

Supporting Information

ABP-Finder: A tool to identify antibacterial peptides and the Gram-staining type of targeted bacteria

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Table of contents

Table S1. Number of peptides per type of Gram staining class in the training, development, validation, and test datasets.

Section S1. ProtDCal's configuration for vicinity operator Autocorrelation of grade 1 (AC1).

Section S2. ProtDCal's configuration for vicinity operator Autocorrelation of grade 2 (AC2).

Section S3. ProtDCal's configuration for vicinity operator Electrotopological State (EC).

Section S4. ProtDCal's configuration for no vicinity operator.

Section S5. List (FASTA format) of all the peptides in the training dataset.

Section S6. List (FASTA format) of all the peptides in the development dataset.

Section S7. List (FASTA format) of all the peptides in the validation dataset.

Section S8. List (FASTA format) of all the peptides in the test dataset.

Table S2. Minimum (Min) and maximum (Max) boundaries of the applicability domains defined for the models derived from the training and the production datasets. The first model distinguishes antibacterial peptides from non-antibacterial peptides (ABP) and the second model categorizes antibacterial peptides as anti-Gram+, anti-Gram- or anti- both types of bacteria (Gram).

Table S3. Values resulting from the radial diffusion assay applied to the peptide Urine-3462 against the *Pseudomonas aeruginosa* strain ATCC 27853.

Table S1. Number of peptides per type of Gram staining class in the training, development, validation and test datasets.

	<i>Gram+</i>	<i>Gram-</i>	<i>Broad Spectrum</i>
<i>Training</i>	351	478	4983
<i>Development</i>	52	105	911
<i>Validation</i>	37	82	546
<i>Test</i>	27	38	315

Section S1. ProtDCal's configuration for vicinity operator Autocorrelation of grade 1 (AC1).

directory:

Datasets/Fasta_Protein_Format

indices:

Gs(U),Gw(U),W(U),Mw,HP,Z1,IP,Z2,ECL,ISA,Z3

groups:

AHR,PCR,ARM,NPR,BSR,NCR,ALR,PLR,RTR,UCR,UFR,PRT

invariants:

N1,N2,N3,Ar,P2,P3,K,CV,Q1,RA,DE,Q2,S,MN,Q3,V,MX,I50,SI,MI,TI

parameters(t_cont,s_cont,A%,HydGroup,n,bins,K,SubG):

4.0,8.0,5.0,9.4,3.0,5,1,3

options(decimals,harmonicMeanType,geometricMeanType,windexID,datasetType,outputOrder):

2,0,0,0,fasta,true

Section S2. ProtDCal's configuration for vicinity operator Autocorrelation of grade 2 (AC2).

directory:

Datasets/Fasta_Protein_Format

indices:

Gs(U),Gw(U),W(U),Mw,HP,Z1,IP,Z2,ECL,ISA,Z3

groups:

AHR,PCR,ARM,NPR,BSR,NCR,ALR,PLR,RTR,UCR,UFR,PRT

invariants:

N1,N2,N3,Ar,P2,P3,K,CV,Q1,RA,DE,Q2,S,MN,Q3,V,MX,I50,SI,MI,TI

parameters(t_cont,s_cont,A%,HydGroup,n,bins,K,SubG):

4.0,8.0,5.0,9.4,3.0,5,2,3

options(decimals,harmonicMeanType,geometricMeanType,windexID,datasetType,outputOrder):

2,0,0,0,fasta,true

Section S3. ProtDCal's configuration for vicinity operator Electrotopological State (EC).

directory:

Datasets/Fasta_Protein_Format

indices:

Gs(U),Gw(U),W(U),Mw,HP,Z1,IP,Z2,ECI,ISA,Z3

groups:

AHR,PCR,ARM,NPR,BSR,NCR,ALR,PLR,RTR,UCR,UFR,PRT

invariants:

N1,N2,N3,Ar,P2,P3,K,CV,Q1,RA,DE,Q2,S,MN,Q3,V,MX,I50,SI,MI,TI

parameters(t_cont,s_cont,A%,HydGroup,n,bins,K,SubG):

4.0,8.0,5.0,9.4,3.0,5,5,3

options(decimals,harmonicMeanType,geometricMeanType,windexID,datasetType,outputOrder):

2,0,0,4,fasta,true

Section S4. ProtDCal's configuration for no vicinity operator

directory:

Datasets/Fasta_Protein_Format

indices:

Gs(U),Gw(U),W(U),Mw,HP,Z1,IP,Z2,ECL,ISA,Z3

groups:

AHR,PCR,ARM,NPR,BSR,NCR,ALR,PLR,RTR,UCR,UFR,PRT

invariants:

N1,N2,N3,Ar,P2,P3,K,CV,Q1,RA,DE,Q2,S,MN,Q3,V,MX,I50,SI,MI,TI

parameters(t_cont,s_cont,A%,HydGroup,n,bins,K,SubG):

4.0,8.0,5.0,9.4,3.0,5,5,3

options(decimals,harmonicMeanType,geometricMeanType,windexID,datasetType,outputOrder):

2,0,0,-1,fasta,true

Section S5. List (FASTA format) of all the peptides in the training dataset.

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>ID00001-ABP_both
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KWCFRVCYRGICYRRCR
>ID00004-ABP_both
LLGDFFRKSKEKIGKEFKRIVQRIKDFLRNLPRTES
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FFHHIFRGIVHVGKTIHRLVTG
>ID00006-ABP_both
FLPLIGRVLSGIL
>ID00007-ABP_both
FWGALAKGALKLIPSLFSSFSKGD
>ID00008-ABP_both
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>ID45045-NO
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>ID45049-ABP_both
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YYVPLGTQ
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Section S6. List (FASTA format) of all the peptides in the development dataset.

