

Supplementary Material

Table S1. Sequence Database found in the search from NCBI. Parameters used for selection were: pathology, isolation region and type of EPIYA.

Number	Accession (GI)	Country	Pathology	EPIYA
1	2073134	Japan	Gastroduodenal Disease	ABCCC
4	6573219	Japan	Gastric Cancer	ABD
7	12225001	Japan	Gastric Cancer	ABBD
8	12225003	Japan	Chronic atrophic gastritis	ABD
9	12225005	Japan	Chronic atrophic gastritis	ABD
10	12225007	Japan	Chronic atrophic gastritis	ABD
11	12225009	Japan	Peptic Ulcer	ABD
12	12225011	Japan	Peptic Ulcer	ABD
13	12225013	Japan	Peptic Ulcer	ABD
14	12225015	Japan	Chronic atrophic gastritis	ABD
15	12225017	Japan	Peptic Ulcer	ABD
19	12225027	Japan	Peptic Ulcer	ABBD
20	12225029	Japan	Gastric Cancer	ABD
21	12225031	Japan	Gastric Cancer	ABD
24	22121670	USA	Duodenal Ulcer	ABD
25	22335392	Japan	Atrophic Gastritis	ABD
26	22335396	Japan	Atrophic Gastritis	ABD
27	22335405	Japan	Atrophic Gastritis	BABD
28	22335409	Japan	Atrophic Gastritis	AABD
29	22335412	East Asia	Atrophic Gastritis	ABABD
30	22335416	Japan	Atrophic Gastritis	ABBD
31	22335420	Japan	Atrophic Gastritis	ABD
32	22335424	Japan	Atrophic Gastritis	ABBD
33	22335428	Japan	Gastric Ulcer	ABCC
34	22335433	Japan	Duodenal Ulcer	ABDD
35	22335437	Japan	Atrophic Gastritis	ABABD
36	22335442	Japan	Atrophic Gastritis	ABD
37	22335446	Japan	Atrophic Gastritis	ABCCC
38	22335449	Japan	Atrophic Gastritis	ABD
39	22335784	Japan	Atrophic Gastritis	ABC
40	22335788	Japan	Atrophic Gastritis	ABD
43	52693781	East Asia	Atrophic Gastritis	ABD
45	52693787	Japan	Atrophic Gastritis	ABCC
46	52693789	East Asia	Duodenal Ulcer	ABD

47	52693791	Japan	Atrophic Gastritis	ABD
48	52693793	Occidental	Duodenal Ulcer	ABC
49	52693795	Occidental	Atrophic Gastritis	ABC
50	52693797	Occidental	Duodenal Ulcer	ABC
51	52693799	Occidental	Atrophic Gastritis	ABC
52	52693801	East Asia	Duodenal Ulcer	ABD
53	52693803	East Asia	Atrophic Gastritis	ABD
54	52693805	Occidental	Atrophic Gastritis	ABC
55	52693807	Occidental	Duodenal Ulcer	ABCCC
56	52693809	Occidental	Duodenal Ulcer	ABC
57	52693811	Occidental	Atrophic Gastritis	AB
58	52693813	Occidental	Duodenal Ulcer	ABC
60	52693817	East Asia	Atrophic Gastritis	ABD
61	52693819	Occidental	Duodenal Ulcer	ABC
62	52693821	Occidental	Duodenal Ulcer	ABD
64	52693825	Occidental	Duodenal Ulcer	ABC
68	67483340	Amsterdam	Dyspepsia	ABBC
70	83701033	China	Chronic atrophic gastritis	ABD
71	110292846	East Asia	Gastric Cancer	ABD
72	110292848	East Asia	Gastric Cancer	ABD
73	110292850	East Asia	Gastric Cancer	ABD
74	110292852	East Asia	Gastric Cancer	ABD
76	110292856	East Asia	Gastric Cancer	ABD
77	110292858	Occidental	Gastric Cancer	ABCC
78	110292860	East Asia	Gastric Cancer	ABD
79	110292862	East Asia	Gastric Cancer	ABD
80	110292864	East Asia	Gastric Cancer	ABD
81	110292866	East Asia	Gastric Cancer	ABD
82	110292868	East Asia	Gastric Cancer	ABD
83	110292870	East Asia	Gastric Cancer	ABD
87	259123326	Vietnam	Gastric Ulcer	ABD
88	259123328	Vietnam	Duodenal Ulcer	ABD
89	259123330	Vietnam	Duodenal Ulcer	ABD
90	259123332	Vietnam	Duodenal Ulcer	ABD
91	259123334	Vietnam	Gastric Cancer	ABD
92	259123336	Vietnam	Gastric Cancer	ABD
93	259123338	Vietnam	Gastric Cancer	ABD
94	259123340	Vietnam	Duodenal Ulcer	ABD
95	259123342	Vietnam	Duodenal Ulcer	ABD

