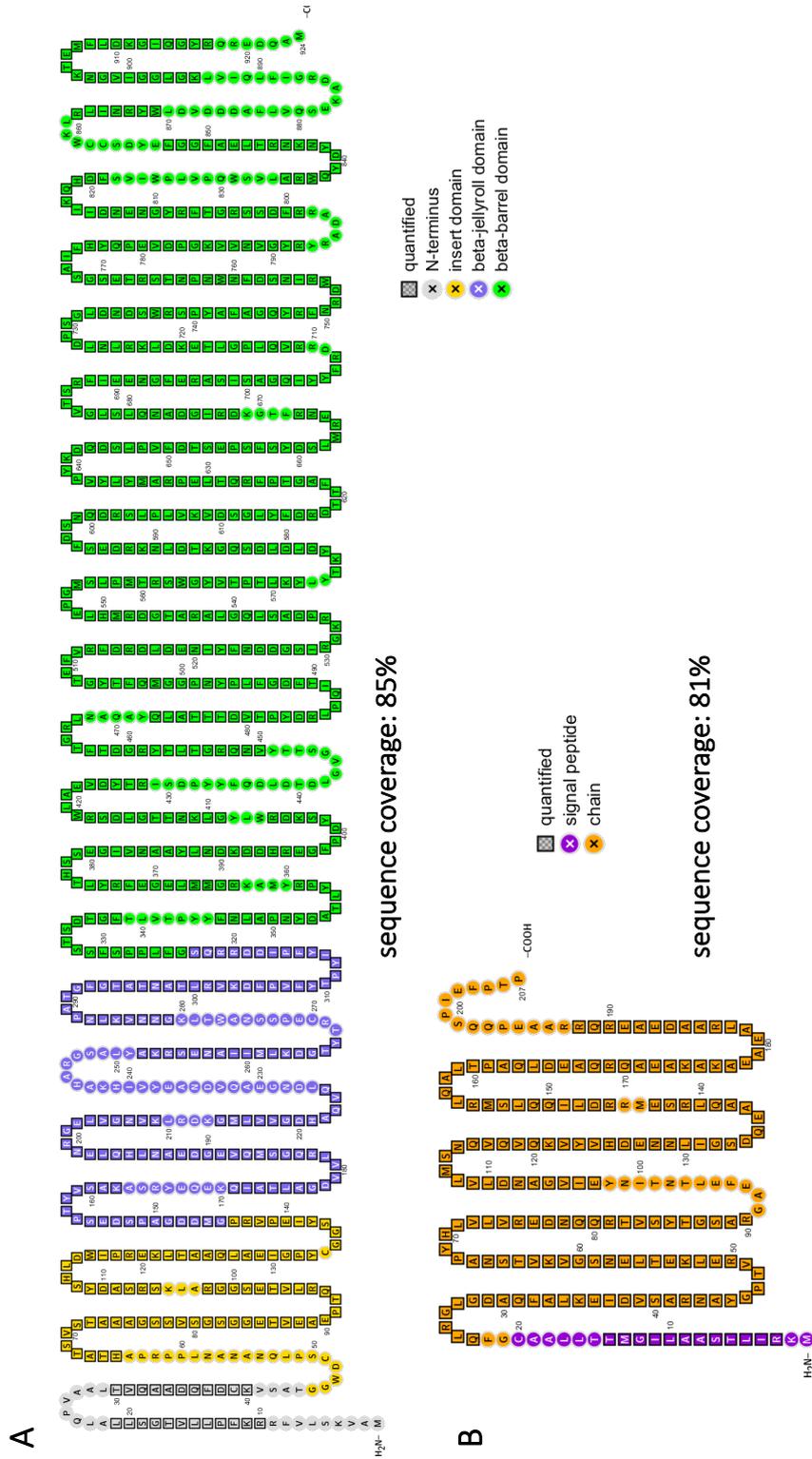
Protein_Entry	Protein_Domain	Sequence	log2 peptide abundance ratio (labeled vs unlabeled)	q-value	res. start	res. end	res. mid	
LptD_Q915U2	LptD_N-term	RKFPLLVTG	↓	-2.040997028	0.115974819	10	18	14
LptD_Q915U2	LptD_N-term	KFPLLVTGSL	↓	-1.882098794	0.117390029	11	21	16
LptD_Q915U2	LptD_N-term	TVQAADQFDCK	↓	-3.214735508	0.051356677	30	40	35
LptD_Q915U2	LptD_N-term	ADQFDCK	↓	-0.630928218	0.214706988	34	40	37
LptD_Q915U2	LptD_insert	HTATSVSTAAAGSSVSGSGGETVEAEPTQR	↓	-0.217327505	0.354243686	65	94	79.5
LptD_Q915U2	LptD_insert	ATSVSTAAAGSSVSGSGGETVEAEPTQR	↓	-0.59875536	0.217521852	67	94	80.5
LptD_Q915U2	LptD_insert	TSVSTAAAGSSVSGSGGETVEAEPTQR	↓	-0.444552869	0.214665569	68	94	81
LptD_Q915U2	LptD_insert	SVSTAAAGSSVSGSGGETVEAEPTQR	↓	-0.983084142	0.047897219	69	94	81.5
LptD_Q915U2	LptD_insert	STAAAGSSVSGSGGETVEAEPTQR	↓	-0.550596356	0.027008595	71	94	82.5
LptD_Q915U2	LptD_insert	TAAAGSSVSGSGGETVEAEPTQR	↓	-0.329122514	0.066812974	72	94	83
LptD_Q915U2	LptD_insert	AAAGSSVSGSGGETVEAEPTQR	↓	-1.136440396	0.010446344	73	94	83.5
LptD_Q915U2	LptD_insert	AAGSSVSGSGGETVEAEPTQR	↓	-0.678272367	0.017491654	74	94	84
LptD_Q915U2	LptD_insert	AGSSVSGSGGETVEAEPTQR	↓	-1.164577842	0.003100856	75	94	84.5
LptD_Q915U2	LptD_insert	GSSVSGSGGETVEAEPTQR	↓	-0.854492605	0.009896912	76	94	85
LptD_Q915U2	LptD_insert	SSVSGSGGETVEAEPTQR	↓	-1.291841507	0.027850968	77	94	85.5
LptD_Q915U2	LptD_insert	SVSGSGGETVEAEPTQR	↓	-1.12938714	0.003100856	78	94	86
LptD_Q915U2	LptD_insert	VSGSGGETVEAEPTQR	↓	-1.547986388	0.028230588	79	94	86.5
LptD_Q915U2	LptD_insert	SGSGGETVEAEPTQR	↓	-2.279568911	0.018926199	80	94	87
LptD_Q915U2	LptD_insert	GSGETVEAEPTQR	↓	-2.481119394	0.010446344	81	94	87.5
LptD_Q915U2	LptD_insert	SGGETVEAEPTQR	↓	-1.491169095	0.012765388	82	94	88
LptD_Q915U2	LptD_insert	GGETVEAEPTQR	↓	-1.692623854	0.018926199	83	94	88.5
LptD_Q915U2	LptD_insert	GETVEAEPTQR	↓	-0.910798073	0.027850968	84	94	89
LptD_Q915U2	LptD_insert	ETVEAEPTQR	↓	-1.175467849	0.048035412	85	94	89.5
LptD_Q915U2	LptD_insert	LVTESGGR	↓	0.463142902	0.214706988	95	102	98.5
LptD_Q915U2	LptD_insert	SADYSHLD	↓	-0.176817909	0.354243686	108	115	111.5
LptD_Q915U2	LptD_insert	SRSADYSHLDWIPR	↓	-0.092073843	0.355569525	106	119	112.5
LptD_Q915U2	LptD_insert	RSADYSHLDWIPR	↓	-0.430961996	0.166074273	107	119	113
LptD_Q915U2	LptD_insert	SADYSHLDWIP	↑	0.612305164	0.300707638	108	118	113
LptD_Q915U2	LptD_insert	SADYSHLDWIPR	↓	0.350829512	0.048035412	108	119	113.5
LptD_Q915U2	LptD_insert	SRSADYSHLDWIPREK	↓	-1.690024734	0.207438575	106	121	113.5
LptD_Q915U2	LptD_insert	RSADYSHLDWIPREK	↓	-1.340161443	0.008871141	107	121	114
LptD_Q915U2	LptD_insert	ADYSHLDWIPR	↓	-0.331701308	0.185066874	109	119	114
LptD_Q915U2	LptD_insert	SADYSHLDWIPREK	↓	-0.8045609	0.012765388	108	121	114.5
LptD_Q915U2	LptD_insert	DYSHLDWIPR	↓	-0.448816329	0.122743975	110	119	114.5
LptD_Q915U2	LptD_insert	SHLDWIPR	↓	-0.563129544	0.19170552	112	119	115.5
LptD_Q915U2	LptD_insert	SHLDWIPREK	↓	-1.572404981	0.048035412	112	121	116.5
LptD_Q915U2	LptD_insert	LTAQLAEIGPY	↓	-1.046897054	0.075861777	122	133	127.5
LptD_Q915U2	LptD_insert	TAAQLAEIGPY	↓	-1.038890004	0.192342847	123	133	128
LptD_Q915U2	LptD_jellyroll	GGSYIEPVRPGMDDGAPSDSPYVSAAK	↓	-0.521354496	0.039970343	135	162	148.5
LptD_Q915U2	LptD_jellyroll	IEPVRPGMDDGAPSDSPYVSAAK	↓	-0.491692424	0.105502071	139	162	150.5
LptD_Q915U2	LptD_jellyroll	EPVRPGMDDGAPSDSPYVSAAK	↓	-0.023788407	0.414187506	140	162	151
