

Predicting the Minimal Inhibitory Concentration for Antimicrobial Peptides with Rana Box Domain

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Supporting Information:

Table S1: The best model details for pre-Rana box sections in the case of training set peptides. Peptide segments with maximal buriability and volume sideways asymmetry moments (SAM) for optimal twist angles in the range from 80 to 120 degrees.

Table S2: Amino acid scales ranking using SAM and correlation among predicted and observed MIC.

Figure S1: ESI-MS characterization of the synthesized peptide.

Figure S2: Peptide purity confirmation by RP-HPLC.

Table S1 Peptide segments with maximal volume and buriability moments for optimal twist angles in the range from 80 to 120 degrees								
TRAINING SET				SAM* (buriability moment)			SAM* (volume moment)	
Name	Sequence	MIC exp µM	ZHOH 040103 vect. norm. ⁺	optimal ZHOH segment	ZHOH twist angle	GRAR 740103 vect. norm. ⁺	optimal GRAR segment	GRAR twist angle
Brevinin-1PRc	FFPMLAGVAARVVPKVICLITKKC	50.00	0.447	FFPMLAGVAARVVPKVI	94	0.413	FFPMLAGVAARVVPK	106
Brevinin-1CHc	FFPTIAGLTKLFCAITKKC	80.00	0.441	FFPTIAGLTKLF	106	0.384	FFPTIAGLT	102
Ranalexin-1Vb	FLGGFLFKLVPSVICAVTKKC	12.50	0.474	FLGGFLFKLVPSVI	97	0.466	FLGGFL	82
Brevinin-1Sb	FLPAIVGAAAKFLPKIFCAISKKC	25.00	0.490	FLPAIVGAAAKFLPKIF	95	0.392	FLPAIVGAAAKFLPKI	102
Brevinin-1JDa	FLPAVIRVAANVLPTVFCAISKKC	50.00	0.437	FLPAVIRVAANVLPTVF	95	0.366	FLPAVI	82
Brevinin-1HSa	FLPAVLRVAAKIVPTVFCAISKKC	24.00	0.441	FLPAVLRVAAKIVPTVF	95	0.396	RVAAKIVPTVF	80
Brevinin-1CHa	FLPIIAGVAAKVLPKLFCAITKKC	10.00	0.475	FLPIIAGVAAKVLPKF	93	0.405	FLPIIAGVAAKVLPKL	100
Brevinin-1CSa	FLPILAGLAAKIVPKLFCLATKKC	32.00	0.475	FLPILAGLAAKIVPKLF	93	0.461	FLPILAGLAAKIVPKL	101
Brevinin-1AUb	FLPILAGLAANILPKVFCSITKKC	25.00	0.469	FLPILAGLAANILPKVF	93	0.438	FLPILAGLAANILPKV	100
Brevinin-1BYa	FLPILASLAAKFGPKLFCLVTKKC	20.00	0.420	FLPILASLAAKFGPKLF	94	0.521	FLPILASLAAKFGPK	105
Brevinin-2PTa	GAIKDALKGAAKTVAVELLKKAQCKLEKTC	18.00	0.408	AIKDALKGAAKTVAVELLKKAQ	90	0.406	IKDALKGAAK	86
Brevinin-2PTb	GFKGAFKNVMFGIAKSAGKSALNALACKIDKSC	9.00	0.445	GFKGAFKNVMFGIAKSAGKSALNALA	92	0.468	FKGAFKNVMFGIAKSAGKSALN	88
Brevinin-2PTe	GFLDSFKNAMIGVAKSVGKTALSTLACKIDKSC	18.00	0.466	FLDSFKNAMIGVAKSVGKTALSTL	96	0.429	FLDSFKNAMIGVAK	87
Palustrin-2ISa	GFMDTAKNVAKNVAVTLLDKLKCKITGGC	100.00	0.392	FMDTAKNVAKNVAVTLLDKL	95	0.304	FMDTAKNVAKNVAVTLLDKL	80
Nigrocin-2JDb	GIFGKILGVGKKVLCGLSGMC	15.00	0.426	IFGKIL	85	0.355	IFGKI	106
Brevinin-2Ej	GIFLDKLNFAKGVAQSLLNKASCKLSGQC	2.00	0.473	FLDKLNFAKGVAQSL	99	0.311	IFLDKLK	80
Esculentin-2PRb	GIFSALAAGVKLLGNTLFKFMAGKAGAEHLACKATNQC	25.00	0.395	LLGNTLF	80	0.391	IFSALAAGVK	87
Esculentin-1ISa	GIFSKFAGKGIKNLLVKGVKKNIGKEVGMDVIRTGIDIAGCKIKGEC	6.30	0.530	IFSKFAGKGIKNLLVKGVKKNIGKEVGMDVIRTGI	90	0.436	IFSKFAGKGIKNLL	118
Esculentin-1ARa	GIFSKINKKKAKTGLFNIIKTVGKEAGMDVIRAGIDTISCKIKGEC	2.00	0.419	IFSKINKKKAKTGLFNIIKTVGKEAGMDVIRAGIDTIS	90	0.527	IFSKINKKKAKTGLFNIIKTVGKEAGMDVIRAGIDTI	111
Esculentin-2HSa	GIFSLIKGAAQLIGKTVAKEAGKTGLELMACKVTKQC	16.00	0.402	IFSLIKGAAQLIGKTV	101	0.438	LIGKTVAKEAGKTGLE	100
Ranatuerin-2PRb	GILDTFKGVAKGVAKDLAVHMLENLKCKMTGC	50.00	0.475	ILDTFKGVAKGVAKDL	99	0.351	ILDTFKGVAKGVAK	87
Nigrocin-2ISb	GILGTVFKAGKGIVCGLTGLC	50.00	0.402	ILGTVF	84	0.379	ILGTVFKAGK	80
Ranatuerin-2CSa	GILSSFKGVAKGVAKDLAGKLLETCLKCKITGC	5.00	0.545	ILSSFKGVAKGVAKDLAGKLLETL	95	0.396	ILSSFKGVAKGVAKDLAGKL	80
Ranatuerin-2PRd	GILSSIKGVAKGVAKNVAAQLLDTLKCKITGC	6.00	0.483	ILSSIKGVAKGVAKNVAAQLLDTL	95	0.371	ILSSIKGVAKGVAK	87
Ranatuerin-2BYb	GIMDSVKGLAKNLAGKLDSLCKITGC	17.00	0.483	IMDSVKGLAKNLAGKLDSL	96	0.400	NLAGKLDSLK	80
Ranatuerin-2VLb	GIMDTIKGAAKDLAQQLLDKLCKITKC	75.00	0.463	IMDTIKGAAKDLAQQLDKL	96	0.372	IMDTIKGAAK	85
Brevinin-2SKb	GLFNVFKKVGKNVLKNVAGSLMDNLKCKVSGEC	3.00	0.538	LFNVFKKVGKNVLKNVAGSLMDNL	95	0.358	NVAGSLMDNLK	81
Esculentin-2JDa	GLFTLIKGAAKLIGKTVAKEAGKTGLELMACKITNQC	34.00	0.406	LFTLIKGAAKLIGKTV	101	0.438	LIGKTVAKEAGKTGLE	100
Brevinin-2HSa	GLDSLKNLAINAAKGAGQSVLNTLSCKLSKTC	36.00	0.417	LLDSLKNLAINAAKGAGQSVLNTL	95	0.355	LLDSLKNLAINAAKGAGQS	86
Nigrocin-2HSa	LLGSLFGAGKKVACALSGLC	28.00	0.425	LLGSLF	84	0.487	LLGSLFGAGKK	80
Ranatuerin-2CHb	GLMDTIKGVAKNVAASLLEKLCKVTGC	20.00	0.454	LMDTIKGVAKNVAASLLEKL	95	0.321	LMDTIKGVAK	86
Ranatuerin-2ARa	GLMDTVKNAAKNLAGQLLDTIKCKMTGC	30.00	0.458	LMDTVKNAAKNLAGQLLDTI	96	0.379	NLAGQLLDTIK	80
Brevinin-2PRa	GLMSLFKGVLTAGKHIFKNVGGSLLDQAKCKITGEC	6.00	0.540	LFKGVLTAGKHIFKNVGGSLL	90	0.434	FKGVLTAGKH	80
Brevinin-2PRc	GLMSVLKGVLTAGKHIFKNVGGSLLDQAKCKISGQC	3.00	0.525	VLKGVLTAGKHIFKNVGGSLL	90	0.424	LMSVLKGVLTAGKH	81
Esculentin-1ISb	RIFSKIGGKAIKNLILKGIKNIGKEVGMDVIRTGIDVAGCKIKGEC	3.10	0.513	IFSKIGGKAIKNLILKGIKNIGKEVGMDVIRTGI	89	0.424	IFSKIGGKAIKNLI	117
Brevinin-2ISb	SFLTTFKDLAIIKAASAGQSVLSTLSCKLSNTC	12.50	0.432	FLTTFKDLAIIKAASAGQSVLSTL	95	0.393	FLTTFKDLAIIKAASAGQSVLSTL	112
Ranatuerin-1	SMSVLKNLGKVG LGFVACKINKQC	20.00	0.396	MSVLKNLGKV	113	0.315	MSVLK	85
Brevinin-2ISc	SVLGTVKDLLIGAGKSAAQSVLTTLSCKLSNSC	50.00	0.419	VLGTVKDLLIGAGKSAAQSVLTTL	95	0.371	VLGTVKDLLIGAGKSAAQ	87

Yellow = 14 MIC values with MIC ≤ 15µM	Orange = 32 winning buriability moments and 12 optimal angles for MIC ≤ 15 µM peptides, all ≤ 100 degrees	Average= 93 St.dev.= 3.29	Green = 6 winning volume moments
	Yellow = eight optimal winning segments longer than 20 AA		

