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The comprehensive computational study on PE11 gene of *Mycobacterium tuberculosis* involved in virulence

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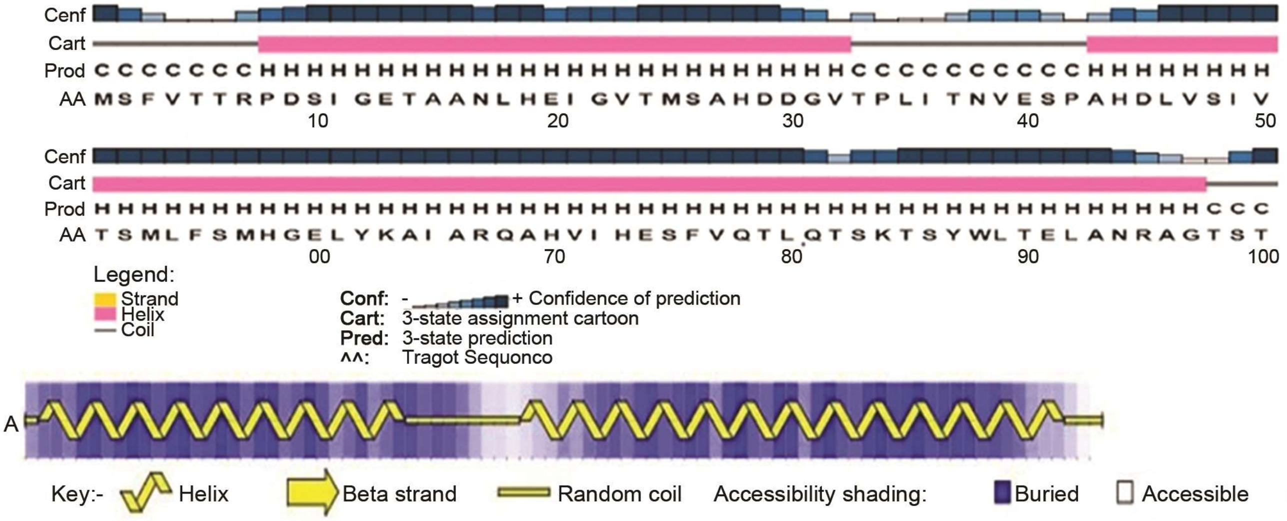
Supplementary Data



Suppl. Fig. 1 — Secondary structure prediction of PE11 gene protein lipX using PSIPRED and PROCECK

Suppl. Table 1 — Emini surface accessibility of uricase from both the sources of predicted peptides and their residue scores

Sr. No.	Position	Residue	Peptide	Score
1.	3	F	MSFVTT	0.498
2.	4	V	SFVTTR	0.986
3.	5	T	FVTTRP	1.137
4.	6	T	VTTRPD	2.193
5.	7	R	TTRPDS	3.96
6.	8	P	TRPDSI	1.923
7.	9	D	RPDSIG	1.319
8.	10	S	PDSIGE	1.166
9.	11	I	DSIGET	1.088
10.	12	G	SIGETA	0.658
11.	13	E	IGETAA	0.496
12.	14	T	GETAAN	1.139
13.	15	A	ETAANL	0.949

14.	16	A	TAANLH	0.746
15.	17	N	AANLHE	0.895
16.	18	L	ANLHEI	0.621
17.	19	H	NLHEIG	0.608
18.	20	E	LHEIGV	0.281
19.	21	I	HEIGVT	0.491
20.	22	G	EIGVTM	0.357
21.	23	V	IGVTMS	0.276
22.	24	T	GVTMSA	0.398
23.	25	M	VTMSAH	0.548
24.	26	S	TMSAHD	1.232
25.	27	A	MSAHDD	1.426
26.	28	H	SAHDDG	1.426
27.	29	D	AHDDGV	0.79
28.	30	D	HDDGVT	1.128
29.	31	G	DDGVTP	1.282
30.	32	V	DGVTPL	0.633
31.	33	T	GVTPLI	0.266
32.	34	P	VTPLIT	0.388
33.	35	L	TPLITN	0.84
34.	36	I	PLITNV	0.432
35.	37	T	LITNVE	0.484
36.	38	N	ITNVES	0.786
37.	39	V	TNVESP	1.734
38.	40	E	NVESPA	1.214
39.	41	S	VESPAH	1.027
40.	42	P	ESPAHD	2.311
41.	43	A	SPAHDL	1.1
42.	44	H	PAHDLV	0.609
43.	45	D	AHDLVS	0.528
44.	46	L	HDLVSI	0.366
45.	47	V	DLVSIV	0.2
46.	48	S	LVSIVT	0.173
47.	49	I	VSIVTS	0.281
48.	50	V	SIVTSM	0.374
49.	51	T	IVTSML	0.23
50.	52	S	VTSMLF	0.285
51.	53	M	TSMLFS	0.514
52.	54	L	SMLFSM	0.352
53.	55	F	MLFSMH	0.358
54.	56	S	LFSMHG	0.358
55.	57	M	FSMHGE	0.751
56.	58	H	SMHGEL	0.715
57.	59	G	MHGELY	0.837
58.	60	E	HGELYK	1.69
59.	61	L	GELYKA	1.255
60.	62	Y	ELYKAI	0.889
61.	63	K	LYKAIA	0.519
62.	64	A	YKAIAR	1.232
63.	65	I	KAIARQ	1.361
64.	66	A	AIARQA	0.688
65.	67	R	IARQAH	0.926
66.	68	Q	ARQAHV	0.981
67.	69	A	RQAHVI	0.68
68.	70	H	QAHVIH	0.473
69.	71	V	AHVIHE	0.473

