

BIOINFORMATICS

Kudari Pavani
be19b023

Q1:

Position	Residue	Set 1				
		Condition 1	Condition 2	Condition 3	Condition 4	Condition 5
'1'	':'	0	1.021	5	1.019	0.943
'2'	'S'	-0.305	0.865	3.008	0.729	0.253
'3'	'L'	0	0.909	4	0.916	0.943
'4'	'S'	0	0.953	4	0.951	0.943
'5'	'D'	-1.121	0.527	1.149	0.492	-1.597
'6'	'K'	-1.16	0.561	1.157	0.439	-1.685
'7'	'D'	0	0.973	6	0.972	0.943
'8'	'K'	0	0.956	5	0.95	0.943
'9'	'A'	-1.169	0.541	1.868	0.465	-1.705
'10'	'A'	-0.305	0.917	4.661	0.77	0.253
'11'	'V'	-0.586	0.744	3.603	0.763	-0.385
'12'	'R'	-0.305	0.871	4.504	0.744	0.253
'13'	'A'	-1.034	0.567	1.909	0.566	-1.399
'14'	'L'	-1.16	0.559	1.521	0.415	-1.685
'15'	'W'	-0.305	0.943	9.306	0.888	0.253
'16'	'S'	-0.916	0.612	2.264	0.604	-1.134
'17'	'K'	0	0.956	5	0.95	0.943
'18'	'I'	-0.689	0.691	3.504	0.719	-0.618
'19'	'G'	-0.305	0.886	4.992	0.831	0.253
'20'	'K'	-1.034	0.613	2.405	0.502	-1.399
'21'	'S'	-0.886	0.713	4.372	0.627	-1.064
'22'	'A'	-0.474	0.74	2.876	0.767	-0.131
'23'	'D'	-1.034	0.624	2.24	0.517	-1.399
'24'	'A'	-0.908	0.665	2.455	0.593	-1.114
'25'	'I'	-0.886	0.757	4.314	0.679	-1.064

'26'	'G'	0	0.977	6	0.977	0.943
'27'	'N'	-0.886	0.65	1.826	0.561	-1.064
'28'	'D'	-0.305	0.922	4.512	0.784	0.253
'29'	'A'	-0.305	0.817	3.347	0.768	0.253
'30'	'L'	0	0.909	4	0.916	0.943
'31'	'S'	-0.886	0.749	3.298	0.628	-1.064
'32'	'R'	0	1.015	5	1.011	0.943
'33'	'M'	-0.305	0.933	4.008	0.944	0.253
'34'	'I'	-0.305	0.904	4.992	0.78	0.253
'35'	'V'	-1.295	0.47	0.959	0.373	-1.991
'36'	'V'	-1.367	0.472	1.132	0.386	-2.154
'37'	'Y'	-0.474	0.83	5.14	0.718	-0.131
'38'	'P'	0	0.993	7	0.993	0.943
'39'	'Q'	-0.474	0.821	3.215	0.715	-0.131
'40'	'T'	0	0.977	5	0.979	0.943
'41'	'K'	0	0.956	5	0.95	0.943
'42'	'T'	0	0.977	5	0.979	0.943
'43'	'Y'	0	1.016	7	1.012	0.943
'44'	'F'	0	0.988	6	0.989	0.943
'45'	'S'	-0.474	0.822	4.521	0.712	-0.131
'46'	'H'	0	0.969	8	0.972	0.943
'47'	'W'	-0.6	0.823	4.24	0.711	-0.417
'48'	'P'	-0.857	0.657	2.295	0.582	-1
'49'	'D'	-0.305	0.888	5.174	0.901	0.253
'50'	'V'	-0.586	0.674	2.81	0.621	-0.385
'51'	'T'	-0.6	0.776	2.752	0.605	-0.417
'52'	'P'	-0.586	0.745	3.959	0.689	-0.385
'53'	'G'	0	0.977	6	0.977	0.943
'54'	'S'	0	0.953	4	0.951	0.943
'55'	'P'	-0.6	0.73	2.322	0.628	-0.417
'56'	'H'	-0.305	0.936	4.198	0.8	0.253
'57'	'I'	-0.305	0.872	3.835	0.748	0.253

'58'	'K'	0	0.956	5	0.95	0.943
'59'	'A'	-0.86	0.596	1.835	0.687	-1.006
'60'	'H'	0	0.969	8	0.972	0.943
'61'	'G'	0	0.977	6	0.977	0.943
'62'	'K'	-0.6	0.777	3.405	0.812	-0.417
'63'	'K'	0	0.956	5	0.95	0.943
'64'	'V'	0	0.956	4	0.956	0.943
'65'	'M'	-0.76	0.66	2.124	0.612	-0.778
'66'	'G'	-0.76	0.704	2.694	0.561	-0.778
'67'	'G'	-0.305	0.817	3.355	0.692	0.253
'68'	'I'	-0.305	0.825	3.669	0.71	0.253
'69'	'A'	-0.86	0.643	2.19	0.545	-1.006
'70'	'L'	-1.673	0.36	0.124	0.382	-2.848

'71'	'A'	0	0.906	4	0.909	0.943
'72'	'V'	-0.586	0.701	2.413	0.682	-0.385
'73'	'S'	-1.594	0.406	0.934	0.359	-2.67
'74'	'K'	-0.305	0.879	6.488	0.745	0.253
'75'	'I'	-0.995	0.543	2.612	0.534	-1.312
'76'	'D'	-0.305	0.888	5.331	0.888	0.253
'77'	'D'	0	0.973	6	0.972	0.943
'78'	'L'	-0.76	0.675	3.14	0.683	-0.778
'79'	'K'	-0.6	0.807	4.446	0.618	-0.417
'80'	'T'	-0.76	0.733	3.149	0.664	-0.778
'81'	'G'	-0.305	0.817	3.355	0.692	0.253
'82'	'L'	0	0.909	4	0.916	0.943
'83'	'M'	-0.305	0.869	3.182	0.749	0.253
'84'	'E'	-1.414	0.451	0.678	0.428	-2.262
'85'	'L'	0	0.909	4	0.916	0.943
'86'	'S'	0	0.953	4	0.951	0.943
'87'	'E'	-0.305	0.888	5.331	0.763	0.253
'88'	'Q'	-0.305	0.826	3.017	0.715	0.253
'89'	'H'	0	0.969	8	0.972	0.943
'90'	'A'	0	0.906	4	0.909	0.943
'91'	'Y'	-0.76	0.731	4.967	0.618	-0.778
'92'	'K'	0	0.956	5	0.95	0.943
'93'	'L'	0	0.909	4	0.916	0.943
'94'	'R'	0	1.015	5	1.011	0.943
'95'	'V'	0	0.956	4	0.956	0.943
'96'	'D'	0	0.973	6	0.972	0.943
'97'	'P'	0	0.993	7	0.993	0.943
'98'	'A'	-0.305	0.86	3.339	0.715	0.253
'99'	'N'	0	1.012	6	1.011	0.943
'100'	'F'	0	0.988	6	0.989	0.943
'101'	'K'	0	0.956	5	0.95	0.943
'102'	'I'	-0.6	0.739	3.058	0.632	-0.417
'103'	'L'	0	0.909	4	0.916	0.943
'104'	'N'	-0.6	0.781	2.926	0.619	-0.417
'105'	'H'	-0.305	0.886	6.653	0.839	0.253

'106'	'C'	-0.305	0.937	7.306	0.962	0.253
'107'	'I'	-0.6	0.739	3.058	0.588	-0.417
'108'	'L'	-0.305	0.825	3.678	0.783	0.253
'109'	'V'	-0.474	0.784	2.215	0.844	-0.131
'110'	'V'	-0.474	0.806	3.479	0.677	-0.131
'111'	'I'	-0.6	0.735	3.24	0.58	-0.417
'112'	'S'	-0.305	0.814	3.504	0.683	0.253
'113'	'T'	-1.72	0.345	0.702	0.355	-2.955
'114'	'M'	-0.305	0.885	6.322	0.769	0.253
'115'	'F'	-0.935	0.559	1.207	0.529	-1.175
'116'	'P'	0	0.993	7	0.993	0.943
'117'	'K'	-1.846	0.302	0.562	0.299	-3.241
'118'	'E'	-0.916	0.633	3.008	0.584	-1.134
'119'	'F'	-0.305	0.893	4.992	0.837	0.253
'120'	'T'	-0.305	0.891	4.182	0.907	0.253
'121'	'P'	0	0.993	7	0.993	0.943
'122'	'E'	-0.76	0.66	2.182	0.589	-0.778
'123'	'A'	-0.886	0.695	2.736	0.519	-1.064
'124'	'H'	0	0.969	8	0.972	0.943
'125'	'V'	-0.305	0.814	3.339	0.685	0.253
'126'	'S'	0	0.953	4	0.951	0.943
'127'	'L'	0	0.909	4	0.916	0.943
'128'	'D'	0	0.973	6	0.972	0.943
'129'	'K'	0	0.956	5	0.95	0.943
'130'	'F'	0	0.988	6	0.989	0.943
'131'	'L'	-0.305	0.822	3.355	0.839	0.253
'132'	'S'	-0.86	0.595	2.289	0.528	-1.006
'133'	'G'	-1.414	0.459	1.496	0.4	-2.262
'134'	'V'	0	0.956	4	0.956	0.943
'135'	'A'	-0.6	0.769	2.909	0.577	-0.417
'136'	'L'	-0.6	0.796	3.231	0.615	-0.417
'137'	'A'	-0.305	0.86	3.339	0.715	0.253
'138'	'L'	0	0.909	4	0.916	0.943
'139'	'A'	-0.305	0.881	4.165	0.738	0.253
'140'	'E'	-0.305	0.868	3.347	0.743	0.253
'141'	'R'	-0.305	0.871	4.504	0.744	0.253
'142'	'Y'	0	1.016	7	1.012	0.943
'143'	'R'	0	1.015	5	1.011	0.943