*SAM=Sideways Asymmetry Moment; ⁺Codes for AA scales are from Kawashima et al. (2008). Vector normalization of scales was used to calculate SAM values as described in the paper

Table S2 Amino acid scales ranking using SAM ^H and correlation among predicted and observed MIC ^{&}									
Scales ranking for pre-Rana-box segments					Scales ranking for Rana-box segments				
Rank	AA scale*	r ²	r	Description	Rank	AA scale*	r ²	r	Description
1	FASG890101	0.504936	-0.71059	Fasman H*	1	SNEP660102	0.646318	-0.80394	Sneath**
2	BIOV880101	0.497963	-0.70567	Biou ***	2	FUKS010106	0.56932	-0.75453	
3	COWR900101	0.47957	-0.69251	Cowan H*	3	WOLS870102	0.554126	-0.7444	
4	RADA880108	0.467705	-0.68389		4	WOLR790101	0.547324	-0.73981	
5	MIYS990105	0.466501	-0.68301		5	NAKH900111	0.529038	-0.72735	
6	NADH010103	0.453422	-0.67337		6	WOLR810101	0.519935	-0.72107	
7	NADH010104	0.44694	-0.66854		7	FUKS010107	0.49847	-0.70602	
8	BIOV880102	0.445472	-0.66744		8	RADA880105	0.496162	-0.70439	
9	NISK860101	0.438289	-0.66203		9	RADA880101	0.493257	-0.70232	
10	FUKS010103	0.438195	-0.66196		10	ROSM880101	0.492192	-0.70156	
11	MEEJ800102	0.431415	-0.65682		11	RADA880104	0.485458	-0.69675	
12	MEEJ810102	0.430904	-0.65643		12	WERD780104	0.482634	-0.69472	
13	GUOD860101	0.429244	-0.65517		13	NAKH920105	0.480753	-0.69336	Nakashima H*
14	MIYS990104	0.419571	-0.64774		14	PARS000102	0.476201	-0.69007	
15	CCS	0.419421	-0.64763	Tossi H*	15	NAKH920108	0.471947	-0.68698	
16	FINA910103	0.413385	-0.64295		16	AURR980116	0.463885	-0.68109	
17	EISD860103	0.411877	-0.64178		17	EISD840101	0.463113	-0.68052	Eisenberg H*
18	QIAN880101	0.408462	-0.63911		18	PRAM820102	0.460215	-0.67839	
19	QIAN880130	0.40845	-0.6391		19	PRAM900101	0.459082	-0.67756	
20	MEEJ810101	0.406432	-0.63752		20	ENG860101	0.458758	-0.67732	
21	CORJ870107	0.406103	-0.63726		21	JACR890101	0.458554	-0.67717	
22	NADH010102	0.404608	-0.63609		22	AURR980112	0.457867	-0.67666	
23	CORJ870103	0.403758	-0.63542		23	QIAN880122	0.457484	-0.67638	
24	GEOR030105	0.401667	-0.63377		24	CHAM830105	0.457295	-0.67624	
25	MIYS850101	0.400213	-0.63262		25	JANJ780103	0.457122	-0.67611	
26	MIYS990103	0.399719	-0.63223		26	ROSM880105	0.453016	-0.67306	
27	RICJ880113	0.395008	-0.6285		27	VHEG790101	0.450675	-0.67132	
28	CORJ870105	0.393601	-0.62738		28	FAUJ880109	0.445613	-0.66754	Fauchere H*
29	PLIV810101	0.392813	-0.62675		29	KUHL950101	0.443858	-0.66623	
30	PONP930101	0.392662	-0.62663		30	GUYH850105	0.438145	-0.66193	
31	RACS770102	0.392239	-0.62629		31	GUYH850104	0.436984	-0.66105	
32	KRIW790101	0.391343	-0.62557		32	RADA880107	0.434472	-0.65914	
33	FAUJ830101	0.390427	-0.62484	Fauchere H*	33	FAUJ880110	0.434278	-0.659	
34	OOBM770103	0.388965	-0.62367		34	JANJ780101	0.43252	-0.65766	
35	PALJ810115	0.388807	-0.62354		35	JANJ790102	0.432262	-0.65747	
36	CIDH920104	0.388684	-0.62345		36	AURR980106	0.431051	-0.65654	
37	MIYS990102	0.388433	-0.62324		37	HOPA770101	0.425706	-0.65246	
38	CORJ870106	0.385368	-0.62078		38	KYTJ820101	0.423148	-0.6505	
39	ROSM880102	0.384318	-0.61993		39	CHAM830106	0.420442	-0.64841	
40	NISK800101	0.384124	-0.61978		40	CHOC760104	0.412312	-0.64212	
41	GUYH850101	0.383501	-0.61927		41	JURD980101	0.409274	-0.63975	
42	CHOC760103	0.383292	-0.61911		42	HOPT810101	0.409157	-0.63965	
43	BASU050103	0.382686	-0.61862		43	ROSM880102	0.406933	-0.63791	
44	BULH740101	0.381746	-0.61786		44	LEVM760101	0.406084	-0.63725	
45	MIYS990101	0.380406	-0.61677		45	KOEP990101	0.405587	-0.63686	
46	RICJ880114	0.379782	-0.61626		46	NADH010102	0.404088	-0.63568	
47	JANJ790101	0.379494	-0.61603		47	CHOC760102	0.404063	-0.63566	
48	GUYH850105	0.376556	-0.61364		48	BIOV880102	0.400208	-0.63262	
49	CORJ870108	0.376464	-0.61357		49	KIDA850101	0.395889	-0.6292	
50	AURR980116	0.376407	-0.61352		50	CHOC760103	0.389646	-0.62422	
51	WILM950101	0.375217	-0.61255		51	CCS	0.38963	-0.6242	Tossi H*
52	WOLS870101	0.373171	-0.61088		52	ZIMJ680103	0.388525	-0.62332	
53	QIAN880127	0.373112	-0.61083		53	OLSK800101	0.387953	-0.62286	
54	CORJ870102	0.372316	-0.61018		54	EISD860103	0.386534	-0.62172	
55	QIAN880139	0.371392	-0.60942		55	ROBB760101	0.385922	-0.62123	
56	KIDA850101	0.37127	-0.60932		56	GRAR740102	0.384912	-0.62041	
57	JANJ780102	0.370039	-0.60831		57	AURR980107	0.383355	-0.61916	

58	SWER830101	0.369758	-0.60808		58	EISD860102	0.383169	-0.61901	
59	CASG920101	0.369195	-0.60761		59	AURR980111	0.383149	-0.61899	
60	GUYH850102	0.363483	-0.6029		60	AURR980115	0.382617	-0.61856	
61	OLSK800101	0.362096	-0.60174		61	COWR900101	0.382544	-0.6185	
62	RADA880107	0.36177	-0.60147		62	AURR980119	0.37488	-0.61227	
63	PRAM820101	0.361187	-0.60099		63	PUNT030101	0.374408	-0.61189	
64	QIAN880122	0.361073	-0.60089		64	FUKS010105	0.373596	-0.61123	
65	EISD840101	0.355651	-0.59636	Eisenberg H*	65	RACS770103	0.372503	-0.61033	
66	JANJ790102	0.354577	-0.59546		66	RACS820109	0.36735	-0.60609	
67	PONP800107	0.35302	-0.59415		67	NAKH900110	0.364872	-0.60405	
68	GUYH850104	0.353016	-0.59415		68	JANJ780102	0.362081	-0.60173	
69	JURD980101	0.349699	-0.59135		69	FUKS010104	0.360948	-0.60079	
70	LEVM760101	0.349624	-0.59129		70	RICJ880113	0.355334	-0.5961	
71	CHOC760102	0.349119	-0.59086		71	QIAN880118	0.354586	-0.59547	
72	KRIW790102	0.347436	-0.58944		72	NAKH920107	0.354339	-0.59526	
73	LAW840101	0.346127	-0.58833		73	MIT020101	0.345021	-0.58738	
74	CIDH920105	0.345543	-0.58783		74	NADH010103	0.342201	-0.58498	
75	GUYH850103	0.345488	-0.58778		75	RICJ880112	0.338419	-0.58174	
76	CORJ870104	0.342284	-0.58505		76	DESM900102	0.336776	-0.58032	
77	MEIH800102	0.341664	-0.58452		77	EISD860101	0.33669	-0.58025	
78	CIDH920102	0.339977	-0.58308		78	KRIW790102	0.335986	-0.57964	
79	ROBB790101	0.337267	-0.58075		79	PUNT030102	0.334769	-0.57859	
80	KYTJ820101	0.336633	-0.5802		80	MIYS990105	0.333781	-0.57774	
81	FUKS010104	0.335591	-0.5793		81	DESM900101	0.333332	-0.57735	
82	PARJ860101	0.328051	-0.57276		82	MAXF760104	0.332513	-0.57664	
83	KUHL950101	0.327953	-0.57267		83	CHAM810101	0.33223	0.576394	
84	ZIMJ680101	0.323229	-0.56853		84	QIAN880102	0.331438	-0.57571	
85	JANJ780101	0.321894	-0.56736		85	NAKH900113	0.327901	-0.57263	
86	SIMZ760101	0.320448	-0.56608		86	LEVM760104	0.319915	-0.56561	
87	PONP800102	0.320111	-0.56578		87	QIAN880110	0.316646	-0.56271	
88	LEVM760103	0.318345	-0.56422		88	FASG760103	0.316245	-0.56236	
89	QIAN880118	0.317608	-0.56357		89	BLAS910101	0.310924	-0.55761	
90	JANJ780103	0.316682	-0.56274		90	FASG760101	0.308112	0.555078	
91	HOPT810101	0.313985	-0.56034		91	CORJ870105	0.306353	-0.55349	
92	ZHOH040103	0.311343	-0.55798	Zhou B ⁺	92	QIAN880106	0.305667	-0.55287	
93	ARGP820101	0.311009	-0.55768		93	WARP780101	0.303753	-0.55114	
94	PONP800108	0.310822	-0.55751		94	CORJ870107	0.303064	-0.55051	
95	JOND750101	0.309466	-0.5563		95	FASG760102	0.302853	-0.55032	
96	RADA880104	0.307549	-0.55457		96	RICJ880106	0.302044	-0.54959	
97	ROSG850102	0.307144	-0.55421		97	FUKS010108	0.301473	-0.54907	
98	BLAS910101	0.306475	-0.5536		98	QIAN880109	0.300881	-0.54853	
99	KRIW710101	0.305585	-0.5528		99	RACS820114	0.299038	-0.54684	
100	GRAR740102	0.30402	-0.55138		100	QIAN880123	0.297902	-0.5458	
101	NAKH900110	0.304015	-0.55138		101	WOEC730101	0.297633	-0.54556	
102	RACS770103	0.303793	-0.55117		102	GEIM800103	0.29722	0.545179	
103	WEBA780101	0.303216	-0.55065		103	RACS820110	0.296795	-0.54479	
104	NAKH920108	0.302822	-0.55029		104	BIOV880101	0.296308	-0.54434	
105	ZIMJ680105	0.302156	-0.54969		105	MUNV940101	0.295988	-0.54405	
106	FAUJ880111	0.299149	-0.54695		106	GEOR030105	0.294456	-0.54264	
107	ROSM880105	0.299111	-0.54691		107	TANS770109	0.294063	-0.54228	
108	NAKH900113	0.298148	-0.54603		108	NADH010104	0.293341	-0.54161	
109	ROBB760105	0.292045	-0.54041		109	LEVM760102	0.293057	-0.54135	
110	MIT020101	0.286489	-0.53525		110	FAUJ830101	0.291884	-0.54026	
111	WOLS870102	0.284626	-0.5335		111	CASG920101	0.291848	-0.54023	
112	OOBM850105	0.283501	-0.53245		112	MAXF760105	0.289797	-0.53833	
113	OOBM850103	0.281312	-0.53039		113	KRIW790101	0.289466	-0.53802	
114	FINA910104	0.279676	-0.52884		114	WOLS870101	0.285368	-0.5342	
115	FAUJ880109	0.279045	-0.52825		115	FAUJ880102	0.284857	0.53372	
116	WERD780101	0.278242	-0.52749		116	FAUJ880111	0.282864	-0.53185	
117	ROSM880101	0.273304	-0.52278		117	LEVM780102	0.282283	-0.5313	

