

Supplementary Data

This supplementary data is a part of paper entitled "Virtual Screening of the Indonesian Medicinal Plant and Zinc Databases for Potential Inhibitors of the RNA-Dependent RNA Polymerase (RdRp) of 2019 Novel Coronavirus".

Table S1. Hydrogen bond occupancy of between ligand and receptor

Remdesivir (RDM)

Acceptor	Donor	Percentage (%)	Distance (Å)	Angle
TYR_560@O	LIG_1079@H34: @O33	97.5	2.6466	158.6022
ASP_559@OD2	LIG_1079@H42: @O41	87.73	2.6095	164.6033
ASP_701@OD1	LIG_1079@H36: @O35	65.33	2.572	167.4986
ASP_559@OD1	LIG_1079@H40: @O39	61.66	2.5706	168.1091
ASP_701@OD2	LIG_1079@H36: @O35	33.79	2.5828	167.1641
LIG_1079@O37	ARG_496@HH22: @NH2	18.55	2.8256	156.0252
LIG_1079@O33	CYS_563@H: @N	14.74	2.922	159.5935
LIG_1079@O37	ARG_496@HH12: @NH1	12.22	2.8363	154.439
ASP_559@OD1	LIG_1079@H42: @O41	10.71	2.5992	166.0198

ZINC1529045114

Acceptor	Donor	Percentage (%)	Distance (Å)	Angle
LIG_1079@O11	ARG_496@HH11: @NH1	45.55	2.8161	160.3069
LIG_1079@N7	ARG_565@HH21: @NH2	30.18	2.8914	151.6928
ASP_701@OD1	LIG_1079@H23: @O15	29.6	2.6544	162.9622
ASP_393@OD2	LIG_1079@H26: @N9	29.58	2.8336	154.8585
ASP_564@OD2	LIG_1079@H15: @N4	28.95	2.7219	159.6432
ASP_559@OD1	LIG_1079@H7: @O7	23.96	2.6534	165.5095
ASP_701@OD2	LIG_1079@H21: @O14	22.52	2.7076	159.0275
ASP_701@OD1	LIG_1079@H21: @O14	19	2.7394	158.8832
LIG_1079@O15	SER_700@HG: @OG	17.66	2.783	158.7613
LIG_1079@O17	ARG_565@HH11: @NH1	13.74	2.914	159.1019
ASP_393@OD1	LIG_1079@H26: @N9	13.26	2.8326	157.1251
TYR_560@O	LIG_1079@H5: @O6	12.98	2.712	158.0925
ASP_564@OD1	LIG_1079@H16: @N4	12.92	2.7262	161.7094
ASP_559@OD2	LIG_1079@H16: @N4	12.63	2.7354	162.14
ASP_564@OD1	LIG_1079@H15: @N4	12.57	2.7371	159.6196
ASP_564@OD1	LIG_1079@H23: @O15	12.47	2.6626	161.8866
ASP_559@OD2	LIG_1079@H15: @N4	12	2.742	163.0233

ZINC169730811

Acceptor	Donor	Percentage (%)	Distance (Å)	Angle
ASP_702@OD2	LIG_1079@H7: @O7	80.78	2.6585	163.4954
ASP_702@OD2	LIG_1079@H5: @O6	45.58	2.6486	162.1343
LYS_492@O	LIG_1079@H25: @N4	32.53	2.8454	160.469
LIG_1079@N5	SER_490@HG: @OG	25.2	2.839	158.8034
ARG_494@O	LIG_1079@H24: @N4	22.69	2.8325	151.8958
LIG_1079@N3	SER_490@HG: @OG	22	2.7854	158.4971
ARG_494@O	LIG_1079@H21: @O11	18.99	2.6927	162.3982
ASP_701@O	LIG_1079@H5: @O6	18.38	2.7158	161.0261
LIG_1079@O1	ARG_777@HH21: @NH2	17.89	2.817	153.8028
LIG_1079@O1	ARG_777@HH11: @NH1	17.45	2.8169	153.3582
LIG_1079@O7	SER_755@H: @N	17.21	2.9072	150.621

9-Ribosyl-trans-zeatin

Acceptor	Donor	Percentage (%)	Distance (Å)	Angle
GLU_752@O	LIG_1079@H3*: @O3*	37.66	2.7351	162.4237
GLU_752@O	LIG_1079@H2*: @O2*	29.31	2.7178	160.6939
ASP_702@OD2	LIG_1079@H3*: @O3*	23.14	2.6916	164.9356
TRP_558@O	LIG_1079@H5*: @O5*	15.34	2.7385	158.6033
ASP_702@OD2	LIG_1079@H2*: @O2*	15.24	2.6704	159.5671

Table S2. The results of cluster analysis

Remdesivir (RDM)

#Cluster	Frames	Frac	AvgDist	Stdev	Centroid	AvgCDist
0	20000	1	1.696	0.337	10516	0

ZINC1529045114

#Cluster	Frames	Frac	AvgDist	Stdev	Centroid	AvgCDist
0	20000	1	1.788	0.32	8765	0

ZINC169730811

#Cluster	Frames	Frac	AvgDist	Stdev	Centroid	AvgCDist
0	20000	1	1.834	0.385	13887	0

9-Ribosyl-trans-zeatin

#Cluster	Frames	Frac	AvgDist	Stdev	Centroid	AvgCDist
0	20000	1	1.821	0.472	14033	0

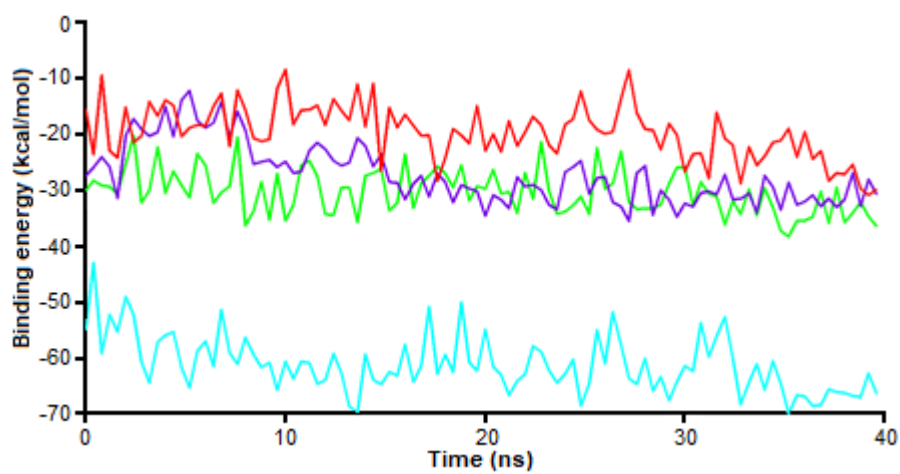


Fig S1. Plot of MM-PBSA binding energy (kcal/mol) versus time in which RDM, ZINC1529045114, ZINC169730811, and 9-Ribosyl-trans-zeatin assigned as red, green, blue, and purple, respectively