Position	Residue	Set 2				
		Condition 1	Condition 2	Condition 3	Condition 4	Condition 5
1	-	-1.216	0.529	1.306	0.494	-1
2	-	-1.216	0.529	1.306	0.494	-1
3	-	-1.216	0.529	1.306	0.494	-1
4	-	-1.216	0.529	1.306	0.494	-1
5	-	-1.216	0.529	1.306	0.494	-1
6	-	-1.216	0.529	1.306	0.494	-1
7	-	-1.216	0.529	1.306	0.494	-1
8	-	-1.216	0.529	1.306	0.494	-1
9	-	-1.216	0.529	1.306	0.494	-1
10	-	-1.216	0.529	1.306	0.494	-1

11	-	-1.216	0.529	1.306	0.494	-1
12	-	-1.216	0.529	1.306	0.494	-1
13	-	-1.216	0.529	1.306	0.494	-1
14	-	-1.216	0.529	1.306	0.494	-1
15	-	-1.216	0.529	1.306	0.494	-1
16	-	-1.216	0.529	1.306	0.494	-1
17	-	-1.216	0.529	1.306	0.494	-1
18	-	-1.216	0.529	1.306	0.494	-1
19	-	-1.216	0.529	1.306	0.494	-1
20	-	-1.216	0.529	1.306	0.494	-1
21	-	-1.216	0.529	1.306	0.494	-1
22	-	-1.216	0.529	1.306	0.494	-1
23	-	-1.216	0.529	1.306	0.494	-1
24	-	-1.216	0.529	1.306	0.494	-1
25	-	-1.216	0.529	1.306	0.494	-1
26	-	-1.216	0.529	1.306	0.494	-1
27	-	-1.216	0.529	1.306	0.494	-1
28	-	-1.216	0.529	1.306	0.494	-1
29	-	-1.216	0.529	1.306	0.494	-1
30	-	-1.216	0.529	1.306	0.494	-1
31	-	-1.216	0.529	1.306	0.494	-1
32	-	-1.216	0.529	1.306	0.494	-1
33	-	-1.216	0.529	1.306	0.494	-1
34	-	-1.216	0.529	1.306	0.494	-1
35	-	-1.216	0.529	1.306	0.494	-1
36	-	-1.216	0.529	1.306	0.494	-1
37	-	-1.216	0.529	1.306	0.494	-1
38	-	-1.216	0.529	1.306	0.494	-1
39	-	-1.216	0.529	1.306	0.494	-1
40	-	-1.216	0.529	1.306	0.494	-1
41	-	-1.216	0.529	1.306	0.494	-1
42	-	-1.216	0.529	1.306	0.494	-1
43	-	-1.216	0.529	1.306	0.494	-1
44	-	-1.216	0.529	1.306	0.494	-1

45	-	-1.216	0.529	1.306	0.494	-1
46	-	-1.216	0.529	1.306	0.494	-1
47	-	-1.216	0.529	1.306	0.494	-1
48	-	-1.216	0.529	1.306	0.494	-1
49	-	-1.216	0.529	1.306	0.494	-1
50	-	-1.216	0.529	1.306	0.494	-1
51	-	-1.216	0.529	1.306	0.494	-1
52	-	-1.216	0.529	1.306	0.494	-1
53	M	-1.216	0.529	1.306	0.494	-1
54	A	-1.216	0.529	1.306	0.494	-1
55	S	-0.974	0.648	1.328	0.666	-0.56
56	K	-1.494	0.426	1.109	0.365	-1.507
57	P	-0.377	0.882	3.5	0.827	0.529
58	Q	-0.736	0.726	2.938	0.641	-0.125
59	P	-0.377	0.884	3.828	0.83	0.529
60	I	-0.736	0.769	3.172	0.713	-0.125
61	A	-0.377	0.801	3.125	0.739	0.529
62	A	-0.377	0.812	4.656	0.754	0.529
63	A	-0.377	0.812	4.656	0.754	0.529
64	N	0	0.995	6	0.994	1.215
65	W	-0.349	0.909	8.963	0.876	0.58
66	K	0	0.962	5	0.966	1.215
67	C	-0.937	0.679	2.395	0.639	-0.492
68	N	0	0.995	6	0.994	1.215
69	G	-0.349	0.835	4	0.81	0.58
70	S	-1.311	0.51	0.79	0.53	-1.173
71	E	-1.303	0.553	1.568	0.515	-1.159
72	S	-1.523	0.401	0.901	0.372	-1.56
73	L	-1.581	0.481	0.519	0.482	-1.666
74	L	-1.061	0.526	2.667	0.514	-0.718
75	V	-1.677	0.317	0.198	0.27	-1.841
76	P	-1.003	0.64	2.025	0.597	-0.612
77	L	-0.687	0.664	3.012	0.656	-0.036
78	I	-0.965	0.55	2.716	0.557	-0.543
79	E	-1.735	0.362	0.136	0.393	-1.946
80	T	-1.003	0.663	1.815	0.595	-0.612
81	L	-0.349	0.859	3.235	0.826	0.58
82	N	-0.349	0.888	4.988	0.885	0.58
83	A	-1.003	0.591	1.951	0.549	-0.612
84	A	-0.684	0.691	2.716	0.676	-0.031
85	T	-1.889	0.305	0.383	0.302	-2.227
86	F	-1.581	0.426	0.457	0.364	-1.666
87	D	-1.149	0.604	1.543	0.553	-0.879
88	H	-1.677	0.372	0.383	0.348	-1.841
89	D	-1.523	0.429	1.259	0.421	-1.56

90	:	-1.216	0.529	1.306	0.494	-1
91	:	-1.216	0.529	1.306	0.494	-1
92	V	-0.687	0.645	2.222	0.684	-0.036
93	Q	-0.849	0.671	3.432	0.623	-0.331
94	C	-0.349	0.829	3.074	0.795	0.58
95	V	0	0.93	4	0.93	1.215
96	V	-1.061	0.545	2.136	0.563	-0.718
97	A	-1.003	0.594	2.062	0.557	-0.612
98	P	-0.349	0.893	5.049	0.894	0.58
99	T	-0.349	0.889	5.395	0.855	0.58
100	F	-1.215	0.498	0.889	0.51	-0.998

101	L	-1.677	0.321	0.593	0.294	-1.841
102	H	-0.684	0.808	5.247	0.771	-0.031
103	I	-0.687	0.664	3.012	0.686	-0.036
104	P	-1.149	0.595	1.272	0.564	-0.879
105	M	-1.465	0.504	1.704	0.492	-1.454
106	T	-1.149	0.509	1.704	0.45	-0.879
107	K	-0.937	0.625	2.37	0.582	-0.492
108	A	-1.215	0.541	1.556	0.505	-0.998
109	R	-1.427	0.462	0.889	0.399	-1.385
110	L	-0.349	0.85	3.407	0.809	0.58
111	T	-1.216	0.529	1.306	0.494	-1
112	N	-1.523	0.455	0.877	0.44	-1.56
113	P	-1.149	0.584	1.667	0.551	-0.879
114	K	-1.427	0.467	1.469	0.421	-1.385
115	F	-1.311	0.477	1.852	0.497	-1.173
116	Q	-1.831	0.321	-0.222	0.292	-2.121
117	I	-1.003	0.611	2.531	0.549	-0.612
118	A	-0.684	0.691	2.716	0.623	-0.031
119	A	-0.349	0.798	3.235	0.793	0.58
120	Q	0	0.994	5	0.993	1.215
121	N	0	0.995	6	0.994	1.215
122	A	-0.687	0.669	3.568	0.649	-0.036
123	I	-0.849	0.723	4	0.666	-0.331
124	:	-1.074	0.596	1.234	0.506	-0.741
125	T	-1.149	0.532	0.827	0.465	-0.879
126	R	-1.523	0.408	0.654	0.38	-1.56
127	S	-1.369	0.453	1.358	0.446	-1.279
128	G	0	0.944	6	0.951	1.215
129	A	0	0.909	4	0.905	1.215
130	F	0	1.001	6	1.006	1.215
131	T	0	0.983	5	0.984	1.215
132	G	0	0.944	6	0.951	1.215
133	E	0	0.962	5	0.96	1.215
134	V	-1.149	0.559	2	0.478	-0.879

