

Supplementary Tables

Table S1: Screen scores of agonist compounds.

<i>agonist</i>	<i>ID</i>	<i>Type</i>	<i>MARV</i>	<i>AIV</i>	<i>Viability</i>
1	Prestw-945	agonist	0.060	0.125	0.737
2	Prestw-101	agonist	0.302	0.614	0.776
3	Prestw-223	agonist	0.475	0.834	0.880
4	Prestw-295	agonist	0.497	0.918	1.001
5	Prestw-956	agonist	0.534	0.808	0.739
6	Prestw-1454	agonist	0.559	0.880	0.995
7	Prestw-908	agonist	0.568	0.740	0.784
8	Prestw-914	agonist	0.633	0.884	0.954
9	Prestw-1004	agonist	0.655	1.460	1.025
10	Prestw-1020	agonist	0.667	0.976	0.515
11	Prestw-1082	agonist	0.673	1.053	0.912
12	Prestw-96	agonist	0.686	0.940	0.999
13	Prestw-997	agonist	0.800	1.334	0.591
14	Prestw-1465	agonist	0.842	0.893	1.018
15	Prestw-1430	agonist	0.850	0.681	0.969
16	Prestw-1119	agonist	0.861	1.213	0.774
17	Prestw-1023	agonist	0.884	0.953	0.969
18	Prestw-598	agonist	0.916	0.758	0.987
19	Prestw-1018	agonist	0.923	1.204	1.040
20	Prestw-1088	agonist	0.935	0.971	1.056
21	Prestw-345	agonist	0.954	1.001	1.050
22	Prestw-1316	agonist	0.954	1.287	0.974
23	Prestw-927	agonist	0.958	1.030	1.061
24	Prestw-1017	agonist	0.963	0.936	1.008
25	Prestw-1352	agonist	0.964	0.959	0.999
26	Prestw-66	agonist	0.965	1.131	0.999
27	Prestw-588	agonist	1.000	0.987	1.005
28	Prestw-505	agonist	1.012	0.991	1.093
29	Prestw-1096	agonist	1.020	0.906	0.988
30	Prestw-1346	agonist	1.021	1.066	1.048
31	Prestw-1158	agonist	1.028	1.079	1.118
32	Prestw-617	agonist	1.030	1.045	1.012
33	Prestw-1392	agonist	1.054	1.075	1.031
34	Prestw-339	agonist	1.057	1.183	0.969
35	Prestw-1016	agonist	1.060	0.997	1.030
36	Prestw-535	agonist	1.072	1.006	0.843
37	Prestw-1041	agonist	1.122	1.177	0.958
38	Prestw-198	agonist	1.146	1.068	0.905
39	Prestw-282	agonist	1.153	0.869	1.051

40	Prestw-1091	agonist	1.158	1.006	0.996
41	Prestw-197	agonist	1.161	0.968	1.105
42	Prestw-1421	agonist	1.174	1.080	0.943
43	Prestw-923	agonist	1.175	1.069	1.062
44	Prestw-68	agonist	1.180	0.994	1.012
45	Prestw-759	agonist	1.189	0.886	1.091
46	Prestw-349	agonist	1.220	0.954	1.127
47	Prestw-352	agonist	1.245	1.191	0.956
48	Prestw-980	agonist	1.257	0.876	1.025
49	Prestw-1511	agonist	1.307	1.090	0.977
50	Prestw-391	agonist	1.345	1.077	1.021
51	Prestw-1038	agonist	1.347	1.144	1.072
52	Prestw-224	agonist	1.364	0.915	1.049
53	Prestw-324	agonist	1.381	1.224	1.070
54	Prestw-749	agonist	1.386	0.859	1.043
55	Prestw-1292	agonist	1.399	1.216	1.036
56	Prestw-880	agonist	1.421	1.130	1.119
57	Prestw-1044	agonist	1.450	1.376	0.735
58	Prestw-983	agonist	1.458	1.353	0.955
59	Prestw-1283	agonist	1.462	1.231	0.980
60	Prestw-949	agonist	1.482	0.971	1.059
61	Prestw-926	agonist	1.489	1.489	0.875
62	Prestw-1480	agonist	1.512	1.145	1.013
63	Prestw-406	agonist	1.546	1.206	1.049
64	Prestw-460	agonist	1.578	1.047	1.147
65	Prestw-1073	agonist	1.591	1.192	1.019
66	Prestw-85	agonist	1.598	0.825	0.959
67	Prestw-726	agonist	1.598	0.965	1.088
68	Prestw-361	agonist	1.605	1.026	0.994
69	Prestw-481	agonist	1.807	1.238	1.052
70	Prestw-968	agonist	1.815	1.238	0.961
71	Prestw-248	agonist	1.856	0.995	1.214
72	Prestw-539	agonist	1.968	1.338	0.976
73	Prestw-739	agonist	2.349	0.980	1.051
74	Prestw-911	agonist	3.332	1.222	1.028

