

Table 2: Preference scale of candidate AMPs based on docking interactions with mutated sortase C protein of *C. striatum* (where 10 represents the most optimum docking interactions and 0 represents no interactions with the protein residues)

Serial Number	Pep ID	DRAMP ID	AMP length (residues)	Sequence	Name of AMP	TORSDOF	Docking Score (kcal/mol)	Interacting Residues	Essential criteria	Preference Score
1	1	--	5	LPMTG	LPMTG Motif of the Piliin Subunit	14	-5.3	HIS168, ASN236, GLN143		STANDARD
2	4707	18641	6	TWWRWW	KCM11	26	-6.2	HIS168, ARG239, ASN236, THR137, THR169	Interactions with two putative catalytic site residues, seen as His168 and Arg239	10
3	4021	04173	5	WLLKW	L2KW2	23	-5.8	HIS168, ARG239, ASN236		10
4	4583	18503	8	WKSYYRRW	TSG-11 (Ixosin-B peptide derivative)	39	-5.6	HIS168, ARG239, LEU96, PRO94, PRO94		10
5	4785	18719	7	DDDDDDD	SAAP fraction 3 (Surfactant-associated anionic peptide)	28	-5.3	HIS168, ARG239, ASN236, GLN143		10
6	1437	18337	6	ATQSHQ	<i>S. amritsarensis</i> lipopeptide (Bacteriocin)	24	-5.1	HIS168, ARG239, GLN143, ASP139		10
7	5494	21437	7	KKLKAF	Peptide 14 (Derived from B1)	33	-5	HIS168, ARG239, LEU96		10
8	5496	21439	7	KKKIAFA	Peptide 16 (Derived from B1)	33	-5	HIS168, ARG239, GLN143, ILE235		10
9	4708	18642	6	KWRWIW	KCM12	29	-6.3	HIS168, HIS168, GLN143, TYR233		Multiple explicit interactions with His168 from the triad
10	1218	04174	7	KWLKKWL	L2K3W2	37	-5	HIS168, HIS168, ASN236, GLN143, GLN143, THR137, PRO94	9	
11	5482	21425	7	KKGKGGG	Peptide 2 (Derived from B1)	29	-4.9	HIS168, HIS168, GLN143, ALA95	9	
12	5508	21451	7	KKKLAYA	Peptide 28 (Derived from B1)	34	-4.9	HIS168, HIS168, GLN143, ILE235	9	
13	4934	20873	5	GLLKR	Pal-ano-5 (Pal-anoplin peptide derivative)	23	-4.5	HIS168, HIS168, GLN143	9	
14	4931	20870	8	GLLKRIKT	Pal-ano-8 (Pal-anoplin peptide derivative)	38	-4.4	HIS168, HIS168, ASN236, ASN236, GLN143	9	
15	4710	18644	6	WRWFIH	KRS22	26	-6	HIS168, GLN143	Only one explicit interaction with His168 from the triad	
16	2442	18309	6	WAVLL	Baceridin (Bacteriocin)	21	-5.9	HIS168, GLN143		8
17	1005	03881	6	RRWWW	LFB-6RW	30	-5.8	HIS168, ASP139		8
18	3475	18218	6	TVVTNA	Fusaricidin A (Bacteriocin)	20	-5.8	HIS168, GLN143		8
19	4709	18643	6	KWWWRW	KCM21	29	-5.8	HIS168, ASN236, GLN143, ASP139, PRO94, PRO94		8
20	696	18371	9	VGVGGFGR	Crinicepsin-1	26	-5.8	HIS168, ASN236, GLN143		8
21	5492	21435	7	AFALKKK	Peptide 12 (Derived from B1)	33	-5.7	HIS168, GLN143, THR137, PRO94		8
