

Supplementary Table S1. Top 10 drugs for each virus and docking parameters

Flaviviridae - Hepatitis C virus									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-8.13943	53123-88-9	
Trabectedin	4	168.72	761.849	12	4	1	-7.73204	114899-77-3	
Digoxin	7	203.06	780.949	13	6	1	-7.35699	20830-75-5	
Tacrolimus	7	178.36	804.031	11	3	1	-7.17397	104987-11-3	
Rifapentine	6	220.15	877.045	13	6	1	-7.04585	61379-65-5	
Rifabutin	5	205.55	847.019	12	5	1	-6.98407	72559-06-9	
Azithromycin	7	180.08	748.996	13	5	1	-6.82006	83905-01-5	
Dalfopristin	7	176.42	690.859	9	2	1	-6.73667	112362-50-2	
Moxidectin	3	116.04	639.83	7	2	1	-6.70568	113507-06-5	
Pimecrolimus	6	158.13	810.466	10	2	1	-6.64757	137071-32-0	
Flaviviridae - Yellow fever virus									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-8.79	53123-88-9	
Tacrolimus	7	178.36	804.031	11	3	1	-7.78344	104987-11-3	
Rifampin	5	220.15	822.953	13	6	1	-7.50406	13292-46-1	
Rifapentine	6	220.15	877.045	13	6	1	-7.48355	61379-65-5	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.44173	137071-32-0	
Rifabutin	5	205.55	847.019	12	5	1	-7.24808	72559-06-9	
Digoxin	7	203.06	780.949	13	6	1	-7.19704	20830-75-5	
Eribulin	4	146.39	729.908	12	2	1	-6.88494	253128-41-5	
Etoposide	5	160.83	588.562	12	3	1	-6.88186	33419-42-0	
Erythromycin	7	193.91	733.937	13	5	1	-6.73789	114-07-8	
Flaviviridae - Zika virus									

Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.34036	137071-32-0	
Sirolimus	6	195.43	914.187	12	3	1	-7.31482	53123-88-9	
Tacrolimus	7	178.36	804.031	11	3	1	-7.28614	104987-11-3	
Ergotamine	5	118.21	581.673	6	3	1	-7.03937	113-15-5	
M Fostamatinib	7	128.75	470.461	8	3	1	-6.89724	841290-80-0	
Conivaptan	6	78.09	498.586	4	3	1	-6.85443	210101-16-9	
Ergoloid	6	118.21	591.753	6	3	1	-6.84152	8067-24-1	
Abemaciclib	7	75	506.605	6	1	1	-6.80595	1231929-97-7	
Dihydroergotamine	5	118.21	583.689	6	3	1	-6.80464	511-12-6	
Eravacycline	6	193.73	558.563	10	8	1	-6.80014	1207283-85-9	
Flaviviridae - Bovine viral diarrhea virus									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Rifampin	5	220.15	822.953	13	6	1	-6.93071	13292-46-1	
Sirolimus	6	195.43	914.187	12	3	1	-6.73035	53123-88-9	
Dalfopristin	7	176.42	690.859	9	2	1	-6.46299	112362-50-2	
Digoxin	7	203.06	780.949	13	6	1	-6.35662	20830-75-5	
Pimecrolimus	6	158.13	810.466	10	2	1	-6.28407	137071-32-0	
Telmisartan	7	75.77	513.621	2	0	1	-6.22064	144701-48-4	
Tacrolimus	7	178.36	804.031	11	3	1	-6.01496	104987-11-3	
Avapritinib	5	105.75	498.57	6	1	1	-6.01013	1703793-34-3	
Irinotecan	6	112.51	586.689	6	1	1	-5.99025	97682-44-5	
Rifamycin	3	201.31	697.778	11	6	1	-5.97969	6998-60-3	
Flaviviridae - West Nile virus									
Drug information						Other relevant docking results			

drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	0	3	1	-7.18091	53123-88-9	
Rifampin	5	220.15	822.953	0	6	1	-6.56624	13292-46-1	
Pimecrolimus	6	158.13	810.466	0	2	1	-6.52908	137071-32-0	
Tacrolimus	7	178.36	804.031	0	3	1	-6.44666	104987-11-3	
Rifamycin	3	201.31	697.778	0	6	1	-6.391	6998-60-3	
Eribulin	4	146.39	729.908	0	2	1	-6.23569	253128-41-5	
Etoposide Phosphate	7	201.04	666.525	0	2	1	-6.16796	117091-64-2	
Vorapaxar	7	77.52	492.591	0	1	1	-6.16266	618385-01-6	
Rifabutin	5	205.55	847.019	0	5	1	-6.14315	72559-06-9	
Naldemedine	7	141.18	570.646	0	4	1	-6.13882	916072-89-4	
Flaviviridae - Dengue virus									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-6.9541	53123-88-9	
Irinotecan	6	112.51	586.689	6	1	1	-6.73786	97682-44-5	
Dalfopristin	7	176.42	690.859	9	2	1	-6.71463	112362-50-2	
Tacrolimus	7	178.36	804.031	11	3	1	-6.6993	104987-11-3	
Rifapentine	6	220.15	877.045	13	6	1	-6.49837	61379-65-5	
Plerixafor	4	78.66	502.796	8	6	1	-6.4804	110078-46-1	
Dasabuvir	6	104.81	493.584	5	2	1	-6.45614	1132935-63-7	
Rifamycin	3	201.31	697.778	11	6	1	-6.44513	6998-60-3	
Rifampin	5	220.15	822.953	13	6	1	-6.37859	13292-46-1	
Acalabrutinib	7	118.5	465.517	5	2	1	-6.33797	1420477-60-6	
Flaviviridae - Tick-borne encephalitis virus									
Drug information						Other relevant docking results			

drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Tacrolimus	7	178.36	804.031	11	3	1	-7.54614	104987-11-3	
Eribulin	4	146.39	729.908	12	2	1	-7.31986	253128-41-5	
Rifapentine	6	220.15	877.045	13	6	1	-7.30403	61379-65-5	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.25235	137071-32-0	
Sirolimus	6	195.43	914.187	12	3	1	-7.07288	53123-88-9	
Rifampin	5	220.15	822.953	13	6	1	-6.77447	13292-46-1	
Dalfopristin	7	176.42	690.859	9	2	1	-6.76605	112362-50-2	
Plerixafor	4	78.66	502.796	8	6	1	-6.61759	110078-46-1	
Digoxin	7	203.06	780.949	13	6	1	-6.52795	20830-75-5	
Rifamycin	3	201.31	697.778	11	6	1	-6.48052	6998-60-3	
Flaviviridae - Classical swine fever virus									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-7.35583	53123-88-9	
Etoposide Phosphate	7	201.04	666.525	12	2	1	-7.07113	117091-64-2	
Dalfopristin	7	176.42	690.859	9	2	1	-7.03491	112362-50-2	
Rifapentine	6	220.15	877.045	13	6	1	-6.98608	61379-65-5	
Tacrolimus	7	178.36	804.031	11	3	1	-6.88011	104987-11-3	
Ciclesonide	6	99.13	540.697	6	1	1	-6.8731	126544-47-6	
Ubrogepant	6	104.29	549.553	5	2	1	-6.78134	1374248-77-7	
Etoposide	5	160.83	588.562	12	3	1	-6.71705	33419-42-0	
Pimecrolimus	6	158.13	810.466	10	2	1	-6.71489	137071-32-0	
Trametinib	6	102.06	615.403	4	2	1	-6.70854	871700-17-3	
Flaviviridae - Japanese encephalitis virus									
Drug information						Other relevant docking results			

drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-9.83446	53123-88-9	
Rifampin	5	220.15	822.953	13	6	1	-9.80233	13292-46-1	
Etoposide Phosphate	7	201.04	666.525	12	2	1	-9.58387	117091-64-2	
Plerixafor	4	78.66	502.796	8	6	1	-9.48926	110078-46-1	
Tacrolimus	7	178.36	804.031	11	3	1	-9.11698	104987-11-3	
Dihydroergotamine	5	118.21	583.689	6	3	1	-9.11423	511-12-6	
Ergoloid	6	118.21	591.753	6	3	1	-9.11336	8067-24-1	
Digoxin	7	203.06	780.949	13	6	1	-8.9296	20830-75-5	
Bromocriptine	6	118.21	654.606	6	3	1	-8.87967	25614-03-3	
Doxorubicin	5	206.07	543.525	12	6	1	-8.86258	23214-92-8	
Caliciviridae - Rabbit Hemorrhagic Disease Virus									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-8.08678	53123-88-9	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.92432	137071-32-0	
Tacrolimus	7	178.36	804.031	11	3	1	-7.73171	104987-11-3	
Rifapentine	6	220.15	877.045	13	6	1	-7.3618	61379-65-5	
Rifampin	5	220.15	822.953	13	6	1	-7.3377	13292-46-1	
Azithromycin	7	180.08	748.996	13	5	1	-7.26007	83905-01-5	
Dalfopristin	7	176.42	690.859	9	2	1	-7.24238	112362-50-2	
Dihydroergotamine	5	118.21	583.689	6	3	1	-7.19197	511-12-6	
Digoxin	7	203.06	780.949	13	6	1	-7.08502	20830-75-5	
Eribulin	4	146.39	729.908	12	2	1	-7.03538	253128-41-5	
Caliciviridae - Norwalk virus									
Drug information						Other relevant docking results			

drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.74191	137071-32-0	
Rifapentine	6	220.15	877.045	13	6	1	-7.44188	61379-65-5	
Tacrolimus	7	178.36	804.031	11	3	1	-7.41875	104987-11-3	
Moxidectin	3	116.04	639.83	7	2	1	-7.24336	113507-06-5	
Digoxin	7	203.06	780.949	13	6	1	-7.23942	20830-75-5	
Sirolimus	6	195.43	914.187	12	3	1	-7.17971	53123-88-9	
Eribulin	4	146.39	729.908	12	2	1	-6.95825	253128-41-5	
Dalfopristin	7	176.42	690.859	9	2	1	-6.59857	112362-50-2	
Rifampin	5	220.15	822.953	13	6	1	-6.51454	13292-46-1	
Azithromycin	7	180.08	748.996	13	5	1	-6.48766	83905-01-5	
Caliciviridae - Sapporo virus									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-8.62551	53123-88-9	
Pimecrolimus	6	158.13	810.466	10	2	1	-8.28292	137071-32-0	
Rifabutin	5	205.55	847.019	12	5	1	-8.05622	72559-06-9	
Tacrolimus	7	178.36	804.031	11	3	1	-7.93186	104987-11-3	
Digoxin	7	203.06	780.949	13	6	1	-7.72827	20830-75-5	
Rifampin	5	220.15	822.953	13	6	1	-7.72705	13292-46-1	
Rifapentine	6	220.15	877.045	13	6	1	-7.30792	61379-65-5	
Naldemedine	7	141.18	570.646	8	4	1	-7.30019	916072-89-4	
Daunorubicinol	4	189	529.542	11	6	1	-7.03214	28008-55-1	
Etoposide	5	160.83	588.562	12	3	1	-7.01744	33419-42-0	
Caliciviridae - Murine norovirus									
Drug information						Other relevant docking results			

drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Tacrolimus	7	178.36	804.031	11	3	1	-8.97221	104987-11-3	
Sirolimus	6	195.43	914.187	12	3	1	-8.28578	53123-88-9	
Digoxin	7	203.06	780.949	13	6	1	-7.52595	20830-75-5	
Rifamycin	3	201.31	697.778	11	6	1	-7.41853	6998-60-3	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.23673	137071-32-0	
Eribulin	4	146.39	729.908	12	2	1	-7.03744	253128-41-5	
Rifampin	5	220.15	822.953	13	6	1	-6.90614	13292-46-1	
Bazedoxifene	7	57.86	470.613	4	2	1	-6.81949	198481-32-2	
Dihydroergotamine	5	118.21	583.689	6	3	1	-6.80512	511-12-6	
Rimegepant	5	113.68	534.567	5	2	1	-6.80287	1289023-67-1	
Picornaviridae - Rhinovirus									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-7.91188	53123-88-9	
Tacrolimus	7	178.36	804.031	11	3	1	-7.16754	104987-11-3	
Rifabutin	5	205.55	847.019	12	5	1	-7.1458	72559-06-9	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.04785	137071-32-0	
Rifapentine	6	220.15	877.045	13	6	1	-6.98402	61379-65-5	
Ergotamine	5	118.21	581.673	6	3	1	-6.88582	113-15-5	
Digoxin	7	203.06	780.949	13	6	1	-6.85786	20830-75-5	
Lurasidone	5	56.75	492.688	4	0	1	-6.8489	367514-87-2	
Dalfopristin	7	176.42	690.859	9	2	1	-6.7067	112362-50-2	
Etoposide Phosphate	7	201.04	666.525	12	2	1	-6.61666	117091-64-2	
Picornaviridae - Foot-and-mouth disease virus									
Drug information						Other relevant docking results			

drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Rifapentine	6	220.15	877.045	13	6	1	-7.85352	61379-65-5	
Digoxin	7	203.06	780.949	13	6	1	-7.84355	20830-75-5	
Rifampin	5	220.15	822.953	13	6	1	-7.77781	13292-46-1	
Sirolimus	6	195.43	914.187	12	3	1	-7.68884	53123-88-9	
Rifabutin	5	205.55	847.019	12	5	1	-7.6784	72559-06-9	
Azithromycin	7	180.08	748.996	13	5	1	-7.60554	83905-01-5	
Eribulin	4	146.39	729.908	12	2	1	-7.56207	253128-41-5	
Trabectedin	4	168.72	761.849	12	4	1	-7.51409	114899-77-3	
Tacrolimus	7	178.36	804.031	11	3	1	-7.3484	104987-11-3	
Dalfopristin	7	176.42	690.859	9	2	1	-7.14579	112362-50-2	
Picornaviridae - Sicinivirus A									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-16.0604	53123-88-9	
Tacrolimus	7	178.36	804.031	11	3	1	-15.9126	104987-11-3	
Digoxin	7	203.06	780.949	13	6	1	-15.4157	20830-75-5	
Avapritinib	5	105.75	498.57	6	1	1	-14.8323	1703793-34-3	
Ubrogepant	6	104.29	549.553	5	2	1	-14.6875	1374248-77-7	
Naldemedine	7	141.18	570.646	8	4	1	-14.6029	916072-89-4	
Eravacycline	6	193.73	558.563	10	8	1	-14.5522	1207283-85-9	
Linagliptin	5	113.48	472.553	6	1	1	-14.4972	668270-12-0	
Ergotamine	5	118.21	581.673	6	3	1	-14.4733	113-15-5	
Dihydroergotamine	5	118.21	583.689	6	3	1	-14.3847	511-12-6	
Picornaviridae - Porcine aichi virus									
Drug information						Other relevant docking results			

drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-7.99736	53123-88-9	
Rifabutin	5	205.55	847.019	12	5	1	-7.7288	72559-06-9	
Digoxin	7	203.06	780.949	13	6	1	-7.66218	20830-75-5	
Rifapentine	6	220.15	877.045	13	6	1	-7.18944	61379-65-5	
Pancuronium	6	52.6	572.875	2	0	1	-7.11239	15500-66-0	
Bromocriptine	6	118.21	654.606	6	3	1	-6.94399	25614-03-3	
Rifampin	5	220.15	822.953	13	6	1	-6.93922	13292-46-1	
Omadacycline	7	176.66	556.66	9	8	1	-6.92493	389139-89-3	
Rifamycin	3	201.31	697.778	11	6	1	-6.87913	6998-60-3	
M Rapacuronium	7	49.77	555.868	3	1	1	-6.84144	736123-17-4	
Picornaviridae - Poliovirus									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-9.15525	53123-88-9	
Tacrolimus	7	178.36	804.031	11	3	1	-8.83313	104987-11-3	
Pimecrolimus	6	158.13	810.466	10	2	1	-8.02572	137071-32-0	
Azithromycin	7	180.08	748.996	13	5	1	-7.87226	83905-01-5	
Bromocriptine	6	118.21	654.606	6	3	1	-7.8623	25614-03-3	
Rifapentine	6	220.15	877.045	13	6	1	-7.85416	61379-65-5	
Dalfopristin	7	176.42	690.859	9	2	1	-7.7517	112362-50-2	
Rifampin	5	220.15	822.953	13	6	1	-7.75135	13292-46-1	
Eribulin	4	146.39	729.908	12	2	1	-7.60214	253128-41-5	
Dihydroergotamine	5	118.21	583.689	6	3	1	-7.59658	511-12-6	
Picornaviridae - Coxsackievirus B									
Drug information						Other relevant docking results			

drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Tacrolimus	7	178.36	804.031	11	3	1	-9.03564	104987-11-3	
Rifapentine	6	220.15	877.045	13	6	1	-8.81769	61379-65-5	
Sirolimus	6	195.43	914.187	12	3	1	-8.17726	53123-88-9	
Rifabutin	5	205.55	847.019	12	5	1	-8.15459	72559-06-9	
Lurbinectedin	4	164.28	784.887	11	4	1	-8.06431	497871-47-3	
Rifampin	5	220.15	822.953	13	6	1	-8.0009	13292-46-1	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.90693	137071-32-0	
Rifamycin	3	201.31	697.778	11	6	1	-7.87144	6998-60-3	
Azithromycin	7	180.08	748.996	13	5	1	-7.81096	83905-01-5	
Ergotamine	5	118.21	581.673	6	3	1	-7.68561	113-15-5	

Picornaviridae - Enterovirus 71

Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-7.57517	53123-88-9	
Digoxin	7	203.06	780.949	13	6	1	-7.55949	20830-75-5	
Tacrolimus	7	178.36	804.031	11	3	1	-7.49484	104987-11-3	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.16251	137071-32-0	
Erythromycin	7	193.91	733.937	13	5	1	-6.74094	114-07-8	
Eribulin	4	146.39	729.908	12	2	1	-6.68329	253128-41-5	
Rifapentine	6	220.15	877.045	13	6	1	-6.63487	61379-65-5	
Omadacycline	7	176.66	556.66	9	8	1	-6.54386	389139-89-3	
Rifabutin	5	205.55	847.019	12	5	1	-6.53503	72559-06-9	
Rifampin	5	220.15	822.953	13	6	1	-6.52943	13292-46-1	

Picornaviridae - Encephalomyocarditis virus

Drug information						Other relevant docking results			
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drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-8.97226	53123-88-9	
Tacrolimus	7	178.36	804.031	11	3	1	-7.88066	104987-11-3	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.54961	137071-32-0	
Digoxin	7	203.06	780.949	13	6	1	-7.41649	20830-75-5	
Lurbinectedin	4	164.28	784.887	11	4	1	-7.41422	497871-47-3	
Rifampin	5	220.15	822.953	13	6	1	-7.19006	13292-46-1	
Rifamycin	3	201.31	697.778	11	6	1	-7.18945	6998-60-3	
Eribulin	4	146.39	729.908	12	2	1	-7.17229	253128-41-5	
Bromocriptine	6	118.21	654.606	6	3	1	-7.13747	25614-03-3	
Pancuronium	6	52.6	572.875	2	0	1	-7.09821	15500-66-0	

Picornaviridae - Enterovirus D68

Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Sirolimus	6	195.43	914.187	12	3	1	-8.50079	53123-88-9	
Rifapentine	6	220.15	877.045	13	6	1	-8.08768	61379-65-5	
Pimecrolimus	6	158.13	810.466	10	2	1	-7.62972	137071-32-0	
Tacrolimus	7	178.36	804.031	11	3	1	-7.6278	104987-11-3	
Rifampin	5	220.15	822.953	13	6	1	-7.5387	13292-46-1	
Eribulin	4	146.39	729.908	12	2	1	-7.33406	253128-41-5	
Suvorexant	4	80.29	450.93	4	0	1	-7.14603	1030377-33-3	
Digoxin	7	203.06	780.949	13	6	1	-6.9897	20830-75-5	
Ergotamine	5	118.21	581.673	6	3	1	-6.91333	113-15-5	
Azithromycin	7	180.08	748.996	13	5	1	-6.78257	83905-01-5	

Permutotetraviridae - Thosea asigna virus

Drug information						Other relevant docking results			
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drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Rifampin	5	220.15	822.953	13	6	1	-8.37307	13292-46-1	
Sirolimus	6	195.43	914.187	12	3	1	-8.22613	53123-88-9	
Rifabutin	5	205.55	847.019	12	5	1	-7.52686	72559-06-9	
Rifapentine	6	220.15	877.045	13	6	1	-7.45106	61379-65-5	
Digoxin	7	203.06	780.949	13	6	1	-7.29813	20830-75-5	
Sildenafil	7	109.13	474.586	7	1	1	-7.18886	139755-83-2	
Irinotecan	6	112.51	586.689	6	1	1	-7.13626	97682-44-5	
Pimecrolimus	6	158.13	810.466	10	2	1	-6.88851	137071-32-0	
Etoposide	5	160.83	588.562	12	3	1	-6.86226	33419-42-0	
Linagliptin	5	113.48	472.553	6	1	1	-6.77978	668270-12-0	
Coronaviridae - Severe acute respiratory syndrome coronavirus 2									
Drug information						Other relevant docking results			
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	cas	
Tacrolimus	7	178.36	804.031	11	3	1	-8.6515	104987-11-3	
Dalfopristin	7	176.42	690.859	9	2	1	-8.35717	112362-50-2	
Pimecrolimus	6	158.13	810.466	10	2	1	-8.02939	137071-32-0	
Rifapentine	6	220.15	877.045	13	6	1	-7.9257	61379-65-5	
Sirolimus	6	195.43	914.187	12	3	1	-7.9229	53123-88-9	
Rifabutin	5	205.55	847.019	12	5	1	-7.88086	72559-06-9	
Ergotamine	5	118.21	581.673	6	3	1	-7.82652	113-15-5	
Bromocriptine	6	118.21	654.606	6	3	1	-7.80572	25614-03-3	
Lurbinedin	4	164.28	784.887	11	4	1	-7.69796	497871-47-3	
Conivaptan	6	78.09	498.586	4	3	1	-7.64096	210101-16-9	

