Table 1. Lipoprotein sequences of different *Leptospira* species retrieved from Uniprot and their accession number.

S.no	**OMPL/LIPL**	***Leptospira* species**	**EMBL id / accession no**
1	OMPL1	*Leptospira interrogans* serovar Paidjan	AY622666 /**Q6GXD5**
2	OMPL1	Leptospira interrogans serovar Paidjan (Fragment)	AY688405 / Q66ML3
3	LipL41	*Leptospira santarosai* serovar Shermani	CP006694 /K8Y7P9
4	LipL41	*Leptospira kmetyi*	RQEW01000016 /A0A2M9XPR1
5	LipL41	*Leptospira borgpetersenii*	AY461937 / Q6S9Q9
6	LipL41	*Leptospira noguchii*	AY461958 /Q6S9N7
7	LipL41	*Leptospira noguchii*	AY461956/ Q6S9N9
8	LipL41	*Leptospira interrogans*	AY461940 / Q6S9Q5
9	LipL41	*Leptospira interrogans* serovar Paidjan	AY776300 / Q5MJS6
10	LipL41	*Leptospira borgpetersenii*	AY461935 /Q6S9R0
11	LipL41	*Leptospira kirschneri*	AY461955 / Q6S9P0
12	LipL41	*Leptospira sp.*	LC131110 /A0A2Z5TS76
13	LipL41	*Leptospira sp.*	LC131112 /A0A2Z5TZU5
14	LipL41	*Leptospira borgpetersenii*	LC131111 / A0A2Z5U283
15	LipL41	*Leptospira interrogans* serovar Pomona	AY776298 /Q5MJS8

16	LipL41	*Leptospira interrogans* serovar Pyrogenes	AY688418/Q66MK0
17	LipL41	*Leptospira interrogans* serovar Pomona	AY688415 /Q66MK3
18	LipL41	*Leptospira interrogans* serovar Wolffi	AY688416/Q66MK2
19	LipL41	*Leptospira interrogans* serovar Linhai	AY688413 /Q66MK5
20	LipL41	*Leptospira mayottensis*	KT338914/A0A1B2BIA3
21	LipL46	*Leptospira mayottensis*	CP024871 /A0A3Q9DVC0
22	LipL32	*Leptospira interrogans* serovar Hebdomadis	GU220823 /D2XNC3
23	LipL32	*Leptospira santarosai*	CP027843 /A0A2P1QX32
24	LipL32	*Leptospira interrogans* serovar Hardjo	JN886739 /H9AES2
25	LipL32	*Leptospira weilii*	AY461930 /Q6S9R5
26	LipL32	*Leptospira borgpetersenii*	AF181554/Q9L958
27	LipL32	*Leptospira interrogans*	AY461910/Q6S9T5
28	LipL32	Major outer membrane lipoprotein *Leptospira interrogans*	JQ013518 /I1ZHS1
29	LipL32	*Leptospira interrogans*	AY461903/Q6S9U2
30	LipL32	*Leptospira interrogans* serovar Autumnalis	EU526391 /B1Q189

31	LipL32	*Leptospira interrogans* serovar Sejroe	DQ149595/Q3YA44
32	LipL32	*Leptospira interrogans* serovar Hardjo	KC800991 / S4WG23
33	LipL32	*Leptospira kirschneri*	AY461916 /Q6S9S9
34	LipL32	*Leptospira interrogans* serovar Australis	AB094437/Q8GQZ1
35	LipL32	*Leptospira interrogans* serovar Sejroe	KC800994/S4WH52
36	LipL32	*Leptospira interrogans*	KP032210 /A0A0C5D0G5
37	LipL32	*Leptospira borgpetersenii* serovar Javanica	EU526389 /B1Q187
38	LipL32	*Leptospira interrogans* serovar Pomona	KC800987/S4WBS1
39	LipL32	*Leptospira borgpetersenii* serovar Javanica	EU526390 /B1Q188
40	LipL32	*Leptospira interrogans* serovar Wolffi	AY776294/Q5MJT2
41	LipL32	*Leptospira interrogans* serovar Canicola	AY763509 / Q5G801
42	LipL32	*Leptospira interrogans* serovar Icterohaemorrhagiae	AY423075 /Q6TEI2
43	LipL32	*Leptospira interrogans*	MT482305 /A0A7T3ISM8

Table 2. Conservancy results for the predicted epitopes of B cell, CTL and HTL.

