Supplementary Material

Table S1. Functional prediction of 81 putative bacteriocins by ProtFun server using predicted functions of azurin as reference. The sequences are sorted by odd score from high to low. The higher of the score, the higher of the odds that the sequence belongs to the same categories with the azurin.

No.	Sequence ID	Cellular envelope Probability (a)	Non enzyme Probability (b)	Immune response Probability (c)	Probability product of (a), (b), and (c)	Log10 (Probability product)	Cellular envelope Odds	Non enzyme Odds	Immune response Odds	Odds product	Log10 (Odds product)
	azurin	0.592	0.818	0.5	2.42E-01	**-0.6**	9.71	1.147	5.877	65.5	**1.8**
1	p2seq07	0.621	0.441	0.345	9.45E-02	**-1.0**	**10.2**	0.6	4.1	**25.5**	**1.4**
2	p1seq19	0.514	0.547	0.189	5.31E-02	**-1.3**	8.4	0.8	2.2	14.4	**1.2**
3	p2seq31	0.237	0.651	0.305	4.71E-02	**-1.3**	3.9	0.9	3.6	12.7	**1.1**
4	p1seq16	0.413	0.515	0.186	3.96E-02	**-1.4**	6.8	0.7	2.2	10.7	**1.0**
5	p1seq02	0.427	0.371	0.18	2.85E-02	**-1.5**	7.0	0.5	2.1	7.7	**0.9**
6	p2seq33	0.416	0.494	0.138	2.84E-02	**-1.5**	6.8	0.7	1.6	7.7	**0.9**
7	p3seq02	0.108	0.486	0.421	2.21E-02	**-1.7**	1.8	0.7	**5.0**	6.0	**0.8**
8	p3seq17	0.1	0.537	0.376	2.02E-02	**-1.7**	1.6	0.8	4.4	5.5	**0.7**
9	p2seq12	0.052	0.778	0.309	1.25E-02	**-1.9**	0.9	1.1	3.6	3.4	**0.5**
10	p3seq29	0.284	0.43	0.091	1.11E-02	**-2.0**	4.7	0.6	1.1	3.0	**0.5**
11	p3seq13	0.041	0.811	0.292	9.71E-03	**-2.0**	0.7	1.1	3.4	2.6	**0.4**
12	p2seq14	0.051	0.721	0.256	9.41E-03	**-2.0**	0.8	1.0	3.0	2.6	**0.4**
13	p2seq24	0.035	0.708	0.363	9.00E-03	**-2.0**	0.6	1.0	4.3	2.4	**0.4**
14	p2seq08	0.175	0.713	0.07	8.73E-03	**-2.1**	2.9	1.0	0.8	2.4	**0.4**

