

In Silico* Evaluation of Antimicrobial Potential of Amaranth, Chia and Quinoa Peptides Released During the Simulated Gastric Digestion and Their Effects on *Helicobacter pylori

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Table S1: Chemical properties and the predicted antibiofilm, antimicrobial, cell-penetrating activities of the resultant peptides

Organism	Protein ID	Peptide Sequence	Charge	pI	Mol wt	SVM score	Biofilm activity	CPP Probability	Uptake Efficiency Probability	AMP Prediction Probability
Chia	Q36769	KAGVKEYKL	2.00	9.55	1035.38	0.93	Biofilm-active	0.56	0.78	Non-AMP
Chia	Q36769	DRYKGRCYHIEPVPGEKDQYICYVAYPL	0.50	7.03	3377.26	-0.17	Biofilm-inactive	Non-CPP		0.99
Chia	Q36769	RIPVAYVKTF	2.00	10.01	1193.59	1.16	Biofilm-active	Non-CPP		Non-AMP
Chia	Q36769	SAKNYGRAVYECL	1.00	8.51	1473.84	0.06	Biofilm-inactive	Non-CPP		0.76
Chia	Q36769	HIHRAMHAVIDRQKNHGMHF	4.50	10.84	2436.13	0.87	Biofilm-active	Non-CPP		Non-AMP
Chia	Q36769	PGVIPVASGGIHVWHMPAL	1.00	7.26	1938.62	0.51	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A0F6PN28	QSRPHHL	2.00	10.11	874.07	-0.08	Biofilm-inactive	0.72	0.83	Non-AMP

Chia	A0A0F6PN28	QQHHPRSHQMVKAAATAVTAGGSL	3.50	11.01	2413.06	0.47	Biofilm-inactive	Non-CPP		0.84
Chia	XP_047958388.1	HRHIIRTRGL	4.00	12.31	1258.65	0.55	Biofilm-active	0.97	0.01	Non-AMP
Chia	XP_047958388.1	KSEKDERGPVIVEKEL	-1.00	5.01	1969.52	0.60	Biofilm-active	Non-CPP		Non-AMP
Chia	XP_047958388.1	RHNGL	1.50	10.11	595.73	-0.01	Biofilm-inactive	0.84	0.68	Non-AMP
Chia	XP_047958388.1	AKAVL	1.00	9.11	500.70	-0.25	Biofilm-inactive	0.53	0.04	Non-AMP
Chia	XP_047958388.1	TNAHSIMYITRGESRVQVNHKGQAVF	3.00	10.00	3043.87	1.02	Biofilm-active	Non-CPP		Non-AMP
Chia	XP_047958388.1	SGRTSAMRGL	2.00	12.01	1035.32	-0.88	Biofilm-inactive	Non-CPP		0.66
Chia	XP_047958388.1	SGSRSSYATQ	1.00	9.10	1043.18	-1.40	Biofilm-inactive	0.77	0.01	Non-AMP
Chia	XP_047974399.1	QCAGVAPMRNTL	1.00	8.60	1260.66	-0.20	Biofilm-inactive	0.74	0.004	Non-AMP
Chia	XP_047974399.1	HQKVHRIRRGDVIAL	4.00	11.72	1798.36	2.18	Biofilm-active	Non-CPP		Non-AMP
Chia	XP_047974399.1	RRRESPHDNGF	1.50	9.86	1484.71	-1.50	Biofilm-inactive	0.91	0.48	Non-AMP
Chia	XP_047974399.1	KVVDMHRL	1.50	9.10	997.34	0.86	Biofilm-active	Non-CPP		Non-AMP
Chia	XP_047974399.1	SPAHRSGKHF	3.00	11.01	1123.37	0.18	Biofilm-inactive	0.71	0.57	0.59
Chia	A0A1Z1EC60	GKRAADKF	2.00	10.01	892.12	-0.19	Biofilm-inactive	0.91	0.003	Non-AMP
Chia	A0A1Z1EC60	AAAAF	0.00	5.88	449.55	-0.74	Biofilm-inactive	0.71	0.15	Non-AMP
Chia	A0A1Z1EC60	WPIYWAAQGTMF	0.00	5.88	1470.88	0.09	Biofilm-inactive	Non-CPP		0.91
Chia	A0A1Z1EC60	VPYHGWRISHRTHHQNHGHVENDSWVPL	2.00	6.68	3526.27	0.88	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A1Z1EC60	WYRSPGKSGSHF	2.50	10.01	1408.70	-0.85	Biofilm-inactive	0.94	0.01	0.74
Chia	A0A1Z1EC60	VITSTICWAAMVACL	0.00	5.82	1582.18	-0.08	Biofilm-inactive	Non-CPP		0.9995
Chia	A0A1Z1EC60	HHHGYDKKL	2.50	8.84	1134.40	0.42	Biofilm-inactive	0.76	0.10	Non-AMP
Chia	A0A1Z1EC60	PWYRSKEWSYL	1.00	8.83	1514.85	-0.65	Biofilm-inactive	0.98	0.08	0.68
Chia	A0A1Z1EC60	NKIHHDIGTHVVHHL	2.50	7.47	1757.24	1.01	Biofilm-active	Non-CPP		0.82
Chia	A0A1Z1EC60	VEATREAKRVL	1.00	9.10	1271.63	1.09	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A1Z1EC60	GNYyrePRKSGAVPF	2.00	9.72	1741.14	-0.64	Biofilm-inactive	0.63	0.003	Non-AMP
Chia	A0A1Z1EC53	AAAAYF	0.00	5.88	612.74	-0.70	Biofilm-inactive	0.72	0.0003	Non-AMP
Chia	A0A1Z1EC53	WPIYWAAQGTMF	0.00	5.88	1470.88	0.09	Biofilm-inactive	Non-CPP		0.91
Chia	A0A1Z1EC53	VPYHGWRISHRTHHQNHGHVEKDESWVPL	3.00	7.51	3540.34	1.12	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A1Z1EC53	WYRSPGKTGSHF	2.50	10.01	1422.73	-0.44	Biofilm-inactive	0.92	0.01	0.86