LptD_Q915U2	LptD_jellyroll	VRPGMDDGAPSDSPYVSAAK	↓	-0.130741015	0.246634107	140	162	152
LptD_Q915U2	LptD_jellyroll	APSDSPYVSAAK	↑	0.633911848	0.127877563	152	162	156
LptD_Q915U2	LptD_jellyroll	SDSPYVSAAK	↓	-0.426079661	0.192196407	152	162	157
LptD_Q915U2	LptD_jellyroll	SDPYVSAAK	↓	-1.902620554	0.033886088	153	162	157.5
LptD_Q915U2	LptD_jellyroll	ESPTYVSAAK	↓	-0.173785254	0.298631471	154	162	158
LptD_Q915U2	LptD_jellyroll	QIATLAGDVVLR	↑	1.048849225	0.075861777	171	182	176.5
LptD_Q915U2	LptD_jellyroll	IATLAGDVVLR	↓	-0.932461739	0.069464716	172	182	177
LptD_Q915U2	LptD_jellyroll	QIATLAGDVVLRQ	↓	-0.607531548	0.135494965	171	183	177
LptD_Q915U2	LptD_jellyroll	ATLAGDVVLR	↓	-0.270619184	0.227557489	173	182	177.5
LptD_Q915U2	LptD_jellyroll	TLAGDVVLR	↓	-2.642323971	0.021529266	174	182	178
LptD_Q915U2	LptD_jellyroll	QGSMSQVEGDEANLH	↓	-0.963671088	0.010446344	183	196	189.5
LptD_Q915U2	LptD_jellyroll	QGSMSQVEGDEANLHQL	↓	-1.067395926	0.091345866	183	198	190.5
LptD_Q915U2	LptD_jellyroll	QGSMSQVEGDEANLHQLENR	↓	-0.573159099	0.012765388	183	201	192
LptD_Q915U2	LptD_jellyroll	GSMQVEGDEANLHQLENR	↓	-2.675170183	0.000192023	184	201	192.5
LptD_Q915U2	LptD_jellyroll	QVEGDEANLHQLENR	↓	-3.816850424	0.000208482	187	201	194
LptD_Q915U2	LptD_jellyroll	RQGSMSQVEGDEANLHQLENRGELVGNVK	↓	-1.801071405	0.215741445	182	209	195.5
LptD_Q915U2	LptD_jellyroll	DEANLHQLENR	↓	-3.769959927	0.075861777	191	201	196
LptD_Q915U2	LptD_jellyroll	QGSMSQVEGDEANLHQLENRGELVGNVK	↓	-1.521563172	0.225693443	183	209	196
LptD_Q915U2	LptD_jellyroll	GSMQVEGDEANLHQLENRGELVGNVK	↓	-2.532865047	0.055274521	184	209	196.5
LptD_Q915U2	LptD_jellyroll	SMQVEGDEANLHQLENRGELVGNVK	↓	-1.673057318	0.061870683	185	209	197
LptD_Q915U2	LptD_jellyroll	QVEGDEANLHQLENRGELVGNVK	↓	-3.490809441	2.77E-05	187	209	198
LptD_Q915U2	LptD_jellyroll	VEGDEANLHQLENRGELVGNVK	↓	-2.8448174	0.048252212	188	209	198.5
LptD_Q915U2	LptD_jellyroll	GDEANLHQLENRGELVGNVK	↓	-3.346674442	0.005553289	190	209	199.5
LptD_Q915U2	LptD_jellyroll	DEANLHQLENRGELVGNVK	↓	-3.348915577	0.000192023	191	209	200
LptD_Q915U2	LptD_jellyroll	NLHQLENRGELVGNVK	↓	-0.813192546	0.098444485	194	209	201.5
LptD_Q915U2	LptD_jellyroll	HQLENRGELVGNVK	↓	-0.315098852	0.289724484	196	209	202.5
LptD_Q915U2	LptD_jellyroll	QLENRGELVGNVK	↓	-1.553606391	0.002792038	197	209	203
LptD_Q915U2	LptD_jellyroll	ENRGELVGNVK	↓	-1.958863497	0.002792038	199	209	204
LptD_Q915U2	LptD_jellyroll	NRGELVGNVK	↓	-0.720071316	0.03871991	200	209	204.5
LptD_Q915U2	LptD_jellyroll	RGELVGNVK	↓	-1.138474107	0.065972922	201	209	205
LptD_Q915U2	LptD_jellyroll	GELVGNVK	↓	-0.1405541	0.234545679	202	209	205.5
LptD_Q915U2	LptD_jellyroll	GMLVVGDDHA	↓	-1.391724944	0.091345866	214	222	218
LptD_Q915U2	LptD_jellyroll	GMLVVGDDHAQ	↓	-1.489968777	0.079018305	214	223	218.5
LptD_Q915U2	LptD_jellyroll	GMLVVGDDHAQVQ	↓	-2.466878891	0.008871141	214	225	219.5
LptD_Q915U2	LptD_jellyroll	RSENAIIM	↓	-0.806384921	0.030361387	254	261	257.5
LptD_Q915U2	LptD_jellyroll	AKRSENAIIMLK	↓	-1.457039475	0.069464716	252	263	257.5
LptD_Q915U2	LptD_jellyroll	KRSENAIIMLK	↓	-2.371243715	0.081530898	253	263	258
LptD_Q915U2	LptD_jellyroll	RSENAIIMLK	↓	-0.94785738	0.012765388	254	263	258.5
LptD_Q915U2	LptD_jellyroll	SENAIIMLK	↓	-0.62841481	0.018926199	255	263	259
LptD_Q915U2	LptD_jellyroll	ENAIIMLK	↓	-0.825141668	0.026849047	256	263	259.5

LptD_Q915U2	LptD_jellyroll	NAIIMLK		-0.487929344	0.217521852	257	263	260