15	p2seq20	0.033	0.8	0.328	8.66E-03	**-2.1**	0.5	1.1	3.9	2.3	**0.4**
16	p3seq09	0.032	0.715	0.369	8.44E-03	**-2.1**	0.5	1.0	4.3	2.3	**0.4**
17	p1seq03	0.029	0.651	0.383	7.23E-03	**-2.1**	0.5	0.9	4.5	2.0	**0.3**
18	p1seq09	0.052	0.653	0.215	7.30E-03	**-2.1**	0.9	0.9	2.5	2.0	**0.3**
19	p2seq30	0.206	0.754	0.047	7.30E-03	**-2.1**	3.4	1.1	0.5	2.0	**0.3**
20	p3seq16	0.03	0.646	0.361	7.00E-03	**-2.2**	0.5	0.9	4.2	1.9	**0.3**
21	p2seq18	0.035	0.535	0.303	5.67E-03	**-2.2**	0.6	0.7	3.6	1.5	**0.2**
22	p2seq32	0.347	0.396	0.041	5.63E-03	**-2.2**	5.7	0.6	0.5	1.5	**0.2**
23	p3seq01	0.035	0.585	0.252	5.16E-03	**-2.3**	0.6	0.8	3.0	1.4	**0.1**
24	p2seq05	0.296	0.415	0.039	4.79E-03	**-2.3**	4.9	0.6	0.5	1.3	**0.1**
25	p1seq18	0.032	0.469	0.297	4.46E-03	**-2.4**	0.5	0.7	3.5	1.2	**0.1**
26	p3seq21	0.032	0.639	0.221	4.52E-03	**-2.3**	0.5	0.9	2.6	1.2	**0.1**
27	p3seq24	0.126	0.788	0.045	4.47E-03	**-2.3**	2.1	1.1	0.5	1.2	**0.1**
28	p3seq04	0.031	0.529	0.263	4.31E-03	**-2.4**	0.5	0.7	3.1	1.2	**0.1**
29	p1seq11	0.029	0.807	0.167	3.91E-03	**-2.4**	0.5	1.1	2.0	1.1	**0.0**
30	p2seq16	0.035	0.493	0.22	3.80E-03	**-2.4**	0.6	0.7	2.6	1.0	**0.0**
31	p2seq01	0.032	0.749	0.138	3.31E-03	**-2.5**	0.5	1.1	1.6	0.9	**0.0**
32	p2seq21	0.06	0.531	0.097	3.09E-03	**-2.5**	1.0	0.7	1.1	0.8	**-0.1**
33	p2seq03	0.032	0.534	0.18	3.08E-03	**-2.5**	0.5	0.7	2.1	0.8	**-0.1**
34	p3seq03	0.048	0.715	0.081	2.78E-03	**-2.6**	0.8	1.0	1.0	0.8	**-0.1**
35	p2seq11	0.033	0.742	0.113	2.77E-03	**-2.6**	0.5	1.0	1.3	0.8	**-0.1**
36	p3seq15	0.032	0.456	0.19	2.77E-03	**-2.6**	0.5	0.6	2.2	0.7	**-0.1**
37	p2seq09	0.032	0.641	0.129	2.65E-03	**-2.6**	0.5	0.9	1.5	0.7	**-0.1**

38	p1seq12	0.037	0.605	0.116	2.60E-03	**-2.6**	0.6	0.8	1.4	0.7	**-0.2**
39	p1seq14	0.033	0.807	0.087	2.32E-03	**-2.6**	0.5	1.1	1.0	0.6	**-0.2**
40	p2seq13	0.033	0.725	0.092	2.20E-03	**-2.7**	0.5	1.0	1.1	0.6	**-0.2**
41	p2seq19	0.046	0.752	0.061	2.11E-03	**-2.7**	0.8	1.1	0.7	0.6	**-0.2**
42	p3seq08	0.092	0.429	0.047	1.85E-03	**-2.7**	1.5	0.6	0.6	0.5	**-0.3**
43	p1seq07	0.032	0.75	0.07	1.68E-03	**-2.8**	0.5	1.1	0.8	0.5	**-0.3**
44	p2seq02	0.171	0.781	0.012	1.60E-03	**-2.8**	2.8	1.1	0.1	0.4	**-0.4**
45	p1seq04	0.039	0.822	0.046	1.47E-03	**-2.8**	0.6	**1.2**	0.5	0.4	**-0.4**
46	p3seq22	0.032	0.687	0.061	1.34E-03	**-2.9**	0.5	1.0	0.7	0.4	**-0.4**
47	p3seq14	0.033	0.804	0.049	1.30E-03	**-2.9**	0.5	1.1	0.6	0.4	**-0.5**
48	p3seq10	0.036	0.581	0.057	1.19E-03	**-2.9**	0.6	0.8	0.7	0.3	**-0.5**
49	p3seq06	0.033	0.759	0.046	1.15E-03	**-2.9**	0.5	1.1	0.5	0.3	**-0.5**
50	p3seq18	0.034	0.774	0.04	1.05E-03	**-3.0**	0.6	1.1	0.5	0.3	**-0.5**
51	p3seq05	0.029	0.703	0.048	9.79E-04	**-3.0**	0.5	1.0	0.6	0.3	**-0.6**
52	p1seq13	0.03	0.631	0.043	8.14E-04	**-3.1**	0.5	0.9	0.5	0.2	**-0.7**
53	p2seq06	0.169	0.3	0.015	7.61E-04	**-3.1**	2.8	0.4	0.2	0.2	**-0.7**
54	p3seq20	0.031	0.627	0.037	7.19E-04	**-3.1**	0.5	0.9	0.4	0.2	**-0.7**
55	p3seq26	0.031	0.82	0.027	6.86E-04	**-3.2**	0.5	1.1	0.3	0.2	**-0.7**
56	p3seq19	0.029	0.784	0.029	6.59E-04	**-3.2**	0.5	1.1	0.3	0.2	**-0.7**
57	p2seq04	0.045	0.744	0.02	6.70E-04	**-3.2**	0.7	1.0	0.2	0.2	**-0.7**
58	p2seq26	0.043	0.78	0.019	6.37E-04	**-3.2**	0.7	1.1	0.2	0.2	**-0.8**
59	p2seq25	0.031	0.808	0.024	6.01E-04	**-3.2**	0.5	1.1	0.3	0.2	**-0.8**
60	p1seq08	0.032	0.784	0.024	6.02E-04	**-3.2**	0.5	1.1	0.3	0.2	**-0.8**