118	FUKS010102	0.273144	-0.52263		118	PRAM900103	0.282283	-0.5313	
119	TANS770110	0.27233	-0.52185		119	WILM950101	0.28216	-0.53119	
120	BASU050102	0.271988	-0.52152		120	GUYH850101	0.281904	-0.53095	
121	CHOC760104	0.271674	-0.52122		121	MIYS990103	0.274199	-0.52364	
122	PALJ810109	0.271404	-0.52096		122	MEEJ800102	0.274	-0.52345	
123	ANDN920101	0.269055	-0.51871		123	FUKS010101	0.272516	-0.52203	
124	NAKH920105	0.26725	-0.51696		124	LEVVM780101	0.272121	0.521652	
125	KARP850103	0.266865	-0.51659		125	PRAM900102	0.272121	0.521652	
126	NAKH900111	0.265819	-0.51558		126	PALJ810109	0.270989	0.520566	
127	CHOP780203	0.263543	-0.51336		127	PALJ810112	0.267931	-0.51762	
128	FUKS010101	0.262954	-0.51279		128	PONP930101	0.267797	-0.51749	
129	WERD780104	0.259493	-0.5094		129	MIYS990104	0.266993	-0.51671	
130	ROSM880104	0.259313	-0.50923		130	OOBM770103	0.26527	-0.51504	
131	VENT840101	0.258155	-0.50809		131	OOBM770105	0.264905	0.514689	
132	PUNT030101	0.257072	-0.50702		132	NISK800101	0.260426	-0.51032	
133	NOZY710101	0.256956	-0.50691		133	ONEK900102	0.25935	-0.50926	
134	BROC820102	0.256916	-0.50687		134	FAUJ880112	0.259222	-0.50914	
135	FUKS010105	0.256837	-0.50679		135	MUNV940102	0.25763	-0.50757	
136	TANS770106	0.254825	-0.5048		136	FUKS010102	0.256996	-0.50695	
137	RADA880101	0.252953	-0.50294		137	NADH010101	0.25676	-0.50672	
138	MEIH800103	0.249528	-0.49953		138	ZIMJ680105	0.255744	-0.50571	
139	CHOP780210	0.249366	-0.49937		139	PARS000101	0.253562	0.50355	
140	WOLR790101	0.247258	-0.49725		140	CORJ870103	0.250821	-0.50082	
141	EISD860101	0.2463	-0.49629		141	PALJ810114	0.248279	-0.49828	
142	DESM900102	0.24514	-0.49512		142	RICJ880115	0.247764	-0.49776	
143	BASU050101	0.244042	-0.49401		143	BEGF750102	0.246644	-0.49663	
144	WOLR810101	0.243248	-0.4932		144	KIMC930101	0.245208	0.495184	
145	CIDH920103	0.243172	-0.49312		145	QIAN880113	0.245147	-0.49512	
146	BHAR880101	0.241436	-0.49136		146	AURR980103	0.244948	-0.49492	
147	VINM940101	0.241405	-0.49133		147	RICJ880108	0.243582	0.49354	
148	PRAM900101	0.241394	-0.49132		148	FUKS010111	0.242698	0.492644	
149	ENGD860101	0.241009	-0.49093		149	AURR980120	0.242011	0.491946	
150	RADA880105	0.240502	-0.49041		150	FASG890101	0.240674	-0.49059	Fasman H*
151	GEIM800104	0.240131	-0.49003		151	NISK860101	0.240196	-0.4901	
152	QIAN880115	0.239691	-0.48958		152	HUTJ700102	0.238961	0.488837	
153	ZIMJ680104	0.237641	-0.48748		153	FINA770101	0.236756	0.486576	
154	JACR890101	0.23758	-0.48742		154	CORJ870108	0.23622	-0.48602	
155	ISOY800106	0.236716	-0.48653		155	CORJ870106	0.236112	-0.48591	
156	VINM940104	0.235959	-0.48576		156	QIAN880128	0.232698	-0.48239	
157	PARS000101	0.235954	-0.48575		157	RADA880102	0.231366	-0.481	
158	FUKS010106	0.235687	-0.48548		158	RADA880108	0.230881	-0.4805	
159	RICJ880108	0.235299	-0.48508		159	LEVVM760103	0.230875	0.480494	
160	KOEP990102	0.234965	-0.48473		160	PALJ810108	0.226221	0.475627	
161	ZIMJ680103	0.231204	-0.48084		161	HUTJ700103	0.226056	0.475453	
162	RADA880102	0.230641	-0.48025		162	SWER830101	0.225488	-0.47486	
163	QIAN880119	0.230014	-0.4796		163	MIYS990102	0.225456	-0.47482	
164	FUKS010107	0.228342	-0.47785		164	PONP800107	0.225347	-0.47471	
165	ROBB760110	0.226976	-0.47642		165	MAXF760102	0.2252	-0.47455	
166	EISD860102	0.225338	-0.4747		166	BURA740101	0.222735	-0.47195	
167	NAGK730102	0.221577	-0.47072		167	GEIM800107	0.222642	-0.47185	
168	TAKK010101	0.220312	-0.46937		168	MIYS990101	0.22094	-0.47004	
169	BUNA790102	0.220236	-0.46929		169	OOBM770101	0.220672	-0.46976	
170	GEIM800101	0.21817	-0.46709		170	CORJ870102	0.220172	-0.46922	
171	QIAN880120	0.21817	-0.46709		171	AURR980110	0.219203	-0.46819	
172	AURR980101	0.215893	-0.46464		172	QIAN880108	0.217952	-0.46685	
173	QIAN880128	0.215767	-0.46451		173	WILM950102	0.217773	-0.46666	
174	CHOP780206	0.214503	-0.46315		174	WERD780103	0.216381	0.465168	
175	ROBB760106	0.21348	-0.46204		175	SUYM030101	0.213063	-0.46159	
176	HOPA770101	0.212819	-0.46132		176	PALJ810104	0.208946	-0.45711	
177	KLEP840101	0.211929	-0.46036		177	NAGK730102	0.208415	-0.45652	