LptD_Q915U2	LptD_jellyroll	RSENAIIMKLDGTY	↓	-0.769421577	0.079018305	254	267	260.5
LptD_Q915U2	LptD_jellyroll	GNNVKLNPA	↓	-0.783953428	0.144246783	281	289	285
LptD_Q915U2	LptD_jellyroll	GNNVKLNPATGF		0.022684852	0.430059779	281	292	286.5
LptD_Q915U2	LptD_jellyroll	GNNVKLNPATGFGTATNATLR	↓	-1.307109237	0.066812974	281	301	291
LptD_Q915U2	LptD_jellyroll	LNPATGFGTAT	↑	0.585244715	0.096036725	286	296	291
LptD_Q915U2	LptD_jellyroll	LNPATGFGTATN		-0.23924762	0.075861777	286	297	291.5
LptD_Q915U2	LptD_jellyroll	LNPATGFGTATNA	↑	1.226473212	0.069474162	286	298	292
LptD_Q915U2	LptD_jellyroll	LNPATGFGTATNATLR		-0.404132217	0.06854365	286	301	293.5
LptD_Q915U2	LptD_jellyroll	NPATGFGTATNATLR	↓	-0.688337505	0.161737201	287	301	294
LptD_Q915U2	LptD_jellyroll	PATGFGTATNATLR		-0.441622168	0.200664428	288	301	294.5
LptD_Q915U2	LptD_jellyroll	TGFGTATNATLR		-0.133532733	0.109326548	290	301	295.5
LptD_Q915U2	LptD_jellyroll	GFGTATNATLR		0.110644333	0.406497531	291	301	296
LptD_Q915U2	LptD_jellyroll	FGTATNATLR	↑	0.998711467	0.097532897	292	301	296.5
LptD_Q915U2	LptD_jellyroll	GSTATNATLR	↓	-1.038866639	0.239044509	293	301	297
LptD_Q915U2	LptD_jellyroll	RVKDFPVFY		-0.148955762	0.378170193	301	309	305
LptD_Q915U2	LptD_jellyroll	VKDFPVFY		-0.506918132	0.160427482	302	309	305.5
LptD_Q915U2	LptD_jellyroll	RVKDFPVFYTPY		-0.472384959	0.261463431	301	312	306.5
LptD_Q915U2	LptD_jellyroll	DFPVFYTPY	↑	0.708630741	0.184737368	304	312	308
LptD_Q915U2	LptD_jellyroll	TPYIFYPDDR		0.01044932	0.4331092	310	320	315
LptD_Q915U2	LptD_jellyroll	TPYIFYPDDRR		0.5734846	0.298788162	310	321	315.5
LptD_Q915U2	LptD_jellyroll	IYFPIDRR		0.08093337	0.14060694	313	320	316.5
LptD_Q915U2	LptD_jellyroll	IYFPIDRR		0.239288807	0.204875249	313	321	317
LptD_Q915U2	LptD_jellyroll	FPIDRR	↑	3.687490463	0.072933362	315	321	318
LptD_Q915U2	LptD_beta-barrel	RQSGFLPPSFSSDSTGFG	↑	0.90501821	0.248415794	321	338	329.5
LptD_Q915U2	LptD_beta-barrel	QSGFLPPSFSSDSTGFG	↑	2.571289301	0.192342847	322	338	330
LptD_Q915U2	LptD_beta-barrel	NLAPNYDATLY	↓	-2.847301722	0.069375849	347	357	352
LptD_Q915U2	LptD_beta-barrel	FNLPAPNYDATLYPR		-0.055968951	0.406497531	346	359	352.5
LptD_Q915U2	LptD_beta-barrel	NLAPNYDATLYPR		0.000874972	0.433766395	347	359	353
LptD_Q915U2	LptD_beta-barrel	LAPNYDATLYPR		0.272662222	0.079528178	348	359	353.5
LptD_Q915U2	LptD_beta-barrel	APNYDATLYPR		0.111144736	0.354243686	349	359	354
LptD_Q915U2	LptD_beta-barrel	YDATLYPR	↑	0.923169136	0.075861777	352	359	355.5
LptD_Q915U2	LptD_beta-barrel	DATLYPR	↑	0.707713187	0.039891336	353	359	356
LptD_Q915U2	LptD_beta-barrel	RGMMLEGEF	↓	-2.374005556	0.200664428	364	372	368
LptD_Q915U2	LptD_beta-barrel	RGMMLEGEFR	★	0.375829458	0.025274617	364	373	368.5
LptD_Q915U2	LptD_beta-barrel	GMMLEGEFR		-0.340908647	0.299953527	365	373	369
LptD_Q915U2	LptD_beta-barrel	MMLEGEFR		0.191819623	0.298631471	366	373	369.5
LptD_Q915U2	LptD_beta-barrel	MLEGEFR	↑	0.940959215	0.047897219	367	373	370
LptD_Q915U2	LptD_beta-barrel	YLTHSSEGIVN		-0.049647253	0.257278096	374	384	379
LptD_Q915U2	LptD_beta-barrel	YLTHSSEGIVNA		0.239104569	0.278682655	374	385	379.5
LptD_Q915U2	LptD_beta-barrel	RYLTHSSEGIVNAAY	↓	-2.281217098	0.197228722	373	387	380
LptD_Q915U2	LptD_beta-barrel	YLTHSSEGIVNAA		0.005476057	0.430540477	374	386	380
LptD_Q915U2	LptD_beta-barrel	YLTHSSEGIVNAAAY		0.337806761	0.121031084	374	387	380.5
LptD_Q915U2	LptD_beta-barrel	YLTHSSEGIVNAAAYL		-0.272196084	0.355569525	374	388	381