61	p3seq23	0.032	0.657	0.026	5.47E-04	**-3.3**	0.5	0.9	0.3	0.1	**-0.8**
62	p2seq10	0.053	0.8	0.012	5.09E-04	**-3.3**	0.9	1.1	0.1	0.1	**-0.9**
63	p3seq07	0.029	0.71	0.022	4.53E-04	**-3.3**	0.5	1.0	0.3	0.1	**-0.9**
64	p2seq28	0.035	0.762	0.017	4.53E-04	**-3.3**	0.6	1.1	0.2	0.1	**-0.9**
65	p3seq25	0.033	0.773	0.017	4.34E-04	**-3.4**	0.5	1.1	0.2	0.1	**-0.9**
66	p2seq17	0.033	0.729	0.017	4.09E-04	**-3.4**	0.5	1.0	0.2	0.1	**-0.9**
67	p3seq12	0.034	0.517	0.023	4.04E-04	**-3.4**	0.6	0.7	0.3	0.1	**-0.9**
68	p2seq29	0.031	0.698	0.019	4.11E-04	**-3.4**	0.5	1.0	0.2	0.1	**-1.0**
69	p2seq23	0.042	0.733	0.011	3.39E-04	**-3.5**	0.7	1.0	0.1	0.1	**-1.1**
70	p3seq11	0.032	0.729	0.013	3.03E-04	**-3.5**	0.5	1.0	0.1	0.1	**-1.1**
71	p1seq10	0.034	0.774	0.011	2.89E-04	**-3.5**	0.6	1.1	0.1	0.1	**-1.1**
72	p1seq01	0.037	0.22	0.035	2.85E-04	**-3.5**	0.6	0.3	0.4	0.1	**-1.1**
73	p2seq27	0.031	0.801	0.011	2.73E-04	**-3.6**	0.5	1.1	0.1	0.1	**-1.1**
74	p1seq06	0.033	0.78	0.01	2.57E-04	**-3.6**	0.5	1.1	0.1	0.1	**-1.1**
75	p2seq22	0.029	0.705	0.012	2.45E-04	**-3.6**	0.5	1.0	0.1	0.1	**-1.2**
76	p2seq15	0.029	0.786	0.011	2.51E-04	**-3.6**	0.5	1.1	0.1	0.1	**-1.2**
77	p1seq17	0.029	0.681	0.012	2.37E-04	**-3.6**	0.5	1.0	0.1	0.1	**-1.2**
78	p3seq27	0.032	0.568	0.012	2.18E-04	**-3.7**	0.5	0.8	0.1	0.1	**-1.2**
79	p1seq05	0.032	0.28	0.024	2.15E-04	**-3.7**	0.5	0.4	0.3	0.1	**-1.2**
80	p1seq15	0.032	0.406	0.014	1.82E-04	**-3.7**	0.5	0.6	0.2	0.0	**-1.3**
81	p3seq28	0.037	0.371	0.01	1.37E-04	**-3.9**	0.6	0.5	0.1	0.0	**-1.4**

Table S2. Model assessments for the 14 most putative anticancer azurin-like bacteriocins