178	PUNT030102	0.211733	-0.46014		178	ISOY800108	0.206828	-0.45478	
179	NAKH920106	0.209402	-0.4576		179	PONJ960101	0.206228	0.454123	
180	LIFS790102	0.20706	-0.45504		180	KANM800104	0.20562	-0.45345	
181	CHAM830108	0.202222	-0.44969		181	HUTJ700101	0.204734	0.452475	
182	PARS000102	0.201916	-0.44935		182	KANM800102	0.203841	-0.45149	
183	CHOP780101	0.198349	-0.44536		183	AURR980114	0.203783	-0.45142	
184	KARP850101	0.198038	-0.44501		184	CORJ870104	0.203145	-0.45072	
185	QIAN880114	0.196533	-0.44332		185	CHOC750101	0.202096	0.449551	
186	MEIH800101	0.194282	-0.44077		186	LEVM780105	0.19969	-0.44687	
187	AVBF000105	0.192872	-0.43917		187	BASU050103	0.199199	-0.44632	
188	GOLD730101	0.192498	-0.43875		188	CHAM830108	0.198581	0.445624	
189	DESM900101	0.190849	-0.43686		189	ROBB760112	0.198285	0.445292	
190	WOEC730101	0.189989	-0.43588		190	WIMW960101	0.197176	-0.44404	
191	VHEG790101	0.189981	-0.43587		191	JANJ790101	0.196581	-0.44337	
192	DAYM780201	0.186637	-0.43201		192	AURR980117	0.19474	-0.44129	
193	VASM830103	0.185598	-0.43081		193	MEIH800103	0.194174	-0.44065	
194	KARP850102	0.185349	-0.43052		194	RACS820102	0.193487	0.439871	
195	VASM830101	0.18501	-0.43013		195	PALJ810103	0.192349	-0.43858	
196	AVBF000106	0.184069	-0.42903		196	TANS770107	0.185322	-0.43049	
197	BEGF750102	0.183977	-0.42893		197	MONM990201	0.185055	-0.43018	
198	CHOP780215	0.18263	-0.42735		198	ARGP820103	0.184639	-0.4297	
199	SUEM840102	0.182103	-0.42674		199	GEOR030109	0.184619	-0.42967	
200	COSI940101	0.179675	-0.42388		200	QIAN880107	0.183596	-0.42848	
201	VELV850101	0.179588	-0.42378		201	GUOD860101	0.182756	-0.4275	
202	MEEJ800101	0.179275	-0.42341		202	FUKS010109	0.181901	-0.4265	
203	BAEK050101	0.179082	-0.42318		203	HARY940101	0.181724	0.42629	
204	FAUJ880101	0.178898	-0.42296		204	BROC820101	0.179293	0.423429	
205	ZHOH040101	0.177102	-0.42084		205	CHOC760101	0.178698	0.422727	
206	CHOP780208	0.174875	-0.41818		206	YANJ020101	0.178283	0.422235	
207	WILM950102	0.174247	-0.41743		207	GEIM800105	0.176575	-0.42021	
208	CHOP780216	0.173129	-0.41609		208	BIGC670101	0.175141	0.418499	
209	CHAM830105	0.170255	-0.41262		209	DAWD720101	0.174741	-0.41802	
210	OOBM770101	0.169871	-0.41215		210	QIAN880121	0.174494	-0.41772	
211	NADH010105	0.168834	-0.41089		211	NOZY710101	0.169523	-0.41173	
212	CHAM830102	0.167357	-0.40909		212	GEIM800104	0.168969	0.411059	
213	QIAN880132	0.166979	-0.40863		213	ROSG850102	0.167541	-0.40932	
214	NADH010101	0.166292	-0.40779		214	LIFS790102	0.166659	-0.40824	
215	RICJ880115	0.162335	-0.40291		215	OOBM770102	0.166486	-0.40803	
216	KANM800104	0.158204	-0.39775		216	QIAN880119	0.166073	-0.40752	
217	MAXF760102	0.157672	-0.39708		217	MIYS850101	0.16572	-0.40709	
218	MONM990201	0.157231	-0.39652		218	RACS820113	0.165466	-0.40678	
219	FAUJ880104	0.153953	-0.39237		219	GOLD730102	0.165174	0.406416	
220	PALJ810101	0.153015	-0.39117		220	KLEP840101	0.164462	-0.40554	
221	RICJ880103	0.15018	-0.38753		221	MEEJ810102	0.163873	-0.40481	
222	SNEP660102	0.149422	-0.38655		222	TSAJ990101	0.161673	0.402085	
223	LEVM780104	0.148731	-0.38566		223	QIAN880112	0.161546	-0.40193	
224	SNEP660104	0.148346	-0.38516		224	GEIM800106	0.16139	-0.40173	
225	AVBF000104	0.147672	0.384281		225	PARJ860101	0.160933	-0.40117	
226	NAKH920107	0.146902	-0.38328		226	CHOP780204	0.160355	-0.40044	
227	WERD780102	0.144662	-0.38034		227	ROBB760106	0.160188	-0.40024	
228	NAKH920103	0.142474	-0.37746		228	CHOP780202	0.158788	-0.39848	
229	NADH010106	0.141688	-0.37642		229	TSAJ990102	0.156485	0.395582	
230	CHOP780207	0.140438	-0.37475		230	RICJ880110	0.155558	-0.39441	
231	PONP800104	0.1403	-0.37457		231	RACS770102	0.154171	0.392646	
232	ISOY800108	0.140125	-0.37433		232	MEIH800102	0.153374	0.39163	
233	FUKS010108	0.140068	-0.37426		233	GEOR030104	0.153102	-0.39128	
234	VINM940103	0.139319	-0.37325		234	QIAN880101	0.152899	-0.39102	
235	LEVM760102	0.139111	-0.37298		235	QIAN880105	0.151895	-0.38974	
236	TANS770109	0.137882	-0.37132		236	WERD780102	0.149243	0.38632	
237	RACS770101	0.137477	-0.37078		237	QIAN880129	0.148371	0.385189	

238	LEVM760107	0.136952	-0.37007		238	CIDH920104	0.148369	-0.38519	
239	AURR980118	0.136797	-0.36986		239	JUKT750101	0.148172	0.384931	
240	ZASB820101	0.135937	-0.3687		240	ARGP820102	0.145657	-0.38165	
241	ROBB760107	0.135468	-0.36806		241	ROBB760102	0.1453	-0.38118	
242	NAGK730103	0.135347	-0.3679		242	MONM990101	0.143854	-0.37928	
243	ROBB760112	0.134894	-0.36728		243	SNEP660104	0.142535	-0.37754	
244	CRAJ730103	0.134272	-0.36643		244	NAKH920106	0.142408	-0.37737	
245	TANS770107	0.133791	-0.36578		245	NAGK730103	0.141281	-0.37587	
246	HUTJ700102	0.133463	-0.36533		246	GUYH850102	0.140594	-0.37496	
247	PALJ810106	0.132266	-0.36368		247	CHAM830102	0.139561	-0.37358	
248	KUMS000101	0.130783	-0.36164		248	MCMT640101	0.138207	0.371762	
249	ZIMJ680102	0.129671	-0.3601		249	ISOY800106	0.138191	0.37174	
250	FAUJ880106	0.129203	-0.35945		250	PONP800108	0.137853	-0.37129	
251	WARP780101	0.128629	-0.35865		251	FAUJ880113	0.137762	0.371163	
252	PALJ810105	0.12843	-0.35837		252	PONP800104	0.137255	-0.37048	
253	PTIO830102	0.128331	-0.35823		253	NAKH920103	0.136648	0.369659	
254	FAUJ880110	0.125765	-0.35463		254	PALJ810111	0.136131	-0.36896	
255	AVBF000103	0.12485	-0.35334		255	RICJ880105	0.136107	0.368926	
256	LEVM780101	0.124583	-0.35296		256	BAEK050101	0.135343	-0.36789	
257	PRAM900102	0.124583	-0.35296		257	QIAN880127	0.133521	-0.3654	
258	HUTJ700103	0.123969	-0.35209		258	FAUJ880106	0.132753	0.364353	
259	QIAN880121	0.123852	-0.35193		259	MUNV940103	0.132019	0.363344	
260	RACS820113	0.12207	-0.34939		260	KOEP990102	0.130122	-0.36072	
261	MAXF760104	0.122038	-0.34934		261	RACS820106	0.127875	-0.3576	
262	QIAN880106	0.121243	-0.3482		262	QIAN880117	0.12735	0.356861	
263	CHAM830101	0.120801	-0.34757		263	BURA740102	0.126641	-0.35587	
264	BROC820101	0.120596	-0.34727		264	JOND750102	0.126047	-0.35503	
265	VINM940102	0.120249	-0.34677		265	VINM940101	0.122097	0.349424	
266	VASM830102	0.116049	-0.34066		266	TANS770103	0.121465	-0.34852	
267	WERD780103	0.115347	-0.33963		267	QIAN880125	0.120733	0.347467	
268	ROBB760113	0.114872	-0.33893		268	ROBB760111	0.120696	-0.34741	
269	MONM990101	0.114685	-0.33865		269	VASM830101	0.120311	0.346859	
270	MAXF760106	0.113618	-0.33707		270	PALJ810105	0.119091	-0.3451	
271	CHAM830106	0.113056	-0.33624		271	MEIH800101	0.118841	0.344734	
272	AVBF000109	0.113054	-0.33623		272	AVBF000102	0.117152	0.342275	
273	LEVM760105	0.112101	-0.33482		273	QIAN880130	0.11712	-0.34223	
274	DIGM050101	0.112019	-0.33469		274	LIFS790101	0.115597	-0.34	
275	AURR980115	0.110211	-0.33198		275	PONP800102	0.114014	-0.33766	
276	CHOP780205	0.109696	-0.3312		276	AVBF000105	0.113659	-0.33713	
277	QIAN880104	0.108317	-0.32912		277	ROBB760105	0.113512	-0.33692	
278	GARJ730101	0.108293	-0.32908		278	ROBB790101	0.113387	-0.33673	
279	PONP800103	0.10667	-0.3266		279	CEDJ970102	0.113074	0.336265	
280	PALJ810116	0.106357	-0.32612		280	CORJ870101	0.112481	-0.33538	
281	CHOC760101	0.105933	-0.32547		281	BASU050101	0.11242	-0.33529	
282	CHOP780202	0.105362	-0.32459		282	ISOY800102	0.111903	-0.33452	
283	QIAN880138	0.105251	-0.32442		283	QIAN880120	0.111779	-0.33433	
284	QIAN880125	0.104498	-0.32326		284	NADH010105	0.110254	-0.33204	
285	GRAR740101	0.103387	-0.32154		285	CRAJ730101	0.109402	0.33076	
286	RACS820106	0.103369	-0.32151		286	PONP800103	0.109215	-0.33048	
287	ROBB760108	0.102176	-0.31965		287	QIAN880104	0.108936	-0.33005	
288	MAXF760105	0.10177	-0.31901		288	QIAN880126	0.107827	0.32837	
289	ROBB760111	0.101706	-0.31891		289	GEIM800108	0.107625	-0.32806	
290	MAXF760103	0.10076	-0.31743		290	PALJ810116	0.106544	-0.32641	
291	LIFS790101	0.099775	-0.31587		291	CHOP780214	0.10534	-0.32456	
292	CIDH920101	0.098462	-0.31379		292	CEDJ970103	0.104604	-0.32343	
293	PALJ810104	0.09774	-0.31263		293	BROC820102	0.104364	0.323054	
294	QIAN880113	0.097448	-0.31217		294	ROBB760103	0.104223	-0.32284	
295	NAKH900109	0.096991	-0.31143		295	NADH010106	0.103886	-0.32231	
296	PALJ810111	0.096651	-0.31089		296	OOBM850103	0.101145	-0.31803	
297	DAWD720101	0.096603	-0.31081		297	FASG760105	0.100338	-0.31676	