Chia	A0A1Z1EC53	VITSTVCWAAMVAF	0.00	5.85	1499.01	0.07	Biofilm-inactive	Non-CPP		0.99
Chia	A0A1Z1EC53	HHHGDKKL	2.50	8.84	1134.40	0.42	Biofilm-inactive	0.76	0.10	Non-AMP
Chia	A0A1Z1EC53	PWYRSKEWSYL	1.00	8.83	1514.85	-0.65	Biofilm-inactive	0.98	0.08	0.68
Chia	A0A1Z1EC53	NKIHHDIGTHVIHHL	2.50	7.47	1771.27	0.72	Biofilm-active	Non-CPP		0.73
Chia	A0A1Z1EC53	VEATREAKRVL	1.00	9.10	1271.63	1.09	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A1Z1EC53	GNYYREPRKSGPVPF	2.00	9.72	1767.18	-1.09	Biofilm-inactive	0.82	0.02	0.79
Chia	A0A1Z1EC64	MASWVL	0.00	5.88	705.95	-0.48	Biofilm-inactive	0.56	0.001	Non-AMP
Chia	A0A1Z1EC64	PRIYMPRTVSSPNPSKL	3.00	11.01	2040.66	-1.17	Biofilm-inactive	Non-CPP		0.59
Chia	A0A1Z1EC64	CSVGRGRNWGL	2.00	10.38	1204.53	-0.54	Biofilm-inactive	0.59	0.01	0.93
Chia	A0A1Z1EC64	ADIRAAIPKHCWVKNPWKSMYSYVVRDVAVVF	3.50	9.64	3587.71	1.07	Biofilm-active	Non-CPP		0.94
Chia	A0A1Z1EC64	AAAAAYL	0.00	5.88	649.82	-0.73	Biofilm-inactive	0.70	0.14	Non-AMP
Chia	A0A1Z1EC64	NNWAVWPL	0.00	5.88	999.25	0.12	Biofilm-inactive	0.58	0.01	Non-AMP
Chia	A0A1Z1EC64	NSVAGHL	0.50	7.10	696.86	0.56	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A1Z1EC64	VPYHGWRISHRTHHQNHGHVENDESWHPL	2.50	6.75	3564.28	0.71	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A1Z1EC64	SEKIYKQL	1.00	8.83	1008.30	-0.06	Biofilm-inactive	0.77	0.01	Non-AMP
Chia	A0A1Z1EC64	VTKKL	2.00	10.02	587.83	-0.12	Biofilm-inactive	0.67	0.18	Non-AMP
Chia	A0A1Z1EC64	WSRSPGKKGSHF	3.50	11.17	1373.70	-0.39	Biofilm-inactive	0.96	0.66	0.91
Chia	A0A1Z1EC64	VPNERKDVTSTVCWTAMVAIL	0.00	6.39	2447.23	0.76	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A1Z1EC64	HHHGHEDKL	1.00	6.46	1109.31	0.07	Biofilm-inactive	0.55	0.11	Non-AMP
Chia	A0A1Z1EC64	PWYRGKEWSYL	1.00	8.83	1484.83	-0.19	Biofilm-inactive	0.78	0.06	0.65
Chia	A0A1Z1EC64	DRDYGWINNIHHDIGTHVIHHL	0.50	6.17	2663.27	0.15	Biofilm-inactive	Non-CPP		0.98
Chia	A0A1Z1EC52	PRIYPKPRSVQNSF	3.00	11.01	1689.14	-1.14	Biofilm-inactive	Non-CPP		0.98
Chia	A0A1Z1EC52	RISRPNQF	2.00	12.01	1017.26	-1.64	Biofilm-inactive	0.57	0.56	Non-AMP
Chia	A0A1Z1EC52	SDIKAAIPKHCWVKDPWRSVGYYVVRDVAVL	2.50	9.17	3508.60	1.03	Biofilm-active	Non-CPP		0.91
Chia	A0A1Z1EC52	HHHGHEDKL	1.00	6.46	1109.31	0.07	Biofilm-inactive	0.55	0.11	Non-AMP
Chia	A0A1Z1EC52	PWYRGKEWSYL	1.00	8.83	1484.83	-0.19	Biofilm-inactive	0.78	0.06	0.65
Chia	A0A1Z1EC52	INNIHHDIGTHVIHHL	1.50	6.58	1870.38	0.32	Biofilm-inactive	Non-CPP		0.73
Chia	A0A1Z1EC55	GDIKKAIPPHCF	1.50	8.54	1325.76	-0.61	Biofilm-inactive	0.80	0.003	Non-AMP