Supplementary Table S2. Antiviral drug docking parameters.

Flaviviridae - Hepatitis C virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Elbasvir	13	189	882	9	4	1	-8.08897	2.0064008
Pibrentasvir	17	200	1113.2	17	4	1	-8.06932	3.3242452
Faldaprevir	15	227	869.7999	12	4	1	-7.56067	4.3306098
Ritonavir	18	202	720.9	9	4	1	-7.53194	2.3389802
Velpatasvir	13	193	883	10	4	1	-7.03962	3.267632
Daclatasvir	13	175	738.9	8	4	1	-6.937	2.3041263
Simeprevir	8	194	749.9	10	2	1	-6.75098	1.6410096
Lopinavir	15	120	628.8	5	4	1	-6.48458	1.5723376
Asunaprevir	14	191	748.3	10	3	1	-6.46881	2.1620514
TMC310911	15	179	756	12	3	1	-6.45315	2.2789028
Flaviviridae - Yellow fever virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Elbasvir	13	189	882	9	4	1	-8.74685	2.4860983
Velpatasvir	13	193	883	10	4	1	-8.31956	2.9509103
Daclatasvir	13	175	738.9	8	4	1	-8.16457	1.9270446
Pibrentasvir	17	200	1113.2	17	4	1	-7.8953	2.1114364
Faldaprevir	15	227	869.7999	12	4	1	-7.60704	1.209281
Simeprevir	8	194	749.9	10	2	1	-7.46342	1.9784654
Paritaprevir	7	198	765.9	10	3	1	-7.38485	2.7492743
Atazanavir	18	171	704.9	9	5	1	-7.21475	1.8903244
Tipranavir	11	114	602.7	10	2	1	-7.16612	2.5746937
Asunaprevir	14	191	748.3	10	3	1	-6.99591	4.1787357
Flaviviridae - Zika virus								
Drug information						Other relevant docking results		

drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Faldaprevir	15	227	869.7999	12	4	1	-7.59145	4.6088991
Asunaprevir	14	191	748.3	10	3	1	-7.32715	3.2673604
Velpatasvir	13	193	883	10	4	1	-7.15729	2.0988696
TMC310911	15	179	756	12	3	1	-7.05128	2.4796042
Ritonavir	18	202	720.9	9	4	1	-6.89945	3.7855556
Letermovir	7	77.8	572.5	10	1	1	-6.86807	1.1008978
Atazanavir	18	171	704.9	9	5	1	-6.80127	3.1530945
Glecaprevir	7	204	838.9	15	3	1	-6.77939	1.8468144
Elbasvir	13	189	882	9	4	1	-6.76237	3.3429101
Simeprevir	8	194	749.9	10	2	1	-6.74734	2.0395656
Flaviviridae - Bovine viral diarrhea virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Elbasvir	13	189	882	9	4	1	-7.81344	3.0644736
Ritonavir	18	202	720.9	9	4	1	-7.74677	2.3628297
Faldaprevir	15	227	869.7999	12	4	1	-7.37845	1.7347846
Velpatasvir	13	193	883	10	4	1	-7.25284	3.3240459
Cobicistat	20	195	776	10	3	1	-7.2439	3.5859301
Pibrentasvir	17	200	1113.2	17	4	1	-7.0807	4.0254741
Daclatasvir	13	175	738.9	8	4	1	-6.91492	1.2649411
TMC310911	15	179	756	12	3	1	-6.33464	1.524748
Paritaprevir	7	198	765.9	10	3	1	-6.32727	2.2121375
Fosamprenavir	14	186	585.6	11	4	1	-6.26566	2.1523497
Flaviviridae - West Nile virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-8.52122	5.3380089
Elbasvir	13	189	882	9	4	1	-7.46264	2.0807712

Daclatasvir	13	175	738.9	8	4	1	-7.21599	3.2081325
Velpatasvir	13	193	883	10	4	1	-7.02462	3.9562926
Saquinavir	13	167	670.8	7	5	1	-6.88588	6.9203229
Faldaprevir	15	227	869.7999	12	4	1	-6.85665	2.6740346
Paritaprevir	7	198	765.9	10	3	1	-6.77194	3.3090506
Asunaprevir	14	191	748.3	10	3	1	-6.75287	7.287775
Atazanavir	18	171	704.9	9	5	1	-6.63312	6.6349368
TMC310911	15	179	756	12	3	1	-6.30659	3.3974891

