

Applied Microbiology and Biotechnology

**Main Protease Inhibitors and Drug Surface Hotspot for the Treatment of
COVID-19: Drug Repurposing and Molecular Docking Approach**

**Mahmudul Hasan^{1†}, Md. Sorwer Alam Parvez^{2†}, Kazi Faizul Azim³, Md. Abdus Shukur
Imran¹, Topu Raihan², Airin Gulshan⁴, Samuel Muhit⁵, Rubaiat Nazneen Akhand⁶, Md
Bashir Uddin^{7*#}, Syed Sayeem Uddin Ahmed^{8**}**

¹Department of Pharmaceuticals and Industrial Biotechnology, Sylhet Agricultural University, Sylhet 3100, Bangladesh

²Department of Genetic Engineering and Biotechnology, Shahjalal University of Science and Technology, Sylhet-3114

³Department of Microbial Biotechnology, Sylhet Agricultural University, Sylhet 3100, Bangladesh

⁴Faculty of Biotechnology and Genetic Engineering, Sylhet Agricultural University, Sylhet 3100, Bangladesh

⁵School of Health Sciences, Central Michigan University, Mount Pleasant, Michigan 48859, United States

⁶Department of Biochemistry and Chemistry, Sylhet Agricultural University, Sylhet 3100, Bangladesh

⁷Department of Medicine, Sylhet Agricultural University, Sylhet 3100, Bangladesh

⁸Department of Epidemiology and Public Health, Sylhet Agricultural University, Sylhet 3100, Bangladesh

***Correspondence**

bashir.vetmed@sau.ac.bd [MB Uddin]

ahmedssu.eph@sau.ac.bd [SSU Ahmed]

Supplementary Tables

Table S1. List of all approved Main Protease Protein (MPP) inhibitors retrieved from the DrugBank of NCBI.

<i>MPP inhibitors</i>	<i>DrugBank ID</i>	<i>Group</i>	<i>Description</i>
Amprenavir	DB00701	Approved, Investigational	HIV protease inhibitor
Asunaprevir	DB11586	Approved, Investigational, Withdrawn	NS3 protease inhibitor
Atazanavir	DB01072	Approved, Investigational	antiretroviral protease inhibitor
Paritaprevir	DB09297	Approved, Investigational	HCV NS3/4A protease inhibitor
Grazoprevir	DB11575	Approved	HCV NS3/4A protease inhibitor
Glecaprevir	DB13879	Approved, Investigational	HCV NS3/4A protease inhibitor
Ritonavir	DB00503	Approved, Investigational	HIV protease inhibitor
Nelfinavir	DB00220	Approved	HIV-1 protease inhibitor
Lopinavir	DB01601	Approved	antiretroviral protease inhibitor
Simeprevir	DB06290	Approved	HCV NS3/4A protease inhibitor
Telaprevir	DB05521	Approved, Withdrawn	HCV NS3/4A protease inhibitor
Indinavir	DB00224	Approved	specific HIV protease inhibitor
Darunavir	DB01264	Approved	HIV protease inhibitor
Fosamprenavir	DB01319	Approved	HIV protease inhibitor
Saquinavir	DB01232	Approved, Investigational	HIV protease inhibitor
Boceprevir	DB08873	Approved, Withdrawn	HCV NS3/4A protease inhibitor

Table S2. List of the derivatives of Paritaprevir retrieved from NCBI.

<i>PubChem ID</i>	<i>IUPAC Name</i>
CID 131982844	(3S,9Z,12R,15S,17R)-N-cyclopropylsulfonyl-12-methyl-3-[(5-methylpyrazine-2-carbonyl)amino]-2,14-dioxo-17-phenanthridin-6-yloxy-1,13-diazabicyclo[13.3.0]octadec-9-ene-12-carboxamide
CID 117860584	(1S,4R,6S,7Z,14S,18R)-N-cyclopropylsulfonyl-18-(3,9-difluorophenanthridin-6-yl)oxy-14-[(1-methylpyrazole-4-carbonyl)amino]-2,15-dioxo-3,16-diazatricyclo[14.3.0.04,6]nonadec-7-ene-4-carboxamide
CID 144881776	(4S,6R,10S,16Z)-N-cyclopropylsulfonyl-10-[(5-methylpyrazine-2-carbonyl)amino]-3,9-dioxo-6-phenanthridin-6-yloxy-2,8-diazatricyclo[15.2.1.04,8]icos-16-ene-1-carboxamide
CID 144881777	(4S,6R,10S,16Z)-N-cyclopropylsulfonyl-10-[(5-methylpyrazine-2-carbonyl)amino]-3,9-dioxo-6-phenanthridin-6-yloxy-2,8-diazatricyclo[15.2.1.04,8]icos-16-ene-1-carboxamide
CID 89997958	(1R,4S,6R,10S,16Z)-N-cyclopropylsulfonyl-10-[(5-methylpyrazine-2-carbonyl)amino]-3,9-dioxo-6-phenanthridin-6-yloxy-2,8-diazatricyclo[15.2.1.04,8]icos-16-ene-1-carboxamide
CID 90479564	(1S,4R,6S,7Z,14S,18R)-N-cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.04,6]nonadec-7-ene-4-carboxamide;dihydrate
CID 117930281	(1S,4R,6S,7Z,14S)-N-cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.04,6]nonadec-7-ene-4-carboxamide
CID 126760198	(1S,4R,7Z,14S,18R)-N-cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.04,6]nonadec-7-ene-4-carboxamide
CID 130368695	(1S,6S,7Z,14S,18R)-N-cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.04,6]nonadec-7-ene-4-carboxamide