22	3059	18247	8	DWTXWSXL	Bacthuricin F4(Bacteriocin)	28	-5.7	HIS168, GLN143, ILE235		8
23	3366	18226	7	LLDVLE	Gageostatin A (Bacteriocin)	28	-5.6	HIS168, GLN143, ASP139, ALA172		8
24	996	03869	8	RRWVWRR	Bac8d (Bac2A variant)	39	-5.6	HIS168, ASN236, LEU96		8
25	3461	18221	6	TVYTQA	Fusaricidin D (Bacteriocin)	23	-5.5	HIS168, GLN143, ASP139		8
26	1219	04175	7	KWLLKWL	L3K2W2 (LIKmW2 model peptides)	34	-5.5	HIS168, GLN143, ILE235		8
27	3308	18228	7	LLDVLE	Gageostatin C (Bacteriocin)	28	-5.5	HIS168, ASN236, GLN143, ARG98		8
28	3292	02930	6	HSPGGA	Antimicrobial protein 2	15	-5.4	HIS168, ASN236, GLN143, THR137		8
29	1087	03989	7	LLKWLK	L4K2W4	34	-5.4	HIS168, GLN143		8
30	5501	21444	7	AFALKKK	Peptide 21 (Derived from B1)	33	-5.4	HIS168, GLN143, ILE235		8
31	5491	21434	7	AFALKKK	Peptide 11 (Derived from B1)	33	-5.3	HIS168, GLN143, PRO94		8
32	168	01351	12	RVCFAIPLPICH	Tigerinin-2	41	-5.2	HIS168, GLN143, ASP139, ASP139, ASP139		8
33	4020	04172	5	WLKKW	LK2W2 (LIKmW2 model peptides)	26	-5.1	HIS168		8
34	5244	21214	6	IRIKIR	IK6-all D (Derived from IK8-all L)	31	-5.1	HIS168, GLN143		8
35	3296	18230	4	LLLE	Gageotetrin B (Bacteriocin)	17	-5	HIS168, ASN236, ASN236, GLN143		8
36	3298	18232	4	LLEL	Gageopeptide A(Bacteriocin)	17	-5	HIS168, GLN143		8
37	5487	21430	7	KKKLAFA	Peptide 7 (Derived from B1)	33	-5	HIS168, ASN236, GLN143		8
38	5497	21440	7	KKLKAF	Peptide 17 (Derived from B1)	33	-5	HIS168, GLN143, ILE235, GLY234		8
39	3240	18234	4	LLEL	Gageopeptide C(Bacteriocin)	17	-4.9	HIS168, GLN143		8
40	5241	21215	4	IRIK	IK4-all D (Derived from IK8-all L)	21	-4.9	HIS168, GLN143		8
41	5505	21448	7	KKKLAYA	Peptide 25 (Derived from B1)	34	-4.9	HIS168, GLN143, ASP139, THR137, ALA95, PRO94		8
42	782	02999	8	PFKISIH	Jellein-1	32	-4.9	HIS168, ASN236, GLN143		8
43	3297	18231	4	LLLE	Gageotetrin C (Bacteriocin)	17	-4.8	HIS168, ASN236, GLN143		8
44	51	00766	7	KVFLGLK	JCpep7 (Plants)	31	-4.8	HIS168, ARG239, GLN143, ASP139		8
45	5483	21426	7	KKKGGGG	Peptide 3 (Derived from B1)	29	-4.8	HIS168, GLN143		8
46	5499	21442	7	AFALKKK	Peptide 19 (Derived from B1)	33	-4.8	HIS168, GLN143	8	
47	5363	21305	8	RRRRRRRR	R8 (De novo synthesis)	48	-4.8	HIS168, GLN143, ASP139, ILE235	8	
48	5485	21428	7	GGGKGGK	Peptide 5 (Derived from B1)	29	-4.7	HIS168, ASN236, PRO94, GLY170	8	
49	3219	18235	4	LLEL	Gageopeptide D(Bacteriocin)	17	-4.6	HIS168, GLN143	8	
50	3239	18233	4	LLLE	Gageopeptide B(Bacteriocin)	17	-4.6	HIS168, GLN143	8	
51	4674	18612	7	KIKVVK	LL-III/10	35	-4.6	HIS168, GLN143, ASP139	8	