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 ISA_NO_PLR_Q3
 ECI_NO_AHR_I50
 Z3_NO_AHR_I50
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Gs(U)_AC2_PRT_P2
Gs(U)_AC2_PLR_Q3
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Mw_AC2_PLR_Q2
Gs(U)_AC2_NCR_Q3
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Z1_AC2_AHR_Q2
HP_AC2_UCR_Q2
ISA_AC2_RTR_Q3
Mw_AC2_RTR_MN
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Gs(U)_AC2_NCR_I50
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Gs(U)_ES_PCR_CV
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Section S7. List (FASTA format) of all the peptides in the validation dataset.

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Section S8. List (FASTA format) of all the peptides in the test dataset.

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Table S2. Minimum (Min) and maximum (Max) boundaries of the applicability domains defined for the models derived from the training and the production datasets. The first model distinguishes antibacterial peptides from non-antibacterial peptides (ABP) and the second model categorizes antibacterial peptides as anti-Gram+, anti-Gram- or anti- both types of bacteria (Gram).

<i>Descriptor</i>	<i>Training (ABP)</i>		<i>Training (Gram)</i>		<i>Production (ABP)</i>		<i>Production (Gram)</i>	
	Min	Max	Min	Max	Min	Max	Min	Max
<i>ISA_NO_PCR_N2</i>	52,98	581,41	52,98	511,043	52,98	581,41	52,98	511,043
<i>Z3_NO_PLR_I50</i>	-3,44	7,57	-3,44	7,57	-3,44	7,57	-3,44	7,57
<i>Gs(U)_NO_PLR_I50</i>	-1015,71	1338,19	-1015,709	1338,189	-1015,71	1338,19	-1015,709	1338,189
<i>IP_NO_PRT_I50</i>	0	7,99	0	6,52	0	7,99	0	6,52
<i>IP_NO_PLR_Q2</i>	2,77	10,76	2,77	10,76	2,77	10,76	2,77	10,76
<i>Gs(U)_NO_PRT_I50</i>	0	1793,24	0	1793,239	0	1793,24	0	1793,239
<i>IP_NO_AHR_I50</i>	0	9,74	0	9,74	0	9,74	0	9,74
<i>Z3_NO_PRT_N1</i>	-116,18	50,54	-113,52	46,65	-116,18	50,54	-113,52	46,65
<i>IP_NO_PRT_Q1</i>	2,77	10,76	2,77	10,76	2,77	10,76	2,77	10,76
<i>Z2_NO_PLR_I50</i>	-2,09	4,61	-2,09	4,61	-2,09	4,61	-2,09	4,61
<i>Z3_NO_PRT_CV</i>	-	9,45044E+1	-	1,96182E+1	-	9,45044E+1	-	1,96182E+1
	6,38346E+1	6	3,61425E+1	6	6,38346E+1	6	3,61425E+1	6
	6		6		6		6	
<i>Z3_NO_PLR_Q2</i>	-3,44	4,13	-3,44	4,13	-3,44	4,13	-3,44	4,13
<i>Z2_NO_AHR_I50</i>	-1,73	3,47	-1,73	3,47	-1,73	3,47	-1,73	3,47
<i>IP_NO_PRT_RA</i>	0	7,99	0	7,99	0	7,99	0	7,99
<i>ISA_NO_PLR_Q3</i>	17,87	132,16	17,87	132,16	17,87	132,16	17,87	132,16
<i>ECI_NO_AHR_I50</i>	0	1,36	0	1,36	0	1,36	0	1,36
<i>Z3_NO_AHR_I50</i>	-3,14	7,27	-3,14	7,27	-3,14	7,27	-3,14	7,27
<i>Gw(U)_NO_PCR_SI5</i>	0	1	0	1	0	1	0	1
<i>IP_NO_AHR_RA</i>	0	6,52	0	6,52	0	6,52	0	6,52
<i>Z1_NO_PCR_V</i>	0	0,11	0	0,11	0	0,11	0	0,11
<i>Z3_NO_ALR_N3</i>	-3,72	6,5	-3,721	6,004	-3,72	6,5	-3,721	6,004
<i>Z1_NO_NPR_N1</i>	-100,56	55,75	-90,82	55,75	-100,56	55,75	-90,82	55,75