No.	Sequence ID	Before refinement		After refinement	
		Favored rotamers	Ramachandran favored	Favored rotamers	Ramachandran favored
1	p2seq05	73.46%	64.62%	96.21%	88.08%
2	p3seq17	67.74%	50.75%	100.00%	88.06%
3	p3seq16	67.39%	47.06%	95.65%	92.16%
4	p3seq24	83.56%	77.33%	98.63%	96.00%
5	p2seq14	75.00%	54.55%	100.00%	90.91%
6	p2seq08	78.79%	69.57%	96.97%	91.30%
7	p2seq33	72.13%	69.86%	96.86%	89.01%
8	p2seq32	72.89%	70.74%	96.83%	91.48%
9	p2seq18	60.76%	50.00%	100.00%	96.15%
10	p2seq20	74.29%	43.59%	94.29%	79.49%
11	p1seq09	85.71%	69.70%	100.00%	100.00%
12	p1seq16	70.33%	64.76%	96.70%	85.24%
13	p3seq02	78.57%	65.52%	96.43%	93.10%
14	p3seq04	66.67%	34.48%	92.59%	79.31%

Table S3. The binding sites of p28-azurin, azurin and putative bacteriocins with p53 DBD expressed in Figure 2 and Figure 3. The amino acids of p53 DBD which are in binding interface with each bacteriocin are shown in grey color. Note: **SS**: secondary structure, **aaID**: amino acid id of p53 DBD, **azu**: azurin, **p28**: p28-azurin peptide, **109**: p1seq09, **116**: p1seq16, **205**: p2seq05, **208**: p2seq08, **214**: p2seq14, **218**: p2seq18, **220**: p2seq20, **232**: p2seq32, **233**: p2seq33, **302**: p3seq02, **316**: p3seq16, **317**: p3seq17, and **324**: p3seq24

SS	aaID	azu	p28	205	317	316	324	214	208	233	232	218	220	109	116	302
	96															
	97															
	98															
	99															
	100															■
	101						■									
	102						■									■
	103															
	104	■					■							■		■
	105															
	106															
	107															
	108															
	109															
S1	110	■	■				■							■	■	■
S1	111	■	■				■							■	■	■
S1	112		■				■							■		■
Loop 1	113	■	■				■									
Loop 1	114	■	■	■					■					■	■	■
Loop 1	115	■	■					■	■					■		■
Loop 1	116	■	■												■	■
Loop 1	117	■		■										■		
Loop 1	118			■											■	
Loop 1	119	■		■								■				
Loop 1	120		■					■		■	■			■		
Loop 1	121							■		■	■	■				
Loop 1	122	■		■	■								■	■		
Loop 1	123			■	■											
S2	124	■	■	■										■		
S2	125	■	■													
S2	126	■		■			■							■		■
S2	127															
	128		■				■							■	■	■
	129		■											■		
	130		■													
S2'	131						■							■	■	■
S2'	132															
S2'	133		■													
S2'	134															
S2'	135															

Region	Residue
(yellow)	136
	137
	138
	139
	140
S3	141
S3	142
S3	143
S3	144
S3	145
S3	146
	147
	148
	149
	150
	151
	152
	153
	154
S4	155
S4	156
S4	157
S4	158
S4	159
S4	160
S4	161
S4	162
S4	163
Loop 2	164
Loop 2	165
Loop 2	166
Loop 2	167
Loop 2	168
Loop 2	169
Loop 2	170
Loop 2	171
Loop 2	172
Loop 2	173
Loop 2	174
Loop 2	175
Loop 2	176
H1	177
H1	178
H1	179
H1	180
H1	181
Loop 2	182
Loop 2	183
Loop 2	184
Loop 2	185
Loop 2	186
Loop 2	187
Loop 2	188

Section	Row
(green)	189
(green)	190
(green)	191
(green)	192
(green)	193
(green)	194
S5	195
S5	196
S5	197
S5	198
	199
	200
	201
	202
	203
S6	204
S6	205
S6	206
S6	207
S6	208
	209
	210
	211
	212
S7	213
S7	214
S7	215
S7	216
S7	217
S7	218
S7	219
S7	220
	221
	222
	223
	224
	225
	226
	227
	228
	229
S8	230
S8	231
S8	232
S8	233
S8	234
S8	235
S8	236
Loop 3	237
Loop 3	238
Loop 3	239
Loop 3	240
Loop 3	241

