

Table S1. Amino acid sequences of the protegrin peptides activity against *E.coli* with their corresponding experimental and predicted biological activity (*Test set peptides and Bold character is the reference peptide)

Sr. No.	Name	Sequence	Expt Log activity	Pred Log activity	Sr. No.	Name	Sequence	Expt Log activity	Pred Log activity
1	PG-1	RGGRLCYRRRFCVCVGR	6.38	6.32	41	PG-103	RGGRLCYRRRFCVCF	6.45	6.32
2	PG-4	RGGRLCYCRGWICFCVGR	6.00	5.95	42	PG-104*	RGGRLCYRRRFCVCW	6.53	6.32
3	PG-5	RGGRLCYCRPRFCVCVGR	5.86	6.29	43	PG-105	RGGRLCYRRRFCVCE	6.30	6.32
4	PG-6	RGGRLAYCRRRFCVAVGR	6.00	6.17	44	PG-106*	RGGRLCYRRRFCVCR	6.40	5.91
5	PG-10	RCYRRRFCVCVGR	6.21	6.32	45	PG-107	RLCYTRGRFTVCV	6.42	6.63
6	PG-11	RGGRLCYRRRFCVCV	6.18	6.32	46	PG-108	LCYTRGRFTVCVR	6.72	6.63
7	PG-12*	RGGRLCYRRRFCICV	6.01	6.26	47	PG-112	LCYRRRFCYCV	5.46	5.53
8	PG-13	RGGRLCYRRRFCVCR	5.94	5.91	48	PG-113*	LCYRRRFCFCV	5.16	5.65
9	PG-14	RCYRRRFCVCR	5.75	5.91	49	PG-146	LCYRRRFCTCV	6.18	6.19
10	PG-15*	LCYRRRFCVCV	6.01	6.32	50	PG-147	LCYRRRFCGCV	6.32	6.32
11	PG-16	LCYARRRFAVCV	6.39	6.41	51	PG-149	RGGRLCYRRRFCVCVGR	6.26	6.32
12	PG-17	RCYARRRFAVCR	6.19	6.00	52	PG-150	RGGGLCYRRRFCVCVGR	6.41	6.32
13	PG-18	LAYCRRRFCVAV	6.08	6.17					
14	PG-19	RAYCRRRFCVAR	5.72	5.76					
15	PG-20	CYCRRRFCVCVGR	5.93	6.04					
16	PG-21*	RGGRLCYRRRFCVC	6.01	5.91					
17	PG-37	LCYTRRRFTVCV	6.03	5.92					
18	PG-45	LTYCRRRFCVTV	6.48	6.32					
19	PG-64	LCYTRPRFTVCV	6.02	5.89					
20	PG-64a	LCYTRGRFTVCV	6.37	6.63					
21	PG-65	LCYTFRPRFVCV	5.69	5.58					
22	PG-70	LCYRRRFCVC	5.72	5.91					
23	PG-71	CYCRRRFCVC	5.61	5.63					
24	PG-72	CYCFRRFCVC	6.34	6.13					
25	PG-73	LCYCRRRRCVCV	5.04	4.98					
26	PG-74	LCYCFRRRCVCV	5.27	5.49					
27	PG-77	LCYCFRRRCVCV	6.18	6.16					
28	PG-78	LCYCRRFRCVCV	5.93	5.92					
29	PG-80	TCYRRRFCVCVGR	6.19	6.27					
30	PG-91	ACYRRRFCVCVGR	6.38	6.11					
31	PG-92	VCYRRRFCVCVGR	6.39	6.31					
32	PG-93	ICYRRRFCVCVGR	6.39	6.32					
33	PG-94*	FCYRRRFCVCVGR	6.47	6.26					
34	PG-95*	WCYRRRFCVCVGR	6.56	6.21					
35	PG-96*	ECYRRRFCVCVGR	6.46	6.27					
36	PG-97*	RGGRLCYRRRFCVCY	6.53	6.32					
37	PG-98*	RGGRLCYRRRFCVCT	6.44	6.32					
38	PG-100	RGGRLCYRRRFCVCA	6.38	6.32					
39	PG-101	RGGRLCYRRRFCVCL	6.45	6.32					
40	PG-102	RGGRLCYRRRFCVCI	6.39	6.32					

Table S2. Amino acid sequences of the protegrin peptides activity against *P.aeruginosa* with their corresponding experimental and predicted biological activity (* Test set peptides and Bold character is the reference peptide)