Epitope From LIPL 32	Lipoprotein	Epitope sequence	Epitope length	Percent of protein sequence matches at identity <= 100%	Minimum identity	Maximum identity
1	LipL32	YYLYVWIPAVIAEMG	15	75.00% (6/8)	93.33%	100.00%
2		MSAIMPDQIAKAAKA	15	87.50% (7/8)	93.33%	100.00%
3		SSFVLSEDTIPGTNE	15	37.50% (3/8)	86.67%	100.00%
4		INYYGYVKPGQAPDG	15	75.00% (6/8)	86.67%	100.00%
5		KKLLVRGLYRI	11	87.50% (7/8)	27.27%	100.00%
6		GLPSLKSSFVLSE	13	100.00% (8/8)	100.00%	100.00%
7		KTLLPYGSVINYYGYVKPG	19	37.50% (3/8)	84.21%	100.00%
8		AYYLYVWIPAVIAE	14	75.00% (6/8)	92.86%	100.00%
9		FTTYKPGEV	9	87.50% (7/8)	33.33%	100.00%
10		GSVINYYGY	9	75.00% (6/8)	77.78%	100.00%
11		LVDGNKKAY	9	75.00% (6/8)	88.89%	100.00%
12		NIDTKKLLV	9	75.00% (6/8)	33.33%	100.00%
1	LipL41	RMMLIPLDATLIKVE	15	70.00% (7/10)	26.67%	100.00%
2		RIKVFVKDEDEEVKE	15	70.00% (7/10)	26.67%	100.00%
3		KPTGVRMMLIPLDAT	15	70.00% (7/10)	26.67%	100.00%
4		VKKAVVSSPAKIFNS	15	50.00% (5/10)	33.33%	100.00%
5		AEAILYIGYQ	10	100.00% (10/10)	100.00%	100.00%
6		DAVAAG	6	90.00% (9/10)	83.33%	100.00%

7		MLIPLDATLIKV	12	90.00% (9/10)	33.33%	100.00%
8		LIGAEAILY	9	100.00% (10/10)	100.00%	100.00%
9		YTECSTENK	9	50.00% (5/10)	77.78%	100.00%
10		STENKIDAV	9	50.00% (5/10)	66.67%	100.00%
11		AKANLATYY	9	90.00% (9/10)	44.44%	100.00%
1	LipL46	DRGFSFLATKSLEVK	15	90.00% (9/10)	93.33%	100.00%
2		GFSFLATKSLEVKSA	15	90.00% (9/10)	93.33%	100.00%
3		TTRLISALAVISFAVNCG	18	20.00% (2/10)	77.78%	100.00%
4		NPRVAVLVLGKV	12	100.00% (10/10)	100.00%	100.00%
5		LIKILAEALQAEVLVLG	17	50.00% (5/10)	94.12%	100.00%
6		TSDTNGSEW	9	100.00% (10/10)	100.00%	100.00%
7		STAVDNLLA	9	100.00% (10/10)	100.00%	100.00%
1	OMPL1	RMMLIPLDATLIKVE	15	70.00% (7/10)	26.67%	100.00%
2		RIKVFVKDEDEEVKE	15	70.00% (7/10)	26.67%	100.00%
3		KPTGVRMMLIPLDAT	15	70.00% (7/10)	26.67%	100.00%
4		VKKAVVSSPAKIFNS	15	50.00% (5/10)	33.33%	100.00%
5		AEAILYIGYQ	10	100.00% (10/10)	100.00%	100.00%
6		DAVAAG	6	90.00% (9/10)	83.33%	100.00%
7		MLIPLDATLIKV	12	90.00% (9/10)	33.33%	100.00%
8		LIGAEAILY	9	100.00% (10/10)	100.00%	100.00%
9		YTECSTENK	9	50.00% (5/10)	77.78%	100.00%
10		STENKIDAV	9	50.00% (5/10)	66.67%	100.00%
11		AKANLATYY	9	90.00% (9/10)	44.44%	100.00%

Table 3. Binding affinity analysis for all docked complexes.