Group	Row
S8 (red)	242
	243
	244
	245
	246
	247
	248
	249
	250
S9	251
	252
	253
	254
	255
	256
	257
	258
	259
	260
	261
	262
S10	263
	264
	265
	266
	267
	268
	269
	270
	271
	272
	273
	274
	275
	276
	277
H2	278
	279
	280
	281
	282
	283
	284
	285
	286
	287
	288
	289

Figure S1. Plot of probability score versus odds score for 81 putative bacteriocins expressed in Table S1
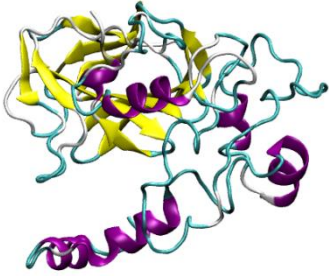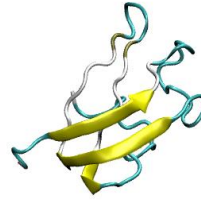
p2seq05	p3seq17
p3seq16	p3seq24
p2seq14	p2seq08
p2seq33	p2seq32
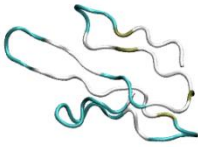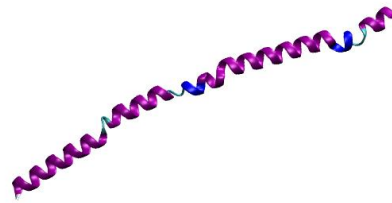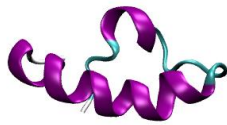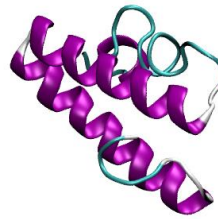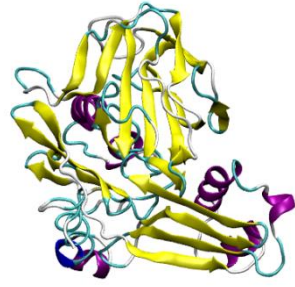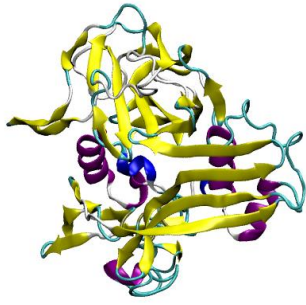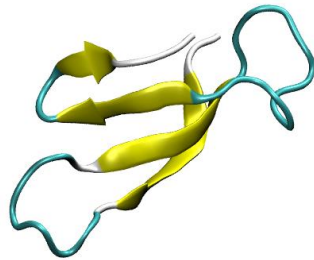
p2seq18	p2seq20
p1seq09	p1seq16
p3seq02	p3seq04
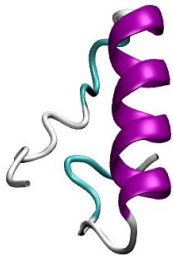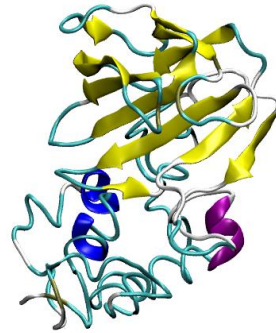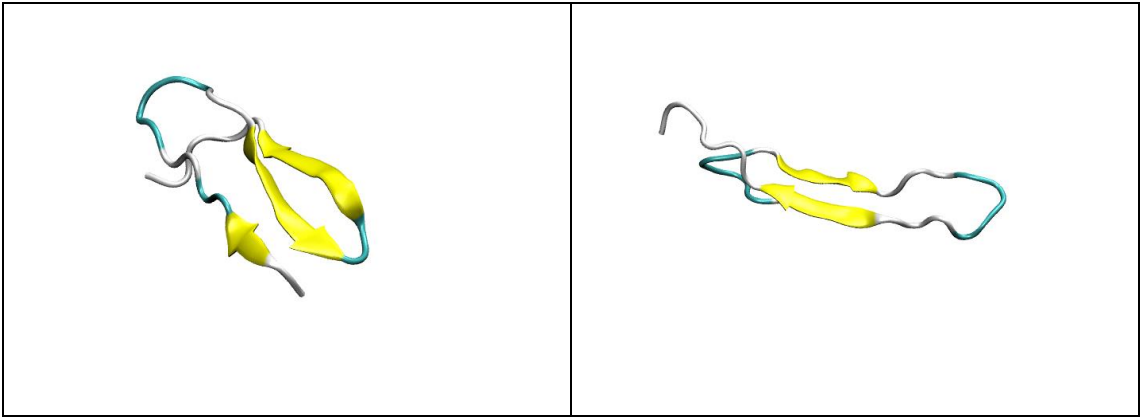
Figure S2. Models of 14 most putative anticancer azurin-like bacteriocins
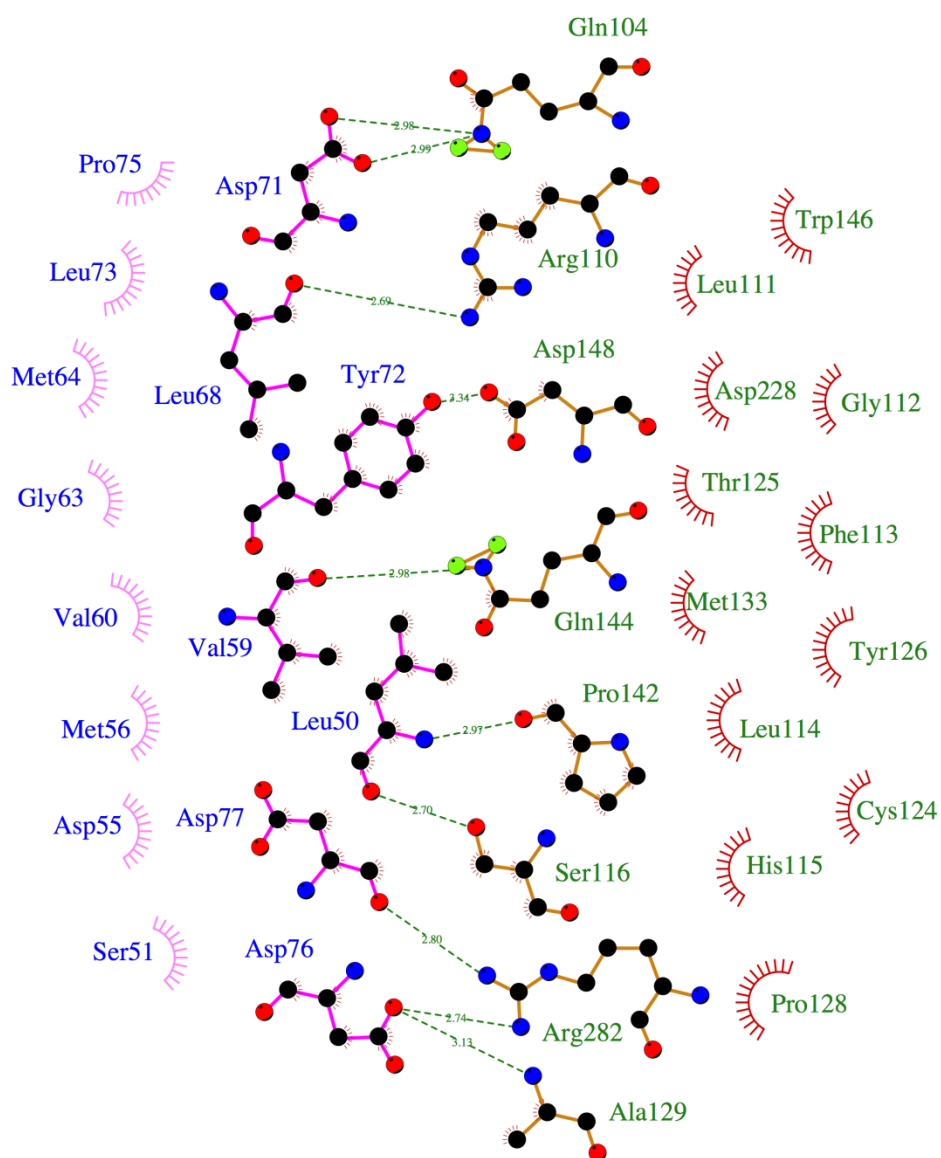