135	S	-0.349	0.873	3.235	0.84	0.58
136	L	-1.149	0.562	1.568	0.469	-0.879
137	Q	-1.465	0.391	0.741	0.375	-1.454
138	I	-0.684	0.811	3.235	0.744	-0.031
139	L	-0.937	0.601	2.914	0.557	-0.492
140	K	-0.349	0.849	3.605	0.848	0.58
141	D	-0.349	0.883	5.012	0.878	0.58
142	Y	-1.523	0.43	1.123	0.415	-1.56
143	G	0	0.944	6	0.951	1.215
144	I	-1.003	0.58	1.778	0.529	-0.612
145	S	-1.677	0.406	0.778	0.368	-1.841
146	W	0	1.013	11	1.013	1.215
147	V	0	0.93	4	0.93	1.215
148	V	-0.687	0.644	3.506	0.676	-0.036
149	L	0	0.963	4	0.959	1.215
150	G	0	0.944	6	0.951	1.215
151	H	0	1.017	8	1.017	1.215
152	S	0	0.979	4	0.977	1.215
153	E	0	0.962	5	0.96	1.215
154	R	0	0.999	5	1	1.215
155	R	0	0.999	5	1	1.215
156	L	-1.149	0.592	1.728	0.522	-0.879
157	Y	-1.273	0.484	1.827	0.463	-1.104
158	:	-1.216	0.529	1.306	0.494	-1
159	:	-1.216	0.529	1.306	0.494	-1
160	Y	-0.849	0.703	3.346	0.65	-0.331
161	G	-0.684	0.735	3.074	0.682	-0.031
162	E	0	0.962	5	0.96	1.215
163	T	-0.684	0.768	2.704	0.7	-0.031
164	N	-0.53	0.796	4.272	0.765	0.25
165	E	-1.149	0.546	1.605	0.484	-0.879
166	I	-1.149	0.577	1.642	0.508	-0.879
167	V	-0.53	0.762	3.654	0.726	0.25
168	A	-0.687	0.601	2.42	0.643	-0.036
169	E	-1.311	0.505	1.914	0.499	-1.173
170	K	0	0.962	5	0.966	1.215
171	V	-0.995	0.535	1.679	0.492	-0.598
172	A	-1.303	0.475	1.21	0.465	-1.159
173	Q	-1.149	0.638	3.346	0.569	-0.879
174	A	0	0.909	4	0.905	1.215
175	C	-0.349	0.861	3.074	0.824	0.58
176	A	-1.427	0.419	1.136	0.381	-1.385
177	:	-1.216	0.529	1.306	0.494	-1
178	A	-1.061	0.514	1.63	0.491	-0.718

179	G	-0.349	0.837	4.79	0.813	0.58
180	F	-1.003	0.642	2.444	0.566	-0.612
181	H	-0.937	0.592	1.444	0.573	-0.492
182	V	0	0.93	4	0.93	1.215
183	I	-0.349	0.858	3.802	0.849	0.58
184	V	-1.303	0.492	0.901	0.401	-1.159
185	C	0	1.017	9	1.018	1.215
186	V	-0.53	0.762	3.654	0.726	0.25
187	G	0	0.944	6	0.951	1.215
188	E	0	0.962	5	0.96	1.215
189	T	-0.965	0.592	1.333	0.598	-0.543
190	N	-0.349	0.859	2.642	0.819	0.58

191	E	-0.637	0.706	3.778	0.782	0.056
192	E	-0.349	0.857	4.407	0.85	0.58
193	R	-0.349	0.89	4.407	0.856	0.58
194	E	-0.349	0.853	4.21	0.816	0.58
195	A	-0.349	0.802	3.407	0.766	0.58
196	G	0	0.944	6	0.951	1.215
197	R	-1.677	0.414	-0.222	0.387	-1.841
198	T	0	0.983	5	0.984	1.215
199	A	-1.831	0.35	-0.062	0.283	-2.121
200	A	-1.311	0.452	0.988	0.454	-1.173
201	V	0	0.93	4	0.93	1.215
202	V	-0.684	0.726	1.84	0.692	-0.031
203	L	-1.273	0.497	0.395	0.44	-1.104
204	T	-1.215	0.533	1.309	0.562	-0.998
205	Q	0	0.994	5	0.993	1.215
206	L	-0.965	0.604	1.543	0.623	-0.543
207	A	-1.427	0.481	0.951	0.424	-1.385
208	A	-0.637	0.629	2.222	0.712	0.056
209	V	-1.149	0.562	2.407	0.491	-0.879
210	A	-1.003	0.581	1.852	0.507	-0.612
211	Q	-0.995	0.612	3.037	0.569	-0.598
212	K	-1.215	0.519	1.593	0.511	-0.998
213	L	-1.215	0.484	1.802	0.458	-0.998
214	S	-1.216	0.529	1.306	0.494	-1
215	K	-1.216	0.529	1.306	0.494	-1
216	E	-1.003	0.635	2.136	0.568	-0.612
217	A	-0.684	0.766	3.407	0.718	-0.031
218	W	0	1.013	11	1.013	1.215
219	S	-1.003	0.658	2.086	0.617	-0.612
220	R	-1.215	0.549	2	0.558	-0.998
221	V	-0.349	0.822	3.802	0.815	0.58
222	V	0	0.93	4	0.93	1.215

223	I	-1.099	0.495	2.667	0.518	-0.787
224	A	0	0.909	4	0.905	1.215
225	Y	0	1.013	7	1.011	1.215
226	E	0	0.962	5	0.96	1.215
227	P	0	0.995	7	0.997	1.215
228	V	0	0.93	4	0.93	1.215
229	W	0	1.013	11	1.013	1.215
230	A	0	0.909	4	0.905	1.215
231	I	0	0.971	4	0.97	1.215
232	G	0	0.944	6	0.951	1.215
233	T	0	0.983	5	0.984	1.215
234	G	0	0.944	6	0.951	1.215
235	K	-0.684	0.75	2.914	0.718	-0.031

236	V	-0.937	0.591	2.037	0.535	-0.492
237	A	0	0.909	4	0.905	1.215
238	T	-0.349	0.876	4.198	0.87	0.58
239	P	-0.349	0.884	5.21	0.88	0.58
240	Q	-1.215	0.53	2.185	0.514	-0.998
241	Q	-0.349	0.888	4.025	0.853	0.58
242	A	0	0.909	4	0.905	1.215
243	Q	-0.349	0.885	4.407	0.852	0.58
244	E	-0.684	0.753	3.852	0.689	-0.031
245	V	-0.349	0.822	3.802	0.788	0.58
246	H	0	1.017	8	1.017	1.215
247	E	-0.637	0.669	2.222	0.641	0.056
248	L	-1.677	0.389	-0.074	0.351	-1.841
249	L	-0.849	0.656	2.914	0.592	-0.331
250	R	0	0.999	5	1	1.215
251	R	-1.677	0.35	0.383	0.319	-1.841
252	W	-0.53	0.822	7.296	0.792	0.25
253	V	-0.349	0.85	3.407	0.808	0.58
254	R	-1.149	0.545	1.827	0.476	-0.879
255	S	-1.303	0.564	1.778	0.525	-1.159
256	K	-0.637	0.724	3.222	0.69	0.056
257	L	-1.149	0.516	2.173	0.471	-0.879
258	G	-0.849	0.673	2.296	0.656	-0.331
259	T	-1.215	0.555	1.42	0.532	-0.998
260	D	-1.677	0.333	0.543	0.319	-1.841
261	I	-0.684	0.707	3.012	0.633	-0.031
262	A	-0.349	0.802	3.407	0.796	0.58
263	A	-1.465	0.426	1.012	0.405	-1.454
264	Q	-1.003	0.651	2.099	0.575	-0.612
265	L	-0.637	0.713	2.222	0.68	0.056
266	R	0	0.999	5	1	1.215
267	I	0	0.971	4	0.97	1.215
268	L	-0.937	0.612	1.963	0.586	-0.492
269	Y	0	1.013	7	1.011	1.215
270	G	0	0.944	6	0.951	1.215
271	G	0	0.944	6	0.951	1.215
272	S	0	0.979	4	0.977	1.215
273	V	-0.349	0.815	3.21	0.776	0.58
274	T	-0.684	0.773	3.346	0.711	-0.031
275	A	-0.965	0.53	1.765	0.521	-0.543
276	K	-1.003	0.592	1.642	0.518	-0.612
277	N	-0.637	0.733	3.222	0.814	0.056
278	A	-0.687	0.669	3.568	0.65	-0.036
279	R	-1.303	0.523	1.593	0.429	-1.159
280	T	-0.849	0.666	2.272	0.596	-0.331