Flaviviridae - Dengue virus

Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Elbasvir	13	189	882	9	4	1	-7.47441	3.6113799
Cobicistat	20	195	776	10	3	1	-7.29492	1.6891743
Pibrentasvir	17	200	1113.2	17	4	1	-7.1638	4.9325747
Simeprevir	8	194	749.9	10	2	1	-6.96879	2.2444115
Faldaprevir	15	227	869.7999	12	4	1	-6.94016	1.4080107
Asunaprevir	14	191	748.3	10	3	1	-6.841	1.5653238
Atazanavir	18	171	704.9	9	5	1	-6.75269	3.0114336
Velpatasvir	13	193	883	10	4	1	-6.71179	4.6408563
TMC310911	15	179	756	12	3	1	-6.70028	3.8594439
Ritonavir	18	202	720.9	9	4	1	-6.67118	1.5103495

Flaviviridae - Tick-borne encephalitis virus

Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-7.9361	3.6355605
Elbasvir	13	189	882	9	4	1	-7.35491	1.5658795
Atazanavir	18	171	704.9	9	5	1	-7.31605	1.8775066
Velpatasvir	13	193	883	10	4	1	-7.21685	3.4438629
Lopinavir	15	120	628.8	5	4	1	-7.14208	1.2830409

Cobicistat	20	195	776	10	3	1	-7.10795	1.6422734
Simeprevir	8	194	749.9	10	2	1	-7.06164	3.2029386
Asunaprevir	14	191	748.3	10	3	1	-6.99644	2.7037504
Daclatasvir	13	175	738.9	8	4	1	-6.91545	3.1354208
Glecaprevir	7	204	838.9	15	3	1	-6.77664	2.2999425
Flaviviridae - Classical swine fever virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-8.17737	1.9282414
Elbasvir	13	189	882	9	4	1	-8.04305	2.0867991
Velpatasvir	13	193	883	10	4	1	-7.8723	2.206986
Daclatasvir	13	175	738.9	8	4	1	-7.38332	1.8605771
Ritonavir	18	202	720.9	9	4	1	-7.30125	2.6110983
Simeprevir	8	194	749.9	10	2	1	-7.07934	3.0122824
TMC310911	15	179	756	12	3	1	-6.93911	1.7837961
Asunaprevir	14	191	748.3	10	3	1	-6.90742	1.9378501
Boceprevir	10	151	519.7	5	4	1	-6.54773	1.0166123
Tipranavir	11	114	602.7	10	2	1	-6.4515	1.6823635
Flaviviridae - Japanese encephalitis virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Paritaprevir	7	198	765.9	10	3	1	-9.65753	2.6597826
Lopinavir	15	120	628.8	5	4	1	-9.35441	2.3489921
Pibrentasvir	17	200	1113.2	17	4	1	-9.34248	4.4087238
Simeprevir	8	194	749.9	10	2	1	-9.32398	1.6303653
Adefovir Dipivoxil	15	167	501.5	12	1	1	-9.26969	1.8219789
Glecaprevir	7	204	838.9	15	3	1	-9.20661	1.988206
Cobicistat	20	195	776	10	3	1	-9.05017	3.0318975
Faldaprevir	15	227	869.7999	12	4	1	-9.02734	2.9768815

Elbasvir	13	189	882	9	4	1	-8.87797	1.4862188
Saquinavir	13	167	670.8	7	5	1	-8.86738	1.851944
Caliciviridae - Rabbit Hemorrhagic Disease Virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-9.03996	3.1416593
Glecaprevir	7	204	838.9	15	3	1	-8.36509	1.6655881
Velpatasvir	13	193	883	10	4	1	-8.03527	2.2849107
Faldaprevir	15	227	869.7999	12	4	1	-7.85356	2.5907347
Cobicistat	20	195	776	10	3	1	-7.84596	2.5260308
Saquinavir	13	167	670.8	7	5	1	-7.84541	1.5516382
Daclatasvir	13	175	738.9	8	4	1	-7.62798	3.5254316
Indinavir	12	118	613.8	7	4	1	-7.60335	2.6847534
Asunaprevir	14	191	748.3	10	3	1	-7.57237	1.6743689
Grazoprevir	8	204	766.9	11	3	1	-7.48074	2.325218
Caliciviridae - Norwalk virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Simeprevir	8	194	749.9	10	2	1	-8.54072	2.4460149
Pibrentasvir	17	200	1113.2	17	4	1	-8.45626	2.0636055
TMC310911	15	179	756	12	3	1	-7.82328	2.9477968
Velpatasvir	13	193	883	10	4	1	-7.68513	3.6971467
Ritonavir	18	202	720.9	9	4	1	-7.48472	1.7189808
Daclatasvir	13	175	738.9	8	4	1	-7.14448	2.4726825
Asunaprevir	14	191	748.3	10	3	1	-7.07972	3.0797808
Lopinavir	15	120	628.8	5	4	1	-6.93793	3.0241423
Elbasvir	13	189	882	9	4	1	-6.92616	2.4678748
Tipranavir	11	114	602.7	10	2	1	-6.70262	2.3889825