<i>Gw(U)_NO_PCR_M</i>	-35,07	-1,72	-34,315	-1,718	-35,072	-1,718	-34,315	-1,718
<i>X</i>								
<i>Z3_NO_AHR_RA</i>	0	7,27	0	7,27	0	7,27	0	7,27
<i>ISA_NO_PRT_Q1</i>	17,87	189,42	17,87	189,42	17,87	189,42	17,87	189,42
<i>IP_NO_PLR_N3</i>	2,77	33,38	2,77	31,037	2,77	33,38	2,77	31,037
<i>Mw_NO_AHR_I50</i>	0	137	0	137	0	137	0	137
<i>ECI_NO_PLR_MN</i>	0,15	1,69	0,15	1,69	0,15	1,69	0,15	1,69
<i>ECI_NO_PLR_TI5</i>	0	75,86	0	74,98	0	79,338	0	79,338
<i>IP_NO_AHR_MX</i>	3,22	9,74	3,22	9,74	3,22	9,74	3,22	9,74
<i>Z3_NO_PLR_SI5</i>	0	1	0	1	0	1	0	1
<i>Gw(U)_NO_AHR_I50</i>	-28,91	30,86	-28,359	28,912	-28,91	30,86	-28,359	28,912
<i>ECI_NO_PCR_MN</i>	0,53	1,69	0,53	1,69	0,53	1,69	0,53	1,69
<i>IP_NO_AHR_DE</i>	0	4,61	0	4,61	0	4,61	0	4,61
<i>Gs(U)_NO_AHR_P2</i>	185,74	818,65	185,74	818,649	185,74	818,65	185,74	818,649
<i>Gs(U)_NO_BSR_N1</i>	-4052,65	14716,69	-2472,433	14716,693	-4052,65	14716,69	-2472,433	14716,693
<i>Mw_NO_PLR_Q2</i>	87	163	87	163	87	163	87	163
<i>Z2_NO_RTR_P3</i>	-5,36	1,45	-5,36	1,45	-5,36	1,45	-5,36	1,45
<i>Z2_NO_NPR_SI5</i>	0	1	0	1	0	1	0	1
<i>Mw_NO_RTR_P3</i>	57	115	57	115	57	115	57	115
<i>ECI_NO_PLR_Q3</i>	0,15	1,69	0,53	1,69	0,15	1,69	0,53	1,69
<i>Z2_NO_PLR_MI5</i>	0	2,58	0	2,55	0	2,58	0	2,561
<i>ISA_NO_PLR_N2</i>	17,87	581,41	17,87	513,006	17,87	581,41	17,87	513,006
<i>Z2_NO_PRT_RA</i>	0	9,01	0	9,01	0	9,01	0	9,01
<i>Z3_NO_NPR_I50</i>	-1,29	3,52	-1,29	3,52	-1,29	3,52	-1,29	3,52
<i>ECI_NO_PLR_CV</i>	0	1,44	0	1,263	0	1,44	0	1,263
<i>Z2_NO_RTR_I50</i>	-5,36	6,81	-5,36	6,81	-5,36	6,81	-5,36	6,81
<i>Mw_NO_PRT_I50</i>	0	115	0	99	0	115	0	99
<i>HP_NO_PLR_Ar</i>	-4,5	2,5	-4,5	1,3	-4,5	2,5	-4,5	1,3
<i>ECI_NO_RTR_I50</i>	0	1,31	0	1,31	0	1,31	0	1,31
<i>Gw(U)_NO_PCR_P3</i>	-37,77	-1,72	-37,77	-1,718	-37,77	-1,718	-37,77	-1,718
<i>Z1_NO_PRT_MX</i>	-4,92	3,64	-4,92	3,64	-4,92	3,64	-4,92	3,64

<i>Z2_NO_AHR_P2</i>	0,27	1,74	0,27	1,74	0,27	1,74	0,27	1,74
<i>Mw_NO_PRT_RA</i>	0	129	0	129	0	129	0	129
<i>ISA_NO_AHR_DE</i>	0	95,33	0	95,332	0	95,332	0	95,332
<i>Mw_NO_PRT_Q2</i>	57	186	57	186	57	186	57	186
<i>Z3_NO_PLR_P2</i>	0,01	4,13	0,01	3,869	0,01	4,13	0,01	3,879
<i>Gs(U)_NO_PCR_Q1</i>	-1015,71	-583,48	-1015,709	-583,484	-1015,71	-583,48	-1015,709	-583,484
<i>ISA_NO_PLR_CV</i>	0	1,24	0	1,208	0	1,24	0	1,208
<i>Z3_NO_PLR_N2</i>	0,01	19,46	0,01	16,852	0,01	19,46	0,01	16,852
<i>Z3_NO_RTR_I50</i>	0	2,36	0	2,36	0	2,36	0	2,36
<i>Z1_NO_PRT_SI5</i>	0	1	0	1	0	1	0	1
<i>Z1_NO_NPR_I50</i>	-4,92	7,15	-4,92	7,15	-4,92	7,15	-4,92	7,15
<i>Z1_NO_PRT_P2</i>	0,9	4,92	0,901	4,92	0,9	4,92	0,901	4,92
<i>Z1_NO_PLR_N1</i>	-4,17	108,88	-1,39	97,02	-4,17	108,88	-1,39	102,74
<i>ECI_NO_ALR_P3</i>	0,01	0,34	0,01	0,34	0,01	0,34	0,01	0,34
<i>ISA_NO_NPR_SI5</i>	0	1	0	1	0	1	0	1
<i>Mw_NO_RTR_RA</i>	0	58	0	58	0	58	0	58
<i>Z2_NO_PCR_Q3</i>	1,41	2,52	1,41	2,52	1,41	2,52	1,41	2,52
<i>ISA_NO_PLR_V</i>	0	6531,1	0	5198,94	0	6531,1	0	5198,94
<i>ISA_NO_NPR_I50</i>	0	189,42	0	189,42	0	189,42	0	189,42
<i>Z1_NO_AHR_Q2</i>	-4,19	3,08	-4,19	3,08	-4,19	3,08	-4,19	3,08
<i>Z1_NO_PRT_Q1</i>	-4,92	3,64	-4,92	3,64	-4,92	3,64	-4,92	3,64
<i>Mw_NO_ALR_SI5</i>	0	1	0	1	0	1	0	1
<i>IP_AC1_PRT_Q2</i>	15,35	231,56	15,346	231,555	15,35	231,56	15,346	231,555
<i>IP_AC1_AHR_Q1</i>	8,92	209,6	10,368	209,605	8,919	209,6	10,368	209,605
<i>Z1_AC1_PCR_Q3</i>	-28,34	20,97	-27,946	19,757	-28,34	20,97	-27,946	19,757
<i>Z1_AC1_PCR_MN</i>	-28,34	20,97	-28,339	19,354	-28,34	20,97	-28,339	19,354
<i>ECI_AC1_PCR_Q3</i>	0,01	5,71	0,005	5,712	0,005	5,712	0,005	5,712
<i>HP_AC1_PCR_MN</i>	-40,5	36	-40,5	31,5	-40,5	36	-40,5	31,5
<i>Z2_AC1_PCR_MI5</i>	0	2,58	0	2,585	0	2,585	0	2,585
<i>Z1_AC1_PCR_CV</i>	-6194,93	4647,27	-2936,387	2488,821	-32640,381	4647,27	-3155,779	2674,221
<i>IP_AC1_RTR_Q3</i>	14,04	139,45	14,044	139,45	14,04	139,45	14,044	139,45