70.	72	I	HVIHES	0.627
71.	73	H	VIHESF	0.399
72.	74	E	IHESFV	0.399
73.	75	S	HESFVQ	0.986
74.	76	F	ESFVQT	1.046
75.	77	V	SFVQTL	0.498
76.	78	Q	FVQTLQ	0.644
77.	79	T	VQTLQT	1.073
78.	80	L	QTLQTS	1.936
79.	81	Q	TLQTSK	2.236
80.	82	T	LQTSKT	2.236
81.	83	S	QTSKTS	3.634
82.	84	K	TSKTSY	3.288
83.	85	T	SKTSYW	2.395
84.	86	S	KTSYWL	1.474
85.	87	Y	TSYWLT	1.064
86.	88	W	SYWLTE	1.277
87.	89	L	YWLTEL	0.786
88.	90	T	WLTELA	0.506
89.	91	E	LTELAN	0.775
90.	92	L	TELANR	1.84
91.	93	A	ELANRA	1.288
92.	94	N	LANRAG	0.736
93.	95	R	ANRAGT	1.288
94.	96	A	NRAGTS	1.708
95.	97	G	RAGTST	1.533

Suppl. Table 2 — Karplus & Schulz Flexibility scores and sequence of predict the peptides which can act as B-cell epitopes (PE11 from mycobacteria tuberculosis)

Sr. No.	Position	Residue	Start	End	Peptide	Score
1.	4	V	1	7	MSFVTTR	0.973
2.	5	T	2	8	SFVTTRP	1.005
3.	6	T	3	9	FVTTRPD	1.029
4.	7	R	4	10	VTTRPDS	1.042
5.	8	P	5	11	TTRPDSI	1.045
6.	9	D	6	12	TRPDSIG	1.04
7.	10	S	7	13	RPDSIGE	1.039
8.	11	I	8	14	PDSIGET	1.04
9.	12	G	9	15	DSIGETA	1.04
10.	13	E	10	16	SIGETAA	1.034
11.	14	T	11	17	IGETAAN	1.014
12.	15	A	12	18	GETAANL	0.989
13.	16	A	13	19	ETAANLH	0.968
14.	17	N	14	20	TAANLHE	0.951
15.	18	L	15	21	AANLHEI	0.95
16.	19	H	16	22	ANLHEIG	0.951
17.	20	E	17	23	NLHEIGV	0.955
18.	21	I	18	24	LHEIGVT	0.959
19.	22	G	19	25	HEIGVTM	0.955
20.	23	V	20	26	EIGVTMS	0.953
21.	24	T	21	27	IGVTMSA	0.948
22.	25	M	22	28	GVTMSAH	0.943
23.	26	S	23	29	VTMSAHD	0.951
24.	27	A	24	30	TMSAHDD	0.965