298	GEIM800102	0.094976	-0.30818		298	CHOP780215	0.09974	-0.31582	
299	AURR980117	0.094741	-0.3078		299	NAKH900112	0.098414	-0.31371	
300	YUTK870101	0.094642	-0.30764		300	AVBF000107	0.098	-0.31305	
301	WOLS870103	0.094638	-0.30763		301	CHAM830101	0.097897	-0.31288	
302	BEGF750103	0.094535	-0.30747		302	PTIO830101	0.097713	0.312592	
303	GOLD730102	0.09369	-0.30609		303	JOND920101	0.097293	0.311918	
304	RICJ880116	0.093399	-0.30561		304	ZHOH040103	0.097013	-0.31147	
305	PALJ810112	0.092914	-0.30482		305	MEEJ810101	0.09606	-0.30994	
306	AURR980107	0.092773	-0.30459		306	LEVM760107	0.094288	0.307063	
307	FAUJ880112	0.091042	-0.30173		307	OOBM770104	0.092957	0.304888	
308	ROSM880103	0.090783	-0.3013		308	VENT840101	0.092889	-0.30478	
309	LEVM760104	0.089273	-0.29879		309	LIFS790103	0.091824	-0.30303	
310	FAUJ880108	0.088931	-0.29821		310	ISOY800105	0.091517	-0.30252	
311	CHOP780212	0.086909	-0.2948		311	GUYH850103	0.091468	-0.30244	
312	BURA740102	0.086476	-0.29407		312	ZIMJ680102	0.091434	0.302381	
313	GEOR030109	0.086356	0.293865		313	WERD780101	0.090841	-0.3014	
314	JOND920102	0.085837	-0.29298		314	KRIW710101	0.090482	-0.3008	
315	RICJ880105	0.084914	-0.2914		315	TAKK010101	0.087927	0.296526	
316	SNEP660103	0.084501	-0.29069		316	PONP800105	0.087854	-0.2964	
317	BIGC670101	0.084178	-0.29013		317	AVBF000106	0.087126	-0.29517	
318	CHOP780211	0.083923	-0.28969		318	GEOR030103	0.086938	0.294853	
319	AURR980103	0.083602	-0.28914		319	LEVM780103	0.086719	-0.29448	
320	WILM950103	0.083161	-0.28838		320	AURR980104	0.086401	-0.29394	
321	KANM800102	0.082757	-0.28768		321	GEOR030106	0.085808	0.292931	
322	QIAN880131	0.080996	-0.2846		322	PLIV810101	0.08548	0.292369	
323	CEDJ970105	0.079053	-0.28116		323	RADA880106	0.084758	0.291132	
324	PALJ810114	0.078923	-0.28093		324	FAUJ880108	0.08229	0.286863	
325	NAGK730101	0.078755	-0.28063		325	FAUJ880107	0.081051	0.284694	
326	ISOY800103	0.078583	-0.28033		326	AVBF000103	0.0794	-0.28178	
327	RACS820108	0.078524	-0.28022		327	AURR980118	0.079001	0.281071	
328	CHAM810101	0.078139	-0.27953		328	NAKH900101	0.078891	0.280876	
329	QIAN880133	0.078133	-0.27952		329	NAGK730101	0.078814	0.280739	
330	KUMS000102	0.077793	-0.27891		330	PTIO830102	0.077778	-0.27889	
331	KIMC930101	0.077621	-0.27861		331	PRAM900104	0.077703	-0.27875	
332	FINA910101	0.077581	-0.27853		332	SUEM840101	0.076957	0.277412	
333	NADH010107	0.076893	-0.2773		333	RADA880103	0.076468	-0.27653	
334	FINA770101	0.076825	-0.27717		334	WOLS870103	0.075737	-0.2752	
335	CHAM820101	0.07635	-0.27631		335	PALJ810110	0.075443	-0.27467	
336	JUNJ780101	0.076256	-0.27614		336	CIDH920105	0.07515	-0.27414	
337	NAKH900106	0.075863	-0.27543		337	SNEP660103	0.075095	-0.27403	
338	GEIM800107	0.075242	-0.2743		338	QIAN880133	0.075007	0.273874	
339	RACS820104	0.07478	0.273459		339	GEIM800111	0.074846	-0.27358	
340	KOEP990101	0.07455	-0.27304		340	RICJ880109	0.07468	0.273276	
341	CEDJ970103	0.074031	-0.27209		341	CHOP780209	0.074471	-0.27289	
342	RICJ880106	0.073839	-0.27173		342	NAKH900109	0.073348	-0.27083	
343	FINA910102	0.073647	0.27138		343	PONP800101	0.072288	-0.26886	
344	FAUJ880103	0.073147	-0.27046		344	DAYM780101	0.072011	0.268349	
345	BUNA790101	0.072909	0.270016		345	QIAN880116	0.071831	0.268012	
346	GEIM800103	0.07209	-0.2685		346	RACS820103	0.071734	-0.26783	
347	AURR980114	0.071274	-0.26697		347	TANS770105	0.071311	-0.26704	
348	PTIO830101	0.070465	0.265452		348	LEVM780104	0.069472	0.263576	
349	PONP800101	0.070183	-0.26492		349	RACS820107	0.06756	-0.25992	
350	FUKS010109	0.069349	-0.26334		350	ZHOH040102	0.066775	0.258409	
351	BLAM930101	0.068358	0.261454		351	KANM800101	0.066654	0.258175	
352	PALJ810103	0.068318	-0.26138		352	GEOR030101	0.06623	0.257352	
353	AURR980108	0.068314	-0.26137		353	CHAM820101	0.065333	0.255603	
354	HARY940101	0.067541	-0.25989		354	NAKH900104	0.064399	-0.25377	
355	TSAJ990101	0.06701	-0.25886		355	CHOP780213	0.063701	-0.25239	
356	MUNV940105	0.066999	0.258842		356	MANP780101	0.063598	-0.25219	
357	LEVM780102	0.065361	-0.25566		357	RACS820111	0.062878	-0.25075	