LptD_Q915U2	LptD_beta-barrel	THSSEGIVNAAAY	↓	-0.726057649	0.265578305	376	387	381.5
LptD_Q915U2	LptD_beta-barrel	YLTHSSEGIVNAAAYLNKD	↑	-0.006207973	0.431316847	374	391	382.5
LptD_Q915U2	LptD_beta-barrel	LNKDHHREGFPDYSK	★	1.466746926	0.012765388	388	403	395.5
LptD_Q915U2	LptD_beta-barrel	DHREGFPDYSK		0.145248413	0.353549019	392	403	397.5
LptD_Q915U2	LptD_beta-barrel	EGFPDYSK	↓	-0.588537693	0.108957314	396	403	399.5
LptD_Q915U2	LptD_beta-barrel	EGFPDYSKDR		-0.539537191	0.075861777	396	405	400.5
LptD_Q915U2	LptD_beta-barrel	GLKNTTGLDSR	↓	-0.654536903	0.225693443	409	419	414
LptD_Q915U2	LptD_beta-barrel	NTTGLDSRW		0.123312972	0.354243686	412	420	416
LptD_Q915U2	LptD_beta-barrel	WLAEDVYTR	↑	2.441585541	0.091529665	420	428	424
LptD_Q915U2	LptD_beta-barrel	LAEDVYTR	↑	1.691240549	0.075861777	421	428	424.5
LptD_Q915U2	LptD_beta-barrel	AEVDYTR		0.371827334	0.284727388	422	428	425
LptD_Q915U2	LptD_beta-barrel	VNQRGTLTY	↓	-1.155394673	0.298631471	450	458	454
LptD_Q915U2	LptD_beta-barrel	GTLTYRGDTF	↓	-0.969043791	0.248920816	454	463	458.5
LptD_Q915U2	LptD_beta-barrel	TYRGDTF		-0.056044251	0.295769172	457	463	460
LptD_Q915U2	LptD_beta-barrel	GTLTYRGDTFTGR		0.072179228	0.420965192	454	466	460
LptD_Q915U2	LptD_beta-barrel	TYRGDTFTGR	↓	-0.925630748	0.151070422	457	466	461.5
LptD_Q915U2	LptD_beta-barrel	RGDTFTGR	↑	0.707967997	0.144246783	459	467	463
LptD_Q915U2	LptD_beta-barrel	GDTFTGR	↑	2.219792128	0.133036388	460	467	463.5
LptD_Q915U2	LptD_beta-barrel	QLATTTDVTVPYDR		0.536112726	0.244270274	473	485	479
LptD_Q915U2	LptD_beta-barrel	DRLPQITF	★	0.216809675	0.030765467	484	491	487.5
LptD_Q915U2	LptD_beta-barrel	DGPLPYPNGMQF		0.474513501	0.276982421	492	504	498
LptD_Q915U2	LptD_beta-barrel	NPGGMQFTY		-0.074114792	0.410431973	498	506	502
LptD_Q915U2	LptD_beta-barrel	TYGTEFVR	↑	1.079380631	0.088746937	505	512	508.5
LptD_Q915U2	LptD_beta-barrel	YGTTEFVR	↓	-1.605264664	0.19170552	506	512	509
LptD_Q915U2	LptD_beta-barrel	TYGTEFVRF		-0.468804568	0.225693443	505	513	509
LptD_Q915U2	LptD_beta-barrel	GTEFVRF	↓	-1.138354421	0.075861777	507	513	510
LptD_Q915U2	LptD_beta-barrel	TYGTEFVRFDOR		-0.160229325	0.298788162	505	515	510
LptD_Q915U2	LptD_beta-barrel	GTEFVRFDOR		-0.198910326	0.278682655	507	515	511
LptD_Q915U2	LptD_beta-barrel	FDRDLDENIY		0.264987707	0.298788162	513	522	517.5
LptD_Q915U2	LptD_beta-barrel	DRDLDENIY		-0.468898296	0.248099014	514	522	518
LptD_Q915U2	LptD_beta-barrel	IYFNDDGSIR	↑	1.085234284	0.119013716	521	530	525.5
LptD_Q915U2	LptD_beta-barrel	YFNDDGSIR		0.107036799	0.35671197	522	530	526
LptD_Q915U2	LptD_beta-barrel	FNDDGSIR		0.252874345	0.243319698	523	530	526.5
LptD_Q915U2	LptD_beta-barrel	FNDDGSIRGK		0.043595772	0.403778287	523	532	527.5
LptD_Q915U2	LptD_beta-barrel	GKRPDASLQ		-0.037007317	0.415039126	531	539	535
LptD_Q915U2	LptD_beta-barrel	GKRPDASLQGLA	↑	0.727592051	0.018926199	531	542	536.5
LptD_Q915U2	LptD_beta-barrel	GKRPDASLQGLAR	↑	0.651716709	0.082048537	531	543	537
LptD_Q915U2	LptD_beta-barrel	RPDASLQGL		-0.341858953	0.117390029	533	541	537
LptD_Q915U2	LptD_beta-barrel	RPDASLQGLA	↑	0.753582358	0.127877563	533	542	537.5
LptD_Q915U2	LptD_beta-barrel	RPDASLQGLAR		-0.398887753	0.134910573	533	543	538
LptD_Q915U2	LptD_beta-barrel	DASLQGLAR		-0.107186846	0.358931697	535	543	539
LptD_Q915U2	LptD_beta-barrel	ASLQGLAR	↓	-2.034970045	0.096036725	536	543	539.5
LptD_Q915U2	LptD_beta-barrel	ATGDRMHLEPGMSLPM	★	-0.510388732	0.048035412	544	559	551.5