Construct no	**Receptor**	**Binding affinity (kcal mol^{-1})**	**Dissociation constant**
1	TLR 4	-11.8	2.2E-09
2	TLR 4	-9.3	1.6E-07
3	TLR 4	-6.0	4.0E-05
4	TLR 4	-7.4	3.6E-06
5	TLR 4	-9.4	1.2E-07
6	TLR 4	-16.7	5.6E-13
1	MHC I	-4.3	6.8E-04
2	MHC I	-5.5	8.8E-05
3	MHC I	-20.1	1.8E-15
4	MHC I	-7.9	1.7E-06
5	MHC I	-4.2	7.8E-04
6	MHC I	-3.9	1.4E-03
1	MHC II	-8.6	4.8E-07
2	MHC II	-3.8	1.6E-03
3	MHC II	-6.6	1.3E-05
4	MHC II	-4.9	2.7E-04
5	MHC II	-8.3	7.8E-07
6	MHC II	-3.9	1.3E-03
1	TLR2	-143.9	2.7E-106
2	TLR 2	-4.1	1.0E-03

3	TLR 2	-10.1	4.0E-08
4	TLR 2	-148.6	1.1E-109
5	TLR 2	-7.6	2.5E-04
6	TLR 2	-12.2	1.1E-09

Table 4. Epitope prediction against selected mice alleles.

mice alleles	***peptide***
H-2-Db	YAAYNIDTKKL
	AAYLIGAEAI
	YSTENKIDAV
	AAYSTAVDNL
	SSFVLSEDTI
	GSVINYYGYV
	YAAYNIDTK
	AYLIGAEAI
	AAYSTENKI
	YAKANLATY
	TAVDNLLAA
	AAYVTKADI
	GGPGPGYYL
	MSAIMPDQI
	SFVLSEDTI
	MLIPLDATL
	AVVSSPAKI
	FSFLATKSL
	FSFLATKSL
	IGYQKKDAV
	MLIPLDATL
	RLISALAVI
	SALAVISFA
	SSIVIPATV
	SAIMPDQI
H-2-Dd	IAGGPGPGYYL
	AKAGPGPGSSF
	AGPGPGSSFVL
	GGPGPGRMMLI

	KGPGPGGFSF
	KGPGPGGFSFL
	VGPGPGEGNYI
	IGVAPRKAKKF
	AGGPGPGYYL
	GGPGPGMSAI
	KAGPGPGSSF
	AGPGPGSSFV
	GPGPGSSFVL
	GGPGPGRMML
	GPGPGRMMLI
	GPGPGRIKVF
	PGPGDRGFSF
	KGPGPGGFSF
	GPGPGGFSFL
	KGLPSLKSSF
	KNPRVAVLVL
	TSDTNGSEW
	GGPGPGYYL
	PGPGYYLYV
	PGPGMSAIM
	AGPGPGSSF
	PGPGSSFVL
	GGPGPGRMM
	PGPGRMMLI
	PGPGRIKVF
	PGDRGFSFL
	FSFLATKSL
	PGPGGFSFL
	FSFLATKSL
	PGPGEGNYI
	IGYQKKDAV
	VAAGKKMLI
	ISALAVISF
	KNPRVAVLV
	VGPSDPACF
	VAPRKAKKF
	VAAEKKSSI
	SSIVIPATV
	KAYAAYNI
	GPGPGYYL
	PGPGRMML
	KGPGPGGF
	PGPGGFSF
	GPGGFSFL
	KNPRVAVL
H-2-Kb	INYYGYAAYL
	SVINYYGYA