52	5489	21432	7	KKKLAF	Peptide 9 (Derived from B1)	33	-4.5	HIS168, GLN143, ALA95	8	
53	5502	21445	7	KKKLAYA	Peptide 22 (Derived from B1)	34	-4.5	HIS168, GLN143, THR137, PRO94, GLY170, ILE235	8	
54	4932	20871	7	GLLKRIK	Pal-ano-7 (Pal-anoplin peptide derivative)	34	-4.3	HIS168, GLN143	8	
55	5509	21452	7	KKKLAF	Peptide 29 (Derived from B1)	33	-4.3	HIS168, ASN236, GLN143	8	
56	1245	04240	8	KLKLLLLL	Synthetic 1	38	-4.2	HIS168, GLN143	8	
57	4844	20778	8	FFFLSRIF	Temporin-SHf	34	-6.1	ARG239, GLN143, PRO94, ILE235, GLY234	Interaction with	7
58	3349	18227	7	LLDVLE	Gageostatin B (Bacteriocin)	28	-5.4	ARG239, GLN143, GLN143, ALA95		7
59	5490	21433	7	AFALKKK	Peptide 10 (Derived from B1)	33	-5.3	ARG239, ASN236		7
60	4886	20820	7	FRIRVRV	FV7	32	-5.1	ARG239, GLN143, ASP139, THR137, GLY234, GLY234		7

61	5498	21441	7	AFAKLKK	Peptide 18 (Derived from B1)	33	-5.1	ARG239, ASN236, ASN236, PRO94, GLY170, TYR233	Arg239 from the triad	7
62	26	00201	14	SCNCVCGVCCSCSP	Amythiamicin A/B (Bacteriocin)	49	-4.5	ARG239, GLN143, THR169		7
63	5484	21427	7	GGGGKKK	Peptide 4 (Derived from B1)	29	-4.3	ARG239, ASN236, ASP139, ALA95, ILE235		7
64	88	01827	13	VLPLISMALGKLL	Temporin-1La	48	-4.2	ARG239, ASN236, GLN143		7
65	1326	00031	7	GSEIQPR	Lantibiotic carnocin-UI49 (Bacteriocin)	27	-5	ASN236, ASN236, GLN143, ILE235	Multiple explicit interactions with Asn236 near the triad	6
66	5240	21217	8	IRIKIRIK	IK8-2D (Derived from IK8-all L)	42	-5	ASN236, ASN236, GLN143, ASP139, ASP139, ARG98		6
67	5245	21212	8	IRIKIRIK	IK8-all L (De novo synthesis)	42	-4.6	ASN236, ASN236, GLN143, ASP139		6
68	72	01082	16	ILGKLLSTAAGLLSNL	Alyteserin-2a	59	-4.5	ASN236, ASN236, GLN143, GLN143, GLN143, ASP140		6
69	113	01192	18	FLPKLFAKTKKNMAHIR	Andersonin-Y1	80	-4	ASN236, ASN236, GLN143, GLN143, THR137, LEU96, ARG98, THR237		6
70	5481	21424	7	KKGKGGG	B1 (De Novo Synthesis)	29	-4.9	ASN236, GLN143, LEU96, GLY170	Interactions with Asn236 and Gln143 near the triad	5
71	3052	18248	8	KYGDVPLY	Bifidin I (Bacteriocin)	31	-4.9	ASN236, GLN143, ILE235		5
72	1089	03991	8	KLLKWLLK	L4K3W5 (LIKmWn model peptide)	41	-4.8	ASN236, GLN143, ASP139, PRO94, THR237		5
73	2533	04395	5	AMVGT	EP3	16	-4.7	ASN236, GLN143, THR137		5
74	3983	04037	7	LKLLKKL	Immobilized peptide E07LKK	37	-4.5	ASN236, GLN143, ASP139, THR137		5
75	109	01188	19	LALKSGGWRLFLGDKDKKH	Chensinin-1ZHa	82	-3.9	ASN236, GLN143, ASP139, THR137, GLY234		5
