

IUCrJ

Volume 8 (2021)

Supporting information for article:

VirusMED: an atlas of hotspots of viral proteins

**HuiHui Zhang, Pei Chen, Haojie Ma, Magdalena Woinska, Dejian Liu,
David Cooper, Guo Peng, Yousong Peng, Lei Deng, Wladek Minor and
Heping Zheng**

Table S2 The list of drugs in complex with viral proteins in virusMED.

family	species	drug_name	component_name
Caliciviridae	Norwalk virus	Fluorouracil, Ribavirin	RNA Dependent RNA Polymerase
Coronaviridae	Severe acute respiratory syndrome-related coronavirus	Chlorzoxazone, Dalfampridine, Histamine, Kinetin, Nicotinamide, Pyrazinamide, Salicylamide	Non-Structural Protein 3
		Clonidine, Ifenprodil, Masitinib, Sulfapyridine	3c-Like Proteinase
		Tipiracil	Uridylate-Specific Endoribonuclease
Filoviridae	Zaire ebolavirus	Benzatropine, Bepidil, Paroxetine, Sertraline	Envelope Glycoprotein, Virion Spike Glycoprotein, Ebov-Gp1
		Clomipramine, Imipramine, Thioridazine	Ebola Surface Glycoprotein, Gp1
		Ibuprofen, Toremifene	Envelope Glycoprotein
		Benzatropine	Virion Spike Glycoprotein, Virion Spike Glycoprotein, Ebola Virus (Makona) Gp2
Flaviviridae	Hepacivirus C	Asunaprevir, Grazoprevir, Simeprevir	Non-Structural Protein 4a, Serine Protease Ns3
		Asunaprevir, Grazoprevir	Ns3 Protease
Herpesviridae	Human α -herpesvirus 8	Acyclovir, Ganciclovir, Idoxuridine, Penciclovir	Thymidine Kinase
	Human γ -herpesvirus 8	Raltitrexed	Thymidylate Synthase
Myoviridae	Escherichia virus T4	Glucosamine, Guaiacol, Toluene	Tail-Associated Lysozyme
		Toluene	Lysozyme
	Escherichia virus RB69	Foscarnet	Dna Polymerase
	Escherichia virus RB43	Phylloquinone	Vitamin K Epoxide Reductase-Like Protein, Termini Restrained By Green Fluorescent Protein
Nimaviridae	White spot syndrome virus	Methotrexate	Thymidylate Synthase
Orthomyxoviridae	Influenza A virus	Phentermine, Rimantadine	Matrix Protein 2
		Peramivir, Zanamivir	Neuraminidase
		Taurine	Hemagglutinin

	Influenza B virus	Peramivir, Zanamivir	Neuraminidase
Paramyxo- viridae	Human respirovirus 3	Zanamivir	Hemagglutinin-Neuraminidase
Poxviridae	Vaccinia virus	Rifabutin, Rifampicin, Rifapentine, Rifaximin	Scaffold Protein D13
		Cysteamine	Envelope Protein H3
Retroviridae	Human immunodeficiency virus 1	Amprenavir, Atazanavir, Indinavir, Lopinavir, Nelfinavir, Oxygen, Ritonavir, Saquinavir, Tipranavir	Protease, Tethered Dimer
		Delavirdine, Doravirine, Efavirenz, Etravirine, Foscarnet, Nevirapine, Ralpivirine	Reverse Transcriptase/Ribonuclease H
		Amphetamine, Amprenavir, Lopinavir, Saquinavir	Protease
		Acepromazine	HIV-1 trans activating region RNA
		Dolutegravir	Integrase
		Human immunodeficiency virus 2	Amprenavir, Indinavir
	Western chimpanzee simian foamy virus	Dolutegravir, Elvitegravir, Raltegravir	Pfv Integrase
	Murine leukemia virus	Amprenavir	Gag-Pro-Pol Polyprotein
	Primate T- lymphotropic virus 1	Indinavir	Protease
	Simian immunodeficiency virus	Dolutegravir	Pol Protein
	Feline immunodeficiency virus	Lopinavir	Feline Immunodeficiency Virus Protease
Togaviridae	Aura virus	Piperazine	Capsid Protein
	Sindbis virus	Formaldehyde	Capsid