Caliciviridae - Sapporo virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Cobicistat	20	195	776	10	3	1	-8.55555	3.5620697
Lopinavir	15	120	628.8	5	4	1	-8.09583	3.3545964
Ritonavir	18	202	720.9	9	4	1	-8.07278	2.7049119
Velpatasvir	13	193	883	10	4	1	-7.86397	3.151207
Faldaprevir	15	227	869.7999	12	4	1	-7.63169	2.8498564
Simeprevir	8	194	749.9	10	2	1	-7.57209	6.178628
Atazanavir	18	171	704.9	9	5	1	-7.55074	1.588237
Pibrentasvir	17	200	1113.2	17	4	1	-7.47146	2.2140079
Asunaprevir	14	191	748.3	10	3	1	-7.25966	4.0166941
Saquinavir	13	167	670.8	7	5	1	-7.02118	1.8621677
Caliciviridae - Murine norovirus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Faldaprevir	15	227	869.7999	12	4	1	-8.49482	2.2890763
Elbasvir	13	189	882	9	4	1	-8.03277	1.8270922
TMC310911	15	179	756	12	3	1	-7.66716	1.883667
Cobicistat	20	195	776	10	3	1	-7.63866	2.32495
Asunaprevir	14	191	748.3	10	3	1	-7.4724	2.0450752
Daclatasvir	13	175	738.9	8	4	1	-7.38686	1.5950013
Indinavir	12	118	613.8	7	4	1	-7.33512	3.1546149
Velpatasvir	13	193	883	10	4	1	-7.21816	3.6524951
Ritonavir	18	202	720.9	9	4	1	-7.17162	1.8828226
Saquinavir	13	167	670.8	7	5	1	-6.958	1.4695296
Picornaviridae - Rhinovirus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine

Pibrentasvir	17	200	1113.2	17	4	1	-8.41877	1.8659644
Daclatasvir	13	175	738.9	8	4	1	-7.99065	3.3949578
TMC310911	15	179	756	12	3	1	-7.80537	2.014998
Faldaprevir	15	227	869.7999	12	4	1	-7.36557	2.2707524
Asunaprevir	14	191	748.3	10	3	1	-7.20985	1.5784526
Elbasvir	13	189	882	9	4	1	-7.02102	2.5762348
Velpatasvir	13	193	883	10	4	1	-6.81942	2.5264175
Atazanavir	18	171	704.9	9	5	1	-6.6754	1.4590093
Paritaprevir	7	198	765.9	10	3	1	-6.58898	2.9824302
Nelfinavir	10	127	567.8	6	4	1	-6.44515	2.6811311

Picornaviridae - Foot-and-mouth disease virus

Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-8.11791	2.5394499
Ritonavir	18	202	720.9	9	4	1	-8.04774	5.0281134
Faldaprevir	15	227	869.7999	12	4	1	-7.77907	3.9540565
Cobicistat	20	195	776	10	3	1	-7.74635	3.7080991
Velpatasvir	13	193	883	10	4	1	-7.55509	2.0866845
TMC310911	15	179	756	12	3	1	-7.50971	1.8903565
Elbasvir	13	189	882	9	4	1	-7.45923	1.7902089
Grazoprevir	8	204	766.9	11	3	1	-7.23185	3.4524331
Simeprevir	8	194	749.9	10	2	1	-7.0612	2.5247068
Nelfinavir	10	127	567.8	6	4	1	-6.89386	1.5721376

Picornaviridae - Sicinivirus A

Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Elbasvir	13	189	882	9	4	1	-9.60662	3.9389417
Pibrentasvir	17	200	1113.2	17	4	1	-9.45904	1.5180686
Simeprevir	8	194	749.9	10	2	1	-9.05039	2.0904777

Faldaprevir	15	227	869.7999	12	4	1	-9.01861	1.0372427
TMC310911	15	179	756	12	3	1	-8.96993	4.0140924
Glecaprevir	7	204	838.9	15	3	1	-8.93224	1.7932105
Ritonavir	18	202	720.9	9	4	1	-8.75001	2.0592415
Paritaprevir	7	198	765.9	10	3	1	-8.54128	5.9056072
Asunaprevir	14	191	748.3	10	3	1	-8.38819	1.7741857
Atazanavir	18	171	704.9	9	5	1	-8.21476	2.2124505

Picornaviridae - Porcine aichi virus

Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-9.53585	3.3291364
Elbasvir	13	189	882	9	4	1	-8.64773	4.9959693
Cobicistat	20	195	776	10	3	1	-7.71308	2.4279871
Grazoprevir	8	204	766.9	11	3	1	-7.66645	3.9634478
Asunaprevir	14	191	748.3	10	3	1	-7.66037	3.969944
Faldaprevir	15	227	869.7999	12	4	1	-7.44145	3.0836513
Velpatasvir	13	193	883	10	4	1	-7.40925	1.6757953
Ritonavir	18	202	720.9	9	4	1	-7.36326	2.9577777
Daclatasvir	13	175	738.9	8	4	1	-7.2574	1.7913272
Indinavir	12	118	613.8	7	4	1	-7.24389	2.8436437

Picornaviridae - Poliovirus

Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Daclatasvir	13	175	738.9	8	4	1	-8.89528	2.0335491
Velpatasvir	13	193	883	10	4	1	-8.57167	4.1986799
TMC310911	15	179	756	12	3	1	-8.50119	2.0121818
Indinavir	12	118	613.8	7	4	1	-8.38184	2.4691854
Atazanavir	18	171	704.9	9	5	1	-8.32909	1.8969368
Faldaprevir	15	227	869.7999	12	4	1	-8.16512	2.3023481

Asunaprevir	14	191	748.3	10	3	1	-7.91606	4.277133
Glecaprevir	7	204	838.9	15	3	1	-7.90509	3.0035627
Fosamprenavir	14	186	585.6	11	4	1	-7.85395	1.9007305
Grazoprevir	8	204	766.9	11	3	1	-7.853	2.4681702