Sr. No	Name	Sequences	Expt Log activity	Pred Log activity
1	PG-1*	RGGRLCYCRRRFCVCVGR	6.38	6.29
2	PG-12	RGGRLCYCRRRFCICV	5.80	5.91
3	PG-15*	LCYCRRRFCVCV	5.70	5.54
4	PG-16	LCYARRRFAVCV	6.26	6.45
5	PG-17*	RCYARRRFAVCR	6.41	6.08
6	PG-37	LCYTRRRFTVCV	6.03	5.92
7	PG-45	LTYCRRRFCVTV	6.48	6.44
8	PG-71	CYCRRRFCVC	5.14	5.50
9	PG-72	CYCFRRFCVC	6.03	5.57
10	PG-73	LCYCRRRRCVCV	5.33	5.31
11	PG-74	LCYCFRRRCVCV	5.20	5.36
12	PG-77	LCYCFRRRCVCV	5.69	5.57
13	PG-78	LCYCRRFRCVCV	5.61	5.66
14	PG-80	TCYCRRRFCVCVGR	5.62	5.90
15	PG-98	RGGRLCYCRRRFCVCT	5.66	5.89
16	PG-100	RGGRLCYCRRRFCVCA	6.20	6.21
17	PG-101	RGGRLCYCRRRFCVCL	6.15	5.91
18	PG-102	RGGRLCYCRRRFCVCI	6.21	5.91
19	PG-103	RGGRLCYCRRRFCVCF	6.45	6.36
20	PG-104	RGGRLCYCRRRFCVCW	6.31	6.41
21	PG-105*	RGGRLCYCRRRFCVCE	6.45	6.10
22	PG-107	RLCYTRGRFTVCV	6.50	6.52
23	PG-108	LCYTRGRFTVCVR	6.59	6.50
24	PG-112*	LCYCRRRFCYCV	5.42	5.78
25	PG-147*	LCYCRRRFCGCV	6.22	5.88
26	PG-148*	LCYCRRRFCWCV	5.79	5.98
27	PG-149	RGGRLCYCRRRFCVCVGR	6.33	6.29
28	PG-150*	RGGGLCYCRRRFCVCVGR	6.36	6.26

Table S3. Amino acid sequences of the protegrin peptides activity against *N.Gonorrhoeae* F-62 with their corresponding experimental and predicted biological activity (*Test set peptides and Bold character is the reference peptide)

Sr. No	Name	Sequences	Expt Log activity	Pred Log activity
1	PG-1*	RGGRLCYCRRRFCVCVGR	6.26	5.93
2	PG-3*	RGGGLCYCRRRFCVCVGR	6.17	5.93
3	PG-4	RGGRLCYCRGWICFCVGR	6.24	5.90
4	PG-5*	RGGRLCYCRPRFCVCVGR	6.18	5.93
5	PG-6	RGGRLAYCRRRFCVAVGR	6.28	5.91
6	PG-7	RGGRLCYARRRFAVCVGR	5.55	5.90
7	PG-9	LCYCRRRFCVCVGR	6.24	5.93
8	PG-10	RCYCRRRFCVCVGR	6.35	6.28
9	PG-11*	RGGRLCYCRRRFCVCV	6.11	5.93
10	PG-12*	RGGRLCYCRRRFCICV	6.18	5.93
11	PG-13	RGGRLCYCRRRFCVCR	6.22	5.93
12	PG-14	RCYCRRRFCVCR	6.17	6.28
13	PG-15	LCYCRRRFCVCV	5.82	5.93
14	PG-16	LCYARRRFAVCV	5.03	5.90
15	PG-17	RCYARRRFAVCR	6.11	6.25
16	PG-18	LAYCRRRFCVAV	5.96	5.91
17	PG-19	RAYCRRRFCVAR	4.05	4.11
18	PG-20	CYCRRRFCVCVGR	5.67	5.55
19	PG-37	LCYTRRRFTVCV	5.93	5.91
20	PG-45	LYCRRRFCVTV	5.88	6.02
21	PG-64	LCYTRPRFTVCV	6.05	5.91
22	PG-064a	LCYTRGRFTVCV	6.31	5.91
23	PG-66	LCYTFRGRFVCV	4.39	4.53
24	PG-70	LCYCRRRFCVC	5.65	5.93
25	PG-71	CYCRRRFCVC	5.49	5.55
26	PG-72*	CYCFRRFCVC	5.86	5.55
27	PG-73	LCYCRRRRCVCV	4.68	4.53