Chia	A0A1Z1EC55	KRSIPRSF	3.00	12.01	990.27	-1.96	Biofilm-inactive	0.89	0.05	Non-AMP
Chia	A0A1Z1EC55	TGVVWIAHECGHHAF	0.50	6.29	1664.10	1.31	Biofilm-active	Non-CPP		0.91
Chia	A0A1Z1EC55	SWKYSHRRHHSNTGSL	4.50	11.01	1953.34	-0.28	Biofilm-inactive	0.88	0.92	Non-AMP
Chia	A0A1Z1EC55	VPKVKTGVSWAAKYMNNPPGRL	4.00	10.47	2414.19	0.26	Biofilm-inactive	Non-CPP		0.98
Chia	A0A1Z1EC55	NVSGRPYDRF	1.00	9.10	1210.44	-1.34	Biofilm-inactive	0.80	0.03	Non-AMP
Chia	A0A1Z1EC55	SVAKGL	1.00	9.11	573.77	0.50	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A1Z1EC55	HNITDTHVAHHL	1.00	6.46	1394.70	0.53	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A1Z1EC46	MGAGGRMSVPPADKAKSDVIQRVPHAKPPF	4.50	10.45	3274.31	-0.23	Biofilm-inactive	Non-CPP		0.78
Chia	A0A1Z1EC46	GEIKKAIPPHCF	1.50	8.54	1339.79	-0.24	Biofilm-inactive	0.78	0.06	Non-AMP
Chia	A0A1Z1EC46	KRSIPRSF	3.00	12.01	990.27	-1.96	Biofilm-inactive	0.89	0.05	Non-AMP
Chia	A0A1Z1EC46	SWKYSHRRHHSNTGSL	4.50	11.01	1953.34	-0.28	Biofilm-inactive	0.88	0.92	Non-AMP
Chia	A0A1Z1EC46	VPKVKGSVSWTAKYMNNPPGRVITL	4.00	10.47	2743.64	0.25	Biofilm-inactive	Non-CPP		0.93
Chia	A0A1Z1EC46	NVSGRPYDRF	1.00	9.10	1210.44	-1.34	Biofilm-inactive	0.80	0.03	Non-AMP
Chia	A0A1Z1EC46	HNITDTHVAHHL	1.00	6.46	1394.70	0.53	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A2R4LNR5	ISATMSGVTCCL	0.00	5.82	1185.60	-0.92	Biofilm-inactive	Non-CPP		0.88
Chia	A0A2R4LNR5	NVQKNSSYF	1.00	8.94	1200.41	-1.53	Biofilm-inactive	0.75	0.06	Non-AMP
Chia	A0A2R4LNR5	RRKAF	3.00	12.01	676.87	0.36	Biofilm-inactive	0.95	0.29	Non-AMP
Chia	A0A2R4LNR9	KYDSVHGQWKHHEL	1.50	7.34	1764.15	0.97	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A2R4LNR9	KVKDECTL	1.00	8.83	960.25	0.18	Biofilm-inactive	0.84	0.34	Non-AMP
Chia	A0A2R4LNR9	TDKDKAAHL	0.50	7.09	1069.31	-0.44	Biofilm-inactive	0.56	0.04	Non-AMP
Chia	A0A2R4LNR9	DIVSNASCTTNCL	-1.00	3.80	1340.66	-1.17	Biofilm-inactive	Non-CPP		0.92
Chia	A0A2R4LNR9	NIIPSSTGAAGVKGVL	2.00	10.02	1626.18	0.52	Biofilm-active	Non-CPP		0.99
Chia	A0A2R4LNR9	IKHIHSTQ	2.00	9.11	963.23	0.01	Biofilm-inactive	0.85	0.01	Non-AMP
Chia	A0A2R4LNR7	RVHIMQTKEL	1.50	9.10	1254.67	1.43	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A2R4LNR7	GTCPVRIQGGCSF	1.00	8.39	1324.72	-1.05	Biofilm-inactive	Non-CPP		0.95
Chia	A0A2R4LNR7	RCDVTGKIL	1.00	8.57	1004.34	0.66	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A2R4LNR7	KSRPAKSGKTIEL	3.00	10.30	1414.85	0.36	Biofilm-inactive	0.54	0.79	Non-AMP
Chia	A0A2R4LNR7	MKYRITEGVNL	1.00	8.93	1323.74	0.75	Biofilm-active	Non-CPP		Non-AMP

Chia	A0A2R4LNR7	GRTRMEVNVKVSFV	3.00	11.01	1750.31	0.89	Biofilm-active	Non-CPP		Non-AMP
Chia	A0A2R4LNR7	VVKIRKF	3.00	11.17	976.33	1.75	Biofilm-active	0.80	0.03	Non-AMP
Chia	A0A2R4LNR7	KVWEKSGYNTVEWVRYITKAGSYEVR	2.00	9.05	3253.09	0.86	Biofilm-active	Non-CPP		Non-AMP
Amaranth	Q8LL67	NKKEPKTIL	2.00	9.72	1070.43	-0.22	Biofilm-inactive	0.96	0.17	Non-AMP
Amaranth	Q8LL67	SYTNHTVTDPR	0.50	7.09	1403.68	-0.37	Biofilm-inactive	0.79	0.29	Non-AMP
Amaranth	Q8LL67	NQVVTEIEYKRRSVTVKTEGDNVYKAKYVIVSPSL	2.00	9.26	4015.12	0.84	Biofilm-active	Non-CPP		Non-AMP
Amaranth	Q8LL67	WKRRASEF	2.00	10.84	1192.50	-0.02	Biofilm-inactive	0.98	0.26	Non-AMP
Amaranth	Q8LL67	YVHARRGYAIWQQL	2.50	9.72	1924.42	0.53	Biofilm-active	Non-CPP		Non-AMP
Amaranth	Q8LL67	TNWPVGTYNKKHKNL	3.50	10.01	1800.28	0.15	Biofilm-inactive	0.92	0.01	0.75
Amaranth	Q0GPA4	ARVVKAKEQVAGTL	2.00	10.01	1569.10	0.63	Biofilm-active	Non-CPP		Non-AMP
Amaranth	Q0GPA4	TIEAIDAGKKL	1.00	8.83	1286.71	0.32	Biofilm-inactive	0.80	0.21	Non-AMP
Amaranth	Q0GPA4	GAIREGHAPGWKEVPVHDEPVQNAAEHAVKTIQQRNSL	0.50	6.32	4258.29	0.85	Biofilm-active	Non-CPP		Non-AMP
Amaranth	Q0GPA4	KVKRGNKDEIF	2.00	9.72	1333.71	0.96	Biofilm-active	Non-CPP		Non-AMP
Amaranth	Q8S390	VHIKSRYTNYL	3.50	10.01	1521.96	0.74	Biofilm-active	0.98	0.01	Non-AMP
Amaranth	Q8S390	YVEEGNMKKVRL	1.00	8.83	1465.91	0.90	Biofilm-active	Non-CPP		Non-AMP
Amaranth	J9PE35	NRQNSRIF	2.00	12.01	1034.25	-1.65	Biofilm-inactive	0.86	0.15	Non-AMP
Amaranth	J9PE35	TKKRAKPAVPL	4.00	11.27	1208.66	0.33	Biofilm-inactive	0.93	0.001	0.70
Amaranth	J9PE35	NSNSKIYVL	1.00	8.94	1150.49	-0.85	Biofilm-inactive	0.67	0.001	Non-AMP
Amaranth	J9PE35	AAQSPENPNWF	-1.00	4.00	1388.62	-0.77	Biofilm-inactive	0.95	0.95	Non-AMP
Amaranth	J9PE35	GITKKPVPDF	1.00	8.94	1101.45	-0.64	Biofilm-inactive	0.71	0.0002	Non-AMP
Amaranth	X4Y205	EKTRPHCL	1.50	8.57	983.26	0.29	Biofilm-inactive	0.68	0.12	Non-AMP
Amaranth	X4Y205	PWTTDCAAKF	0.00	6.16	1139.41	-0.26	Biofilm-inactive	0.57	0.0002	Non-AMP
Amaranth	X4Y205	GRRWHIGPVSL	2.50	12.01	1348.75	0.70	Biofilm-active	0.87	0.18	Non-AMP
Amaranth	X4Y205	NSKKTNSVIYICF	2.00	9.25	1516.96	-1.15	Biofilm-inactive	Non-CPP		0.76
Amaranth	X4Y205	VRRNAIEKAIREVMGEDEAQERRNRAMKL	2.00	9.97	3470.41	0.52	Biofilm-active	Non-CPP		Non-AMP
Amaranth	X4Y205	RHNKL	2.50	11.01	666.85	0.39	Biofilm-inactive	0.53	0.91	Non-AMP
Amaranth	D6RSA4	RKERF	2.00	10.84	734.91	-0.05	Biofilm-inactive	0.83	0.13	Non-AMP
Amaranth	D6RSA4	VGAEVAPWSKTGGL	0.00	6.35	1371.76	0.01	Biofilm-inactive	Non-CPP		0.74