Figure S3. Amino acids involved in binding site of docking model between p53 DBD and p28-azurin. Name of amino acids of p28-azurin are in blue and those of p53 DBD are in green. Hydrogen bonds are shown in dot green line along with molecular details of donors and acceptors.
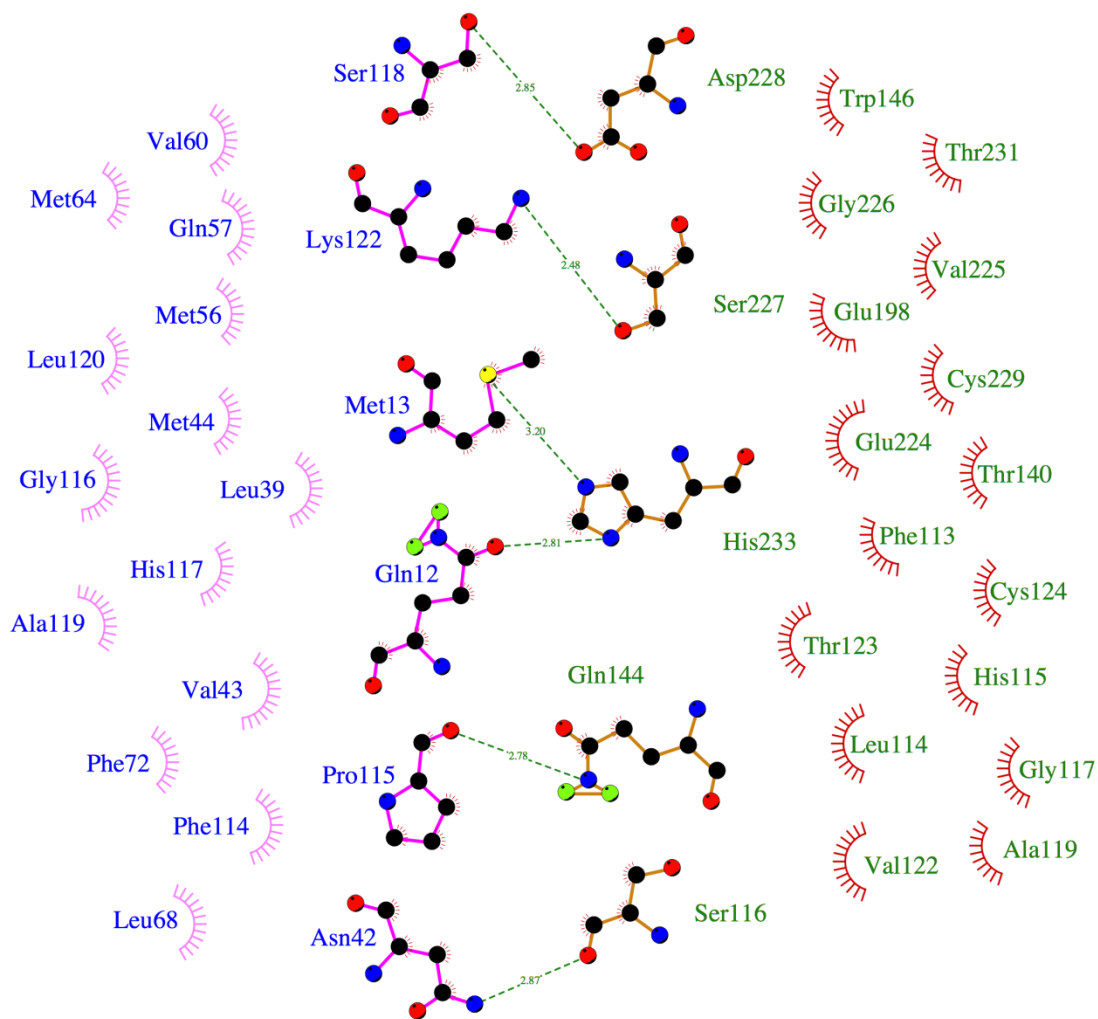
Figure S4. Amino acids involved in binding site of docking model between p53 DBD and azurin. Names of amino acids of azurin are in blue and those of p53 DBD are in green. Hydrogen bonds are shown in dot green line along with molecular details of donors and acceptors.