Table S2: Screen scores of antagonist compounds.

<i>antagonist</i>	<i>ID</i>	<i>Type</i>	<i>MARV</i>	<i>AIV</i>	<i>Viability</i>
1	Prestw-149	antagonist	0.027	1.023	1.174
2	Prestw-509	antagonist	0.198	1.086	1.029
3	Prestw-278	antagonist	0.067	1.298	1.001
4	Prestw-99	antagonist	0.197	1.112	0.987
5	Prestw-499	antagonist	0.091	0.917	0.955
6	Prestw-115	antagonist	0.059	1.350	0.904
7	Prestw-1456	antagonist	0.066	1.298	0.885
8	Prestw-806	antagonist	0.028	0.785	0.884
9	Prestw-559	antagonist	0.039	1.147	0.874
10	Prestw-141	antagonist	0.176	1.027	0.871
11	Prestw-297	antagonist	0.087	0.717	0.867
12	Prestw-263	antagonist	0.179	1.260	0.864
13	Prestw-350	antagonist	0.099	0.989	0.853
14	Prestw-340	antagonist	0.197	1.675	0.849
15	Prestw-888	antagonist	0.055	0.819	0.826
16	Prestw-103	antagonist	0.024	0.996	0.812
17	Prestw-706	antagonist	0.019	1.149	0.807
18	Prestw-1043	antagonist	0.109	1.371	0.793
19	Prestw-858	antagonist	0.031	0.818	0.790
20	Prestw-693	antagonist	0.023	1.735	0.761
21	Prestw-383	antagonist	0.091	0.772	0.723
22	Prestw-294	antagonist	0.017	0.868	0.705
23	Prestw-133	antagonist	0.160	1.153	0.921
24	Prestw-147	agonist	0.027	1.124	1.021
25	Prestw-64	antagonist	0.013	0.136	1.061
26	Prestw-842	antagonist	0.017	0.687	0.852
27	Prestw-932	antagonist	0.024	0.389	0.847
28	Prestw-793	antagonist	0.060	0.412	0.817
29	Prestw-74	antagonist	0.046	0.600	0.756
30	Prestw-288	antagonist	0.144	0.657	0.670
31	Prestw-399	antagonist	0.029	0.806	0.668
32	Prestw-348	antagonist	0.020	1.034	0.624
33	Prestw-312	antagonist	0.052	1.333	0.611
34	Prestw-306	antagonist	0.010	0.441	0.585
35	Prestw-576	antagonist	0.095	0.983	0.565
36	Prestw-146	antagonist	0.013	0.715	0.528
37	Prestw-998	antagonist	0.013	0.501	0.524
38	Prestw-308	antagonist	0.025	0.860	0.513
39	Prestw-1068	antagonist	0.017	0.596	0.424
40	Prestw-947	antagonist	0.053	0.882	0.410