Amaranth	D6RSA4	HTYKRGVDRIF	2.50	10.00	1391.75	0.94	Biofilm-active	0.66	0.06	Non-AMP
Amaranth	D6RSA4	ARVWGITGSKL	2.00	11.01	1187.57	0.96	Biofilm-active	Non-CPP		Non-AMP
Amaranth	D6RSA4	NITVTMTAKPL	1.00	9.11	1188.61	-0.30	Biofilm-inactive	0.92	0.05	Non-AMP
Amaranth	D6RSA4	IKENVQIVVL	0.00	6.35	1154.58	0.83	Biofilm-active	Non-CPP		Non-AMP
Amaranth	D6RSA4	YPEKARGVTKF	2.00	9.72	1295.65	0.69	Biofilm-active	Non-CPP		0.66
Amaranth	A7LIU5	TKPYKIPNL	2.00	9.72	1073.43	-0.70	Biofilm-inactive	0.77	0.06	Non-AMP
Amaranth	A7LIU5	SPEEPRKGCDEL	-1.00	4.68	1329.65	-0.97	Biofilm-inactive	0.75	0.11	Non-AMP
Amaranth	A7LIU5	TRSNIRNVL	2.00	12.01	1185.54	-0.19	Biofilm-inactive	0.88	0.42	Non-AMP
Amaranth	A7LIU5	QETPIVEVTRTSITKHNYL	0.50	7.10	2128.69	0.70	Biofilm-active	Non-CPP		Non-AMP
Amaranth	A7LIU5	ANSRPGPVL	1.00	10.11	967.23	-1.03	Biofilm-inactive	Non-CPP		0.53
Amaranth	A7LIU5	PKPTYSANEEGL	-1.00	4.54	1305.57	-0.83	Biofilm-inactive	0.68	0.02	Non-AMP
Amaranth	A7LIU5	ASRAKIVHIDISAEIGKNKQPHVSICGDVKVAL	2.00	8.49	3613.71	0.90	Biofilm-active	Non-CPP		Non-AMP
Amaranth	A7LIU5	ESRKGKVKL	3.00	10.30	1044.39	1.68	Biofilm-active	0.83	0.79	Non-AMP
Amaranth	A7LIU5	NEQKKKF	2.00	9.72	921.16	-0.33	Biofilm-inactive	0.78	0.54	Non-AMP
Amaranth	A7LIU5	YKYRNPRQWL	3.00	10.29	1423.78	0.19	Biofilm-inactive	0.96	0.99	0.89
Amaranth	A7LIU5	ATIRVENL	0.00	6.36	915.17	0.90	Biofilm-active	Non-CPP		Non-AMP
Amaranth	A7LIU5	YKANRAHTYL	2.50	9.72	1236.53	0.52	Biofilm-active	0.98	0.003	0.60
Amaranth	A7LIU5	DVIVPHQEHVL	-1.00	5.16	1285.64	0.83	Biofilm-active	Non-CPP		Non-AMP
Amaranth	F8RNK2	NWCSDYPPVWL	-1.00	3.80	1379.70	-0.76	Biofilm-inactive	Non-CPP		0.65
Amaranth	F8RNK2	EEEEDIRKL	-3.00	4.26	1160.37	-0.71	Biofilm-inactive	0.64	0.01	Non-AMP
Amaranth	F8RNK2	CRAPVAVAVCSVARL	2.00	9.10	1685.30	0.12	Biofilm-inactive	Non-CPP		0.9997
Amaranth	Q38719	KSNNNQKYL	2.00	9.72	1108.35	-0.98	Biofilm-inactive	0.93	0.19	Non-AMP
Amaranth	Q38719	VHIKSRYTNKYL	3.50	10.01	1521.96	0.74	Biofilm-active	0.98	0.01	Non-AMP
Amaranth	Q38719	YVEEGNMKKVRL	1.00	8.83	1465.91	0.90	Biofilm-active	Non-CPP		Non-AMP
Amaranth	A2I9A6	RCAGVSVIRRTIEPHGL	2.50	10.29	1864.45	1.14	Biofilm-active	Non-CPP		Non-AMP
Amaranth	A2I9A6	QDQHQKIRHL	2.00	9.11	1302.62	-0.11	Biofilm-inactive	0.53	0.002	Non-AMP
Amaranth	A2I9A6	AGRTSAIRSL	2.00	12.01	1031.31	-0.70	Biofilm-inactive	Non-CPP		0.56
Amaranth	Q38712	HPTKMAKSTNYF	2.50	9.72	1424.80	-0.44	Biofilm-inactive	0.98	0.89	Non-AMP