Table S4. Amino acid sequences of the protegrin peptides activity against *N. Gonorrhoeae* FA-19 with their corresponding experimental and predicted biological activity (*Test set peptides and Bold character is the reference peptide)

Sr. No	Name	Sequences	Expt Log activity	Pred Log activity
1	PG-1	RGGRLCYRRRFCVCVGR	6.10	5.98
2	PG-4	RGGRLCYCRGWICFCVGR	5.78	5.39
3	PG-5	RGGRLCYCRPRFCVCVGR	6.12	6.10
4	PG-6	RGGRLAYCRRRFCVAVGR	5.58	5.59
5	PG-7	RGGRLCYARRRFACVGR	4.81	5.47
6	PG-9	LCYRRRFCVCVGR	5.44	5.27
7	PG-10	RCYRRRFCVCVGR	5.99	5.95
8	PG-11*	RGGRLCYRRRFCVCV	5.71	5.63
9	PG-12	RGGRLCYRRRFCICV	5.66	5.59
10	PG-13*	RGGRLCYRRRFCVCR	6.02	6.20
11	PG-14	RCYRRRFCVCR	6.06	6.19
12	PG-15	LCYRRRFCVCV	5.19	4.94
13	PG-16*	LCYARRRFACV	4.48	4.44
14	PG-17	RCYARRRFACVCR	5.81	5.68
15	PG-18	LAYCRRRFCVAV	5.09	4.74
16	PG-20	CYRRRFCVCVGR	4.49	5.12
17	PG-37	LCYTRRRFTVCV	5.18	4.94
18	PG-45*	LYCRRRFCVTV	5.18	5.18
19	PG-64	LCYTRPRFTVCV	5.02	5.07
20	PG-65*	LCYTFRPRFVCV	4.70	4.97
21	PG-66	LCYTFRGRFVCV	3.97	4.28
22	PG-69*	CYRRRFCVCV	4.04	4.77
23	PG-70	LCYRRRFCVC	4.64	4.77
24	PG-71*	CYRRRFCVC	5.00	4.60
25	PG-72	CYCFRRFCVC	5.19	5.32
26	PG-73	LCYRRRRRCVCV	4.20	4.17
27	PG-74	LCYCFRRRCVCV	5.13	4.89

Table S5. Amino acid sequences of the protegrin peptides activity against *L. monocytogenes* with their corresponding experimental and predicted biological activity (*Test set peptides and Bold character is the reference peptide)

Sr. No	Name	Sequences	Expt Log activity	Pred Log activity
1	PG-1*	RGGRLCYCRRRFCVCVGR	6.38	5.85
2	PG-3	RGGGLCYCRRRFCVCVGR	5.87	5.92
3	PG-4	RGGRLCYCRGWICFCVGR	6.04	6.04
4	PG-5*	RGGRLCYCRPRFCVCVGR	5.92	5.85
5	PG-6	RGGRLAYCRRRFCVAVGR	5.91	6.08
6	PG-10	RCYCRRRFCVCVGR	5.35	5.53
7	PG-11	RGGRLCYCRRRFCVCV	5.72	5.85
8	PG-12*	RGGRLCYCRRRFCICV	5.55	5.83
9	PG-13	RGGRLCYCRRRFCVCR	5.87	5.93
10	PG-14	RCYCRRRFCVCR	5.69	5.61
11	PG-15	LCYCRRRFCVCV	5.80	5.92
12	PG-16*	LCYARRRFAVCV	5.99	5.91
13	PG-18	LAYCRRRFCVAV	6.02	6.15
14	PG-21*	RGGRLCYCRRRFCVC	4.71	4.63
15	PG-37*	LCYTRRRFTVCV	5.56	5.87
16	PG-45	LTYCRRRFCVTV	6.70	6.63
17	PG-64	LCYTRPRFTVCV	5.86	5.87
18	PG-064a	LCYTRGRFTVCV	5.56	5.67
19	PG-65*	LCYTFRPRFVCV	5.16	5.68
20	PG-70	LCYCRRRFCVC	4.74	4.70
21	PG-77	LCYCRFRRCVCV	5.64	5.71
22	PG-78*	LCYCRRFRCVCV	5.93	5.71
23	PG-79	YCYCRRRFCVCVGR	5.31	5.59
24	PG-80	TCYCRRRFCVCVGR	5.68	5.57
25	PG-91	ACYCRRRFCVCVGR	6.05	5.92
26	PG-92*	VCYCRRRFCVCVGR	6.09	5.91
27	PG-93	ICYCRRRFCVCVGR	6.09	5.75
28	PG-94*	FCYCRRRFCVCVGR	6.13	5.92
29	PG-95	WCYCRRRFCVCVGR	6.11	5.82
30	PG-96	ECYCRRRFCVCVGR	6.16	5.91
31	PG-97*	RGGRLCYCRRRFCVCY	6.26	6.11