<i>Mw_AC1_PCR_Q2</i>	7296	58032	7296	58032	7296	58032	7296	58032
<i>Mw_AC1_NPR_MX</i>	4959	69192	7171	69192	4959	69192	7171	69192
<i>IP_AC1_RTR_MX</i>	14,04	139,45	14,044	139,45	14,04	139,45	14,044	139,45
<i>IP_AC1_RTR_Q2</i>	14,04	139,45	14,044	139,45	14,04	139,45	14,044	139,45
<i>Mw_AC1_PCR_SI5</i>	0	1	0	1	0	1	0	1
<i>Mw_AC1_PCR_Q1</i>	7296	58032	7296	58032	7296	58032	7296	58032
<i>IP_AC1_ALR_Q2</i>	16,54	139,45	16,537	139,45	16,54	139,45	16,537	139,45
<i>ISA_AC1_PCR_SI5</i>	0	1	0	1	0	1	0	1
<i>Z2_AC1_PCR_MN</i>	-27,01	18,4	-27,014	18,396	-27,014	18,4	-27,014	18,396
<i>Z2_AC1_PCR_Q2</i>	-27,01	18,4	-27,014	18,396	-27,01	18,4	-27,014	18,396
<i>Gs(U)_AC1_BSR_M</i>	-1579487,69	1057312,79	-	893700,369	-	1133208,39	-	893700,369
<i>N</i>			1579487,69		1579487,69	9	1579487,69	
			2		2		2	
<i>ISA_AC1_ALR_MX</i>	356,15	58473,95	367,908	58473,954	356,15	58473,954	367,908	58473,954
<i>ISA_AC1_PCR_P3</i>	946,75	38937,18	1034,699	38937,175	946,75	38937,18	1034,699	38937,175
<i>Gs(U)_AC1_PLR_Q2</i>	-1579487,69	2063330,66	-	2063330,66	-1579487,69	2063330,66	-	2063330,66
			1579487,69	4		4	1579487,69	4
			2				2	
<i>ISA_AC1_PRT_M</i>	470,47	55813,23	511,157	55813,234	470,47	55813,23	511,157	55813,234
<i>IP_AC1_ARM_Q1</i>	15,18	163,34	15,18	163,337	15,18	163,34	15,18	163,337
<i>Z3_AC1_RTR_MN</i>	-16,24	11,69	-16,237	9,747	-16,24	11,69	-16,237	9,747
<i>IP_AC1_BSR_N3</i>	15,18	296,86	15,678	296,859	15,18	300,115	15,678	296,859
<i>Gs(U)_AC1_PCR_Q1</i>	-1579487,69	2063330,66	-	2063330,66	-	2063330,66	-	2063330,66
			1579487,69	4	1579487,69	4	1579487,69	4
			2		2		2	
<i>Z1_AC1_ALR_MN</i>	-32,32	43,69	-32,323	43,69	-32,32	43,69	-32,323	43,69
<i>Gs(U)_AC1_PCR_CV</i>	-4468,31	33259,35	-4468,312	8490,981	-4468,31	33259,35	-4468,312	8490,981
<i>Z3_AC1_PCR_Ar</i>	-28,41	22,19	-28,414	21,977	-28,41	22,19	-28,414	21,977
<i>Z2_AC1_PCR_CV</i>	-	4,74163E+1	-	997,75	-	4,74163E+1	-	997,75
	4,1852E+16	5	4,1852E+16		4,1852E+16	5	4,1852E+16	
<i>Z2_AC1_UFR_Q2</i>	-39,13	57,46	-39,128	57,459	-39,13	57,46	-39,128	57,459
<i>Z2_AC1_PCR_MX</i>	-27,01	18,4	-19,883	18,396	-27,01	18,4	-19,883	18,396