25.	28	H	25	31	MSAHDDG	0.988
26.	29	D	26	32	SAHDDGV	1.012
27.	30	D	27	33	AHDDGVT	1.024
28.	31	G	28	34	HDDGVTP	1.033
29.	32	V	29	35	DDGVTPL	1.031
30.	33	T	30	36	DGVTPLI	1.021
31.	34	P	31	37	GVTPLIT	1.014
32.	35	L	32	38	VTPLITN	0.998
33.	36	I	33	39	TPLITNV	0.989
34.	37	T	34	40	PLITNVE	0.994
35.	38	N	35	41	LITNVES	1.007
36.	39	V	36	42	ITNVESP	1.029
37.	40	E	37	43	TNVESPA	1.048
38.	41	S	38	44	NVESPAH	1.053
39.	42	P	39	45	VESPAHD	1.036
40.	43	A	40	46	ESPAHDL	1.006
41.	44	H	41	47	SPAHDLV	0.977
42.	45	D	42	48	PAHDLVS	0.951
43.	46	L	43	49	AHDLVSI	0.938
44.	47	V	44	50	HDLVSIV	0.93
45.	48	S	45	51	DLVSIVT	0.932
46.	49	I	46	52	LVSIVTS	0.943
47.	50	V	47	53	VSIVTSM	0.954
48.	51	T	48	54	SIVTSML	0.968
49.	52	S	49	55	IVTSMLF	0.964
50.	53	M	50	56	VTSMLFS	0.946
51.	54	L	51	57	TSMLFSM	0.929
52.	55	F	52	58	SMLFSMH	0.914
53.	56	S	53	59	MLFSMHG	0.917
54.	57	M	54	60	LFSMHGE	0.934
55.	58	H	55	61	FSMHGEL	0.957
56.	59	G	56	62	SMHGELY	0.977
57.	60	E	57	63	MHGELYK	0.99
58.	61	L	58	64	HGELYKA	0.99
59.	62	Y	59	65	GELYKAI	0.978
60.	63	K	60	66	ELYKAIA	0.969
61.	64	A	61	67	LYKAIAR	0.957
62.	65	I	62	68	YKAIARQ	0.956
63.	66	A	63	69	KAIARQA	0.965
64.	67	R	64	70	AIARQAH	0.969
65.	68	Q	65	71	IARQAHV	0.969
66.	69	A	66	72	ARQAHVI	0.953
67.	70	H	67	73	RQAHVIH	0.933
68.	71	V	68	74	QAHVIHE	0.926
69.	72	I	69	75	AHVIHES	0.934
70.	73	H	70	76	HVIHESF	0.954
71.	74	E	71	77	VIHESFV	0.972
72.	75	S	72	78	IHESFVQ	0.981
73.	76	F	73	79	HESFVQT	0.982
74.	77	V	74	80	ESFVQTL	0.983
75.	78	Q	75	81	SFVQTLQ	0.992
76.	79	T	76	82	FVQTLQT	1.005
77.	80	L	77	83	VQTLQTS	1.025
78.	81	Q	78	84	QTLQTSK	1.05
79.	82	T	79	85	TLQTSKT	1.07
80.	83	S	80	86	LQTSKTS	1.087

81.	84	K	81	87	QTSKTSY	1.081
82.	85	T	82	88	TSKTSYW	1.049
83.	86	S	83	89	SKTSYWL	1.008
84.	87	Y	84	90	KTSYWLT	0.968
85.	88	W	85	91	TSYWLTE	0.949
86.	89	L	86	92	SYWLTEL	0.959
87.	90	T	87	93	YWLTELA	0.975
88.	91	E	88	94	WLTELAN	0.988
89.	92	L	89	95	LTELANR	0.993
90.	93	A	90	96	TELANRA	0.994
91.	94	N	91	97	ELANRAG	1.002
92.	95	R	92	98	LANRAGT	1.016
93.	96	A	93	99	ANRAGTS	1.04

Suppl. Table 3 — Parker hydrophilicity of PE11 from both the sources of predicted peptides and their residue scores