41	Prestw-144	antagonist	0.010	0.395	0.395
42	Prestw-375	antagonist	0.020	0.336	0.387
43	Prestw-1368	antagonist	0.014	1.237	0.385
44	Prestw-320	antagonist	0.027	0.325	0.354
45	Prestw-283	antagonist	0.024	1.147	0.347
46	Prestw-1341	antagonist	0.013	0.047	0.259
47	Prestw-37	antagonist	0.097	0.354	0.202
48	Prestw-269	antagonist	0.027	0.894	0.199
49	Prestw-125	antagonist	0.021	0.506	0.196
50	Prestw-53	antagonist	0.013	0.650	0.154
51	Prestw-313	antagonist	0.021	0.641	0.119
52	Prestw-78	antagonist	0.029	0.329	0.082
53	Prestw-136	antagonist	0.020	0.386	0.043
54	Prestw-138	antagonist	0.015	0.024	0.024
55	Prestw-430	antagonist	0.202	0.873	0.900
56	Prestw-455	antagonist	0.204	0.926	0.975
57	Prestw-132	antagonist	0.239	0.990	0.887
58	Prestw-844	antagonist	0.256	1.030	0.951
59	Prestw-1074	antagonist	0.290	0.543	0.839
60	Prestw-105	antagonist	0.309	0.466	0.644
61	Prestw-1152	antagonist	0.313	0.900	0.659
62	Prestw-34	antagonist	0.325	1.020	0.145
63	Prestw-377	antagonist	0.330	0.785	0.985
64	Prestw-529	antagonist	0.343	0.947	0.962
65	Prestw-1075	antagonist	0.392	0.853	0.965
66	Prestw-47	antagonist	0.405	0.434	0.925
67	Prestw-707	antagonist	0.414	0.859	0.968
68	Prestw-128	antagonist	0.415	0.474	0.922
69	Prestw-531	antagonist	0.426	1.030	0.955
70	Prestw-457	antagonist	0.464	2.049	1.015
71	Prestw-1258	antagonist	0.468	1.023	0.996
72	Prestw-371	antagonist	0.486	1.188	0.970
73	Prestw-1055	antagonist	0.511	1.230	0.947
74	Prestw-1029	antagonist	0.549	1.102	0.905
75	Prestw-1188	antagonist	0.588	1.388	0.900
76	Prestw-1432	antagonist	0.591	1.358	0.585
77	Prestw-944	antagonist	0.604	0.932	0.786
78	Prestw-227	antagonist	0.608	1.201	0.958
79	Prestw-1424	antagonist	0.630	0.750	0.707
80	Prestw-169	antagonist	0.634	1.181	1.110
81	Prestw-277	antagonist	0.640	1.045	1.001
82	Prestw-807	antagonist	0.643	0.960	0.920
83	Prestw-931	antagonist	0.645	0.871	1.005