LptD_Q915U2	LptD_beta-barrel	ATGDRMHLEPGMSLPMTR	★	-0.637015283	0.002792038	544	561	552.5
LptD_Q915U2	LptD_beta-barrel	MHLEPGMSL		0.206453219	0.416886736	549	557	553
LptD_Q915U2	LptD_beta-barrel	GDRMHLEPGMSLPMTR	★	1.428945541	0.002792038	546	561	553.5
LptD_Q915U2	LptD_beta-barrel	MHLEPGMSLPM		-0.30479753	0.248415794	549	559	554

LptD_Q915U2	LptD_beta-barrel	MHLEPGMSLPMTR		0.206948146	0.188853129	549	561	555
LptD_Q915U2	LptD_beta-barrel	HLEPGMSLPMTR		0.255927503	0.1687179	550	561	555.5
LptD_Q915U2	LptD_beta-barrel	LEPGMSLPMTR	↑	1.073154807	0.109630865	551	561	556
LptD_Q915U2	LptD_beta-barrel	EPGMSLPMTR	↓	-1.078237295	0.246634107	552	561	556.5
LptD_Q915U2	LptD_beta-barrel	SWGYYVPTLK		-0.172339231	0.26653118	562	571	566.5
LptD_Q915U2	LptD_beta-barrel	WGYVPTLTK	↑	2.716914654	0.027850968	563	571	567
LptD_Q915U2	LptD_beta-barrel	SWGYYVPTLKY	↑	0.835783064	0.277942369	562	572	567
LptD_Q915U2	LptD_beta-barrel	GYVPTLTK	↑	0.919792354	0.044414233	564	571	567.5
LptD_Q915U2	LptD_beta-barrel	TKYDLDLDSQGK	↑	1.155433774	0.048252212	575	586	580.5
LptD_Q915U2	LptD_beta-barrel	YDLDLDSQGK	↑	0.633354008	0.314604159	577	586	581.5
LptD_Q915U2	LptD_beta-barrel	DDLDSQGK		0.561847329	0.15421787	578	586	582
LptD_Q915U2	LptD_beta-barrel	YDLDLDSQGKTDLNK	↓	-1.016589046	0.028230588	577	591	584
LptD_Q915U2	LptD_beta-barrel	YDLDLDSQGKTDLNKR	↑	1.500206947	0.014652501	577	592	584.5
LptD_Q915U2	LptD_beta-barrel	DDLDSQGKTDLNK		-0.197909981	0.349417546	578	591	584.5
LptD_Q915U2	LptD_beta-barrel	DDLDSQGKTDLNKR		0.112526841	0.342027627	578	592	585
LptD_Q915U2	LptD_beta-barrel	TDLNKRDESFDSNQDR		0.38822031	0.091529665	587	602	594.5
LptD_Q915U2	LptD_beta-barrel	DLNKRDESFDSNQDR		-0.022067849	0.402069255	588	602	595
LptD_Q915U2	LptD_beta-barrel	NKRDESFDSNQDR		-0.362311244	0.179343952	590	602	596
LptD_Q915U2	LptD_beta-barrel	KRDESFDSNQDR	↓	-0.599866033	0.225693443	591	602	596.5
LptD_Q915U2	LptD_beta-barrel	RDESFDSNQDR	↓	-0.593821193	0.07261745	592	602	597
LptD_Q915U2	LptD_beta-barrel	DESFDSNQDR		0.471219301	0.19170552	593	602	597.5
LptD_Q915U2	LptD_beta-barrel	SLPLVKVDSGL		0.391217202	0.278682655	603	613	608
LptD_Q915U2	LptD_beta-barrel	SLPLVKVDSGLY	↓	-1.299883723	0.079018305	603	614	608.5
LptD_Q915U2	LptD_beta-barrel	VDSGLYFDR		0.332601011	0.234545679	609	617	613
LptD_Q915U2	LptD_beta-barrel	VDSGLYFDRDITFF		-0.141655058	0.24214517	609	621	615
LptD_Q915U2	LptD_beta-barrel	VDSGLYFDRDITFA		0.401721507	0.225344221	609	622	615.5
LptD_Q915U2	LptD_beta-barrel	YFDRDITFF		-0.093545012	0.376287671	614	621	617.5
LptD_Q915U2	LptD_beta-barrel	FDRDITFF		0.152773067	0.04183989	615	621	618
LptD_Q915U2	LptD_beta-barrel	VDSGLYFDRDITFAGTFFPR	↑	1.050641179	0.26653118	609	627	618
LptD_Q915U2	LptD_beta-barrel	FDRDITFAGTFF		0.144447193	0.359456689	615	626	620.5
LptD_Q915U2	LptD_beta-barrel	FDRDITFAGTFFPR	↓	-0.768832564	0.1687179	615	627	621
LptD_Q915U2	LptD_beta-barrel	DITFAGTFFPR		-0.091173127	0.355569525	618	627	622.5
LptD_Q915U2	LptD_beta-barrel	QTLLEPRA	↑	0.630236089	0.155460968	628	634	631
LptD_Q915U2	LptD_beta-barrel	AMYLYVVPYK	↑	0.844182789	0.180575133	634	642	638
LptD_Q915U2	LptD_beta-barrel	YLYVVPYK	↑	1.00317347	0.048035412	636	642	639
LptD_Q915U2	LptD_beta-barrel	KQDQSLPVDFDTSEPSFSY	↑	2.35209322	0.168944987	642	659	650.5
LptD_Q915U2	LptD_beta-barrel	DSLWRENR		0.312277585	0.354243686	660	667	663.5
LptD_Q915U2	LptD_beta-barrel	DRIGDANQL		0.415964037	0.07110223	672	680	676