281	L	-0.349	0.859	3.235	0.823	0.58
282	Y	-1.003	0.59	1.383	0.52	-0.612
283	Q	-1.465	0.444	1.111	0.427	-1.454
284	M	-0.937	0.637	2.457	0.601	-0.492
285	R	-0.684	0.777	3.802	0.707	-0.031
286	D	-0.349	0.883	5.012	0.852	0.58
287	I	-0.687	0.637	3.506	0.638	-0.036
288	N	-0.349	0.883	5.012	0.847	0.58
289	G	0	0.944	6	0.951	1.215
290	F	0	1.001	6	1.006	1.215
291	L	0	0.963	4	0.959	1.215
292	V	0	0.93	4	0.93	1.215
293	G	0	0.944	6	0.951	1.215
294	G	0	0.944	6	0.951	1.215
295	A	0	0.909	4	0.905	1.215
296	S	0	0.979	4	0.977	1.215
297	L	-0.349	0.862	3.617	0.829	0.58
298	K	0	0.962	5	0.966	1.215
299	P	0	0.995	7	0.997	1.215
300	E	-0.684	0.752	3.309	0.713	-0.031
301	F	0	1.001	6	1.006	1.215
302	V	-0.684	0.715	3.259	0.678	-0.031
303	E	-0.849	0.682	3.469	0.628	-0.331
304	I	0	0.971	4	0.97	1.215
305	I	-0.349	0.858	3.802	0.824	0.58
306	E	-0.684	0.782	3.988	0.714	-0.031
307	A	-0.53	0.714	2.963	0.663	0.25
308	T	-1.465	0.462	1.062	0.457	-1.454
309	K	-1.427	0.502	1.519	0.451	-1.385
310	:	-1.216	0.529	1.306	0.494	-1
311	:	-1.216	0.529	1.306	0.494	-1
312	:	-1.216	0.529	1.306	0.494	-1
313	:	-1.216	0.529	1.306	0.494	-1
314	:	-1.216	0.529	1.306	0.494	-1
315	:	-1.216	0.529	1.306	0.494	-1
316	:	-1.216	0.529	1.306	0.494	-1

2)

For Condition 1

Highest Conservation Scores:

Position	Residue	Set 1
117	K	-1.846
113	T	-1.72
70	L	-1.673
73	S	-1.594
84	E	-1.414
133	G	-1.414
36	V	-1.367
35	V	-1.295
9	A	-1.169
6	K	-1.16

Position	Residue	Set 2
85	T	-1.889
116	Q	-1.831
199	A	-1.831
79	E	-1.735
75	V	-1.677
88	H	-1.677
101	L	-1.677
145	S	-1.677
197	R	-1.677
248	L	-1.677

Lowest Conservation Scores:

Position	Residue	Set 1
1	:	0
3	L	0
4	S	0
7	D	0
8	K	0
17	K	0
26	G	0
30	L	0
32	R	0
38	P	0

Position	Residue	Set 2
64	N	0
66	K	0
68	N	0
95	V	0
120	Q	0
121	N	0
128	G	0
129	A	0
130	F	0
131	T	0

3) and 4)

```
import numpy as np
```

```
def Que_3(strings_list):
    t, l = len(strings_list), len(strings_list[0])
    uwf = [[0 for __ in range(20)] for _ in range(l)]

    AA = {'A':1,'C':2,'D':3,'E':4,'F':5,'G':6,'H':7,'I':8,'K':9,'L':10,
           'M':11,'N':12,'P':13,'Q':14,'R':15,'S':16,'T':17,'V':18,'W':19,'Y':20}
```

```
AA_freq = [0]*20
```

```
blossum_62 = {
    ('W', 'F'): 1, ('L', 'R'): -2, ('S', 'P'): -1, ('V', 'T'): 0,
    ('Q', 'Q'): 5, ('N', 'A'): -2, ('Z', 'Y'): -2, ('W', 'R'): -3,
    ('Q', 'A'): -1, ('S', 'D'): 0, ('H', 'H'): 8, ('S', 'H'): -1,
    ('H', 'D'): -1, ('L', 'N'): -3, ('W', 'A'): -3, ('Y', 'M'): -1,
    ('G', 'R'): -2, ('Y', 'I'): -1, ('Y', 'E'): -2, ('B', 'Y'): -3,
    ('Y', 'A'): -2, ('V', 'D'): -3, ('B', 'S'): 0, ('Y', 'Y'): 7,
    ('G', 'N'): 0, ('E', 'C'): -4, ('Y', 'Q'): -1, ('Z', 'Z'): 4,
    ('V', 'A'): 0, ('C', 'C'): 9, ('M', 'R'): -1, ('V', 'E'): -2,
    ('T', 'N'): 0, ('P', 'P'): 7, ('V', 'I'): 3, ('V', 'S'): -2,
    ('Z', 'P'): -1, ('V', 'M'): 1, ('T', 'F'): -2, ('V', 'Q'): -2,
    ('K', 'K'): 5, ('P', 'D'): -1, ('I', 'H'): -3, ('I', 'D'): -3,
    ('T', 'R'): -1, ('P', 'L'): -3, ('K', 'G'): -2, ('M', 'N'): -2,
    ('P', 'H'): -2, ('F', 'Q'): -3, ('Z', 'G'): -2, ('X', 'L'): -1,
    ('T', 'M'): -1, ('Z', 'C'): -3, ('X', 'H'): -1, ('D', 'R'): -2,
    ('B', 'W'): -4, ('X', 'D'): -1, ('Z', 'K'): 1, ('F', 'A'): -2,
    ('Z', 'W'): -3, ('F', 'E'): -3, ('D', 'N'): 1, ('B', 'K'): 0,
    ('X', 'X'): -1, ('F', 'I'): 0, ('B', 'G'): -1, ('X', 'T'): 0,
    ('F', 'M'): 0, ('B', 'C'): -3, ('Z', 'I'): -3, ('Z', 'V'): -2,
    ('S', 'S'): 4, ('L', 'Q'): -2, ('W', 'E'): -3, ('Q', 'R'): 1,
    ('N', 'N'): 6, ('W', 'M'): -1, ('Q', 'C'): -3, ('W', 'I'): -3,
    ('S', 'C'): -1, ('L', 'A'): -1, ('S', 'G'): 0, ('L', 'E'): -3,
    ('W', 'Q'): -2, ('H', 'G'): -2, ('S', 'K'): 0, ('Q', 'N'): 0,
    ('N', 'R'): 0, ('H', 'C'): -3, ('Y', 'N'): -2, ('G', 'Q'): -2,
    ('Y', 'F'): 3, ('C', 'A'): 0, ('V', 'L'): 1, ('G', 'E'): -2,
    ('G', 'A'): 0, ('K', 'R'): 2, ('E', 'D'): 2, ('Y', 'R'): -2,
    ('M', 'Q'): 0, ('T', 'I'): -1, ('C', 'D'): -3, ('V', 'F'): -1,
    ('T', 'A'): 0, ('T', 'P'): -1, ('B', 'P'): -2, ('T', 'E'): -1,
    ('V', 'N'): -3, ('P', 'G'): -2, ('M', 'A'): -1, ('K', 'H'): -1,
    ('V', 'R'): -3, ('P', 'C'): -3, ('M', 'E'): -2, ('K', 'L'): -2,
    ('V', 'V'): 4, ('M', 'I'): 1, ('T', 'Q'): -1, ('I', 'G'): -4,
    ('P', 'K'): -1, ('M', 'M'): 5, ('K', 'D'): -1, ('I', 'C'): -1,
```

```

('Z', 'D'): 1, ('F', 'R'): -3, ('X', 'K'): -1, ('Q', 'D'): 0,
('X', 'G'): -1, ('Z', 'L'): -3, ('X', 'C'): -2, ('Z', 'H'): 0,
('B', 'L'): -4, ('B', 'H'): 0, ('F', 'F'): 6, ('X', 'W'): -2,
('B', 'D'): 4, ('D', 'A'): -2, ('S', 'L'): -2, ('X', 'S'): 0,
('F', 'N'): -3, ('S', 'R'): -1, ('W', 'D'): -4, ('V', 'Y'): -1,
('W', 'L'): -2, ('H', 'R'): 0, ('W', 'H'): -2, ('H', 'N'): 1,
('W', 'T'): -2, ('T', 'T'): 5, ('S', 'F'): -2, ('W', 'P'): -4,
('L', 'D'): -4, ('B', 'I'): -3, ('L', 'H'): -3, ('S', 'N'): 1,
('B', 'T'): -1, ('L', 'L'): 4, ('Y', 'K'): -2, ('E', 'Q'): 2,
('Y', 'G'): -3, ('Z', 'S'): 0, ('Y', 'C'): -2, ('G', 'D'): -1,
('B', 'V'): -3, ('E', 'A'): -1, ('Y', 'W'): 2, ('E', 'E'): 5,
('Y', 'S'): -2, ('C', 'N'): -3, ('V', 'C'): -1, ('T', 'H'): -2,
('P', 'R'): -2, ('V', 'G'): -3, ('T', 'L'): -1, ('V', 'K'): -2,
('K', 'Q'): 1, ('R', 'A'): -1, ('I', 'R'): -3, ('T', 'D'): -1,
('P', 'F'): -4, ('I', 'N'): -3, ('K', 'I'): -3, ('M', 'D'): -3,
('V', 'W'): -3, ('W', 'W'): 11, ('M', 'H'): -2, ('P', 'N'): -2,
('K', 'A'): -1, ('M', 'L'): 2, ('K', 'E'): 1, ('Z', 'E'): 4,
('X', 'N'): -1, ('Z', 'A'): -1, ('Z', 'M'): -1, ('X', 'F'): -1,
('K', 'C'): -3, ('B', 'Q'): 0, ('X', 'B'): -1, ('B', 'M'): -3,
('F', 'C'): -2, ('Z', 'Q'): 3, ('X', 'Z'): -1, ('F', 'G'): -3,
('B', 'E'): 1, ('X', 'V'): -1, ('F', 'K'): -3, ('B', 'A'): -2,
('X', 'R'): -1, ('D', 'D'): 6, ('W', 'G'): -2, ('Z', 'F'): -3,
('S', 'Q'): 0, ('W', 'C'): -2, ('W', 'K'): -3, ('H', 'Q'): 0,
('L', 'C'): -1, ('W', 'N'): -4, ('S', 'A'): 1, ('L', 'G'): -4,
('W', 'S'): -3, ('S', 'E'): 0, ('H', 'E'): 0, ('S', 'I'): -2,
('H', 'A'): -2, ('S', 'M'): -1, ('Y', 'L'): -1, ('Y', 'H'): 2,
('Y', 'D'): -3, ('E', 'R'): 0, ('X', 'P'): -2, ('G', 'G'): 6,
('G', 'C'): -3, ('E', 'N'): 0, ('Y', 'T'): -2, ('Y', 'P'): -3,
('T', 'K'): -1, ('A', 'A'): 4, ('P', 'Q'): -1, ('T', 'C'): -1,
('V', 'H'): -3, ('T', 'G'): -2, ('I', 'Q'): -3, ('Z', 'T'): -1,
('C', 'R'): -3, ('V', 'P'): -2, ('P', 'E'): -1, ('M', 'C'): -1,
('K', 'N'): 0, ('I', 'I'): 4, ('P', 'A'): -1, ('M', 'G'): -3,
('T', 'S'): 1, ('I', 'E'): -3, ('P', 'M'): -2, ('M', 'K'): -1,
('I', 'A'): -1, ('P', 'I'): -3, ('R', 'R'): 5, ('X', 'M'): -1,
('L', 'I'): 2, ('X', 'I'): -1, ('Z', 'B'): 1, ('X', 'E'): -1,
('Z', 'N'): 0, ('X', 'A'): 0, ('B', 'R'): -1, ('B', 'N'): 3,
('F', 'D'): -3, ('X', 'Y'): -1, ('Z', 'R'): 0, ('F', 'H'): -1,
('B', 'F'): -3, ('F', 'L'): 0, ('X', 'Q'): -1, ('B', 'B'): 4
}