<i>IP_AC1_NPR_MN</i>	15,18	139,45	15,18	129,55	15,18	139,45	15,18	129,55
<i>HP_AC1_AHR_MN</i>	-35,1	35,1	-35,1	35,1	-35,1	35,1	-35,1	35,1
<i>IP_AC1_BSR_MN</i>	15,18	129,55	15,18	129,55	15,18	129,55	15,18	129,55
<i>Z2_AC1_PRT_MX</i>	-13,51	57,46	-13,507	57,459	-13,51	57,46	-13,507	57,459
<i>Gw(U)_AC1_PCR_S</i>	-3,68	3,2	-2,584	3,201	-3,68	3,2	-2,584	3,201
<i>Z3_AC1_UCR_N3</i>	-41,54	54,4	-41,541	54,398	-41,54	54,4	-41,541	54,398
<i>HP_AC1_UFR_Q3</i>	-14,4	14,4	-13,92	14,4	-14,4	14,4	-14,4	14,4
<i>IP_AC1_UFR_MN</i>	16,54	139,45	16,537	139,45	16,537	139,45	16,537	139,45
<i>Z3_AC1_PCR_N2</i>	0,01	109,83	0,022	86,609	0,01	109,83	0,022	86,609
<i>Z3_AC1_UFR_N3</i>	-35,87	22,93	-25,566	22,927	-35,87	22,93	-29,715	22,927
<i>Mw_AC1_AHR_Q2</i>	4047	50964	4047	50964	4047	50964	4047	50964
<i>ISA_AC1_BSR_Q2</i>	1062,19	71759,87	2231,999	71759,873	1062,19	71759,87	2231,999	71759,873
<i>ISA_AC1_UFR_Q3</i>	356,15	46351,07	356,149	46351,074	356,149	46351,074	356,149	46351,074
<i>Mw_AC1_ALR_N3</i>	4959	82987,4	5871	76407,394	4959	82987,4	5871	76407,394
<i>ECI_AC1_PRT_MX</i>	0	5,71	0,002	5,712	0	5,712	0,002	5,712
<i>ISA_AC1_UCR_MX</i>	329,88	50067,49	393,618	50067,494	329,88	50067,49	393,618	50067,494
<i>Z3_AC1_RTR_CV</i>	-	77823,08	-479,559	1577,997	-	81603,356	-479,559	1577,997
	1,43686E+16				1,43686E+16			
<i>Gs(U)_AC1_NCR_Q3</i>	-882104,01	1229493,56	-882104,009	1229493,558	-882104,01	1229493,56	-882104,009	1229493,558
<i>ISA_AC1_ARM_Q1</i>	1561,48	65116,91	1561,481	65116,913	1561,48	65116,91	1561,481	65116,913
<i>Gw(U)_AC1_PCR_G</i>	0	2621,92	0	2621,918	0	2621,92	0	2621,918
<i>Z2_AC1_UCR_Q1</i>	-24,87	22,4	-24,87	17,474	-24,87	22,4	-24,87	17,474
<i>Mw_AC1_ARM_Q3</i>	7809	69192	7809	69192	7809	69192	7809	69192
<i>Z2_AC1_NPR_MN</i>	-39,13	28,73	-39,128	22,52	-39,13	28,73	-39,128	22,52
<i>Z2_AC1_PCR_N3</i>	-46,08	33,66	-43,325	32,454	-46,08	33,66	-43,325	32,454
<i>Z3_AC1_ALR_MN</i>	-15,34	11,69	-15,342	9,232	-15,342	11,69	-15,342	9,232
<i>IP_AC1_ARM_Q3</i>	15,18	163,34	15,18	163,337	15,18	163,34	15,18	163,337
<i>Gw(U)_AC1_PCR_M</i>	0	2226,07	0	1884,606	0	2226,07	0	1884,606
<i>N</i>								

<i>ZI_AC1_BSR_Q3</i>	-33,06	48,41	-28,31	48,413	-33,06	48,41	-28,31	48,413
<i>Mw_AC1_ALR_Q3</i>	4959	48732	5871	44802	4959	48732	5871	44802
<i>HP_AC1_ALR_Q2</i>	-40,5	40,5	-40,5	40,5	-40,5	40,5	-40,5	40,5
<i>Gs(U)_AC1_PCR_I5</i>	-1579487,69	2999111,86	-	2999111,85	-	2999111,86	-	2999111,85
<i>0</i>			1480343,05	9	1579487,69		1480343,05	9
			7		2		7	
<i>Z3_AC1_UCR_Q1</i>	-28,41	26,27	-28,414	17,057	-28,414	26,27	-28,414	17,057
<i>ECI_AC1_AHR_Q3</i>	0	4,6	0	4,597	0	4,6	0	4,597
<i>Mw_AC1_UCR_Q3</i>	4959	60636	4959	60636	4959	60636	4959	60636
<i>ZI_AC1_AHR_Q3</i>	-30,5	41,23	-29,26	40,517	-30,5	41,23	-29,26	40,517
<i>IP_AC1_ALR_RA</i>	0	122,91	0	122,913	0	122,913	0	122,913
<i>Gw(U)_AC1_AHR_M</i>	0	2326,26	0	2326,259	0	2326,26	0	2326,259
<i>X</i>								
<i>ISA_AC1_NPR_Q3</i>	393,62	71759,87	787,235	71759,873	393,62	71759,87	787,235	71759,873
<i>Z2_AC1_PLR_Q3</i>	-27,01	22,4	-27,014	18,396	-27,01	22,4	-27,014	18,396
<i>ZI_AC1_PCR_N2</i>	0,17	114,76	0,199	78,499	0,17	114,76	0,199	78,499
<i>Mw_AC1_NCR_MN</i>	6555	47988	6555	47988	6555	47988	6555	47988
<i>W(U)_AC1_UCR_M</i>	0	1104	0	880	0	1104	0	880
<i>N</i>								
<i>ISA_AC1_UCR_Q3</i>	329,88	50067,49	393,618	47355,571	329,88	50067,49	393,618	47355,571
<i>ZI_AC1_UCR_N3</i>	-40,97	39,48	-40,971	32,283	-40,97	39,48	-40,971	32,676
<i>Mw_AC1_PLR_Q2</i>	4959	58032	5757	58032	4959	58032	5757	58032
<i>Z3_AC1_BSR_Q1</i>	-11,56	9,63	-11,564	9,212	-11,564	9,63	-11,564	9,212
<i>ZI_AC1_BSR_MX</i>	-33,06	48,41	-28,31	48,413	-33,06	48,413	-28,31	48,413
<i>Z2_AC1_ARM_Q1</i>	-39,13	22,52	-39,128	22,52	-39,13	22,52	-39,128	22,52
<i>IP_AC2_PRT_Q1</i>	7,67	231,56	7,673	128,69	7,67	231,56	7,673	128,69
<i>ZI_AC2_PCR_MN</i>	-28,34	20,97	-28,339	16,813	-28,34	20,97	-28,339	19,482
<i>IP_AC2_AHR_MX</i>	15,65	209,6	15,651	209,605	15,65	209,605	15,651	209,605
<i>Gs(U)_AC2_AHR_M</i>	-1381198,42	1663019,09	-	1663019,09	-	1663019,09	-	1663019,09
<i>N</i>			1381198,42	3	1381198,42		1381198,42	3
			1		1		1	