H-2-Kd	INYYGYAAY
	NYYGYAAYL
	VAAYAKANL
	FSFLATKSL
	FSFLATKSL
	SVINYYGYV
	IGYQKKDAV
	SSIVIPATV
	IVIPATVGI
	INYYGYAA
	YYGYAAYL
	YGYAAYLV
	KAYAAYNI
	AAYAKANL
	AAYYTQKI
	RGFSFLAT
	TLLPYGSV
	VINYYGYV
	KNPRVAVL
	KAKKFWRV
	AYLTAAGAGAV
	AYYTQKISGGV
	NYIGVAPRKAI
	INYYGYAAYL
	AYNIDTKKLL
	VAAYLIGAEA
	AAYLIGAEAI
	AAYSTAVDNL
	AYSTAVDNLL
	TYKPGEVAA
	AYGSVINYY
	NYYGYAAYL
	YYGYAAYLV
	AYNIDTKKL
	AYLIGAEAI
	AYAKANLAT
	EWAAYSTAV
	AYSTAVDNL
	KYFFAAYYT
	AYYTQKISG
	AYVTKADIA
	LYVWIPAVI
	SFVLSEDTI
	MLIPLDATL
	GYVKPGKKA
	LYVWIPAVI
	MLIPLDATL
	RLISALAVI

	YYGYAAYL
	AYSTENKI
	AYVTKADI
	SFLATKSL
	SFLATKSL
H-2-Kk	AEKKAEAILYI
	GEVAAYGSVI
	SEWAAYSTAV
	AYESDFGKYF
	YESDFGKYFF
	GEVAAYGSV
	SEWAAYSTA
	YESDFGKYF
	VEGPGPGRI
	AEKKAEAIL
	AEALQAEVL
	AEKKSSIVI
	TENKIDAV
	NEGPGPGI
	SEKKKTLL
	AEKKAEAI
	AEALQAEV
H-2-Ld	GPGPGDRGFSF
	VKGPGPGGFSF
	YVKPGKKAYYL
	IVIPATVGIKL
	GPGPGSSFVL
	GPGPGRIKVF
	GPGKPTGVRM
	GPGDRGFSFL
	KGPGPGGFSF
	GPGPGGFSFL
	LPSLKSSFVL
	LPYGSVINYY
	VKPGKKAYYL
	VIPATVGIKL
	NYYGYAAYL
	VAAYAKANL
	YESDFGKYF
	GPGPGYYLY
	GPGPGMSAI
	GPGPGSSFV
	GPGPGINYY
	GPGINYYGY
	GPGPGRMML
	GPGPGRIKV
	KPTGVRMML
	GPGPGDRGF

	GPGDRGFSF
	GPGPGGFSF
	GPGKGGYDI
	IPAKKKKLL
	LPSLKSSFV
	LPYGSVINY
	KPGKKAYYL
	NPRVAVLVL IPATVGIKL
	GPGPGYYL
	IPAVIAEM
	GPGPGSSF
	GPGSSFVL
	IPLDATLI
	KPTGVRMM
	GPGGFSFL
	LPSLKSSF
	IPLDATLI
H-2-Qa1	AAYGSVINYY
	YLVDGNKKAY
	YLIGAEAILY
	YAKANLATYY
	AVDNLLAAAY
	AAYESDFGKY
	KAGPGPGSSF
	YVKPGKKAYY
	ALSEAAAKF
	EAAAKFTTY
	AAYGSVINY
	INYYGYAAY
	LVDGNKKAY
	YAKANLATY
	NLATYYAAY
	YSTAVDNLL
	AGAGAVAAY
	YESDFGKYF
	ESDFGKYFF
	KISGGVAAY
	IAGGPGPGY
	AGGPGPGYY
	AGPGPGSSF
	MLIPLDATL
	VVSSPAKIF
	RIKKGLPSL
	GLPSLKSSF
	GSVINYYGY
	YVKPGKKAY
	MLIPLDATL

	KTTRLISAL
	ISALAVISF
	ALQAEVLVL
	IVIPATVGI
H-2-Qa2	AAYESDFGKYF
	AEKKAEAILYI
	SEAAAKFTTY
	AYESDFGKYF
	YESDFGKYFF
	AEMGGPGPGM
	AEAILYAAY
	YESDFGKYF
	VEGPGPGRI
	GPGPGGFSF
	AEKKAEAIL
	AEAILYIGY
	AEALQAEVL
	AEKKSSIVI
	SDFGKYFF