

IDENTIFICATION OF CD4⁺ T CELL EPITOPES FROM *Staphylococcus aureus* SECRETOME USING IMMUNOINFORMATIC PREDICTION AND MOLECULAR DOCKING

HLA class-II binding profiles of the peptides generated from staphylococcal secretome

Gene ID	Protein	Peptides generated	Strong binding peptides	strong binding non –self peptides	Percentage of strong binding non –self peptides	Alleles bound	peptides binding with glide score better than -10 kcal/mol
SACOL1173	α hemolysin precursor (HLY)	305	119	20	6.56	11	7
SACOL2003	β hemolysin precursor (HLB)	316	100	3	0.95	7	3
SACOL2022	δ hemolysin (HLD)	30	19	0	0	0	0
SACOL2419	γ hemolysin comp A (HLgA)	295	134	20	6.78	11	9
SACOL2422	γ hemolysin comp B (HLgB)	311	150	10	3.22	7	5
SACOL2421	γ hemolysin Comp C(HLgC)	301	126	10	3.32	7	5
SACOL1880	LeukotoxinD LukD	313	127	11	3.51	3	4
SACOL1881	LeukotoxinE LukE	297	115	9	3.03	5	4
SACOL2004	Leukocidin Subunit Precursor ,Putative	276	95	7	2.54	5	5
SACOL2006	Aerolysin/leukocidin family protein	337	121	12	3.56	5	6
SACOL0442	Staphylococcal enterotoxin	189	61	11	5.82	12	7

SUPPLEMENTARY INFORMATION 1

Gene ID	Protein	Peptides generated	Strong binding peptides	strong binding non –self peptides	Percentage of strong binding non –self peptides	Alleles bound	peptides binding with glide score better than -10 kcal/mol
SACOL0886	Staphylococcal enterotoxin (Sek)	228	88	2	0.88	5	2
SACOL0887	Staphylococcal enterotoxin type I(Sei)	228	111	25	10.96	11	12
SACOL0907	Staphylococcal enterotoxin type B (Seb)	252	119	28	11.11	16	13
SACOL1869	Serine protease SplA (SplA)	224	88	1	0.45	3	1
SACOL1868	Serine protease SplB (SplB)	226	119	11	4.87	12	6
SACOL1867	Serine protease SplC (SplC)	225	110	3	1.33	3	2
SACOL1866	Serine protease SplD (SplD)	225	96	0	0	0	0
SACOL1865	Serine protease SplE (SplE)	224	113	11	4.91	8	8
SACOL1864	Serine protease SplF (SplF)	225	100	3	1.33	6	1
SACOL1057	V8 protease (SspA)	322	97	3	0.93	1	3
SACOL1056	Cysteine protease precursor SspB (SspB1)	379	150	10	2.64	7	5
SACOL1970	Cysteine protease precursor SspB (SspB2)	374	193	21	5.61	11	12
SACOL2659	Zinc metalloproteinase aureolysin (Aur)	495	133	5	1.01	3	5
SACOL2694	Lipase1 (Lip1)	666	175	7	1.05	5	4
SACOL0317	Lipase2 (Lip2)	630	225	7	1.11	5	5
SACOL0078	1-Phosphatidylinositol phosphodiesterase (Plc)	314	147	19	6.05	7	7
SACOL0263	Peptidoglycan hydrolase (LytM)	308	112	16	5.19	9	8

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SACOL0507	N-Acetylmuramoyl-L-alanine amidase (Sle1)	320	210	17	5.31	9	10
SACOL0723	LysM domain protein	252	118	13	5.16	9	6
SACOL1062	Bifunctional autolysin (Atl1)	1242	542	43	3.46	10	24
SACOL2088	SceD protein (SceD)	217	91	4	1.84	3	2
SACOL2584	Immunodominant antigen A (IsaA)	219	138	7	3.2	5	5
SACOL2666	N-Acetylmuramoyl-L-alanine amidase domain protein	605	171	9	1.49	9	5
SACOL0303	Acid phosphatase 5-nucleotidase	282	111	8	2.84	7	4
SACOL0860	Thermonuclease precursor (Nuc)	214	119	4	1.87	9	2
SACOL0962	Glycerophosphoryl diester phosphodiesterase (GlpQ)	295	127	1	0.34	1	1
SACOL1071	Chitinase-related protein	91	28	0	0	0	0
SACOL08581	Secretory extracellular matrix and plasma-binding protein (Empbp1)	326	137	32	9.82	12	12
SACOL0985	Surface protein, putative	130	51	0	0	0	0
SACOL1164	Fibrinogen binding-related protein	95	75	7	7.37	5	3
SACOL1168	Fibrinogen-binding protein (Efb)	151	88	10	6.62	4	5
SACOL2002	Map protein (Map)	670	323	23	3.43	9	14

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SACOL2019	SdrH protein, putative (SdrH)	405	113	10	2.47	15	5
SACOL2197	Surface protein, putative	127	52	0	0	0	0
SACOL2418	IgG-binding protein (Sbi)	422	170	21	4.98	13	9
SACOL2660	Immunodominant antigen B (IsaB)	161	90	10	6.21	7	8
SACOL0270	Staphyloxanthin biosynthesis protein, putative	283	91	2	0.71	1	0
SACOL0271	Virulence factor EsxA (EsxA)	83	45	1	1.2	1	1
SACOL0480	Hypothetical protein	88	48	0	0	0	0
SACOL0669	Conserved hypothetical protein	154	78	5	3.25	7	3
SACOL0755	Conserved hypothetical protein	136	46	1	0.74	1	1
SACOL0859	Hypothetical protein	142	52	2	1.41	2	2
SACOL0908	Hypothetical protein	171	43	0	0	0	0
SACOL1166	Hypothetical protein	119	46	0	0	0	0
SACOL2179	Conserved hypothetical protein	275	147	2	0.73	3	2
SACOL2291	Staphylococcal secretory antigen SsaA2	253	135	10	3.95	7	6
SACOL2295	Staphyloxanthin biosynthesis protein	152	69	3	1.97	2	1
SACOL2557	Conserved domain protein	129	94	15	11.63	5	9