Z1_AC2_PCR_N2	0,17	98,8	0,169	78,554	0,17	98,8	0,169	78,554
Gs(U)_AC2_PLR_Q1	-1579487,69	2063330,66	-	1340372,89	-	2063330,66	-	1340372,89
			1579487,69	9	1579487,69		1579487,69	9
			2		2		2	
Z3_AC2_PCR_Q3	-28,41	23,67	-28,414	23,667	-28,414	23,67	-28,414	23,667
HP_AC2_PLR_MN	-40,5	21,35	-40,5	20,25	-40,5	21,35	-40,5	20,25
IP_AC2_NPR_P3	15,18	136,22	16,537	128,69	15,18	136,22	16,537	128,69
HP_AC2_PLR_MX	-40,5	40,5	-40,5	40,5	-40,5	40,5	-40,5	40,5
IP_AC2_NPR_N3	15,18	348,41	16,537	348,408	15,18	348,41	16,537	348,408
IP_AC2_PCR_Q1	21,02	231,56	21,024	189,735	21,02	231,56	21,024	189,735
IP_AC2_ALR_P3	15,9	139,45	16,537	139,45	15,9	139,45	16,537	139,45
Gs(U)_AC2_PCR_Q1	-1579487,69	2063330,66	-	1646412,11	-	2063330,66	-	1646412,11
			1579487,69	1	1579487,69		1579487,69	1
			2		2		2	
IP_AC2_RTR_MN	7,67	139,45	7,673	139,45	7,67	139,45	7,673	139,45
Z1_AC2_PCR_Q3	-28,34	20,97	-28,339	20,966	-28,34	20,97	-28,339	20,966
IP_AC2_RTR_Q2	7,67	139,45	7,673	139,45	7,67	139,45	7,673	139,45
Z3_AC2_PCR_MI5	0	2,58	0	2,585	0	2,585	0	2,585
IP_AC2_ALR_Q2	15,9	139,45	16,537	139,45	15,9	139,45	16,537	139,45
Z1_AC2_PCR_P3	-28,34	20,97	-28,339	17,014	-28,34	20,97	-28,339	19,482
ECI_AC2_PCR_SI5	0	1	0	1	0	1	0	1
Gs(U)_AC2_AHR_N3	-3233254,1	4144046,87	-	3312445,96	-3233254,1	4144046,87	-	3312445,96
			2790877,16	8			2790877,16	8
			8				8	
Z3_AC2_PCR_S	-3,09	3,68	-2,475	2,041	-3,09	3,68	-2,475	2,041
Gs(U)_AC2_PCR_CV	-124046,25	5815,45	-2605,349	3167,065	-124046,25	5815,45	-2605,349	3167,065
IP_AC2_UCR_Q2	8,92	126,32	15,734	126,322	8,92	126,322	15,734	126,322
Z3_AC2_UCR_MX	-25,94	34,11	-25,936	34,114	-25,94	34,114	-25,936	34,114
Gs(U)_AC2_PRT_P2	2826,9	1859861,13	4434,144	1828947,15	2826,9	1859861,13	4434,144	1828947,15
				5				5

<i>Gs(U)_AC2_PLR_Q3</i>	-1579487,69	2063330,66	-	2063330,66	-1579487,69	2063330,66	-	2063330,66
			1579487,69	4		4	1579487,69	4
			2				2	
<i>IP_AC2_ARM_Q2</i>	15,18	163,34	15,18	163,337	15,18	163,34	15,18	163,337
<i>Z2_AC2_PCR_Q1</i>	-27,01	18,4	-27,014	18,396	-27,014	18,4	-27,014	18,396
<i>HP_AC2_PCR_Q3</i>	-40,5	40,5	-40,5	40,5	-40,5	40,5	-40,5	40,5
<i>IP_AC2_BSR_P3</i>	15,18	129,55	16,537	126,753	15,18	129,55	16,537	126,753
<i>IP_AC2_AHR_MN</i>	8,92	209,6	8,919	209,605	8,919	209,6	8,919	209,605
<i>Z2_AC2_ALR_MN</i>	-39,13	37,47	-39,128	28,73	-39,13	37,47	-39,128	28,73
<i>IP_AC2_PCR_V</i>	0	7459,83	0	6571,732	0	7459,83	0	6571,732
<i>Z1_AC2_PRT_N2</i>	0,29	183,29	0,286	126,991	0,29	183,29	0,286	126,991
<i>Gs(U)_AC2_UFR_M</i>	-304785,56	398150,24	-304785,562	398150,235	-304785,562	398150,24	-304785,562	398150,235
<i>X</i>								
<i>Z1_AC2_PRT_MN</i>	-35,82	24,21	-35,818	24,206	-35,82	24,21	-35,818	24,206
<i>HP_AC2_UCR_Q3</i>	-31,5	31,5	-31,5	31,5	-31,5	31,5	-31,5	31,5
<i>IP_AC2_BSR_Q1</i>	15,18	129,55	15,18	128,474	15,18	129,55	15,18	128,474
<i>HP_AC2_AHR_Q1</i>	-35,1	35,1	-35,1	35,1	-35,1	35,1	-35,1	35,1
<i>ISA_AC2_ARM_Q1</i>	1561,48	71759,87	1561,481	58931,099	1561,48	71759,87	1561,481	59055,473
<i>Mw_AC2_PLR_Q2</i>	4959	58032	4959	58032	4959	58032	4959	58032
<i>Gs(U)_AC2_NCR_Q3</i>	-941182,13	1229493,56	-941182,126	1229493,55	-941182,13	1229493,56	-941182,126	1229493,55
				8				8
<i>ISA_AC2_RTR_Q1</i>	319,34	46351,07	319,337	41499,896	319,337	46351,07	319,337	41499,896
<i>Z1_AC2_AHR_Q2</i>	-29,78	41,23	-29,26	39,805	-29,78	41,23	-29,26	39,805
<i>HP_AC2_UCR_Q2</i>	-31,5	31,5	-31,5	31,5	-31,5	31,5	-31,5	31,5
<i>ISA_AC2_RTR_Q3</i>	319,34	46351,07	349,001	46351,074	319,34	46351,074	349,001	46351,074
<i>Mw_AC2_RTR_MN</i>	3249	42780	3249	42780	3249	42780	3249	42780
<i>IP_AC2_UFR_MN</i>	16,54	139,45	16,537	139,45	16,537	139,45	16,537	139,45
<i>ISA_AC2_UCR_MN</i>	319,34	50067,49	319,337	50067,494	319,337	50067,49	319,337	50067,494
<i>Z3_AC2_UFR_Q3</i>	-15,34	18,42	-15,342	18,42	-15,34	18,42	-15,342	18,42
<i>IP_AC2_RTR_MX</i>	7,67	139,45	15,346	139,45	7,67	139,45	15,346	139,45
<i>IP_AC2_ALR_RA</i>	0	123,55	0	116,303	0	123,55	0	116,303