```

```

for i in range(l):
    for i1 in range(t):
        if strings_list[i1][i].isalpha():
            uwf[i][AA[str(strings_list[i1][i])]-1] += 1

```

```

        AA_freq[AA[str(strings_list[i1][i])]-1] += 1
    uwf = np.divide(uwf,t)
    AA_freq = np.divide(AA_freq, t * l)

entropy, variance, sum_of_pairs = [0]*l, [0]*l, [0]*l

for j in range(l):
    for j1 in range(20):
        if uwf[j][j1] == 0:
            entropy[j] += 0
        else:
            entropy[j] += uwf[j][j1]*(np.log(uwf[j][j1]))
    variance[j] += (uwf[j][j1] - AA_freq[j1])**2
    for j2 in range(20):
        p = (list(AA.keys())[list(AA.values()).index(j1+1)],
             list(AA.keys())[list(AA.values()).index(j2+1)])
        if p not in blossom_62:
            p = (list(AA.keys())[list(AA.values()).index(j2+1)],
                 list(AA.keys())[list(AA.values()).index(j1+1)])
        sum_of_pairs[j] += uwf[j][j1] * uwf[j][j2] * blossom_62[p]

for k in range(l):
    variance[k] = variance[k]**0.5
    sum_of_pairs[k] = sum_of_pairs[k]**0.5

return [entropy, variance, sum_of_pairs]

class Que_4():
    A =
    ['-----MAAQIPESDQIKQFK-----EFLGTYNKLTETCFLDCVKD-FTTREVKPEETTCSEHCLQK
YLKMTQRISMRFQEYHIQQNEALAAKAGLLGQPR----',
     '-----MAAQIPESDQIKQFK-----EFLGTYNKLTETCFLDCVKD-FTTREVKPEEVTCSEHCLQK
YLKMTQRISVRFQEYHIQQNEALAAKAGLLGQPR----',
     '---02-----MTSEQNIQTFR-----DFLTQYNLVAEQCFNCSVNE-FGSRTVSGKEESCANNCLD
KFLKMTQRVSQRFQEHLNAQANGAAIKVENGGKINKIQ',
     '---MSFLGFGGGQPQLSSQQKIQAAE--AELDLVTDMFNKLVNNCYKKCINTSYSEGELNKNESS
CLDRCVAKYFETNVQVGENMQKMGQSFNAAG---KF-----',
     'MDSYSSPPMGGSGSSVSPEVMMESVKTQLAQAYAEELIETLRTKCFDKCVTKP--GSSLGGSE
SSCISRCVERYMEATAIISRSLFTQR-----']

```

B =

[M---SFLFGGGQPQLSSQQKIQAAEAELDL--VTDMFNKLVNNCYKKCINTSYSEGELNKNESS
 CLDRCVAKYFETNVQVGENM--QKM---GQSFNA----AGKF----',

'MDSYSSPPMGGSGSSVSPEVMMESVKTQLAQAYAELIETLRTKCFDKCVTKPGS--SLGGSE
 SSCISRCVERYMEATAIISRSLFTQR-----',

'M-----AAQIPESDQIKQFKEFLGT-----YNKLTETCFLDCVKDFTR-EVKPEETTCSEHCLQK
 YLKMTQRISMRF--QEYHIQQNEALAA----KAGLLGQPR',

'M-----AAQIPESDQIKQFKEFLGT-----YNKLTETCFLDCVKDFTR-EVKPEEVTCSEHCLQK
 YLKMTQRISVRF--QEYHIQQNEALAA----KAGLLGQPR',

'M-----TSEQNIQTFRDFLTQ-----YNLVAEQCFNSCVNEFSR-TVSGKEESCANNCLDKF
 LKMTQRVSQRF--QEHQQLNAQANGAAIKVENGGKINKIQ']

C =

[--MSFLFGGGQPQLSSQQKIQAAEAELDL--VTDMFNKLVNNCYKKCINTSYSEGELNKNESS
 CLDRCVAKYFETNVQVGENMQKMGQSFNAAGKF-----',

'MDSYSSPPMGGSGSSVSPEVMMESVKTQLAQAYAELIETLRTKCFDKCVT-KPGS-SLGGSE
 SSCISRCVERYMEATAIISRSLFTQR-----',

'-----MAAQIPESDQIKQFKEFLGT-----YNKLTETCFLDCVK-DFTTREVKPEETTCSEHCLQK
 YLKMTQRISMRFQEYHIQQNEALAA----KAGLLGQPR',

'-----MAAQIPESDQIKQFKEFLGT-----YNKLTETCFLDCVK-DFTTREVKPEEVTCSEHCLQK
 YLKMTQRISVRFQEYHIQQNEALAA----KAGLLGQPR',

'-----MTSEQNIQTFRDFLTQ-----YNLVAEQCFNSCVN-EFGSRTVSGKEESCANNCLDKF
 LKMTQRVSQRFQEHQQLNAQANGAAIKVENGGKINKIQ']

```

def part_1(self, x, y, z):
    similar, dissimilar = [], []
    for i in range(len(x)):
        if x[i] == y[i] == z[i]:
            similar.append((i, x[i]))
        elif x[i] != y[i] != z[i]:
            dissimilar.append((i, x[i], y[i], z[i]))

results = f"\tSimilar:\n\t\tTotal number of scores: {len(similar)}\n" \
    f"\t\tSimilar residues (format: position, common conservation score)\n\t\t{similar}\n" \
    + \
    f"\n\tDissimilar:\n\t\tTotal number of scores: {len(dissimilar)}\n"