84	Prestw-311	antagonist	0.677	0.859	0.833
85	Prestw-1058	antagonist	0.686	1.034	1.020
86	Prestw-461	antagonist	0.689	0.901	0.756
87	Prestw-704	antagonist	0.698	0.948	1.032
88	Prestw-1117	antagonist	0.710	1.226	0.973
89	Prestw-392	antagonist	0.713	0.864	0.972
90	Prestw-1433	antagonist	0.713	0.971	1.071
91	Prestw-1012	antagonist	0.716	0.819	1.000
92	Prestw-1323	antagonist	0.725	1.244	0.926
93	Prestw-1325	antagonist	0.734	0.493	1.065
94	Prestw-180	antagonist	0.745	0.946	0.913
95	Prestw-1066	antagonist	0.749	1.011	0.949
96	Prestw-928	antagonist	0.758	0.830	0.873
97	Prestw-110	antagonist	0.775	0.854	1.055
98	Prestw-922	antagonist	0.778	0.830	0.998
99	Prestw-584	antagonist	0.801	1.147	1.089
100	Prestw-1490	antagonist	0.808	0.848	1.028
101	Prestw-1187	antagonist	0.821	0.962	0.997
102	Prestw-1497	antagonist	0.824	1.049	0.993
103	Prestw-785	antagonist	0.834	0.721	0.773
104	Prestw-213	antagonist	0.836	1.082	1.029
105	Prestw-751	antagonist	0.844	1.239	1.058
106	Prestw-510	antagonist	0.871	1.360	1.076
107	Prestw-119	antagonist	0.878	1.006	1.134
108	Prestw-1144	antagonist	0.886	1.189	1.024
109	Prestw-921	antagonist	0.889	1.013	1.008
110	Prestw-1307	antagonist	0.889	0.973	1.010
111	Prestw-209	antagonist	0.918	0.800	1.066
112	Prestw-65	antagonist	0.920	1.376	0.881
113	Prestw-915	antagonist	0.921	1.044	1.033
114	Prestw-1199	antagonist	0.931	0.788	1.023
115	Prestw-1256	antagonist	0.936	1.320	0.981
116	Prestw-117	antagonist	0.937	1.169	0.976
117	Prestw-935	antagonist	0.938	1.044	0.901
118	Prestw-847	antagonist	0.949	1.100	1.040
119	Prestw-1510	antagonist	0.954	0.939	0.956
120	Prestw-484	antagonist	0.959	1.318	0.918
121	Prestw-258	antagonist	0.963	0.807	1.109
122	Prestw-1022	antagonist	0.968	0.965	0.961
123	Prestw-1189	antagonist	0.977	1.019	0.960
124	Prestw-208	antagonist	0.982	1.156	1.042
125	Prestw-59	antagonist	0.987	1.148	1.099
126	Prestw-1350	antagonist	0.993	0.936	0.800

127	Prestw-443	antagonist	0.999	1.067	1.004
128	Prestw-683	antagonist	1.002	1.064	1.021
129	Prestw-116	antagonist	1.003	1.192	1.008
130	Prestw-874	antagonist	1.007	1.138	1.014
131	Prestw-109	antagonist	1.009	1.048	1.090
132	Prestw-216	antagonist	1.016	1.116	0.976
133	Prestw-1364	antagonist	1.031	0.979	0.991
134	Prestw-857	antagonist	1.032	1.106	1.024
135	Prestw-228	antagonist	1.039	1.045	1.077
136	Prestw-56	antagonist	1.057	0.710	1.118
137	Prestw-129	antagonist	1.059	1.038	1.057
138	Prestw-1102	antagonist	1.067	1.063	1.044
139	Prestw-42	antagonist	1.077	1.134	1.060
140	Prestw-262	antagonist	1.093	0.955	0.914
141	Prestw-289	antagonist	1.114	0.769	1.037
142	Prestw-62	antagonist	1.117	1.258	1.048
143	Prestw-981	antagonist	1.123	0.801	1.077
144	Prestw-52	antagonist	1.131	0.919	0.984
145	Prestw-1095	antagonist	1.136	0.921	1.055
146	Prestw-75	antagonist	1.136	0.974	1.038
147	Prestw-475	antagonist	1.137	1.166	0.980
148	Prestw-104	antagonist	1.139	1.124	1.011
149	Prestw-877	antagonist	1.151	1.133	1.081
150	Prestw-157	antagonist	1.161	1.020	1.063
151	Prestw-93	antagonist	1.161	1.260	0.947
152	Prestw-1190	antagonist	1.166	1.007	1.061
153	Prestw-69	antagonist	1.174	1.015	1.081
154	Prestw-201	antagonist	1.178	1.273	1.049
155	Prestw-1036	antagonist	1.185	1.166	1.028
156	Prestw-337	antagonist	1.191	0.939	1.054
157	Prestw-948	antagonist	1.191	1.064	1.102
158	Prestw-35	antagonist	1.200	0.909	1.034
159	Prestw-503	antagonist	1.209	1.080	1.032
160	Prestw-303	antagonist	1.213	1.000	1.023
161	Prestw-360	antagonist	1.219	1.121	0.968
162	Prestw-382	antagonist	1.219	1.123	1.029
163	Prestw-820	antagonist	1.222	0.830	1.007
164	Prestw-827	antagonist	1.235	0.895	1.003
165	Prestw-27	antagonist	1.250	1.108	1.073
166	Prestw-250	antagonist	1.257	0.995	1.079
167	Prestw-1507	antagonist	1.267	0.969	1.073
168	Prestw-111	antagonist	1.274	1.017	1.012
169	Prestw-342	antagonist	1.274	0.895	1.070