LptD_Q915U2	LptD_beta-barrel	DRIGDANQLSL		-0.094817623	0.225693443	672	682	677
LptD_Q915U2	LptD_beta-barrel	DRIGDANQLSLGVTSR	↑	0.676760554	0.079018305	672	687	679.5
LptD_Q915U2	LptD_beta-barrel	IGDANQLSLGVTSR		-0.034312196	0.419732568	674	687	680.5
LptD_Q915U2	LptD_beta-barrel	ANQLSLGVTSR	↑	0.716999233	0.248415794	677	687	682
LptD_Q915U2	LptD_beta-barrel	SRFIEENGFER	↓	-1.146912098	0.069464716	686	696	691
LptD_Q915U2	LptD_beta-barrel	FIEENGFER		-0.245429292	0.31133005	688	696	692
LptD_Q915U2	LptD_beta-barrel	IEENGFER	↑	0.623226643	0.047321439	689	696	692.5
LptD_Q915U2	LptD_beta-barrel	FIEENGFERA		-0.01076164	0.427493701	688	697	692.5
LptD_Q915U2	LptD_beta-barrel	ASISAGQIY		-0.323325276	0.265707509	697	705	701
LptD_Q915U2	LptD_beta-barrel	ASISAGQIYY	↓	-3.084347486	0.168944987	697	706	701.5
LptD_Q915U2	LptD_beta-barrel	ASISAGQIYYFR		-0.454708338	0.217521852	697	708	702.5
LptD_Q915U2	LptD_beta-barrel	RVQLPGLTEK	↓	-1.442379355	0.227557489	711	720	715.5
LptD_Q915U2	LptD_beta-barrel	VQLPGLTEK		0.451734364	0.060953824	712	720	716
LptD_Q915U2	LptD_beta-barrel	QLPGLTEK	↑	0.82327944	0.075105573	713	720	716.5
LptD_Q915U2	LptD_beta-barrel	RVQLPGLTEKDLK		-0.21536617	0.301540116	711	723	717
LptD_Q915U2	LptD_beta-barrel	VQLPGLTEKDLK		-0.165921167	0.146472426	712	723	717.5
LptD_Q915U2	LptD_beta-barrel	VQLPGLTEKDLKR		-0.168745965	0.349417546	712	724	718
LptD_Q915U2	LptD_beta-barrel	RNLNPSGLDNDNSWR	↑	1.07182014	0.051356677	724	738	731
LptD_Q915U2	LptD_beta-barrel	LNLDPGSLDNDNSW	↑	1.160336852	0.214706988	725	737	731
LptD_Q915U2	LptD_beta-barrel	LNLDPGSLDNDNSWR		0.542779803	0.168911375	725	738	731.5
LptD_Q915U2	LptD_beta-barrel	NLDPSGLDNDNSWR		-0.113032863	0.393820025	726	738	732
LptD_Q915U2	LptD_beta-barrel	LDPGSLDNDNSWR	↑	0.611316085	0.051356677	727	738	732.5
LptD_Q915U2	LptD_beta-barrel	RNLNPSGLDNDNSWRSPY		-0.288519323	0.298788162	724	741	732.5
LptD_Q915U2	LptD_beta-barrel	DPSGLDNDNSWR	↓	-0.725672483	0.094479441	728	738	733
LptD_Q915U2	LptD_beta-barrel	PSGLDNDNSWR	↑	0.769068062	0.248099014	729	738	733.5
LptD_Q915U2	LptD_beta-barrel	SPYAFAGQYR	↑	0.861299038	0.260512643	739	748	743.5
LptD_Q915U2	LptD_beta-barrel	YAFAGQYR		0.42359972	0.234545679	741	748	744.5
LptD_Q915U2	LptD_beta-barrel	AFAGQYR		0.52125144	0.109326548	742	748	745
LptD_Q915U2	LptD_beta-barrel	RFNRDW		0.227481306	0.383116072	748	753	750.5
LptD_Q915U2	LptD_beta-barrel	FNRDWR	↑	1.026957035	0.018926199	749	754	751.5
LptD_Q915U2	LptD_beta-barrel	RINSDFNWNPNPNTSR	↓	-0.695811272	0.185066874	754	767	760.5
LptD_Q915U2	LptD_beta-barrel	INSDFNWNPNPNTSR		0.183201849	0.143716644	755	767	761
LptD_Q915U2	LptD_beta-barrel	NSDFNWNPNPNTSR		0.28691569	0.310351479	756	767	761.5
LptD_Q915U2	LptD_beta-barrel	SDFNWNPNPNTSR		0.043111909	0.382344886	757	767	762
LptD_Q915U2	LptD_beta-barrel	NWNPNPNTSR	↑	0.605584383	0.19170552	760	767	763.5
LptD_Q915U2	LptD_beta-barrel	INSDFNWNPNPNTSRTEGSGS		0.484191418	0.246634107	755	772	763.5
LptD_Q915U2	LptD_beta-barrel	NWNPNPNTSRTEGSGSAIF	↓	-1.430130124	0.108957314	760	775	767.5
LptD_Q915U2	LptD_beta-barrel	AIFHYQPEVDPGK	↑	3.290810585	0.103415096	773	785	779
LptD_Q915U2	LptD_beta-barrel	HYQPEVDPGK		0.333617598	0.107408623	776	785	780.5
LptD_Q915U2	LptD_beta-barrel	HYQPEVDPGKVVNVGY		0.561069608	0.091345866	776	791	783.5
LptD_Q915U2	LptD_beta-barrel	HYQPEVDPGKVVNVGYR		0.373797894	0.021513377	776	792	784
LptD_Q915U2	LptD_beta-barrel	DPGKVVNVGYR		0.150778919	0.314604159	782	792	787