```

```

f"\t\tDissimilar residues (format: position, conservation scores (in the order Clustal
Omega, MAFFT, MUSCLE))\n\t\t{dissimilar}"
print(results)

def part_2(self):
    Co_entropy, Co_variance, Co_sum_of_pairs = Que_3(self.A)
    MAFFT_entropy, MAFFT_variance, MAFFT_sum_of_pairs = Que_3(self.B)
    MUSCLE_entropy, MUSCLE_variance, MUSCLE_sum_of_pairs = Que_3(self.C)

    print(f"\nComparison of \033[1mentropy\033[0m based conservation scores (all alignments:
Clustal Omega, MAFFT, MUSCLE):")
    self.part_1(Co_entropy, MAFFT_entropy, MUSCLE_entropy)

    print(f"\nComparison of \033[1mvariance\033[0m based conservation scores (all
alignments: Clustal Omega, MAFFT, MUSCLE):")
    self.part_1(Co_variance, MAFFT_variance, MUSCLE_variance)

    print(f"\nComparison of \033[1msum of all pairs\033[0m based conservation scores (all
alignments: Clustal Omega, MAFFT, MUSCLE):")
    self.part_1(Co_sum_of_pairs, MAFFT_sum_of_pairs, MUSCLE_sum_of_pairs)

if __name__ == "__main__":
    s = ['AAANWKCNGSESLLVPLIETLNAATFDHD--VQCVVAPTFHLIPMTKARLTNPKFQIAAQ',
        '--NWKCNLSKADIAELVSAFNAAPPIDAAHVQVVVAPPAYLDSTRQAL-RADFDTSAQ',
        'VGGNFKLNGSKQSIKEIVERLNTASIPEN--VEVICPPATYLDYSVSLVKKPQVTVGAAQ',
        'VGGNWKCNGTTDQVEKIVKTLNEGQVPPSDVVEVVVSPPYVFLPVVSQL-RQEFHVAAQ',
        'VGGNWKMNGDYASVDGIVTFLNASADNSS--VDVVVAPPAPLAYAKSKL-KAGVLVAAQ',]
    entropy, variance, sum_of_pairs = Que_3(s)

    print(f"Entropy of each position in alignment:\n")
    for d in range(len(entropy)):
        if d % 4 == 0 and d != 0:
            print(f"{entropy[d]}", end="\n")
        elif d == len(entropy) - 1:
            print(f"{entropy[d]}\n")
        else:
            print(f"{entropy[d]}\t", end="")

    print(f"Variance of each position in alignment:\n")
    for d1 in range(len(variance)):
        if d1 % 4 == 0 and d1 != 0:
            print(f"{variance[d1]}", end="\n")

```

```

        elif d1 == len(variance) - 1:
            print(f"{variance[d1]}\n")
        else:
            print(f"{variance[d1]},{t", end="")

    print(f"Sum of all pairs for each position in alignment:\n")
    for d2 in range(len(sum_of_pairs)):
        if d2 % 4 == 0 and d2 != 0:
            print(f"{sum_of_pairs[d2]},", end="\n")
        elif d2 == len(sum_of_pairs) - 1:
            print(f"{sum_of_pairs[d2]}\n")
        else:
            print(f"{sum_of_pairs[d2]},{t", end="")

call = Que_4()
call.part_2()

```

Output:

Entropy of each position in alignment:

```

-0.6283829567464145,      -0.6283829567464145,      -0.6283829567464145,      0.0,
-0.5004024235381879,
0.0,      -0.9502705392332347,      0.0,      -0.5004024235381879,
-0.9502705392332347,      -1.3321790402101223,      -1.3321790402101223,
-1.3321790402101223,
-1.0549201679861442,      -1.6094379124341005,      -1.3321790402101223,
-0.6730116670092565,
-0.5004024235381879,      -1.3321790402101223,      -1.3321790402101223,
-0.5004024235381879,
0.0,      -0.9502705392332347,      -0.9502705392332347,      -1.6094379124341005,
-1.6094379124341005,      -1.3321790402101223,      -1.6094379124341005,
-1.3321790402101223,
-0.6437751649736402,      -0.6437751649736402,      0.0,      -1.0549201679861442,
-0.5004024235381879,      0.0,      -0.5004024235381879,      -0.9502705392332347,
0.0,      -0.5004024235381879,      -0.9502705392332347,      -1.3321790402101223,
-0.9502705392332347,      -0.5004024235381879,      -1.0549201679861442,
-1.3321790402101223,
-1.3321790402101223,      -0.9502705392332347,      -0.9502705392332347,
-1.6094379124341005,
-0.5004024235381879,      -0.6437751649736402,      -1.0549201679861442,
-1.0549201679861442,
-1.6094379124341005,      -0.6730116670092565,-1.6094379124341005,
-0.9502705392332347,
-0.9502705392332347,      0.0,      0.0

```

Variance of each position in alignment:

0.5057228050578257, 0.6031215097768903, 0.6031215097768903, 0.9735273779178248,
0.8452350100547317,
0.973527377917825, 0.6760834925428137, 0.9735273779178248, 0.8031742581089668,
0.6280304309682948, 0.5070393366287165, 0.43330769154903714,
0.48002314759001175,
0.5109685791600975, 0.3282614134429382, 0.4990880572493083, 0.6983949853453671,
0.7172323348972928, 0.500422044100999, 0.4937160677510461, 0.7897819670994999,
0.9735273779178248, 0.5748236444529942, 0.5654693232665726, 0.3592894221778438,
0.3756180092712394, 0.48691774345251465, 0.4208193066969348, 0.4543371239753827,
0.2847611084556473, 0.29623564193991847, 0.8913036644276866, 0.582885542414251,
0.7227878127239158, 0.8913036644276866, 0.7172323348972928, 0.5759822528130146,
0.9666551723454555, 0.7889374006993346, 0.5851685417229999, 0.4063113201584333,
0.6800163396729686, 0.7880919292118711, 0.5376698697982704, 0.49640932930619086,
0.4271091455614387, 0.6119005002630921, 0.6031215097768903, 0.3756180092712394,
0.762291865946954, 0.32417416443771224, 0.5851685417229999, 0.5083524586566118,
0.4144340183377271, 0.6651482708556208, 0.4208193066969348, 0.5571554740126154,
0.5654693232665726, 0.9098107251266913, 0.9837456762576167

Sum of all pairs for each position in alignment:

1.2649110640673518, 1.5231546211727818, 1.5231546211727818, 2.449489742783178,
2.7568097504180447,
2.23606797749979, 1.8110770276274832, 2.449489742783178, 1.6492422502470645,
1.42828568570857, 0.8717797887081349, 0.9591663046625439, 0.66332495807108,
1.6970562748477143, 0.4898979485566357, 0.8944271909999159, 1.7435595774162693,
1.9183326093250879, 1.1661903789690602, 0.66332495807108, 1.6733200530681513,
2.449489742783178, 1.232882800593795, 1.4422205101855958, 0.8246211251235323,
nan, 0.6324555320336759, 0.8944271909999159, 1.1661903789690602,
0.48989794855663565, 0.48989794855663565, 2.0, 1.6733200530681513,
1.61245154965971, 2.0, 1.9183326093250879, 1.4560219778561037,
2.6457513110645907, 2.08806130178211, 1.1135528725660044, 0.8485281374238571,
2.04939015319192, 1.8330302779823362, 1.2000000000000002, 0.9165151389911681,
1.1661903789690602, 1.3856406460551018, 1.4, 0.66332495807108,
1.7435595774162698, 0.5656854249492381, 1.5748015748023623, 1.1489125293076057,
0.9591663046625439, 1.5231546211727818, nan, 1.5620499351813308,
1.4422205101855958, 2.0, 2.23606797749979

Comparison of **entropy** based conservation scores (all alignments: Clustal Omega, MAFFT, MUSCLE):

Similar:

Total number of scores: 28

Similar residues (format: position, common conservation score)

$[(1, -0.3218875824868201), (2, -0.3218875824868201), (4, -0.366516292749662), (5, -0.6437751649736402), (6, -0.6437751649736402), (7, -0.6437751649736402), (8, -0.6437751649736402), (9, -0.366516292749662), (10, -0.366516292749662), (12, -1.0102914577233022), (13, -1.0102914577233022), (14, -0.6283829567464145), (20, -1.3321790402101223), (23, -1.3321790402101223), (25, -0.9502705392332347), (39, -0.9502705392332347), (40, -0.5004024235381879), (41, -1.3321790402101223), (43, -1.3321790402101223), (46, -1.3321790402101223), (47, -1.0549201679861442), (59, -1.3321790402101223), (63, -1.3321790402101223), (67, -1.3321790402101223), (68, -1.0549201679861442), (71, -1.3321790402101223), (73, -0.5004024235381879), (89, -1.0102914577233022)]$

Dissimilar:

Total number of scores: 28

Dissimilar residues (format: position, conservation scores (in the order Clustal Omega, MAFFT, MUSCLE))