<i>IP_AC2_BSR_MN</i>	15,18	129,55	15,18	126,753	15,18	129,55	15,18	126,753
<i>Z2_AC2_PCR_N2</i>	0,13	68,95	0,212	68,951	0,127	68,95	0,212	68,951
<i>Z3_AC2_UFR_Q1</i>	-15,34	18,42	-15,342	18,42	-15,342	18,42	-15,342	18,42
<i>Z3_AC2_PCR_Ar</i>	-28,41	21,52	-28,414	20,286	-28,414	21,52	-28,414	20,286
<i>Z3_AC2_RTR_N3</i>	-31,15	25,63	-31,148	24,654	-31,15	25,63	-31,148	24,654
<i>Z1_AC2_ARM_Q2</i>	-35,82	48,41	-35,818	48,413	-35,82	48,41	-35,818	48,413
<i>ECI_AC2_ARM_MX</i>	0	3,65	0,001	3,65	0	3,65	0,001	3,65
<i>HP_AC2_NCR_P2</i>	0	31,5	0	31,5	0	31,5	0	31,5
<i>Z3_AC2_PLR_MN</i>	-28,41	15,2	-28,414	15,205	-28,414	15,2	-28,414	15,205
<i>ECI_AC2_PLR_Q2</i>	0	5,71	0,005	5,712	0	5,712	0,005	5,712
<i>HP_AC2_ALR_Q1</i>	-40,5	28,88	-40,5	25,2	-40,5	28,88	-40,5	25,2
<i>Z1_AC2_UFR_MN</i>	-21,94	16,23	-21,943	14,54	-21,943	16,23	-21,943	14,54
<i>Z1_AC2_AHR_Q3</i>	-29,78	41,23	-29,26	41,23	-29,78	41,23	-29,26	41,23
<i>HP_AC2_ALR_N3</i>	-97,43	81,23	-97,433	65,602	-97,43	81,23	-97,433	65,602
<i>HP_AC2_RTR_Q1</i>	-31,5	31,5	-31,5	31,5	-31,5	31,5	-31,5	31,5
<i>Gs(U)_AC2_UCR_Q2</i>	-1001308,09	1308037,85	-	1308037,84	-1001308,09	1308037,85	-	1308037,84
			1001308,08	6			1001308,08	6
			6				6	
<i>ECI_AC2_PLR_Q3</i>	0	5,71	0,005	5,712	0	5,712	0,005	5,712
<i>Gs(U)_AC2_NCR_I50</i>	-941182,13	1787105,08	-941182,126	1767297,89	-941182,13	1787105,08	-941182,126	1767297,89
				2				2
<i>Z1_AC2_AHR_N2</i>	0,01	183,29	0,013	99,909	0,01	183,29	0,013	99,909
<i>Mw_AC2_AHR_Q3</i>	4047	50964	4047	50964	4047	50964	4047	50964
<i>Z2_AC2_AHR_N2</i>	0,01	53,23	0,01	50,224	0,01	53,23	0,01	50,224
<i>Mw_AC2_UCR_MX</i>	4959	60636	4959	60636	4959	60636	4959	60636
<i>Z1_AC2_UCR_Ar</i>	-30,72	20,99	-30,722	18,547	-30,722	20,99	-30,722	18,547
<i>Z1_AC2_NPR_N3</i>	-67,75	111,6	-62,551	84,284	-67,75	111,6	-62,551	84,284
<i>Z1_AC2_RTR_Q2</i>	-35,2	26,5	-34,58	23,587	-35,2	26,5	-34,58	23,587
<i>ECI_AC2_RTR_RA</i>	0	4,43	0	4,427	0	4,43	0	4,427
<i>ECI_AC2_BSR_MX</i>	0	3,65	0,001	3,65	0	3,65	0,001	3,65