Amaranth	Q38712	QDQHQKIRHL	2.00	9.11	1302.62	-0.11	Biofilm-inactive	0.53	0.002	Non-AMP
Amaranth	Q38712	AGRTSAIRSL	2.00	12.01	1031.31	-0.70	Biofilm-inactive	Non-CPP		0.56
Quinoa	XP_021755284.1	KEGDIVAAKL	0.00	6.42	1043.37	0.71	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021755284.1	PRYSOSSKVAYVL	1.00	8.83	1484.84	-0.96	Biofilm-inactive	Non-CPP		0.55
Quinoa	XP_021755284.1	GETSKAHKRGFE	1.50	8.94	1346.63	0.53	Biofilm-active	0.79	0.03	Non-AMP
Quinoa	XP_021755284.1	AGKTSVWKAL	2.00	10.02	1060.40	0.76	Biofilm-active	Non-CPP		0.87
Quinoa	XP_021755284.1	RSKRTSDEIF	1.00	9.10	1238.49	-2.18	Biofilm-inactive	0.78	0.02	Non-AMP
Quinoa	Q06AW2	MAKSTTTL	1.00	9.11	852.12	-0.89	Biofilm-inactive	0.61	0.77	Non-AMP
Quinoa	Q06AW2	QDQHQKIRHL	2.00	9.11	1302.62	-0.11	Biofilm-inactive	0.53	0.002	Non-AMP
Quinoa	Q06AW2	DKDYPKRF	1.00	8.83	1068.29	-1.37	Biofilm-inactive	0.90	0.001	Non-AMP
Quinoa	Q06AW2	SAEKGVL	0.00	6.35	702.90	0.51	Biofilm-active	Non-CPP		Non-AMP
Quinoa	Q06AW2	NAHSIIYGVRGRGRIQIVNAQGNSVF	3.50	11.72	2827.61	0.29	Biofilm-inactive	Non-CPP		0.75
Quinoa	Q06AW2	AGRTSAIRAMPL	2.00	12.01	1243.65	-0.38	Biofilm-inactive	0.84	0.04	Non-AMP
Quinoa	Q06AW2	RPENQGRQRDL	2.00	11.53	1524.83	-0.34	Biofilm-inactive	0.86	0.03	Non-AMP
Quinoa	Q06AW1	MAKSTTTL	1.00	9.11	852.12	-0.89	Biofilm-inactive	0.61	0.77	Non-AMP
Quinoa	Q06AW1	QDQHQKIRHL	2.00	9.11	1302.62	-0.11	Biofilm-inactive	0.53	0.002	Non-AMP
Quinoa	Q06AW1	DKDYPKRF	1.00	8.83	1068.29	-1.37	Biofilm-inactive	0.90	0.001	Non-AMP
Quinoa	Q06AW1	QAKQDERGNIVL	0.00	6.42	1370.71	0.60	Biofilm-active	Non-CPP		Non-AMP
Quinoa	Q06AW1	SAEKGVL	0.00	6.35	702.90	0.51	Biofilm-active	Non-CPP		Non-AMP
Quinoa	Q06AW1	NAHSIIYGVRGRGRIQIVNAQGNSVF	3.50	11.72	2827.61	0.29	Biofilm-inactive	Non-CPP		0.75
Quinoa	XP_021768828.1	MAKSTTTL	1.00	9.11	852.12	-0.89	Biofilm-inactive	0.61	0.77	Non-AMP
Quinoa	XP_021768828.1	QDQHQKIRHL	2.00	9.11	1302.62	-0.11	Biofilm-inactive	0.53	0.002	Non-AMP
Quinoa	XP_021768828.1	SAEKGVL	0.00	6.35	702.90	0.51	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021768828.1	NAHSIIYGVRGRGRIQIVNAQGNSVF	3.50	11.72	2827.61	0.29	Biofilm-inactive	Non-CPP		0.75
Quinoa	XP_021768828.1	AGRTSAIRAMPL	2.00	12.01	1243.65	-0.38	Biofilm-inactive	0.84	0.04	Non-AMP
Quinoa	XP_021768828.1	RPENQGRQRDL	2.00	11.53	1524.83	-0.34	Biofilm-inactive	0.86	0.03	Non-AMP
Quinoa	XP_021752668.1	PSGQSSPQHSRL	1.50	10.11	1280.53	-1.29	Biofilm-inactive	0.79	0.03	Non-AMP
Quinoa	XP_021752668.1	QCAGVTVIRREIEPKGL	1.00	8.57	1869.47	1.17	Biofilm-active	Non-CPP		Non-AMP