$[(0, -0.3218875824868201, 0.0, -0.3218875824868201), (3, -0.6437751649736402, -0.3218875824868201, -0.6437751649736402), (11, -1.0102914577233022, -0.6437751649736402, -1.0102914577233022), (52, -0.9656627474604602, -0.9502705392332347, -1.3321790402101223), (53, -1.0102914577233022, -1.0549201679861442, -0.9502705392332347), (54, -0.688403875236482, -0.6730116670092565, -1.0549201679861442), (55, -1.3321790402101223, -0.6283829567464145, -1.0549201679861442), (56, -1.0549201679861442, -0.3218875824868201, -0.6283829567464145), (85, -0.9502705392332347, -0.3218875824868201, -0.5004024235381879), (86, -1.3321790402101223, -0.3218875824868201, -0.9502705392332347), (87, -1.0549201679861442, 0.0, -1.3321790402101223), (88, -1.3321790402101223, -0.9502705392332347, -1.3321790402101223), (90, -0.6283829567464145, -0.688403875236482, -1.0102914577233022), (91, -1.0102914577233022, -0.688403875236482, -1.0102914577233022), (92, -0.6283829567464145, -0.688403875236482, -0.6283829567464145), (93, -1.0102914577233022, -0.688403875236482, -1.0102914577233022), (94, -0.17851484105136778, -1.0102914577233022, -0.17851484105136778), (95, -1.0102914577233022, -0.733032585499324, -1.0102914577233022), (96, -0.30649537425959444, -0.6283829567464145, -1.0102914577233022), (97, -0.688403875236482, -1.0102914577233022, -0.6283829567464145), (98, -0.688403875236482, -1.0102914577233022, -0.3218875824868201), (99, -0.30649537425959444, -0.17851484105136778, -0.3218875824868201), (103, -0.688403875236482, -0.3218875824868201, -0.688403875236482), (104, -0.688403875236482, -0.3218875824868201, -0.688403875236482), (106, -0.688403875236482, -0.6283829567464145, -0.688403875236482), (107, -0.3218875824868201, -0.17851484105136778, -0.688403875236482), (108, -0.3218875824868201, -0.733032585499324, -0.688403875236482), (109, -0.3218875824868201, -1.0102914577233022, -0.688403875236482)]$

Comparison of **variance** based conservation scores (all alignments: Clustal Omega, MAFFT, MUSCLE):

Similar:

Total number of scores: 0

Similar residues (format: position, common conservation score)

[]

Dissimilar:

Total number of scores: 112

Dissimilar residues (format: position, conservation scores (in the order Clustal Omega, MAFFT, MUSCLE))

[(0, 0.26011428022219424, 0.9909252759070775, 0.26079988809938753), (1, 0.26420124132631806, 0.26258416991731715, 0.2648762706916386), (2, 0.23102754054397048, 0.22980447213658295, 0.23179919617405662), (3, 0.3136458583973267, 0.2625841699173172, 0.3142146835317197), (4, 0.38426480293608756, 0.3841183899779295, 0.38472923158067035), (5, 0.27609937947583074, 0.2756229129640996, 0.27674538876751253), (6, 0.2948646351484432, 0.29409914304582613, 0.29546961928152166), (7, 0.3055711447270438, 0.3046474936938978, 0.30615497276206177), (8, 0.3008597374735494, 0.3000051297396661, 0.30145269030114147), (9, 0.4041951564402967, 0.4037146690553426, 0.4046367103303144), (10, 0.4041951564402967, 0.4037146690553426, 0.4046367103303144), (11, 0.4611501260712288, 0.2743469259256438, 0.46153719420286493), (12, 0.4389298791099898, 0.4387017417574167, 0.4385228567798575), (13, 0.4517610100529722, 0.4520940640866618, 0.45215611580650383), (14, 0.5761468155437679, 0.5750694151631425, 0.5745950215373522), (15, 0.46423763487318975, 0.4628321555228239, 0.4929671202348621), (16, 0.5403194916539885, 0.5583524548482134, 0.5582006898993244), (17, 0.4657737144378421, 0.5326230265360575, 0.5319930278045504), (18, 0.4372995167467474, 0.5138464416432328, 0.5128514225705659), (19, 0.48234784002368064, 0.5570942066321426, 0.5569195981248193), (20, 0.44779077886067853, 0.4605522131398444, 0.4599869674285149), (21, 0.6356791723850024, 0.8101350920332968, 0.8103011848714538), (22, 0.4453916529188619, 0.517249395861645, 0.5163216150850957), (23, 0.45412648826834445, 0.44426512233433935, 0.4433824649262549), (24, 0.4711105529079395, 0.626465656058647, 0.6263403993982565), (25, 0.5974488706669588, 0.6048078633370473, 0.6042842367425367), (26, 0.28501029340523615, 0.46055221313984446, 0.4599869674285149), (27, 0.2812259059974412, 0.61000683686989, 0.6095801917747014), (28, 0.2721911280774626, 0.9585275205724015, 0.9581318185054983), (29, 0.26420124132631806, 0.482867448278465, 0.48271791103361084), (30, 0.2601142802221943, 0.5279914844906832, 0.5272727772535324), (31, 0.29847614679247253, 0.24025481496887402, 0.24234452200728362), (32, 0.4340204194387586, 0.2625841699173172, 0.2648762706916386), (33, 0.4572614243560041, 0.28807209863238187, 0.2893628644918673), (34, 0.4603750135066243, 0.26391703370023584, 0.2648762706916386), (35, 0.477884635126299, 0.284394568957584, 0.28563615003021176), (36, 0.5455817434404402, 0.28807209863238187, 0.2893628644918673), (37, 0.5005163150514207, 0.6490232261218026, 0.6492980904053866), (38, 0.6116273458602727, 0.7908487051018939, 0.7906702465475165), (39, 0.6133766113465191, 0.6019001409075262, 0.6013218856852639), (40, 0.778149459700804, 0.7796780198980983, 0.7792960258581892), (41, 0.4748858616895781, 0.4792204092869287, 0.4790043351173604), (42, 0.458041805863141, 0.5978055694979308, 0.5971499059734345), (43, 0.46500630893240447, 0.4582609277148925, 0.457651781446576), (44, 0.795847802340244, 0.9838179784453115, 0.9838783368042276), (45, 0.6254845060806373, 0.8009881554920367, 0.8009918914721184), (46, 0.47186803110139836, 0.47035215322729473, 0.46997204649829544), (47, 0.5610724515767703, 0.5539360821730895, 0.553703901199984), (48, 0.803440465518543, 0.9838179784453115, 0.9838783368042276), (49, 0.6294687183227923, 0.8040486962493562, 0.8041069644046629), (50, 0.4680683819743453, 0.545639419503144, 0.5452543405772827), (51, 0.4904248990749277, 0.4770188020605024, 0.24234452200728362), (52, 0.33028474110088957, 0.62814367892934, 0.47148944412188837), (53, 0.4549122476491752, 0.5596078739679742, 0.6409943248499131), (54, 0.4146626979380042, 0.6645163844771135,

0.5445989443655594), (55, 0.4626964557937327, 0.61000683686989, 0.5272727772535324), (56, 0.5585205037070927, 0.24602722137923588, 0.6188833344279462), (57, 0.6495730544451676, 0.590125996635635, 0.5893235918562632), (58, 0.5546705677927307, 0.6827469727119314, 0.6825494300706696), (59, 0.4642376348731898, 0.45978972002649615, 0.45920989154176106), (60, 0.49621655287478955, 0.5689352233747087, 0.568973520778374), (61, 0.5235341538085951, 0.44347462671136056, 0.4425762357942369), (62, 0.7661234581066062, 0.9474821244307083, 0.9468833139326523), (63, 0.4556966521442858, 0.45209406408666175, 0.4513655584412027), (64, 0.5269339985002963, 0.6645163844771135, 0.6639832260605654), (65, 0.795847802340244, 0.9838179784453115, 0.9838783368042276), (66, 0.6045796735192583, 0.45902596032912873, 0.4584314984547967), (67, 0.46115012607122885, 0.4597897200264962, 0.45920989154176106), (68, 0.5878065852239605, 0.5913139611721776, 0.5917427133269241), (69, 0.803440465518543, 0.9838179784453115, 0.9838783368042276), (70, 0.5514417559489685, 0.6760330034323495, 0.6757129643599282), (71, 0.4485876361949121, 0.45364363938484187, 0.4529452933583814), (72, 0.6075261395232978, 0.7810269379926112, 0.7806696824273534), (73, 0.8201581791188273, 0.8153158406258136, 0.8155730738416456), (74, 0.4665398576493869, 0.6151618734135698, 0.6148305308234563), (75, 0.5255766997755311, 0.6560136851187606, 0.6553206490423025), (76, 0.4801214238426078, 0.635363902339777, 0.6353981958952503), (77, 0.6133766113465191, 0.7877368809822145, 0.787502024616769), (78, 0.46653985764938694, 0.600733111671556, 0.6001328509384487), (79, 0.48308769854944134, 0.6325966459495379, 0.6325815668951398), (80, 0.6328637939024898, 0.7005032706962037, 0.700623810964055), (81, 0.6092871797001302, 0.7742588469501916, 0.7737770139691014), (82, 0.48603587043235685, 0.3795236034681007, 0.379118539967302), (83, 0.5527355440286549, 0.6314863479875675, 0.6314513974542607), (84, 0.47111055290793946, 0.626465656058647, 0.6263403993982564), (85, 0.6063492712748241, 0.24744928378468276, 0.768683110579253), (86, 0.4469925009643533, 0.24025481496887408, 0.5905343913329171), (87, 0.5610724515767704, 0.9493319482907718, 0.5079533262344613), (88, 0.5026524035310188, 0.5978055694979308, 0.5037170508796965), (89, 0.47337935126500996, 0.49506645732503374, 0.4489855345154024), (90, 0.5761468155437679, 0.4513172812960188, 0.41681034937599476), (91, 0.4282215834002251, 0.43468430646984096, 0.43607274482075836), (92, 0.6045796735192583, 0.399345417002174, 0.6078200005439311), (93, 0.42988637559053605, 0.4088961485832977, 0.41681034937599476), (94, 0.772159871624354, 0.45595812824449045, 0.7723910992522388), (95, 0.4307163586777882, 0.49718815384746884, 0.4433824649262549), (96, 0.5804697692914115, 0.5930914464355611, 0.4425762357942368), (97, 0.4257121883936832, 0.44426512233433935, 0.6001328509384486), (98, 0.4155230905443285, 0.4513172812960188, 0.24234452200728362), (99, 0.5804697692914115, 0.7724440073796811, 0.25804652720794685), (100, 0.4453916529188619, 0.24025481496887402, 0.234860466608389), (101, 0.4485876361949121, 0.25581570389900216, 0.2538604992140851), (102, 0.4077141981179203, 0.23283815019429985, 0.2255520438608259), (103, 0.4340204194387586, 0.25166726287589974, 0.41766631784383157), (104, 0.39526050567560983, 0.2236136799708682, 0.42445192752007876), (105, 0.4549122476491752, 0.41738903218209195, 0.588110299595064), (106, 0.4421725699686188, 0.5995638098489936, 0.40815194499607815), (107, 0.24744871659990234, 0.7796780198980984, 0.42192011285627645), (108, 0.23409890200162697, 0.5124789330474788, 0.4327843526727455), (109, 0.25873761431462666, 0.448196687685853, 0.399305839002167), (110, 0.2503186744421757, 0.43225592319050044,