<i>Gs(U)_AC2_BSR_Q1</i>	-1579487,69	1057312,79	-	1057312,79	-	1057312,79	-	1057312,79
			1579487,69	3	1579487,69		1579487,69	3
			2		2		2	
<i>Gs(U)_AC2_ARM_Q3</i>	-1138695,5	1185300,96	-	1185300,96	-	1185300,96	-	1185300,96
			1138695,50	2	1138695,50	2	1138695,50	2
			1		1		1	
<i>ISA_AC2_PRT_CV</i>	0,19	1,87	0,196	1,829	0,19	1,87	0,196	1,829
<i>Z3_AC2_ALR_N3</i>	-31,31	26,03	-31,312	25,089	-31,31	26,03	-31,312	25,089
<i>Gw(U)_AC2_PCR_CV</i>	0	3,46	0	3,464	0	3,46	0	3,464
<i>Z2_AC2_RTR_MN</i>	-39,13	33,93	-39,128	28,73	-39,13	34,25	-39,128	34,25
<i>Z3_ES_PCR_TI5</i>	0	69,5	0	44,29	0	69,5	0	44,29
<i>Z3_ES_PCR_S</i>	-3,06	3,86	-2,406	3,37	-3,06	3,86	-2,406	3,37
<i>Gs(U)_ES_PRT_P2</i>	65,44	2009,9	195,996	1890,971	65,44	2009,9	195,996	1890,971
<i>Gs(U)_ES_PCR_CV</i>	-0,7	0	-0,617	0	-0,7	0	-0,617	0
<i>ISA_ES_PCR_CV</i>	-10838,16	354,9	-10838,162	354,895	-10838,16	354,9	-10838,162	354,895
<i>HP_ES_PCR_S</i>	-2,68	3,32	-2,406	2,238	-2,68	3,32	-2,406	2,238
<i>IP_ES_PCR_SI5</i>	0	1	0	1	0	1	0	1
<i>ISA_ES_PCR_S</i>	-3,61	3,32	-3,607	2,556	-3,61	3,32	-3,607	2,556
<i>HP_ES_PCR_SI5</i>	0	1	0	1	0	1	0	1
<i>HP_ES_PLR_Q1</i>	-12,14	4,06	-12,01	2,271	-12,14	4,06	-12,01	2,271
<i>Z2_ES_PCR_SI5</i>	0	1	0	1	0	1	0	1
<i>IP_ES_PCR_P3</i>	8,01	17,79	8,401	17,204	8,01	17,79	8,401	17,204
<i>IP_ES_BSR_Ar</i>	1,46	7,67	1,55	7,349	1,46	7,67	1,55	7,349
<i>IP_ES_BSR_MN</i>	0,55	7,51	0,547	7,349	0,55	7,51	0,547	7,349
<i>Z3_ES_AHR_MN</i>	-10,04	10,19	-8,839	10,193	-10,04	10,19	-9,157	10,193
<i>Z1_ES_PCR_CV</i>	0	0,62	0	0,577	0	0,635	0	0,577
<i>ISA_ES_RTR_Q2</i>	-114,28	204,1	-114,276	204,102	-114,28	204,247	-114,276	204,247
<i>Z3_ES_UCR_MX</i>	-3,89	11,54	-3,235	11,54	-3,89	11,577	-3,235	11,577
<i>IP_ES_UCR_Q3</i>	-4,32	7,71	-2,376	7,176	-4,32	7,71	-2,561	7,176
<i>Gs(U)_ES_PLR_Q3</i>	-2314,66	1098,63	-2253,505	1098,627	-2474,666	1098,63	-2474,666	1098,627

<i>Z3_ES_RTR_Q2</i>	-1,3	7,69	-0,819	7,519	-1,322	7,69	-0,819	7,519
<i>Z3_ES_ARM_Ar</i>	-2,96	5,61	-2,228	4,908	-2,96	5,61	-2,228	4,908
<i>ECI_ES_AHR_I50</i>	-1,42	3,29	-1,25	3,148	-1,42	3,29	-1,25	3,148
<i>Z1_ES_NPR_N3</i>	-30,9	7,49	-24,947	7,49	-30,9	7,49	-24,959	7,49
<i>ECI_ES_RTR_MX</i>	-1,34	2,78	-1,34	2,785	-1,34	2,78	-1,34	2,785
<i>IP_ES_UCR_P3</i>	-4,51	7,15	-3,085	6,776	-4,51	7,15	-3,085	6,776
<i>Z3_ES_RTR_Q1</i>	-2,42	7,69	-2,422	7,509	-2,42	7,69	-2,422	7,509
<i>ISA_ES_PCR_MN</i>	-60,58	181,29	-60,582	171,078	-60,58	181,29	-60,582	172,277
<i>IP_ES_ARM_Q2</i>	1,07	11,1	1,071	10,402	1,07	11,1	1,071	10,402
<i>Gs(U)_ES_PRT_Q3</i>	-1052,65	2023,94	-1046,549	1982,117	-1052,65	2023,94	-1046,549	1982,117
<i>Z3_ES_ALR_Q3</i>	-4,91	7,69	-4,908	7,39	-4,91	7,69	-4,908	7,39
<i>ISA_ES_RTR_MN</i>	-132,12	195,41	-132,116	195,413	-132,12	195,41	-132,116	195,413
<i>Z1_ES_PCR_Q1</i>	2,04	9,89	2,125	9,89	2,04	9,89	2,125	9,89
<i>Z3_ES_ARM_N1</i>	-6,91	61,37	-4,621	32,974	-6,91	61,37	-4,621	32,974
<i>ISA_ES_PCR_Q1</i>	-59,37	181,29	-59,373	171,078	-59,37	181,29	-59,373	172,277
<i>Z2_ES_PLR_Ar</i>	-4,01	8,28	-3,257	8,21	-4,01	8,28	-3,257	8,21
<i>Z1_ES_AHR_P2</i>	0,01	10,82	0,111	9,966	0,01	10,82	0,111	10,016
<i>Gs(U)_ES_ALR_MX</i>	-661,06	2504,44	-516,742	2446,231	-661,06	2504,44	-516,742	2446,231

Table S3. Values resulting from the radial diffusion assay applied to the peptide Urine-3462 against the *Pseudomonas aeruginosa* strain ATCC 27853.

EXPERIMENTS	1000	500	250	125	62.5	31.25	15.6	7.8	LL 37
1	1.2	1.1	0.9	0.8	0.6	0.4	0	0	0.7
2	1.3	1.1	0.9	0.7	0.6	0.4	0	0	0.7
3	1.1	1	0.9	0.8	0.5	0.3	0	0	0.6
4	1.3	1	0.9	0.8	0.6	0.3	0	0	0.6
5	1.2	1.1	1	0.8	0.6	0.4	0.3	0	0.7
6	1.2	1.1	0.9	0.8	0.6	0.4	0	0	0.7