Quinoa	XP_021752668.1	SEESRRSERF	0.00	6.58	1282.45	-1.39	Biofilm-inactive	0.92	0.19	Non-AMP
Quinoa	XP_021752668.1	HKGHVIGL	2.00	9.11	860.16	1.39	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021752668.1	TKGSGRVQIANHEGEL	0.50	7.11	1696.10	0.78	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021752668.1	KYGRQEL	1.00	8.93	893.11	0.58	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021752233.1	RCAGVAARYVIEPKGL	2.00	9.36	1802.41	0.96	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021752233.1	NGHKL	1.50	9.11	567.72	0.66	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021752233.1	KWVSF	1.00	9.11	665.85	-0.10	Biofilm-inactive	0.58	0.001	Non-AMP
Quinoa	XP_021752233.1	SPRTRSF	2.00	12.01	850.02	-1.61	Biofilm-inactive	0.89	0.34	Non-AMP
Quinoa	XP_021746146.1	IVCYSMQVVVSQYDHEEERRAKEEDWKRREKTAEERRRHRHSWD EDEDEDEEGGREG RPKPRPEPYGPGGGGKGEMF	-5.50	5.02	9456.35	-0.52	Biofilm-inactive	Non-CPP		0.53
Quinoa	XP_021746146.1	KDSKKVVSTQAGEMRVVKGYGGKIVESPL	3.00	9.71	3092.06	0.64	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021746146.1	YIRRGAEKL	2.00	10.00	1105.43	0.91	Biofilm-active	0.58	0.01	Non-AMP
Quinoa	XP_021746146.1	SERKL	1.00	9.10	631.79	-0.41	Biofilm-inactive	0.91	0.08	Non-AMP
Quinoa	XP_021746146.1	TIICSDPSEGL	-2.00	3.67	1247.60	-1.54	Biofilm-inactive	0.75	0.01	Non-AMP
Quinoa	XP_021746146.1	KGEERL	0.00	6.49	730.90	0.19	Biofilm-inactive	0.59	0.62	Non-AMP
Quinoa	XP_021746146.1	KKSGIGL	2.00	10.02	701.97	0.80	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021746146.1	CQIASRSGSF	1.00	8.60	1055.30	-1.70	Biofilm-inactive	0.70	0.03	0.55
Quinoa	XP_021758596.1	EQGRGSSSQCRRL	2.00	10.29	1591.92	-1.04	Biofilm-inactive	0.95	0.9994	0.61
Quinoa	XP_021764389.1	KGKVSIL	2.00	10.02	843.20	0.84	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021764389.1	CKEHCRQQRQL	2.50	9.03	1428.81	0.12	Biofilm-inactive	0.91	0.15	Non-AMP
Quinoa	XP_021764389.1	DSRQRHCETACEEYIREKERREQRDEPQSRHDPGKEYRECRQRC QEEKEGKRQEVCQCESECRKIEQEREIRRRRDEDEIVGRKKERSE DEEEEEESSGGRPYVF	-8.00	5.02	13680.26	-0.40	Biofilm-inactive	Non-CPP		0.91
Quinoa	XP_021764389.1	KAEEGRVRVL	1.00	9.10	1156.49	1.22	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021764389.1	TKRSKL	3.00	11.17	731.97	0.09	Biofilm-inactive	0.85	0.52	Non-AMP
Quinoa	XP_021764389.1	VYTDRESF	0.00	6.42	1172.37	-0.71	Biofilm-inactive	0.71	0.08	Non-AMP
Quinoa	XP_021764389.1	NIERGHVMVIPAGVTAYL	0.50	7.10	1940.57	1.06	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021764389.1	INPVSNIGKF	1.00	9.11	1088.42	-0.73	Biofilm-inactive	Non-CPP		0.90

Quinoa	XP_021764389.1	THEKGSHPWF	1.00	7.26	1225.47	0.32	Biofilm-inactive	0.93	0.04	Non-AMP
Quinoa	XP_021764389.1	GGKSGRSGPFP	2.00	11.01	1006.24	-0.88	Biofilm-inactive	0.65	0.001	0.94
Quinoa	XP_021764389.1	EMACPHVSKSGHKQHHHHHNEKSRREEETSPVHYEKINSEL	3.00	6.82	5067.16	0.40	Biofilm-inactive	0.92	0.84	Non-AMP
Quinoa	XP_021764389.1	KNIEKEAKEL	0.00	6.57	1201.53	-0.14	Biofilm-inactive	0.87	0.01	Non-AMP
Quinoa	XP_021717850.1	VKKEERIPVATEF	0.00	6.57	1645.13	0.87	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021717850.1	KKVDL	1.00	8.94	601.81	-0.40	Biofilm-inactive	0.95	0.16	Non-AMP
Quinoa	XP_021717850.1	QRGDIVYRL	1.00	9.10	1006.24	0.01	Biofilm-inactive	0.52	0.06	Non-AMP
Quinoa	XP_021717850.1	RIVAVF	1.00	10.11	703.96	0.73	Biofilm-active	Non-CPP		Non-AMP
Quinoa	XP_021717850.1	ANPKEDKVQGPL	0.00	6.42	1295.63	-0.38	Biofilm-inactive	0.52	0.00	Non-AMP
Quinoa	XP_021717850.1	KSCSGWSTAVTDHNL	0.50	7.06	1605.95	-0.58	Biofilm-inactive	Non-CPP		0.71
Quinoa	XP_021717850.1	TNKECKNSRF	2.00	9.36	1226.50	-1.09	Biofilm-inactive	0.96	0.29	Non-AMP
Quinoa	XP_021717850.1	SSTTKKNHPQF	2.50	10.02	1274.55	-1.13	Biofilm-inactive	0.57	0.41	Non-AMP
Quinoa	XP_021717850.1	KRTTKVSDVRW	3.00	11.01	1375.74	0.65	Biofilm-active	0.93	0.06	Non-AMP

Table S2: The non-bond interactions between SWKYSRRHHSNTGSL and the target enzymes

PROTEIN	NAME	DISTANCE	CATEGORY	TYPES	FROM	FROM CHEMISTRY	TO	TO CHEMISTRY
Shikimate dehydrogenase	B:ARG7:NE - A:ASP33:OD2	4.83552	Electrostatic	Attractive Charge	B:ARG7:NE	Positive	A:ASP33:OD2	Negative
Shikimate dehydrogenase	A:SER16:HG - B:HIS9:O	2.43332	Hydrogen bond	Conventional hydrogen bond	A:SER16:HG	H-Donor	B:HIS9:O	H-Acceptor
Shikimate dehydrogenase	A:ARG45:HN - B:SER5:O	1.54557	Hydrogen bond	Conventional hydrogen bond	A:ARG45:HN	H-Donor	B:SER5:O	H-Acceptor
Shikimate dehydrogenase	A:ARG45:HE - B:TYR4:O	2.27618	Hydrogen bond	Conventional hydrogen bond	A:ARG45:HE	H-Donor	B:TYR4:O	H-Acceptor
Shikimate dehydrogenase	A:ARG116:HH12 - B:ARG8:O	2.44312	Hydrogen bond	Conventional hydrogen bond	A:ARG116:HH12	H-Donor	B:ARG8:O	H-Acceptor
Shikimate dehydrogenase	A:ARG116:HH22 - B:ARG8:O	1.37884	Hydrogen bond	Conventional hydrogen bond	A:ARG116:HH22	H-Donor	B:ARG8:O	H-Acceptor
Shikimate dehydrogenase	B:ARG7:HH11 - A:ASP33:OD2	2.55857	Hydrogen bond	Conventional hydrogen bond	B:ARG7:HH11	H-Donor	A:ASP33:OD2	H-Acceptor
Shikimate dehydrogenase	B:ARG8:HN - B:HIS6:O	2.78565	Hydrogen bond	Conventional hydrogen bond	B:ARG8:HN	H-Donor	B:HIS6:O	H-Acceptor
Shikimate dehydrogenase	B:THR13:HG1 - B:HIS10:O	3.02285	Hydrogen bond	Conventional hydrogen bond	B:THR13:HG1	H-Donor	B:HIS10:O	H-Acceptor
Shikimate dehydrogenase	A:LYS115:HE2 - B:HIS6:O	1.63966	Hydrogen bond	Carbon hydrogen bond	A:LYS115:HE2	H-Donor	B:HIS6:O	H-Acceptor