LptD_Q915U2	LptD_beta-barrel	PGKVVNVGYR	↑	1.039623857	0.109326548	783	792	787.5
LptD_Q915U2	LptD_beta-barrel	GKVVNVGYR		0.510811508	0.225693443	784	792	788
LptD_Q915U2	LptD_beta-barrel	VNVNVGYR	↑	1.341169119	0.109326548	786	792	789
LptD_Q915U2	LptD_beta-barrel	RFDSSRGTF		-0.150891796	0.406497531	799	807	803
LptD_Q915U2	LptD_beta-barrel	RFDSSRGTFR	↓	-1.024472475	0.090460135	799	808	803.5
LptD_Q915U2	LptD_beta-barrel	FDSSRGTF	↓	-0.855354726	0.319324646	800	807	803.5
LptD_Q915U2	LptD_beta-barrel	RYGNENDIIK		-0.508812964	0.234545679	808	817	812.5
LptD_Q915U2	LptD_beta-barrel	YGNENDIIK		0.382027537	0.109326548	809	817	813
LptD_Q915U2	LptD_beta-barrel	YGNENDIIKQ		0.436732888	0.225693443	809	818	813.5
LptD_Q915U2	LptD_beta-barrel	GNENDIIKHDF	↓	-0.68250984	0.21024202	810	821	815.5
LptD_Q915U2	LptD_beta-barrel	WQYDYNK	↑	0.843273818	0.051356677	837	843	840

LptD_Q9I5U2	LptD_beta-barrel	ARWQYDYNKNR	↑	0.881101847	0.217521852	835	845	840
LptD_Q9I5U2	LptD_beta-barrel	WQYDYNKNR	↑	2.012160778 ★	0.026849047	837	845	841
LptD_Q9I5U2	LptD_beta-barrel	NRTLEAFGGF		-0.430461735	0.246634107	844	853	848.5
LptD_Q9I5U2	LptD_beta-barrel	RLINRY		0.523261726	0.205204127	863	868	865.5
LptD_Q9I5U2	LptD_beta-barrel	LINRYW	↑	0.823237956	0.065496864	864	869	866.5
LptD_Q9I5U2	LptD_beta-barrel	KGLGGIVGNK		-0.036972288	0.410768798	895	904	899.5
LptD_Q9I5U2	LptD_beta-barrel	GLGGIVGNK	↑	0.803203404 ★	0.03871991	896	904	900
LptD_Q9I5U2	LptD_beta-barrel	GLGGIVGNKTEM	↑	0.912104011	0.07261745	896	907	901.5
LptD_Q9I5U2	LptD_beta-barrel	GLGGIVGNKTEMF	↑	0.803023815 ★	0.018926199	896	908	902
LptD_Q9I5U2	LptD_beta-barrel	KGLGGIVGNKTEMFDDK		0.158829018	0.355569525	895	911	903
LptD_Q9I5U2	LptD_beta-barrel	GLGGIVGNKTEMFDDK	↑	0.644001722	0.055274521	896	911	903.5
LptD_Q9I5U2	LptD_beta-barrel	GGIVGNKTEMFDDK		0.119273081	0.33924152	898	911	904.5
LptD_Q9I5U2	LptD_beta-barrel	KTEMFDDK		0.577573717 ★	0.047897219	904	911	907.5
LptD_Q9I5U2	LptD_beta-barrel	TEMFDDK	↑	1.476521969 ★	0.021485715	905	911	908
LptD_Q9I5U2	LptD_beta-barrel	TEMFDDKGIQGYR	↑	1.106205583	0.19170552	905	917	911
LptD_Q9I5U2	LptD_beta-barrel	FLDKGIQGYR		0.264457405	0.161737201	908	917	912.5
LptD_Q9I5U2	LptD_beta-barrel	LDKGIQGYR		0.547606051	0.094479441	909	917	913
LptE_Q9HX32	LptE_signal peptide	RILTSAALIGMT	↓	-5.870284081	0.269511868	3	14	8.5
LptE_Q9HX32	LptE_chain	QRGLGDAQF	↑	1.027638316	0.121031084	23	32	27.5
LptE_Q9HX32	LptE_chain	ALKEIDVSAR	↑	1.231087446	0.075861777	33	42	37.5
LptE_Q9HX32	LptE_chain	EIDVSARN	↑	0.763617396	0.072163074	36	43	39.5
LptE_Q9HX32	LptE_chain	NAYGPTVR	↑	1.207088709	0.075861777	43	50	46.5
LptE_Q9HX32	LptE_chain	ELKETLENSGVK	↑	1.194216967 ★	0.002792038	51	62	56.5
LptE_Q9HX32	LptE_chain	LKETLENSGVK		-0.450332135	0.096036725	52	62	57
LptE_Q9HX32	LptE_chain	ELKETLENSGVKVT	↑	1.239287853	0.117390029	51	64	57.5
LptE_Q9HX32	LptE_chain	ETLENSGVKVT	↓	-2.371898943 ★	0.048252212	54	64	59
LptE_Q9HX32	LptE_chain	ELKETLENSGVKVTSNAPY	↑	0.759512365	0.217521852	51	69	60
LptE_Q9HX32	LptE_chain	VTSNAPYHLVLR		0.040338036	0.420420043	63	75	69
LptE_Q9HX32	LptE_chain	HLVLVREDNQQR		-0.020183044	0.3983820025	70	81	75.5
LptE_Q9HX32	LptE_chain	VLVREDNQQR		-0.546850204	0.055274521	72	81	76.5
LptE_Q9HX32	LptE_chain	VTSYTSGAR		-0.02596996	0.430059779	82	90	86
LptE_Q9HX32	LptE_chain	VSYTSGAR		0.34624666	0.349795519	83	90	86.5
LptE_Q9HX32	LptE_chain	EIVGANDLVMSNQVQVQK	↑	1.351752996 ★	0.012765388	103	121	112