358	PRAM900103	0.065361	-0.25566		358	RACS770101	0.062542	0.250085	
359	GEIM800105	0.064863	-0.25468		359	CEDJ970101	0.061494	0.247981	
360	MANP780101	0.063639	-0.25227		360	LEVM780106	0.060394	-0.24575	
361	FUKS010111	0.062866	-0.25073		361	NAKH900107	0.058539	-0.24195	
362	PALJ810108	0.062811	-0.25062		362	JUNJ780101	0.05645	0.237592	
363	RACS820105	0.062456	-0.24991		363	MUNV940105	0.056422	-0.23753	
364	RADA880103	0.062318	-0.24964		364	LEVM760106	0.05432	0.233067	
365	CHOP780214	0.061747	-0.24849		365	BASU050102	0.05428	-0.23298	
366	LEWP710101	0.061496	-0.24798		366	FAUJ880105	0.052339	0.228778	
367	TSAJ990102	0.060875	-0.24673		367	KUMS000102	0.051519	0.226979	
368	KANM800101	0.060602	-0.24617		368	CHAM830103	0.051352	0.226609	
369	RICJ880101	0.060262	-0.24548		369	AVBF000108	0.05079	0.225366	
370	RICJ880102	0.060262	-0.24548		370	ISOY800107	0.050383	0.224463	
371	FASG760101	0.059746	-0.24443		371	ROBB760108	0.050181	-0.22401	
372	QIAN880124	0.059713	-0.24436		372	VASM830103	0.049308	0.222053	
373	NAKH900104	0.059677	-0.24429		373	CIDH920103	0.049136	-0.22167	
374	SUYM030101	0.059476	-0.24388		374	NAKH900108	0.048673	-0.22062	
375	LIFS790103	0.058953	-0.2428		375	PALJ810101	0.048616	0.220491	
376	KRIW790103	0.058756	-0.2424		376	RACS820104	0.047861	-0.21877	
377	MCMT640101	0.058082	-0.241		377	TANS770110	0.046315	-0.21521	
378	GRAR740103	0.057822	-0.24046		378	ROBB760113	0.045836	-0.21409	
379	ONEK900102	0.05706	0.238872		379	RACS820101	0.044595	0.211176	
380	KHAG800101	0.056285	-0.23725		380	LEWP710101	0.043487	-0.20854	
381	RICJ880110	0.055177	-0.2349		381	NAKH900106	0.042745	-0.20675	
382	TANS770104	0.054908	0.234324		382	GARJ730101	0.042675	-0.20658	
383	OOBM850104	0.054528	-0.23351		383	MEEJ800101	0.042424	-0.20597	
384	LEVM780105	0.054257	-0.23293		384	MUNV940104	0.042393	-0.2059	
385	CORJ870101	0.052556	-0.22925		385	ROBB760107	0.04193	0.204767	
386	TANS770103	0.051977	-0.22798		386	PALJ810106	0.041824	-0.20451	
387	TANS770101	0.051959	-0.22795		387	CHOP780212	0.041653	-0.20409	
388	QIAN880108	0.051921	0.227863		388	YUTK870102	0.040955	-0.20237	
389	BURA740101	0.051858	-0.22772		389	KHAG800101	0.040057	-0.20014	
390	ISOY800102	0.050252	-0.22417		390	ZASB820101	0.039982	-0.19996	
391	NAKH920102	0.050086	0.223799		391	KARP850102	0.039619	0.199046	
392	CHOC750101	0.050056	-0.22373		392	DAYM780201	0.039615	-0.19903	
393	AURR980119	0.049826	0.223218		393	SIMZ760101	0.039348	0.198363	
394	RACS820109	0.049723	-0.22299		394	PALJ810102	0.03908	-0.19769	
395	GEIM800108	0.048867	-0.22106		395	AVBF000109	0.038362	0.195862	
396	NAKH900107	0.048433	-0.22008		396	CHOP780101	0.038148	-0.19532	
397	FAUJ880107	0.048142	-0.21941		397	ONEK900101	0.03578	0.189155	
398	MUNV940104	0.047889	0.218836		398	PRAM820101	0.035403	0.188156	
399	QIAN880129	0.047409	-0.21774		399	WILM950104	0.034868	0.186729	
400	RACS820111	0.047209	-0.21728		400	GEOR030107	0.03433	0.185282	
401	AURR980111	0.046672	-0.21604		401	KARP850103	0.034225	0.185001	
402	RACS820103	0.046652	-0.21599		402	FINA910103	0.034057	-0.18454	
403	TANS770105	0.046564	-0.21579		403	FAUJ880104	0.033944	0.184239	
404	ZHOH040102	0.045751	-0.21389		404	CRAJ730103	0.033734	-0.18367	
405	ISOY800105	0.044867	-0.21182		405	YUTK870101	0.031934	-0.1787	
406	HUTJ700101	0.044688	-0.2114		406	OOBM850102	0.030971	-0.17599	
407	ARGP820103	0.043968	-0.20969		407	FASG760104	0.030493	-0.17462	
408	AVBF000102	0.043747	-0.20916		408	QIAN880114	0.030075	0.17342	
409	QIAN880102	0.041915	-0.20473		409	ROSG850101	0.029318	0.171226	
410	FAUJ880113	0.041732	0.204285		410	CIDH920102	0.029002	-0.1703	
411	FASG760102	0.040055	-0.20014		411	QIAN880135	0.02828	0.168166	
412	QIAN880109	0.039904	0.199759		412	BULH740101	0.028268	-0.16813	
413	LEVM780106	0.039712	-0.19928		413	AURR980105	0.028134	0.167732	
414	GEIM800111	0.038769	-0.1969		414	MAXF760106	0.027947	0.167172	
415	PRAM900104	0.038545	-0.19633		415	JOND750101	0.027813	0.166772	
416	ISOY800107	0.037563	-0.19381		416	CEDJ970105	0.027343	-0.16536	
417	AVBF000108	0.037115	-0.19265		417	ARGP820101	0.026832	0.163805	

418	FUKS010110	0.03705	-0.19248		418	NAKH900103	0.02654	-0.16291	
419	ROBB760104	0.036878	0.192036		419	ISOY800104	0.026298	0.162166	
420	FODM020101	0.036847	0.191955		420	FUKS010112	0.026288	-0.16214	
421	QIAN880137	0.03682	0.191885		421	NADH010107	0.026072	0.161469	
422	AVBF000107	0.0357	-0.18895		422	BUNA790103	0.025961	0.161124	
423	CRAJ730101	0.035249	-0.18775		423	RACS820112	0.025549	-0.15984	
424	ISOY800104	0.034391	0.185449		424	ROSM880104	0.025473	-0.1596	
425	ROBB760101	0.033744	-0.18369		425	AURR980109	0.025466	0.15958	
426	QIAN880136	0.033352	0.182625		426	BEGF750103	0.024722	-0.15723	
427	PONP800105	0.033338	-0.18259		427	KUMS000103	0.024411	-0.15624	
428	LEVM780103	0.033284	-0.18244		428	CHOP780208	0.023376	-0.15289	
429	AURR980112	0.032851	-0.18125		429	GRAR740103	0.022912	0.151366	
430	RICJ880117	0.032581	-0.1805		430	CHAM830107	0.022629	-0.15043	
431	QIAN880117	0.03228	-0.17967		431	CHAM820102	0.022563	0.15021	
432	GEOR030102	0.032095	0.17915		432	CRAJ730102	0.022471	-0.1499	
433	MUNV940101	0.031657	0.177925		433	MAXF760101	0.022107	0.148685	
434	COHE430101	0.031294	-0.1769		434	TANS770101	0.021839	-0.14778	
435	AURR980106	0.031281	-0.17686		435	FINA910102	0.021629	-0.14707	
436	JOND750102	0.031075	-0.17628		436	DIGM050101	0.020905	-0.14459	
437	ROBB760102	0.030981	-0.17601		437	PONP800106	0.020532	-0.14329	
438	LEVM760106	0.030637	-0.17503		438	WILM950103	0.020396	-0.14282	
439	CHAM830107	0.030568	-0.17484		439	FAUJ880101	0.01995	0.141243	
440	PALJ810107	0.029699	-0.17233		440	AURR980113	0.018813	0.137162	
441	PALJ810113	0.029212	-0.17092		441	GEIM800110	0.018024	0.134252	
442	OOBM770102	0.028734	0.169512		442	ANDN920101	0.0178	0.133418	
443	ONEK900101	0.028655	0.169277		443	TANS770102	0.017365	0.131775	
444	PONJ960101	0.027999	-0.16733		444	ROBB760110	0.017312	-0.13157	
445	NAKH900112	0.027898	-0.16703		445	SNEP660101	0.016991	0.13035	
446	ROBB760103	0.027402	0.165537		446	GEOR030102	0.016831	0.129735	
447	OOBM850102	0.027323	-0.1653		447	QIAN880111	0.016781	0.129541	
448	YUTK870103	0.027182	-0.16487		448	CHAM830104	0.016729	-0.12934	
449	CHOP780209	0.027022	-0.16438		449	CHOP780201	0.015948	-0.12629	
450	GEIM800110	0.026974	-0.16424		450	AURR980101	0.015927	0.126201	
451	TANS770108	0.026739	-0.16352		451	VINM940104	0.015879	0.126012	
452	YUTK870104	0.026513	-0.16283		452	MAXF760103	0.015848	-0.12589	
453	MAXF760101	0.026512	-0.16282		453	KANM800103	0.015725	0.125398	
454	CRAJ730102	0.026018	-0.1613		454	COSI940101	0.015094	-0.12286	
455	ARGP820102	0.025545	-0.15983		455	VELV850101	0.014918	-0.12214	
456	ISOY800101	0.025326	-0.15914		456	TANS770108	0.014309	0.119619	
457	WILM950104	0.025307	-0.15908		457	GOLD730101	0.01423	0.119289	
458	RACS820110	0.02438	-0.15614		458	NAKH900105	0.013925	-0.118	
459	AURR980102	0.023612	0.153664		459	QIAN880124	0.013878	-0.11781	
460	FASG760105	0.02339	-0.15294		460	GEIM800102	0.013564	0.116464	
461	DAYM780101	0.022939	-0.15146		461	ROBB760109	0.013477	-0.11609	
462	FASG760103	0.022029	0.148421		462	RICJ880111	0.01275	0.112917	
463	RACS820107	0.021808	0.147676		463	PALJ810115	0.012256	0.110706	
464	GEIM800109	0.0209	-0.14457		464	LAW840101	0.01143	-0.10691	
465	CHOP780204	0.020038	-0.14156		465	QIAN880132	0.011062	0.105178	
466	AURR980120	0.020032	0.141535		466	FODM020101	0.010953	0.104656	
467	OOBM770105	0.019638	-0.14014		467	ISOY800103	0.010914	0.104471	
468	QIAN880126	0.019619	-0.14007		468	RICJ880116	0.010834	0.104085	
469	MUNV940102	0.018709	0.136781		469	PRAM820103	0.010828	0.104056	
470	CHAM830103	0.017708	0.133072		470	ZIMJ680101	0.01075	0.103683	
471	QIAN880135	0.017215	0.131206		471	QIAN880138	0.010641	0.103156	
472	BUNA790103	0.017132	0.130889		472	YUTK870104	0.010399	-0.10197	
473	PALJ810102	0.016953	-0.1302		473	GEOR030108	0.009773	0.098857	
474	JUKT750101	0.016771	-0.1295		474	RICJ880103	0.009747	0.098728	
475	ROSG850101	0.016524	-0.12854		475	ZHOH040101	0.009677	-0.09837	
476	WIMW960101	0.015543	-0.12467		476	NAKH920104	0.009591	0.097935	
477	MUNV940103	0.014526	-0.12053		477	QIAN880131	0.009437	-0.09714	