Sr. No.	Position	Residue	Start	End	Peptide	Score
1.	4	V	1	7	MSFVTTR	0.571
2.	5	T	2	8	SFVTTRP	1.471
3.	6	T	3	9	FVTTRPD	1.971
4.	7	R	4	10	VTTRPDS	4.214
5.	8	P	5	11	TTRPDSI	3.6
6.	9	D	6	12	TRPDSIG	3.671
7.	10	S	7	13	RPDSIGE	4.043
8.	11	I	8	14	PDSIGET	4.186
9.	12	G	9	15	DSIGETA	4.186
10.	13	E	10	16	SIGETAA	3.057
11.	14	T	11	17	IGETAAN	3.129
12.	15	A	12	18	GETAANL	2.957
13.	16	A	13	19	ETAANLH	2.443
14.	17	N	14	20	TAANLHE	2.443
15.	18	L	15	21	AANLHEI	0.557
16.	19	H	16	22	ANLHEIG	1.071
17.	20	E	17	23	NLHEIGV	0.243
18.	21	I	18	24	LHEIGVT	-0.014
19.	22	G	19	25	HEIGVTM	0.7
20.	23	V	20	26	EIGVTMS	1.329
21.	24	T	21	27	IGVTMSA	0.514
22.	25	M	22	28	GVTMSAH	1.957
23.	26	S	23	29	VTMSAHD	2.571
24.	27	A	24	30	TMSAHDD	4.529
25.	28	H	25	31	MSAHDDG	4.6
26.	29	D	26	32	SAHDDGV	4.671
27.	30	D	27	33	AHDDGVT	4.486
28.	31	G	28	34	HDDGVTP	4.486
29.	32	V	29	35	DDGVTPL	2.871
30.	33	T	30	36	DGVTPLI	0.3
31.	34	P	31	37	GVTPLIT	-0.386
32.	35	L	32	38	VTPLITN	-0.2
33.	36	I	33	39	TPLITNV	-0.2
34.	37	T	34	40	PLITNVE	0.171
35.	38	N	35	41	LITNVES	0.8
36.	39	V	36	42	ITNVESP	2.414
37.	40	E	37	43	TNVESPA	3.857
38.	41	S	38	44	NVESPAH	3.414

39.	42	P	39	45	VESPAHD	3.843
40.	43	A	40	46	ESPAHDL	3.057
41.	44	H	41	47	SPAHDLV	1.414
42.	45	D	42	48	PAHDLVS	1.414
43.	46	L	43	49	AHDLVSI	-0.029
44.	47	V	44	50	HDLVSIV	-0.857
45.	48	S	45	51	DLVSIVT	-0.414
46.	49	I	46	52	LVSIVTS	-0.914
47.	50	V	47	53	VSIVTSM	-0.2
48.	51	T	48	54	SIVTSML	-0.986
49.	52	S	49	55	IVTSMLF	-3.229
50.	53	M	50	56	VTSMLFS	-1.157
51.	54	L	51	57	TSMLFSM	-1.229
52.	55	F	52	58	SMLFSMH	-1.671
53.	56	S	53	59	MLFSMHG	-1.786
54.	57	M	54	60	LFSMHGE	-0.071
55.	58	H	55	61	FSMHGEL	-0.071
56.	59	G	56	62	SMHGELY	0.971
57.	60	E	57	63	MHGELYK	0.857
58.	61	L	58	64	HGELYKA	1.757
59.	62	Y	59	65	GELYKAI	0.314
60.	63	K	60	66	ELYKAIA	-0.2
61.	64	A	61	67	LYKAIAR	-0.714
62.	65	I	62	68	YKAIARQ	1.457
63.	66	A	63	69	KAIARQA	2.029
64.	67	R	64	70	AIARQAH	1.514
65.	68	Q	65	71	IARQAHV	0.686
66.	69	A	66	72	ARQAHVI	0.686
67.	70	H	67	73	RQAHVIH	0.686
68.	71	V	68	74	QAHVIHE	1.2
69.	72	I	69	75	AHVIHES	1.271
70.	73	H	70	76	HVIHESF	-0.343
71.	74	E	71	77	VIHESFV	-1.171
72.	75	S	72	78	IHESFVQ	0.214
73.	76	F	73	79	HESFVQT	2.1
74.	77	V	74	80	ESFVQTL	0.486
75.	78	Q	75	81	SFVQTLQ	0.229
76.	79	T	76	82	FVQTLQT	0.043
77.	80	L	77	83	VQTLQTS	2.286
78.	81	Q	78	84	QTLQTSK	3.629
79.	82	T	79	85	TLQTSKT	3.514
80.	83	S	80	86	LQTSKTS	3.7
81.	84	K	81	87	QTSKTSY	4.743
82.	85	T	82	88	TSKTSYW	2.457
83.	86	S	83	89	SKTSYWL	0.4
84.	87	Y	84	90	KTSYWLT	0.214
85.	88	W	85	91	TSYWLTE	0.514
86.	89	L	86	92	SYWLTEL	-1.543
87.	90	T	87	93	YWLTELA	-2.171
88.	91	E	88	94	WLTELAN	-0.9
89.	92	L	89	95	LTELANR	1.129
90.	93	A	90	96	TELANRA	2.743
91.	94	N	91	97	ELANRAG	2.814
92.	95	R	92	98	LANRAGT	2.443
93.	96	A	93	99	ANRAGTS	4.686
94.	97	G	94	100	NRAGTST	5.129

Suppl. Table 4 — T-cell epitope of peptide binding to MHC class I molecule, their Score and ranks