Shikimate dehydrogenase	B:HIS6:HE1 - A:ASP31:OD2	3.0013	Hydrogen bond	Carbon hydrogen bond	B:HIS6:HE1	H-Donor	A:ASP31:OD2	H-Acceptor
Shikimate dehydrogenase	B:HIS9:HA - A:GLU112:OE2	2.01842	Hydrogen bond	Carbon hydrogen bond	B:HIS9:HA	H-Donor	A:GLU112:OE2	H-Acceptor
Shikimate dehydrogenase	B:SER11:HB1 - B:ASN12:OD1	2.73319	Hydrogen bond	Carbon hydrogen bond	B:SER11:HB1	H-Donor	B:ASN12:OD1	H-Acceptor
Shikimate dehydrogenase	A:ARG116 - B:ARG7	4.01517	Hydrophobic	Alkyl	A:ARG116	Alkyl	B:ARG7	Alkyl
Shikimate dehydrogenase	B:TRP2 - A:LYS111	4.76692	Hydrophobic	Pi-Alkyl	B:TRP2	Pi-Orbitals	A:LYS111	Alkyl
Shikimate dehydrogenase	B:TYR4 - A:LYS111	4.66998	Hydrophobic	Pi-Alkyl	B:TYR4	Pi-Orbitals	A:LYS111	Alkyl
Shikimate dehydrogenase	B:HIS6 - B:ARG8	5.13845	Hydrophobic	Pi-Alkyl	B:HIS6	Pi-Orbitals	B:ARG8	Alkyl
Shikimate dehydrogenase	B:HIS9 - A:LYS14	5.20172	Hydrophobic	Pi-Alkyl	B:HIS9	Pi-Orbitals	A:LYS14	Alkyl
Type II dehydroquinase	B:LYS3:NZ - A:ASP18:OD2	5.45601	Electrostatic	Attractive Charge	B:LYS3:NZ	Positive	A:ASP18:OD2	Negative
Type II dehydroquinase	B:ARG8:NE - A:ASP18:OD2	5.2412	Electrostatic	Attractive Charge	B:ARG8:NE	Positive	A:ASP18:OD2	Negative
Type II dehydroquinase	B:ARG8:NE - A:GLU110:OE2	4.15746	Electrostatic	Attractive Charge	B:ARG8:NE	Positive	A:GLU110:OE2	Negative
Type II dehydroquinase	A:ASP18:HN - B:SER5:O	2.53832	Hydrogen bond	Conventional hydrogen bond	A:ASP18:HN	H-Donor	B:SER5:O	H-Acceptor
Type II dehydroquinase	A:ARG113:HH12 - B:ARG8:O	2.15996	Hydrogen bond	Conventional hydrogen bond	A:ARG113:HH12	H-Donor	B:ARG8:O	H-Acceptor
Type II dehydroquinase	B:ARG7:HE - A:ASN10:OD1	2.27313	Hydrogen bond	Conventional hydrogen bond	B:ARG7:HE	H-Donor	A:ASN10:OD1	H-Acceptor
Type II dehydroquinase	B:ARG7:HH11 - B:HIS9:O	2.80244	Hydrogen bond	Conventional hydrogen bond	B:ARG7:HH11	H-Donor	B:HIS9:O	H-Acceptor
Type II dehydroquinase	B:ARG8:HN - B:HIS6:O	2.66073	Hydrogen bond	Conventional hydrogen bond	B:ARG8:HN	H-Donor	B:HIS6:O	H-Acceptor
Type II dehydroquinase	B:SER11:HG - B:ASN12:O	2.22814	Hydrogen bond	Conventional hydrogen bond	B:SER11:HG	H-Donor	B:ASN12:O	H-Acceptor
Type II dehydroquinase	B:ASN12:HD22 - A:GLU55:OE1	2.61227	Hydrogen bond	Conventional hydrogen bond	B:ASN12:HD22	H-Donor	A:GLU55:OE1	H-Acceptor
Type II dehydroquinase	B:ARG8:HD1 - A:GLU110:OE2	2.45241	Hydrogen bond	Carbon hydrogen bond	B:ARG8:HD1	H-Donor	A:GLU110:OE2	H-Acceptor
Type II dehydroquinase	B:ARG8:HD2 - A:GLU110:OE2	2.53103	Hydrogen bond	Carbon hydrogen bond	B:ARG8:HD2	H-Donor	A:GLU110:OE2	H-Acceptor
Type II dehydroquinase	B:HIS10:HE1 - B:SER11:O	2.81646	Hydrogen bond	Carbon hydrogen bond	B:HIS10:HE1	H-Donor	B:SER11:O	H-Acceptor
Type II dehydroquinase	B:ARG7:HN - B:HIS6	2.11193	Hydrogen bond	Pi-Donor hydrogen bond	B:ARG7:HN	H-Donor	B:HIS6	Pi-Orbitals
Type II dehydroquinase	A:MET13:SD - B:HIS6	5.80445	Other	Pi-Sulfur	A:MET13:SD	Sulfur	B:HIS6	Pi-Orbitals
Type II dehydroquinase	B:TYR4 - A:PRO19	3.52856	Hydrophobic	Pi-Alkyl	B:TYR4	Pi-Orbitals	A:PRO19	Alkyl
Type II dehydroquinase	B:TYR4 - A:ARG20	4.93794	Hydrophobic	Pi-Alkyl	B:TYR4	Pi-Orbitals	A:ARG20	Alkyl
Type II dehydroquinase	B:HIS6 - A:ARG17	3.77193	Hydrophobic	Pi-Alkyl	B:HIS6	Pi-Orbitals	A:ARG17	Alkyl
Type II dehydroquinase	B:HIS9 - A:ALA79	3.93735	Hydrophobic	Pi-Alkyl	B:HIS9	Pi-Orbitals	A:ALA79	Alkyl
D-alanine-D-alanine ligase	B:ARG8:NE - A:GLU13:OE2	4.62676	Electrostatic	Attractive Charge	B:ARG8:NE	Positive	A:GLU13:OE2	Negative