Table S6. Amino acid sequences of the protegrin peptides activity against *C. albicans* with their corresponding experimental and predicted biological activity (*Test set peptides and Bold character is the reference peptide)

Sr. No	Name	Sequences	Expt Log activity	Pred Log activity	Sr. No	Name	Sequences	Expt Log activity	Pred Log activity
1	PG-1*	RGGRLCYRRRFCVCVGR	5.61	5.21	41	PG-146	LCYCRRRFCTCV	5.14	5.01
2	PG-3	RGGGLCYRRRFCVCVGR	5.33	5.21	42	PG-147	LCYCRRRFCGCV	5.19	5.14
3	PG-4	RGGRLCYCRGWICFCVGR	4.84	4.82	43	PG-148	LCYCRRRFCWCV	4.81	4.90
4	PG-5	RGGRLCYCRPRFCVCVGR	5.13	5.21	44	PG-149*	RGGRLCYRRRFCVCVGR	4.88	5.21
5	PG-6	RGGRLAYCRRRFCVAVGR	5.12	5.02	45	PG-150	RGGGLCYRRRFCVCVGR	5.31	5.21
6	PG-7	RGGRLCYARRRFAVCVGR	5.05	5.02					
7	PG-10	RCYCRRRFCVCVGR	4.75	5.08					
8	PG-11	RGGRLCYRRRFCVCV	5.23	5.21					
9	PG-12	RGGRLCYRRRFCICV	4.98	5.25					
10	PG-13	RGGRLCYRRRFCVCR	5.29	5.38					
11	PG-14*	RCYCRRRFCVCR	5.21	5.25					
12	PG-15	LCYCRRRFCVCV	5.24	5.21					
13	PG-16	LCYARRRFAVCV	4.76	5.02					
14	PG-17	RCYARRRFAVCR	5.17	5.06					
15	PG-19	RAYCRRRFCVAR	4.72	4.89					
16	PG-20*	CYCRRRFCVCVGR	4.38	4.32					
17	PG-37	LCYTRRRFTVCV	4.74	4.70					
18	PG-45	LTYCRRRFCVTV	5.75	5.68					
19	PG-64	LCYTRPRFTVCV	4.71	4.70					
20	PG- 64a*	LCYTRGRFTVCV	5.07	4.70					
21	PG-71	CYCRRRFCVC	4.61	4.62					
22	PG-72	CYCFRRFCVC	4.66	4.62					
23	PG-74*	LCYCFRRRCVCV	4.74	4.65					
24	PG-77	LCYCFRRRCVCV	4.64	4.65					
25	PG-91	ACYCRRRFCVCVGR	5.28	5.21					
26	PG-92	VCYCRRRFCVCVGR	5.19	5.21					
27	PG-93	ICYCRRRFCVCVGR	5.17	5.21					
28	PG-94	FCYCRRRFCVCVGR	5.31	5.21					
29	PG-95	WCYCRRRFCVCVGR	5.26	5.21					
30	PG-96	ECYCRRRFCVCVGR	5.27	5.06					
31	PG-97	RGGRLCYRRRFCVCY	5.27	5.53					
32	PG-98*	RGGRLCYRRRFCVCT	4.95	5.23					
33	PG-100*	RGGRLCYRRRFCVCA	5.69	5.69					
34	PG-101*	RGGRLCYRRRFCVCL	5.65	5.14					
35	PG-102*	RGGRLCYRRRFCVCI	5.74	5.16					
36	PG-103	RGGRLCYRRRFCVCF	6.12	5.99					
37	PG-104	RGGRLCYRRRFCVCW	5.75	5.91					
38	PG-105	RGGRLCYRRRFCVCE	5.65	5.36					
39	PG-106	RGGRLCYRRRFCVCR	5.43	5.38					
40	PG-107*	RLCYTRGRFTVCV	4.69	4.70					