76	50	00765	17	RPRCWIKIFRCKSLKF	Piceain 2	83	-3.8	ASN236, GLN143, ASP139, ASP139, LEU96, PRO94, ALA172		5
77	115	01195	15	FIFPKNIINSLFGR	Andersonin-D1	63	-3.6	ASN236, ASP139, ARG98, ARG98	Only one interaction with Asn236 near the triad	4
78	49	00764	20	KSLRPRCWIKIFRCKSLKF	Piceain 1	98	-2.8	ASN236, THR137, PRO94, ARG98, ARG98		4
79	4819	02842	6	RRWQWR	LfcinB (20-25)	31	-5.8	GLN143, GLN143, ASP139, LEU96, LEU96, PRO94	Only one interaction with Gln143 near the triad	3
80	3469	18220	6	TVYTNA	Fusaricidin C (Bacteriocin)	22	-5.6	GLN143, GLY170, ILE235		3
81	5486	21429	7	KKLKFAFA	Peptide 6 (Derived from B1)	33	-5.4	GLN143, ASP139, THR137, LEU96, PRO94		3
82	187	03542	10	HKTDSFVGLM	Neurokinin A	41	-5.2	GLN143, ASP139, THR237, THR237		3
83	3470	18219	6	TVVTQA	Fusaricidin B (Bacteriocin)	21	-5	GLN143, ILE235		3
84	5235	21222	8	IIRKIIRK	Control-4D (Derived from IK12-all L)	42	-5	GLN143, GLY170, GLY170, ILE235		3
85	5243	21213	8	IRIKIRIK	IK8-all D (Derived from IK8-all L)	42	-5	GLN143, ASP139, THR137, THR137, ILE235, THR237		3
86	995	03868	8	RIWVIWRR	Bac8c (Bac2A variant)	37	-4.9	GLN143, THR169, TYR233, GLY234		3
87	1086	03988	7	LLKWLLK	L3K3W4 (LIKmWn model peptide)	37	-4.8	GLN143, ASP139		3
88	5242	21216	8	IRIKIRIK	IK8-4D (Derived from IK8-all L)	42	-4.7	GLN143, PRO94, GLY170, ILE235		3
89	5495	21438	7	KKKLFAFA	Peptide 15 (Derived from B1)	33	-4.6	GLN143, ASP139, LEU96, PRO94		3
90	4933	20872	6	GLLKRI	Pal-ano-6 (Pal-anoplin peptide derivative)	27	-4.5	GLN143, GLY170, GLY170		3
91	5238	21220	8	IIRKIIRK	Control-all L (Derived from IK12-all L)	42	-4.5	GLN143		3
92	1088	03990	8	LLKWLLK	L4K3W4 (LIKmWn model peptide)	41	-4.3	GLN143		3
93	5488	21431	7	KKKLFAFA	Peptide 8 (Derived from B1)	33	-4.2	GLN143, ASP139, ASP139, ASP139, PRO94, ARG98		3
94	5500	21443	7	AFAKLKK	Peptide 20 (Derived from B1)	33	-5.3	ASP139, ASP139, ILE235	Interactions with Asp139 away from the triad	2
95	994	03867	8	RIWVIRWR	Bac8b (Bac2A variant)	37	-5	ASP139, PRO94, PRO94, GLY234		2
96	167	01350	11	FCTMIPIRCY	Tigerinin-1	42	-5	ASP139, THR237, THR237		2
97	2534	04394	5	AMVSS	EP2	18	-4.5	ASP139, THR169		2
98	5236	21221	8	IIRKIIRK	Control-all D (From IK12-all L)	42	-4.3	THR137	Interactions with residues away from the triad	1
99	5493	21436	7	AFALKKK	Peptide 13 (Derived from B1)	33	-4.3	GLY170, ILE235		1
100	3309	18229	2	LE	Gageotetrin A (Bacteriocin)	9	-4.3	THR231, THR231	1	
101	993	03866	8	KIWVIRWR	Bac8a (Bac2A variant)	38	-4.5	No H interaction with any residues	No interactions	0