478	NAKH920101	0.01443	0.120125		478	OOBM850105	0.009396	-0.09693	
479	AURR980109	0.014398	-0.11999		479	OOBM850104	0.008888	0.094275	
480	RICJ880112	0.014247	-0.11936		480	YUTK870103	0.008668	-0.0931	
481	GEOR030103	0.013167	-0.11475		481	QIAN880134	0.008653	0.093023	
482	FAUJ880105	0.012479	-0.11171		482	CHOP780211	0.008227	0.090703	
483	OOBM770104	0.012295	-0.11088		483	LEV760105	0.00817	0.09039	
484	GEOR030107	0.012255	0.1107		484	AVBF000104	0.007504	-0.08662	
485	QIAN880116	0.011936	-0.10925		485	CIDH920101	0.007115	-0.08435	
486	KANM800103	0.011604	-0.10772		486	KRIW790103	0.007096	0.08424	
487	QIAN880111	0.010994	0.104853		487	VINM940103	0.006784	0.082367	
488	KUMS000103	0.010676	0.103323		488	BUNA790102	0.006223	0.078888	
489	GEOR030101	0.01018	0.100896		489	ZIMJ680104	0.006181	0.078619	
490	NAKH900108	0.008324	-0.09124		490	VINM940102	0.00539	0.073419	
491	CHAM820102	0.008312	0.091171		491	TANS770104	0.005349	0.073139	
492	NAKH920104	0.008255	-0.09085		492	RICJ880101	0.005234	0.072346	
493	SNEP660101	0.006633	0.081445		493	RICJ880102	0.005234	0.072346	
494	QIAN880105	0.006423	-0.08014		494	BULH740102	0.004756	0.068961	
495	AURR980110	0.006226	-0.0789		495	QIAN880136	0.004609	0.067892	
496	YANJ020101	0.006051	0.077788		496	FINA910101	0.004605	-0.06786	
497	QIAN880107	0.006041	0.077726		497	RICJ880107	0.004326	-0.06577	
498	BULH740102	0.005292	-0.07275		498	NAKH920102	0.003826	-0.06186	
499	GEOR030104	0.005067	0.071181		499	FUKS010110	0.003684	0.060693	
500	CHOP780201	0.005015	-0.07082		500	BLAM930101	0.003566	-0.05971	
501	FASG760104	0.004946	0.070329		501	PALJ810113	0.00351	0.059244	
502	AURR980105	0.004721	-0.06871		502	QIAN880139	0.0034	-0.05831	
503	QIAN880103	0.004464	-0.06681		503	FUKS010103	0.003399	-0.0583	
504	GEOR030108	0.004115	-0.06415		504	OOBM850101	0.003335	0.057751	
505	RICJ880107	0.003955	-0.06289		505	CEDJ970104	0.003247	0.056979	
506	QIAN880134	0.003848	0.062032		506	AURR980102	0.003152	0.056138	
507	QIAN880123	0.003728	-0.06106		507	NAKH920101	0.003061	-0.05533	
508	ROBB760109	0.003653	-0.06044		508	JOND920102	0.003045	-0.05518	
509	OOBM850101	0.003609	-0.06008		509	GRAR740101	0.002873	0.053598	
510	PRAM820103	0.003457	0.058798		510	KUMS000104	0.002798	-0.0529	
511	FAUJ880102	0.002612	-0.05111		511	AVBF000101	0.002673	-0.0517	
512	PRAM820102	0.002418	-0.04918		512	QIAN880115	0.002455	0.049548	
513	NAKH900101	0.002276	0.047707		513	NAKH900102	0.002307	-0.04803	
514	CHOP780213	0.002197	0.046874		514	GEIM800109	0.002036	-0.04512	
515	YUTK870102	0.002065	0.045441		515	RICJ880114	0.00177	-0.04208	
516	KUMS000104	0.001642	0.040525		516	BHAR880101	0.001659	0.040736	
517	PALJ810110	0.001542	-0.03927		517	CHOP780207	0.001645	-0.04056	
518	QIAN880110	0.001412	-0.03757		518	FAUJ880103	0.001416	-0.03763	
519	NAKH900103	0.001067	-0.03267		519	BEGF750101	0.001337	-0.03657	
520	RICJ880111	0.001004	-0.03169		520	KARP850101	0.00133	0.036465	
521	TANS770102	0.000991	-0.03147		521	ISOY800101	0.001322	0.03636	
522	AVBF000101	0.00095	-0.03082		522	CHOP780203	0.001319	0.036316	
523	RACS820101	0.00088	-0.02966		523	ROBB760104	0.001166	0.034148	
524	BEGF750101	0.000723	-0.02689		524	CHOP780205	0.00111	-0.03332	
525	AURR980104	0.000692	-0.0263		525	COHE430101	0.001059	0.032536	
526	JOND920101	0.000488	-0.02208		526	GEIM800101	0.000997	-0.03158	
527	CEDJ970104	0.000469	0.021654		527	BUNA790101	0.000976	-0.03124	
528	SUEM840101	0.000429	-0.02071		528	FINA910104	0.000941	-0.03067	
529	PONP800106	0.000422	-0.02054		529	WEBA780101	0.000933	0.030546	
530	RACS820114	0.000369	-0.0192		530	SUEM840102	0.000829	0.028793	
531	RADA880106	0.000339	0.018399		531	RACS820108	0.000814	-0.02853	
532	GEIM800106	0.000323	0.017982		532	QIAN880137	0.000726	-0.02695	
533	AURR980113	0.00029	0.017042		533	AURR980108	0.000523	-0.02286	
534	CEDJ970102	0.000246	-0.0157		534	RICJ880104	0.0004	-0.02	
535	RACS820102	0.000203	-0.01426		535	CHOP780216	0.000384	0.019607	
536	QIAN880112	0.000116	-0.01076		536	CHOP780206	0.000382	0.019547	
537	NAKH900105	5.15E-05	0.007179		537	PALJ810107	0.000301	0.017341	

538	RACS820112	1.92E-05	0.004379		538	QIAN880103	0.000287	0.016954	
539	GEOR030106	1.91E-05	-0.00437		539	KUMS000101	0.000264	0.016253	
540	CEDJ970101	1.87E-06	-0.00137		540	RACS820105	0.000244	-0.01562	
541	CHAM830104	1.79E-06	-0.00134		541	VASM830102	0.000212	-0.01456	
542	RICJ880104	9.89E-07	0.000994		542	ROSM880103	0.000168	-0.01296	
543	RICJ880109	9.74E-07	-0.00099		543	TANS770106	0.000142	-0.01193	
544	FUKS010112	8.79E-08	-0.0003		544	RICJ880117	0.000108	0.010377	
545	NAKH900102	4.30E-08	0.000207		545	CHOP780210	4.14E-05	0.006432	

Linear QSAR model is used for predicting MIC by using the training set of 38 Rana box peptides with Sideways Asymmetry Moment (SAM) as the only descriptor applied either to pre-Rana box (left part of the Table) or to peptide Rana box segment alone (right part of the Table).

&MIC = Minimal Inhibitory Concentration against *E. coli* cells

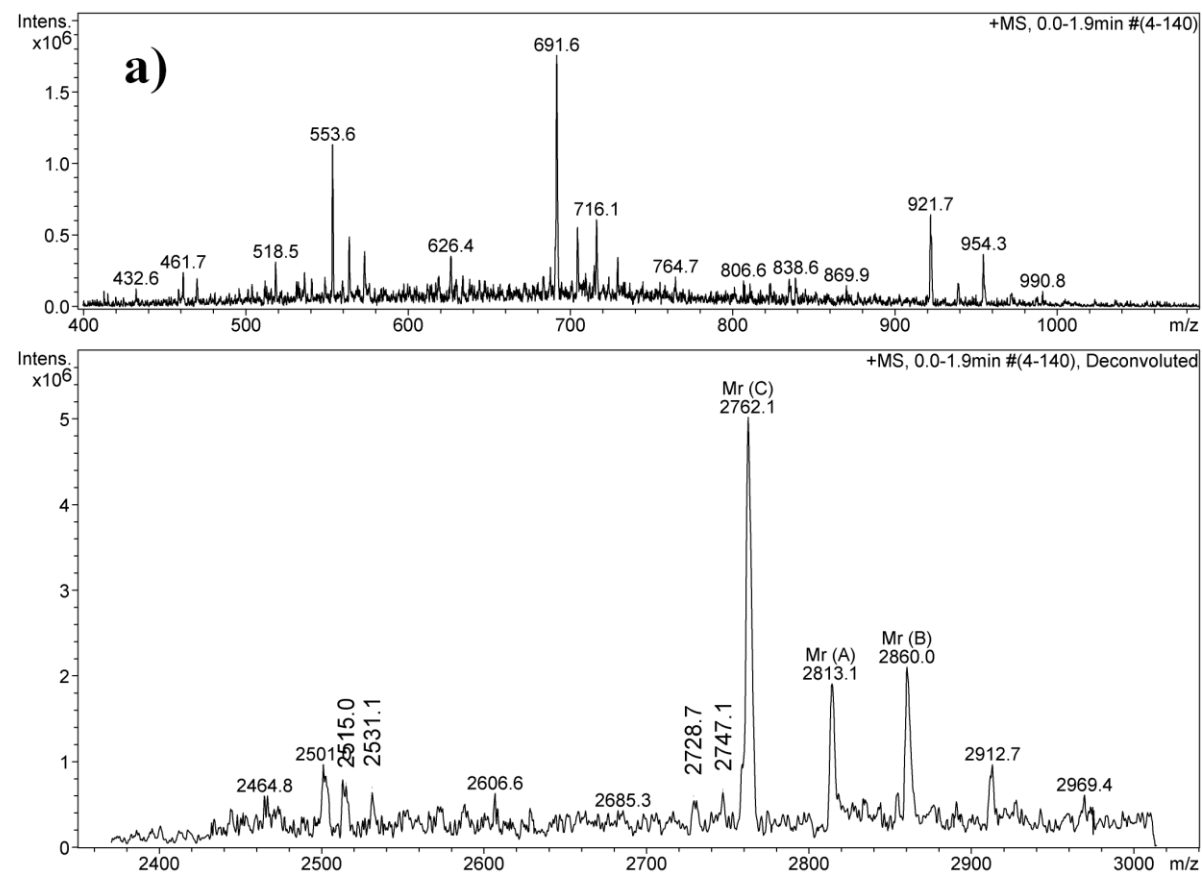
Codes for AA scales are from Kawashima et al. 2008, reference No. 28 from the manuscript. H = Hydrophobicity scales: FASG890101, Fasman's hydrophobicity index (1989); COWR900101, The hydrophobicity index determined by HPLC (Cowan and Whittaker, 1990); NAKH920105, AA membrane composition of single spanning integral membrane proteins (Nakashima and Nishikawa, 1992); CCS, Extended consensus hydrophobicity scale (Tossi et. al., 2002), reference No. 42 from the manuscript; EISD840101, Consensus normalized hydrophobicity scale (Eisenberg et al., 1984); FAUJ880109, Hydrophobic parameters π of amino-acid side chains from the partitioning of N-acetyl-amino-acid amides (Fauchère and Pliska, 1983)