Picornaviridae - Coxsackievirus B

Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-10.2691	3.1064909
Faldaprevir	15	227	869.7999	12	4	1	-9.36034	2.706239
Elbasvir	13	189	882	9	4	1	-9.27429	2.6072867
Atazanavir	18	171	704.9	9	5	1	-8.92829	3.235029
Daclatasvir	13	175	738.9	8	4	1	-8.81252	2.2757351
Simeprevir	8	194	749.9	10	2	1	-8.67508	1.9548296
Ritonavir	18	202	720.9	9	4	1	-8.51379	1.693522
Asunaprevir	14	191	748.3	10	3	1	-8.30589	2.8585947
Grazoprevir	8	204	766.9	11	3	1	-8.26416	2.5908279
Lopinavir	15	120	628.8	5	4	1	-8.26413	2.3035035

Picornaviridae - Enterovirus 71

Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Lopinavir	15	120	628.8	5	4	1	-8.05083	2.3307419
Velpatasvir	13	193	883	10	4	1	-7.81302	1.482374
Faldaprevir	15	227	869.7999	12	4	1	-7.71272	1.406225
Ritonavir	18	202	720.9	9	4	1	-7.69824	2.0875652
Elbasvir	13	189	882	9	4	1	-7.648	2.7108085
Atazanavir	18	171	704.9	9	5	1	-7.59563	2.3386309
Asunaprevir	14	191	748.3	10	3	1	-7.53451	1.7668103
Simeprevir	8	194	749.9	10	2	1	-7.40489	2.9410374
Remdesivir	14	204	602.6	13	4	1	-7.24998	1.988232

Daclatasvir	13	175	738.9	8	4	1	-7.06726	1.8579408
Picornaviridae - Encephalomyocarditis virus								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-9.10627	1.8265388
Cobicistat	20	195	776	10	3	1	-8.69375	1.9722017
Elbasvir	13	189	882	9	4	1	-8.33936	1.7930715
Faldaprevir	15	227	869.7999	12	4	1	-7.78355	2.7007823
Grazoprevir	8	204	766.9	11	3	1	-7.74204	1.4567504
Simeprevir	8	194	749.9	10	2	1	-7.69588	1.1795809
Paritaprevir	7	198	765.9	10	3	1	-7.66112	5.6915388
Glecaprevir	7	204	838.9	15	3	1	-7.61538	2.0355229
Asunaprevir	14	191	748.3	10	3	1	-7.59181	3.0439818
TMC310911	15	179	756	12	3	1	-7.5566	2.6050415
Picornaviridae - Enterovirus D68								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-8.90819	2.6152112
Tmc310911	15	179	756	12	3	1	-7.92275	1.8912758
Grazoprevir	8	204	766.9	11	3	1	-7.82144	1.916132
Asunaprevir	14	191	748.3	10	3	1	-7.72846	3.4367688
Velpatasvir	13	193	883	10	4	1	-7.72295	2.8790085
Daclatasvir	13	175	738.9	8	4	1	-7.70067	1.68752
Cobicistat	20	195	776	10	3	1	-7.58851	3.2509
Atazanavir	18	171	704.9	9	5	1	-7.42024	2.6924884
Elbasvir	13	189	882	9	4	1	-7.41226	2.8252082
Faldaprevir	15	227	869.7999	12	4	1	-7.32369	1.5882791
Permutotetraviridae - Thosea asigna virus								

Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Pibrentasvir	17	200	1113.2	17	4	1	-8.36022	4.3056946
Elbasvir	13	189	882	9	4	1	-7.57189	4.549839
Daclatasvir	13	175	738.9	8	4	1	-7.36794	2.5047803
Velpatasvir	13	193	883	10	4	1	-7.34419	1.8090734
Asunaprevir	14	191	748.3	10	3	1	-7.21125	1.3827612
Saquinavir	13	167	670.8	7	5	1	-7.06066	4.2023182
Tmc310911	15	179	756	12	3	1	-6.98785	2.0409074
Faldaprevir	15	227	869.7999	12	4	1	-6.94982	1.6306881
Cobicistat	20	195	776	10	3	1	-6.92816	2.6698358
Beclabuvir	6	113	659.8	7	1	1	-6.80299	1.6370478
Coronaviridae - Severe acute respiratory syndrome coronavirus 2								
Drug information						Other relevant docking results		
drug name	rotatable bond count	TPSA	Weight	H2 acceptor count	H2 donor count	rseq	S-score	rmsd_refine
Cobicistat	20	195	776	10	3	1	-8.97678	2.7672822
Pibrentasvir	17	200	1113.2	17	4	1	-8.34582	2.4019134
Faldaprevir	15	227	869.7999	12	4	1	-8.26969	2.1635737
Ritonavir	18	202	720.9	9	4	1	-8.19398	3.2771966
Velpatasvir	13	193	883	10	4	1	-8.13801	2.666265
Asunaprevir	14	191	748.3	10	3	1	-7.5965	2.9216647
Saquinavir	13	167	670.8	7	5	1	-7.5766	2.3707156
Daclatasvir	13	175	738.9	8	4	1	-7.46685	1.8453356
Tipranavir	11	114	602.7	10	2	1	-7.46614	3.5127912
Beclabuvir	6	113	659.8	7	1	1	-7.3573	1.7283682