96	259123344	Vietnam	Duodenal Ulcer	AABD
97	259123346	Vietnam	Gastric Cancer	ABD
98	259123348	Vietnam	Gastric Cancer	AD
99	259123350	Vietnam	Gastric Cancer	ABD
100	259123352	Vietnam	Duodenal Ulcer	ABD
101	259123354	Vietnam	Gastric Cancer	ABD
102	259123356	Vietnam	Gastric Ulcer	ABD
104	259123360	Occidental	Gastric Cancer	ABCC
105	259123362	Vietnam	Duodenal Ulcer	ABD
106	259123364	Vietnam	Gastric Cancer	ABD
107	259123366	Vietnam	Gastric Cancer	ABD
108	259123368	Vietnam	Duodenal Ulcer	ABD
109	307135428	Japan	Gastric Cancer	ABD
110	307135430	Japan	Gastritis	ABD
111	307135432	Japan	Gastritis	ABD
112	307135434	Japan	Gastric Cancer	ABCC
113	307135436	Japan	Gastric Ulcer	ABC
114	307135438	Japan	Gastric Ulcer	ABC
115	307135440	Japan	Gastric Ulcer	ABC
116	307135442	Japan	Duodenal Ulcer	ABC
117	307135444	Japan	Gastritis	ABC
118	307135446	Japan	Gastritis	ABD
119	307135448	Japan	Gastric Ulcer	ABC
120	307135450	Japan	Gastritis	ABC
121	307135452	Japan	Gastritis	ABCC
122	307135454	Japan	Gastritis	ABCC
123	307135456	Japan	Duodenal Ulcer	ABD
124	307135458	Japan	Gastritis	ABC
125	307135460	Japan	Gastric Ulcer	ABCC
126	307135462	Japan	Gastric Ulcer	ABC
127	307135464	Japan	Duodenal Ulcer	ABC
135	335335488	Colombia	Gastric Cancer	ABCCC
136	335335490	Colombia	Gastric Cancer	AACC
137	335335492	Colombia	Gastritis	ABCC
138	335335494	Colombia	Atrophic Gastritis	ABC
139	335335496	Colombia	Duodenal Ulcer	ABCC
140	335335498	Colombia	Atrophic Gastritis	ABABC
150	345421953	Senegal	Dolor abdominal	BC
170	377652613	Colombia	Duodenal Ulcer	ABCC

171	377652609	Colombia	Duodenal Ulcer	ABCC
172	377652607	Colombia	Gastric Cancer	ABCC
174	548691481	Colombia	Gastric Cancer	ABCC
175	548691483	Colombia	Gastritis	ABCC
176	548691485	Colombia	Atrophic Gastritis	ABCC
177	548691487	Colombia	Metaplasia	ABCC
178	548691489	Colombia	Metaplasia	ABCC
179	548691491	Colombia	Duodenal Ulcer	ABCC
180	548691493	Colombia	Gastric Cancer	ABC
181	548691495	Colombia	Gastric Cancer	ABCC
182	548691497	Colombia	Duodenal Ulcer	ABCC
183	548691499	Colombia	Duodenal Ulcer	ABD
186	52693783	Japan	Peptic Ulcer	ABD
187	6573221	Japan	Gastric Ulcer	ABCCC
188	12225025	Japan	Chronic atrophic gastritis	AB

S2 Table. Energy and total of Hydrogen bonds for Crystal and Mutation Models. Only models the docking models obtained in SwissDock that presented an interaction with the N-terminal were selected to run the statistical tests in R. Were Cluster is the number of interacting model using the same location reference of PS to the N-Terminal CagA protein. The difference between models in the same cluster is the rotation of the allowed angles in the PS. ΔG is the Gibbs Free Energy (Kcal/mol). HBonds are the number of hydrogen bonds in each model.