** SNEP660102, Principal component II for relations between chemical structure and biological activity in peptides (Sneath, 1966)

*** BIOV880101, Information value for accessibility for average fraction 35% (Biou et al., 1988)

+ ZHOH040103, Buriability index (Zhou and Zhou, 2004)

Figure S1.



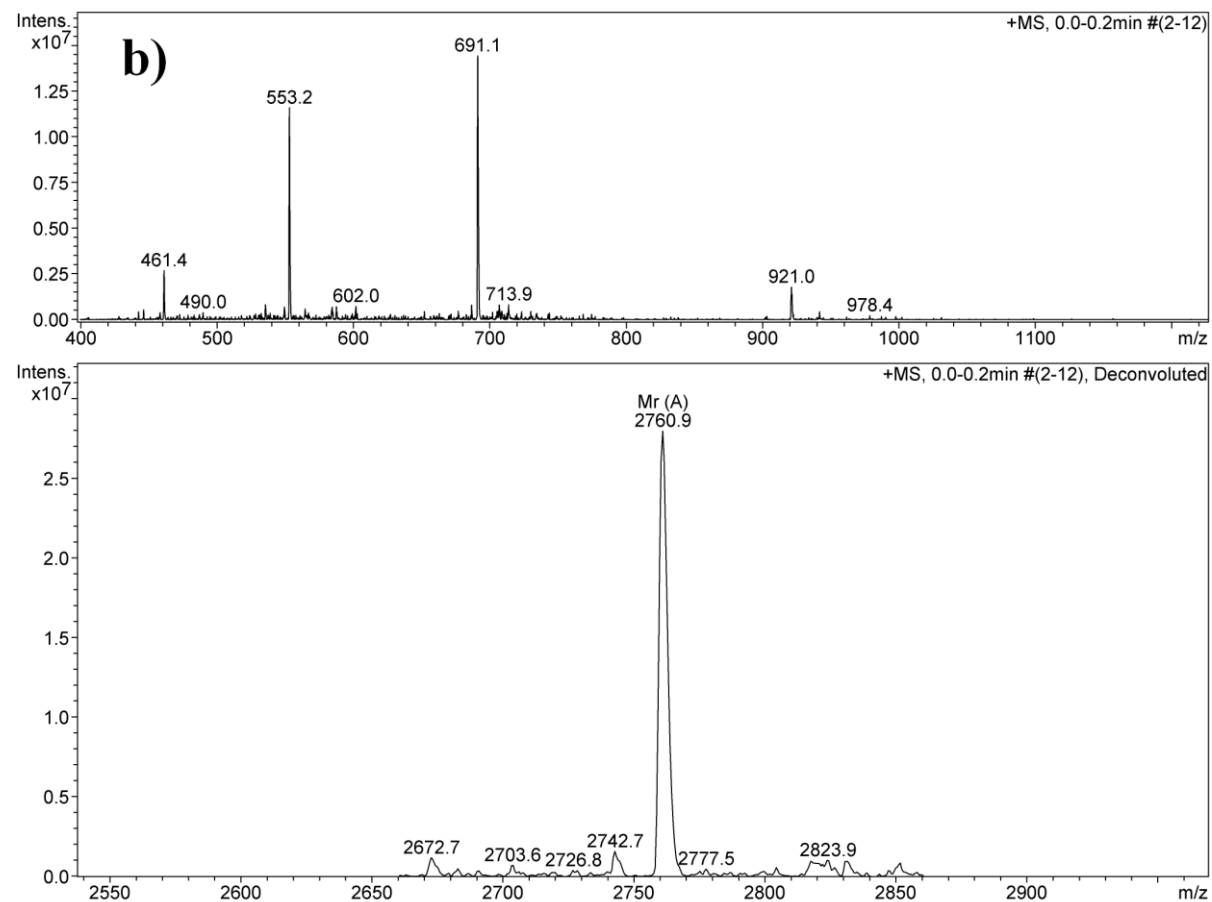


Figure S1: ESI-MS spectra of ranaboxin-1. a) Crude peptide in reduced form (calculated molecular weight 2762.4). This peptide was used for folding in 0.1 M ammonium acetate buffer (pH 7.5) in the presence of the cysteine and cystine pair (peptide:Cys:Cys₂ ratio = 1:50:5). After folding for 24 hours the oxidized peptide solution was purified directly by RP-HPLC. b) ESI-MS of the main purified peptide fraction (calculated molecular weight 2760.4). MS spectra were obtained on Bruker Daltonics, Esquire 4000 with an electrospray ionization (ESI) ion source. The mass range of the analysis was 400 – 1500 m/z. Molecular weight is presented in Daltons (Da).

Figure S2.

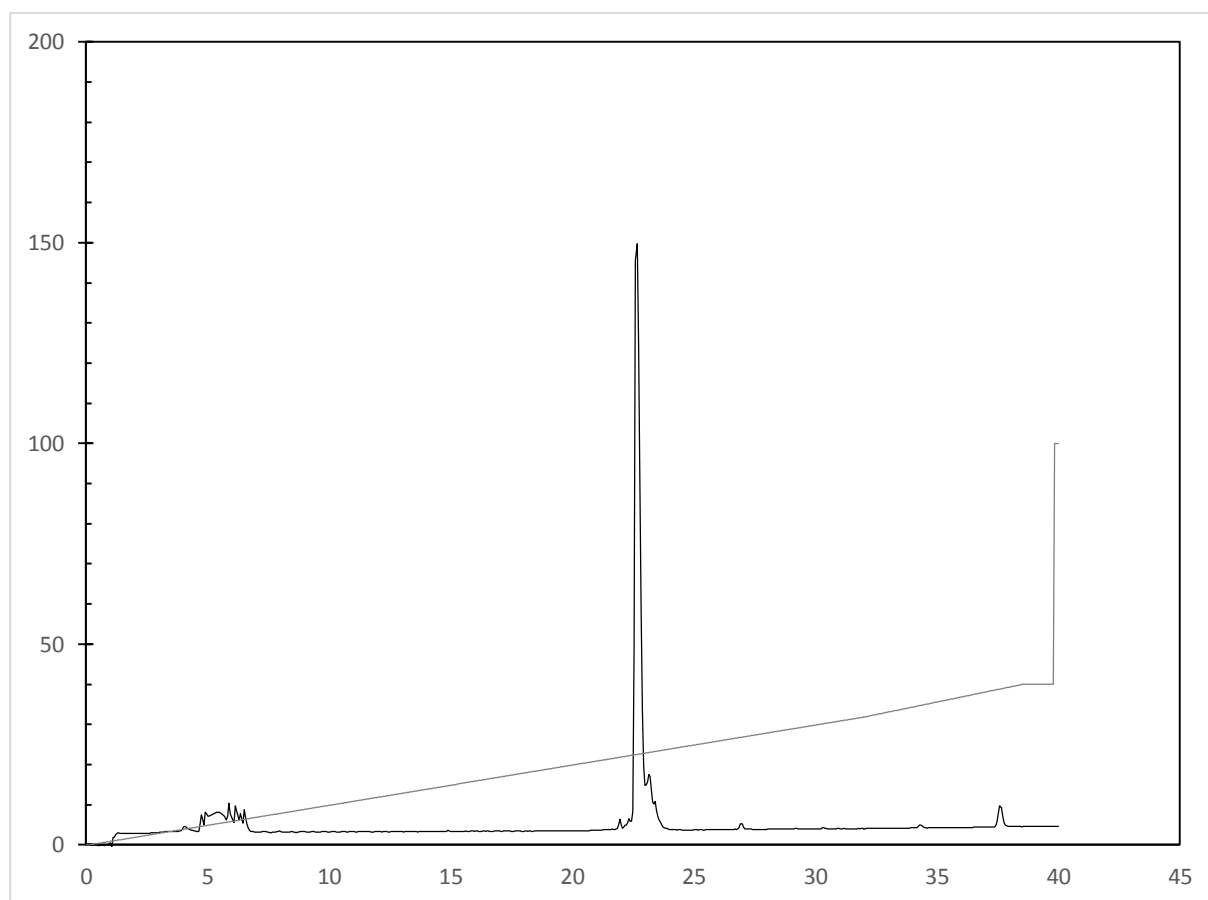


Figure S2. Analytical RP-HPLC of oxidized and purified ranaboxin-1. Waters Symmetry® analytical column (C₁₈, 3.5 µm, 100 Å, 4.6 x 75 mm) was used with a gradient of 0-40 % solvent B (0.05% TFA v/v in acetonitrile) in 40 min with flow of 0.8 mL/min.