0.45920989154176106), (111, 0.23409890200162697, 0.399345417002174, 0.43113075103707915)]

Comparison of **sum of all pairs** based conservation scores (all alignments: Clustal Omega, MAFFT, MUSCLE):

Similar:

Total number of scores: 13

Similar residues (format: position, common conservation score)

[(1, 0.48989794855663565), (2, 0.4), (4, 0.8), (5, 0.48989794855663565), (6, 0.4472135954999579), (7, 0.6000000000000001), (8, 0.66332495807108), (9, 0.9797958971132713), (10, 0.9797958971132713), (12, 0.8717797887081347), (13, 1.0), (14, 1.4), (63, 0.8944271909999161)]

Dissimilar:

Total number of scores: 33

Dissimilar residues (format: position, conservation scores (in the order Clustal Omega, MAFFT, MUSCLE))

[(0, 0.447213595499958, 2.23606797749979, 0.447213595499958), (3, 0.6324555320336759, 0.5291502622129182, 0.6324555320336759), (11, 0.7483314773547883, 0.6324555320336759, 0.7483314773547883), (46, nan, nan, nan), (51, 0.692820323027551, 1.2165525060596438, 0.447213595499958), (52, 0.7211102550927979, 1.0392304845413265, 1.32664991614216), (53, 1.131370849898476, 0.7745966692414834, 1.4966629547095767), (54, 1.0583005244258363, 1.6492422502470643, 1.2000000000000002), (55, 0.2000000000000001, 1.414213562373095, 1.3416407864998738), (56, 1.0583005244258363, 0.48989794855663565, 1.2489995996796797), (85, 1.2328828005937953, 0.48989794855663565, 1.5748015748023623), (86, 0.692820323027551, 0.447213595499958, 1.4560219778561037), (87, 1.2806248474865698, 2.23606797749979, 1.2961481396815722), (88, 1.131370849898476, 1.61245154965971, 1.1661903789690602), (89, 0.447213595499958, 1.2806248474865698, 0.8246211251235321), (90, 1.4, 1.216552506059644, 0.8), (91, 0.6324555320336759, 1.0583005244258363, 0.7483314773547883), (92, 1.2649110640673518, 0.8, 1.3564659966250538), (93, 0.938083151964686, 1.019803902718557, 1.1135528725660044), (94, 1.6, 1.019803902718557, 1.6), (95, nan, 1.4966629547095767, 0.0), (96, 1.2, 1.3564659966250538, 0.8717797887081347), (97, 0.7483314773547883, 0.6324555320336759, 1.0954451150103321), (98, 0.8485281374238571, 0.8944271909999161, 0.4), (99, 1.2, 1.6, 0.4), (100, 0.959166304662544, 0.4, 0.447213595499958), (103, 0.8, 0.4, 1.019803902718557), (104, 1.148912529307606, 0.447213595499958, 0.938083151964686), (106, 0.8485281374238571, 1.296148139681572, 0.7211102550927979), (107, 0.48989794855663565, 1.9595917942265426, 1.0583005244258363), (108, 0.447213595499958, 0.894427190999916, 1.0954451150103324), (109, 0.4, 1.1661903789690602, 1.077032961426901), (110, 0.48989794855663565, 1.0954451150103324, 0.8944271909999159)]

5)

5th Set - 1

Position

C'

9 A, S, T, T, A, S, T, T, G, T, T

$$f(A) = \frac{2}{11}, f(S) = \frac{2}{11}, f(T) = \frac{6}{11}, f(G) = \frac{1}{11}$$

$$= 0.182 \quad = 0.182 \quad = 0.55 \quad = 0.091$$

$$\begin{aligned} C' &= (0.182) \ln(0.182) + (0.182) \ln(0.182) + (0.545) \ln(0.545) \\ &\quad + (0.091) \ln(0.091) \\ &= 2(0.182 \times (-1.704)) + (0.545 \times (-0.607)) + \\ &\quad (0.091 \times (-2.397)) \\ &= -1.1692 \end{aligned}$$

$$= -1.1692$$

11 U, V, I, I, V, I, V, V, V, V

$$f(I) = \frac{3}{11}, f(V) = \frac{8}{11}$$

$$= 0.273 \quad = 0.727$$

$$\begin{aligned} C' &= (0.273 \times \ln(0.273)) + (0.727 \times \ln(0.727)) \\ &= (-0.273 \times -1.298) + (0.727 \times -0.319) \\ &= -0.5863 \end{aligned}$$

20 K, S, G, G, G, G, G, G, G, A, A

$$f(K) = \frac{1}{11}, f(S) = \frac{1}{11}, f(A) = \frac{2}{11}, f(G) = \frac{7}{11}$$

$$= 0.091 \quad = 0.091 \quad = 0.182 \quad = 0.636$$

$$\begin{aligned} C' &= 2 \times (0.091 \times \ln(0.091)) + (0.182 \times \ln(0.182)) \\ &\quad + (0.636 \times \ln(0.636)). \end{aligned}$$

$$C^e = 2 \times (0.091 \times (-2.397) + (0.182 \times (-1.704)) \\ + (0.636 \times (-0.458)))$$

$$C^e = -1.0345$$

22

A, A, A, G, A, G, A, A, A, A, A

$$f(G) = \frac{2}{11} \quad f(A) = \frac{9}{11}$$

$$= 0.182 \quad = 0.818$$

$$C^e = (0.182 \times \ln(0.182)) + (0.818 \times \ln(0.818)) \\ = (0.182 \times (-1.704)) + (0.818 \times (-0.201)) \\ = -0.4745$$

30

L, L, L, L, L, L, L, L, L, L

$$C^e = \ln(1)$$

$$= 0.$$

Set-2

9 $-,-,-,-,-,-,-, G_1, -,-$

$$f(G_1) = \frac{1}{9} = 0.111$$
$$C^e = (0.111 \times \ln(0.111)) = (0.111 \times (-2.198))$$
$$= -0.244$$

11 $-,-,-,-,-,-,-, G_1, -,-$

$$C^e = (0.111 \times \ln(0.111))$$
$$= (0.111 \times (-2.198))$$
$$= -0.244.$$

20 $-,-,-,-,-,-,-, K_1 E_1 E$

$$f(K_1) = \frac{1}{9} = 0.111 \quad f(E_1) = \frac{2}{9} = 0.222$$

$$C^e = (0.111 \times \ln(0.111)) + (0.222 \times \ln(0.222))$$
$$= (0.111 \times (-2.198)) + (0.222 \times (-1.505))$$
$$= -0.5781$$

22 $-,-,-,-,-,-,-, F_1 E_1 E$

$$f(E_1) = \frac{3}{9} = 0.333$$

$$C^e = (0.333 \times \ln(0.333)) = 0.333 \times (-0.996)$$
$$= -0.3662$$

30 $-,-,-,-,-,-,-, I_1 I_1 I_1$

$$f(I_1) = 0.333$$

$$C^e = (0.333 \times \ln(0.333)) = (0.333 \times (-1.0996))$$
$$= -0.3662$$

6)

- Open ConSurf server
- Select analyze Amino acids
- yes , known protein structure
- Enter PDB ID '1BTM'

- No for MSA
- Then submit

Alignment Details:

The average number of replacements between any two sequences in the alignment: the expected replacement for every 100 positions is 1

Average pairwise distance: 0.99628

Lower bound: 0.10971

Upper bound: 1.89437