Alleles	Start	End	Length	Peptide	Core	Icore	Score	Rank
HLA-A*02:01	4	17	14	VTTRPDSIGETAAN	VTIGETAAN	VTTRPDSIGETAAN	0.0	100
HLA-A*02:01	8	17	10	PDSIGETAAN	PSIGETAAN	PDSIGETAAN	0.0	100
HLA-A*02:01	11	24	14	IGETAANLHEIGVT	IGLHEIGVT	IGETAANLHEIGVT	0.0	100
HLA-A*02:01	18	29	12	LHEIGVTMSAHD	LHVTMSAHD	LHEIGVTMSAHD	0.0	100
HLA-A*02:01	18	30	13	LHEIGVTMSAHDD	LHIGVTMSA	LHEIGVTMSA	0.0	100
HLA-B*35:01	4	17	14	VTTRPDSIGETAAN	VPDSIGETA	VTTRPDSIGETA	0.0	100
HLA-B*35:01	8	20	13	PDSIGETAANLHE	DSIGETAAE	DSIGETAANLHE	0.0	100
HLA-B*35:01	8	21	14	PDSIGETAANLHEI	DSIGETHEI	DSIGETAANLHEI	0.0	100
HLA-B*35:01	9	22	14	DSIGETAANLHEIG	DSIGETAAG	DSIGETAANLHEIG	0.0	100
HLA-B*35:01	10	22	13	SIGETAANLHEIG	SAANLHEIG	SIGETAANLHEIG	0.0	100
HLA-B*08:01	34	45	12	PLITNVESPAHD	PLITNSPAH	PLITNVESPAH	0.0	100
HLA-B*08:01	8	20	13	PDSIGETAANLHE	DSIGETAAE	DSIGETAANLHE	1e-06	100
HLA-B*08:01	11	24	14	IGETAANLHEIGVT	IANLHEIGV	IGETAANLHEIGV	1e-06	100
HLA-B*08:01	18	30	13	LHEIGVTMSAHDD	LHEIGTMSA	LHEIGVTMSA	1e-06	100
HLA-B*08:01	18	31	14	LHEIGVTMSAHDDG	LHEIGVTMG	LHEIGVTMSAHDDG	1e-06	100
HLA-B*07:02	8	17	10	PDSIGETAAN	PSIGETAAN	PDSIGETAAN	0.0	100
HLA-B*07:02	8	20	13	PDSIGETAANLHE	DSIGETAAE	DSIGETAANLHE	0.0	100
HLA-B*07:02	9	22	14	DSIGETAANLHEIG	DSIGETHEI	DSIGETAANLHEI	0.0	100
HLA-B*07:02	11	24	14	IGETAANLHEIGVT	IGETAANVT	IGETAANLHEIGVT	0.0	100

Suppl. Table 5 — Association of functional protein partners of PE11 (lipX) with their score summary calculated through STRING network tool

Sr. No.	Associated Protein	Identifier	Score
1.	PPE17	Rv1168c, PPE17	0.901
2.	PPE41	Rv2430c, PPE41	0.731
3.	Rv774C	Rv0774c	0.730
4.	PE_PGRS17	Rv0978c, PE_PGRS17	0.630
5.	Rv1167c	Rv1167c	0.602
6.	PE25	Rv2431c, PE25	0.578
7.	mshB	Rv1170, mshB	0.577
8.	PE12	Rv1172c, PE12	0.570
9.	tgs4	Rv3088, tgs4	0.570
10.	PPE37	Rv2123, PPE37	0.555

Suppl. Table 6 — T-cell epitope of peptide binding to MHC class II molecule, their Score and ranks

Alleles	Start	End	Length	Peptide	Rank	Adjusted Rank
HLA-DRB1*15:01	1	43	57	15	AHDLVSIVTSMLFSM	4.20
HLA-DRB1*15:01	1	44	58	15	HDLVSIVTSMLFSMH	4.20
HLA-DRB1*04:01	1	84	98	15	KTSYWLTELANRAGT	4.60
HLA-DRB1*04:01	1	83	97	15	SKTSYWLTELANRAG	4.60
HLA-DRB1*01:01	1	86	100	15	SYWLTELANRAGTST	8.20
HLA-DRB1*01:01	1	85	99	15	TSYWLTELANRAGTS	8.20
HLA-DRB1*03:02	1	59	73	15	GELYKAIARQAHVIH	13.00
HLA-DRB1*03:02	1	58	72	15	HGELYKAIARQAHVI	14.00