170	Prestw-1111	antagonist	1.284	0.916	1.076
171	Prestw-1057	antagonist	1.298	1.053	0.975
172	Prestw-900	antagonist	1.305	0.898	1.091
173	Prestw-971	antagonist	1.306	0.973	1.008
174	Prestw-150	antagonist	1.313	1.275	1.135
175	Prestw-1034	antagonist	1.316	1.207	1.046
176	Prestw-1317	antagonist	1.323	1.230	1.094
177	Prestw-801	antagonist	1.328	1.044	0.998
178	Prestw-974	antagonist	1.366	1.152	0.953
179	Prestw-653	antagonist	1.427	0.966	0.976
180	Prestw-162	antagonist	1.429	1.144	1.002
181	Prestw-565	antagonist	1.452	1.091	1.082
182	Prestw-334	antagonist	1.461	1.016	1.135
183	Prestw-310	antagonist	1.471	0.919	1.156
184	Prestw-1035	antagonist	1.498	0.993	1.038
185	Prestw-760	antagonist	1.503	0.962	1.080
186	Prestw-1259	antagonist	1.527	0.758	0.933
187	Prestw-332	antagonist	1.533	1.051	1.015
188	Prestw-953	antagonist	1.555	1.021	1.017
189	Prestw-90	antagonist	1.594	0.971	1.060
190	Prestw-818	antagonist	1.611	1.078	1.054
191	Prestw-322	antagonist	1.639	1.254	0.998
192	Prestw-1039	antagonist	1.691	1.163	1.030
193	Prestw-330	antagonist	1.696	1.089	1.098
194	Prestw-733	antagonist	1.781	1.011	0.998
195	Prestw-966	antagonist	1.801	1.304	0.930
196	Prestw-80	antagonist	1.809	1.284	1.109
197	Prestw-882	antagonist	1.832	1.130	1.032
198	Prestw-167	antagonist	1.834	1.163	0.670
199	Prestw-230	antagonist	1.845	1.022	1.109

Table S3: Screen scores of compounds which have both agonist and antagonist activity.

<i>Both</i>	<i>ID</i>	<i>Type</i>	<i>MARV</i>	<i>AIV</i>	<i>Viability</i>
1	Prestw-364	both	0.029	1.267	0.599
2	Prestw-299	both	0.187	0.323	0.544
3	Prestw-975	both	0.366	1.194	0.875
4	Prestw-905	both	0.906	0.995	1.056
5	Prestw-26	both	0.966	1.039	1.023
6	Prestw-60	both	1.063	0.969	0.924
7	Prestw-374	both	1.190	0.946	1.025
8	Prestw-978	both	1.283	1.252	0.990
9	Prestw-543	both	1.566	1.220	1.084

Table S4: Summary of infectious filovirus assay data of six lead compounds.

Drug name	Infectious virus IC₅₀ (µM)		CC₅₀ (µM)	Selectivity index	
	EBOV	MARV		EBOV	MARV
Benztropine mesylate	3.7	13.2	68	18.4	5.2
Cyproheptadine hydrochloride	7.8	10.2	111	14.2	10.9
Dilazep dihydrochloride	10	21.7	48	4.8	2.2
Propafenone hydrochloride	13.6	23.7	51	3.8	2.2
Trimipramine maleate	11.1	10.9	73	6.6	6.7
Promethazine hydrochloride	19.4	19.1	37	1.9	1.9