D-alanine-D-alanine ligase	B:ARG8:NE - A:GLU101:OE2	5.58178	Electrostatic	Attractive Charge	B:ARG8:NE	Positive	A:GLU101:OE2	Negative
D-alanine-D-alanine ligase	A:SER177:HG - B:HIS10:O	2.76315	Hydrogen bond	Conventional hydrogen bond	A:SER177:HG	H-Donor	B:HIS10:O	H-Acceptor
D-alanine-D-alanine ligase	B:HIS6:HD1 - A:TYR311:OH	1.98194	Hydrogen bond	Conventional hydrogen bond	B:HIS6:HD1	H-Donor	A:TYR311:OH	H-Acceptor
D-alanine-D-alanine ligase	B:ARG7:HH22 - A:VAL19:O	2.887	Hydrogen bond	Conventional hydrogen bond	B:ARG7:HH22	H-Donor	A:VAL19:O	H-Acceptor
D-alanine-D-alanine ligase	B:ARG8:HE - A:GLU13:OE1	2.17839	Hydrogen bond	Conventional hydrogen bond	B:ARG8:HE	H-Donor	A:GLU13:OE1	H-Acceptor
D-alanine-D-alanine ligase	B:ARG8:HH21 - A:GLU13:OE1	2.80439	Hydrogen bond	Conventional hydrogen bond	B:ARG8:HH21	H-Donor	A:GLU13:OE1	H-Acceptor
D-alanine-D-alanine ligase	B:ARG8:HH22 - A:GLU101:OE1	2.08367	Hydrogen bond	Conventional hydrogen bond	B:ARG8:HH22	H-Donor	A:GLU101:OE1	H-Acceptor
D-alanine-D-alanine ligase	B:HIS10:HN - B:ARG7:O	2.20613	Hydrogen bond	Conventional hydrogen bond	B:HIS10:HN	H-Donor	B:ARG7:O	H-Acceptor
D-alanine-D-alanine ligase	B:ASN12:HN - B:ASN12:OD1	2.4825	Hydrogen bond	Conventional hydrogen bond	B:ASN12:HN	H-Donor	B:ASN12:OD1	H-Acceptor
D-alanine-D-alanine ligase	B:ASN12:HD22 - A:PHE12:O	2.73113	Hydrogen bond	Conventional hydrogen bond	B:ASN12:HD22	H-Donor	A:PHE12:O	H-Acceptor
D-alanine-D-alanine ligase	B:GLY14:HN - B:SER11:O	1.59964	Hydrogen bond	Conventional hydrogen bond	B:GLY14:HN	H-Donor	B:SER11:O	H-Acceptor
D-alanine-D-alanine ligase	A:SER177:HA - B:ARG8:O	3.07123	Hydrogen bond	Carbon hydrogen bond	A:SER177:HA	H-Donor	B:ARG8:O	H-Acceptor
D-alanine-D-alanine ligase	B:TRP2:HD1 - A:ASN310:OD1	2.60648	Hydrogen bond	Carbon hydrogen bond	B:TRP2:HD1	H-Donor	A:ASN310:OD1	H-Acceptor
D-alanine-D-alanine ligase	B:TRP2:HD1 - A:ASN310:O	2.56664	Hydrogen bond	Carbon hydrogen bond	B:TRP2:HD1	H-Donor	A:ASN310:O	H-Acceptor
D-alanine-D-alanine ligase	B:HIS10:HD2 - B:HIS6:O	2.97844	Hydrogen bond	Carbon hydrogen bond	B:HIS10:HD2	H-Donor	B:HIS6:O	H-Acceptor
D-alanine-D-alanine ligase	B:SER11:HB2 - A:SER177:O	2.81738	Hydrogen bond	Carbon hydrogen bond	B:SER11:HB2	H-Donor	A:SER177:O	H-Acceptor
D-alanine-D-alanine ligase	B:SER1:N - B:TRP2	4.71145	Electrostatic	Pi-Cation	B:SER1:N	Positive	B:TRP2	Pi-Orbitals
D-alanine-D-alanine ligase	B:SER1:N - B:TRP2	4.21702	Electrostatic	Pi-Cation	B:SER1:N	Positive	B:TRP2	Pi-Orbitals
D-alanine-D-alanine ligase	B:ARG8:NE - A:HIS96	4.13537	Electrostatic	Pi-Cation	B:ARG8:NE	Positive	A:HIS96	Pi-Orbitals
D-alanine-D-alanine ligase	B:HIS9:HD1 - B:HIS10	2.53168	Hydrogen bond	Pi-Donor hydrogen bond	B:HIS9:HD1	H-Donor	B:HIS10	Pi-Orbitals
D-alanine-D-alanine ligase	A:GLU233:OE1 - B:HIS6	2.8139	Other	Pi-Lone Pair	A:GLU233:OE1	Lone Pair	B:HIS6	Pi-Orbitals
D-alanine-D-alanine ligase	B:HIS9 - B:HIS10	4.54445	Hydrophobic	Pi-Pi T-shaped	B:HIS9	Pi-Orbitals	B:HIS10	Pi-Orbitals
D-alanine-D-alanine ligase	A:ALA23 - B:LYS3	4.7562	Hydrophobic	Alkyl	A:ALA23	Alkyl	B:LYS3	Alkyl
D-alanine-D-alanine ligase	B:ARG7 - A:VAL19	4.68609	Hydrophobic	Alkyl	B:ARG7	Alkyl	A:VAL19	Alkyl
D-alanine-D-alanine ligase	B:ARG8 - A:ILE16	4.87383	Hydrophobic	Alkyl	B:ARG8	Alkyl	A:ILE16	Alkyl