Mutation	Cluster	ΔG	Hbonds
4DVY	28	-6.59372	3
4DVY	28	-6.63488	3
4DVY	28	-6.63488	3
4DVY	28	-6.63488	3
4DVY	28	-6.63488	3
4DVY	28	-6.67062	3
4DVY	28	-6.67062	3
4DVY	28	-6.67062	3
4DVY	10	-7.29307	1
4DVY	10	-7.30221	1
4DVY	10	-7.30221	1
4DVY	10	-7.30221	1
4DVY	10	-7.21762	1
4DVY	10	-7.1835	1
4DVY	10	-8.91991	1
K636N	0	-8.50848	4
K636N	0	-8.5151	4
K636N	0	-8.51094	4
K636N	0	-8.5151	4
K636N	0	-8.5151	4
K636N	0	-8.50848	4
K636N	0	-8.5151	4
K636N	0	-8.51094	4
K636N	6	-7.91795	1
K636N	6	-7.85934	1
K636N	6	-7.61327	2
K636N	6	-6.7117	2
K636N	18	-7.73668	0
K636N	18	-7.73668	0
K636N	18	-7.73668	0
K636N	18	-7.73668	0
K636N	18	-7.70981	0
K636N	18	-7.72128	0
K636N	18	-7.72128	0

K636N	18	-7.72128	0
K636N	21	-7.84754	2
K636N	21	-7.84754	2
K636N	21	-7.84754	2
K636N	21	-7.83932	2
K636N	21	-7.83932	2
K636N	21	-7.83932	2
K636N	21	-7.76492	1
K636N	21	-7.76492	1
K636N	25	-8.36419	2
K636N	25	-8.37319	2
K636N	25	-7.52496	1
K636N	30	-8.46167	4
K636N	30	-8.51244	4
K636N	30	-8.04953	4
K636N	30	-6.87024	2
K636R	7	-8.48093	1
K636R	7	-8.51774	1
K636R	7	-8.51051	1
K636R	7	-8.51051	1
K636R	7	-8.51051	1
K636R	8	-8.65689	3
K636R	8	-8.67863	3
K636R	8	-8.65689	3
K636R	8	-8.67863	3
K636R	8	-8.70192	3
K636R	8	-8.70192	3
K636R	8	-8.70192	3
K636R	8	-8.70192	3
K636R	9	-7.77946	0
K636R	9	-7.77946	0
K636R	9	-7.77946	0
K636R	9	-7.97347	2
K636R	9	-7.97347	2
K636R	9	-7.97347	2
K636R	9	-7.93328	1
K636R	9	-7.93328	1
K636R	28	-6.08855	0
K636R	28	-6.08855	0
K636R	28	-6.08855	0
K636R	28	-6.08855	0

K636R	28	-6.08855	0
K636R	28	-5.95155	0
K636R	28	-5.95155	0
K636R	28	-5.95155	0
K636R	29	-6.6821	0
K636R	29	-6.68549	0
K636R	29	-6.68549	0
K636R	29	-6.68549	0
K636R	29	-6.68549	0
K636R	29	-6.7039	0
K636R	29	-6.7039	0
K636R	29	-6.7039	0
K636R	33	-7.64615	3
K636R	33	-7.59375	3
K636R	33	-7.62225	3
K636A	7	-8.10353	2
K636A	7	-8.13613	2
K636A	7	-8.10676	2
K636A	7	-8.32935	2
K636A	7	-6.12246	1
K636A	7	-6.11635	1
K636A	7	-8.26822	3
K636A	7	-8.28707	3
K636A	8	-8.49543	2
K636A	8	-8.49543	2
K636A	8	-8.49543	2
K636A	8	-8.48028	1
K636A	8	-8.48028	1
K636A	8	-8.48028	1
K636A	8	-8.66526	1
K636A	8	-8.66526	1
K636A	15	-6.75848	0
K636A	15	-6.75848	0
K636A	15	-6.73222	0
K636A	15	-6.67188	0
K636A	15	-6.67188	0
K636A	15	-6.67188	0
K636A	15	-6.67188	0
K636A	15	-6.67188	0
K636A	17	-6.2147	0
K636A	17	-6.2147	0

K636A	17	-6.19683	0
K636A	17	-6.19683	0
K636A	17	-6.19683	0
K636A	17	-6.19683	0
K636A	17	-6.1852	0
K636A	17	-6.1852	0
K636A	18	-6.14987	0
K636A	18	-6.14987	0
K636A	18	-6.14987	0
K636A	18	-6.21486	0
K636A	18	-6.1918	0
K636A	18	-5.7124	0
K636A	18	-5.76062	0
K636A	18	-5.39119	0
K636A	31	-5.9708	0
K636A	31	-5.96028	0
K636A	31	-5.96028	0
K636A	31	-5.96028	0
K636A	31	-5.96028	0
K636A	31	-5.93288	0
K636A	31	-5.93288	0
K636A	31	-5.93288	0