LptE_Q9HX32	LptE_chain	VLSMNQVQVQK	↑	0.872299373 ★	0.018926199	111	121	116
LptE_Q9HX32	LptE_chain	MSNQVQVQK	↑	1.072729468 ★	0.03871991	113	121	117
LptE_Q9HX32	LptE_chain	MSNQVQVQVYVHDENNL	↑	1.897056341	0.267952649	113	130	121.5
LptE_Q9HX32	LptE_chain	VYVHDENNLIGSDQEAQAQ	↑	1.194699645	0.110275497	122	139	130.5
LptE_Q9HX32	LptE_chain	VYVHDENNLIGSDQEAQAQLR	↑	1.227746964 ★	0.027850968	122	141	131.5
LptE_Q9HX32	LptE_chain	VYVHDENNLIGSDQEAQAQLR		0.346918851	0.265578305	123	141	132
LptE_Q9HX32	LptE_chain	VYVHDENNLIGSDQEAQAQL	↓	-1.564569831	0.205774239	124	140	132
LptE_Q9HX32	LptE_chain	VYVHDENNLIGSDQEAQAQLRSE	↑	1.20427525 ★	0.018926199	122	143	132.5
LptE_Q9HX32	LptE_chain	VYVHDENNLIGSDQEAQAQLR		-0.196592867	0.1687179	124	141	132.5
LptE_Q9HX32	LptE_chain	HDENNLIGSDQEAQAQLR		0.158003435	0.327472688	125	141	133
LptE_Q9HX32	LptE_chain	DENNLIGSDQEAQAQLR		0.470982403	0.248920816	126	141	133.5
LptE_Q9HX32	LptE_chain	NLIGSDQEAQAQLR	↓	-1.040130258	0.160427482	129	141	135
LptE_Q9HX32	LptE_chain	LIGSDQEAQAQLR		0.446872681	0.107408623	130	141	135.5
LptE_Q9HX32	LptE_chain	GSQEAQAQLR	↑	1.130748749	0.096970269	132	141	136.5
LptE_Q9HX32	LptE_chain	RDLIQQL		-0.146960422	0.146953423	146	152	149
LptE_Q9HX32	LptE_chain	DUIQQLSM	↑	2.393887997	0.096461635	147	154	150.5
LptE_Q9HX32	LptE_chain	DLIQQLSMR	↓	-1.328466654	0.074846657	147	155	151
LptE_Q9HX32	LptE_chain	RLQALTPAQLDEAQR		0.52057147	0.123873576	155	169	162
LptE_Q9HX32	LptE_chain	LQALTPAQLDEAQR		0.117787793	0.19170552	156	169	162.5
LptE_Q9HX32	LptE_chain	QALTPAQLDEAQR	↑	0.915397823 ★	0.027850968	157	169	163
LptE_Q9HX32	LptE_chain	ALTPAQLDEAQR	↑	0.675958455 ★	0.047897219	158	169	163.5
LptE_Q9HX32	LptE_chain	LTPAQLDEAQR		0.07412982	0.399831839	159	169	164
LptE_Q9HX32	LptE_chain	TPAQLDEAQR		0.170436874	0.260512643	160	169	164.5
LptE_Q9HX32	LptE_chain	RLQALTPAQLDEAQRQAEAK		-0.129322007	0.248415794	155	174	164.5
LptE_Q9HX32	LptE_chain	LQALTPAQLDEAQRQAEAK		-0.254166782	0.234545679	156	174	165
LptE_Q9HX32	LptE_chain	QALTPAQLDEAQRQAEAK		-0.359755039	0.088746937	157	174	165.5
LptE_Q9HX32	LptE_chain	ALTPAQLDEAQRQAEAK		0.115570195	0.378205953	158	174	166
LptE_Q9HX32	LptE_chain	QLDEAQRQAEAK		-0.018595796	0.420420043	163	174	168.5
LptE_Q9HX32	LptE_chain	AKAEAEAL		0.301512808	0.299122762	175	182	178.5
LptE_Q9HX32	LptE_chain	AKAEAEALR		-0.281902552	0.255624397	175	183	179
LptE_Q9HX32	LptE_chain	AKAEAEALRA	↑	1.546369195 ★	0.018926199	175	184	179.5
LptE_Q9HX32	LptE_chain	AKAEAEALRAADEAER		0.430291444	0.065496864	175	190	182.5
LptE_Q9HX32	LptE_chain	KAEAEALRAADEAER	↑	0.733445227 ★	0.044414233	176	190	183
LptE_Q9HX32	LptE_chain	AEAEALRAADEAER		0.031132117	0.380267337	177	190	183.5
LptE_Q9HX32	LptE_chain	EAEALRAADEAER		0.407705933	0.292279534	178	190	184
LptE_Q9HX32	LptE_chain	AEALRAADEAER		0.341715336	0.146953423	179	190	184.5
LptE_Q9HX32	LptE_chain	AEAEALRAADEAERQR		-0.189107805	0.170819546	177	192	184.5
LptE_Q9HX32	LptE_chain	EALRAADEAER	↑	0.612682521	0.107408623	180	190	185
LptE_Q9HX32	LptE_chain	ALRAADEAERQR	↓	-0.597052515	0.134388672	181	192	186.5

Figure S4. MS identified peptide fragments of recombinant *Pa* LptD (A) and LptE (B) colored according to annotated protein domains and visualized using Protter webtool. MS detectable peptides are uniformly distributed across all domains of LptD/E with >80% of protein sequence covered by MS.



References

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