CID 129606829	(1R,4S,6R,7Z,14R,18S)-N-cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 134503655	(1S,4R,7Z,14S)-N-cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 91971755	(1S,4R,6S,7Z,14S,18R)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-N-(2,2,3,3-tetradeuteriocyclopropyl)sulfonyl-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 129190351	(1S,4R,7Z,18R)-N-cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 134689630	(7Z)-N-cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 76528926	N-cyclopropylsulfonyl-8,8-difluoro-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadecane-4-carboxamide
CID 57415626	(1S,4R,6S,14S,18R)-N-cyclopropylsulfonyl-8,8-difluoro-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadecane-4-carboxamide
CID 132247343	(3S,9Z,12R,15S,17R)-N-cyclopropylsulfonyl-11-methyl-3-[(5-methylpyrazine-2-carbonyl)amino]-2,14-dioxo-17-phenanthridin-6-yloxy-1,13-diazabicyclo[13.3.0]octadec-9-ene-12-carboxamide
CID 123539122	N-cyclopropylsulfonyl-9,9-difluoro-12-methyl-3-[(5-methylpyrazine-2-carbonyl)amino]-2,14-dioxo-17-phenanthridin-6-yloxy-1,13-diazabicyclo[13.3.0]octadecane-12-carboxamide
CID 68500653	(1S,4R,6S,14S,18R)-N-cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide

CID 139266795	<i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide;dihydrate
CID 140642412	(7 <i>Z</i>)- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-14-(pyrazine-2-carbonylamino)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 75093025	<i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 123207199	<i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2-oxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 45110641	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-14-(pyridazine-4-carbonylamino)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 126970090	(1 <i>R</i> ,4 <i>R</i> ,6 <i>S</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 134693118	(1 <i>S</i> ,4 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 145142292	(1 <i>S</i> ,4 <i>R</i> ,8 <i>Z</i> ,15 <i>S</i> ,19 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-15-[(5-methylpyrazine-2-carbonyl)amino]-2,16-dioxo-19-phenanthridin-6-yloxy-3,17-diazatricyclo[15.3.0.0 ^{4,7}]icosa-5,8-diene-4-carboxamide
CID 134322927	(3 <i>S</i> ,9 <i>Z</i> ,12 <i>R</i> ,15 <i>S</i> ,17 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-11,12-dimethyl-3-[(5-methylpyrazine-2-carbonyl)amino]-2,14-dioxo-17-(phenanthridin-6-yloxymethyl)-1,13-diazabicyclo[13.3.0]octadec-9-ene-12-carboxamide
CID 67985746	(1 <i>S</i> ,4 <i>R</i> ,7 <i>Z</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-14-(pyrazine-2-carbonylamino)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide

CID 68496388	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-14-(pyridazine-4-carbonylamino)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 45110639	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-14-(pyrazine-2-carbonylamino)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 144678769	(1 <i>S</i> ,4 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-5-methylidene-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-(phenanthridin-6-yloxymethyl)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 68498031	(1 <i>S</i> ,4 <i>R</i> ,6 <i>R</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 132207185	(1 <i>S</i> ,4 <i>R</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-(phenanthridin-6-yloxymethyl)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 123457581	<i>N</i> -cyclopropylsulfonyl-8,8-difluoro-5-methyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadecane-4-carboxamide
CID 68494543	<i>N</i> -ethylethanamine;(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylic acid
CID 68494548	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylic acid
CID 140642415	(7 <i>Z</i>)- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-14-(pyridazine-4-carbonylamino)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 144411760	(1 <i>S</i> ,4 <i>S</i> ,15 <i>S</i> ,19 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-9,9-difluoro-15-[(5-methylpyrazine-2-carbonyl)amino]-2,16-dioxo-19-phenanthridin-6-yloxy-3,17-diazatricyclo[15.3.0.0 ^{4,7}]icos-5-yne-4-carboxamide

CID 144411796	(1 <i>S</i> ,4 <i>R</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-8,8-difluoro-5-methyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadecane-4-carboxamide
CID 123172379	<i>N</i> -cyclopropylsulfonyl-12-methyl-3-[(5-methylpyrazine-2-carbonyl)amino]-2,14-dioxo-17-phenanthridin-6-yloxy-1,13-diazabicyclo[13.3.0]octadec-9-ene-12-carboxamide
CID 58001490	<i>N</i> -[(2 <i>S</i>)-1-[(2 <i>S</i>)-2-[[1 <i>R</i> ,2 <i>S</i>)-1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(7-methoxy-2-phenylquinolin-4-yl)oxypyrrolidin-1-yl]-3-[methyl(prop-2-enoyl)amino]-1-oxopropan-2-yl]pyrazine-2-carboxamide
CID 123747270	<i>N</i> -cyclopropylsulfonyl-6-methylidene-15-[(5-methylpyrazine-2-carbonyl)amino]-2,16-dioxo-19-phenanthridin-6-yloxy-3,17-diazatricyclo[15.3.0.0 ^{4,7}]icos-8-ene-4-carboxamide
CID 139598190	(1 <i>S</i> ,4 <i>R</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylic acid
CID 77506125	3- <i>O</i> - <i>tert</i> -butyl 4- <i>O</i> -ethyl 14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-3,4-dicarboxylate
CID 87473268	(1 <i>S</i> ,4 <i>R</i> ,6 <i>R</i> ,7 <i>E</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 133548468	(1 <i>R</i> ,4 <i>S</i> ,6 <i>R</i> ,7 <i>E</i> ,14 <i>R</i> ,18 <i>S</i>)- <i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 123942813	ethyl (1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylate
CID 68499876	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)-14-amino- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide

CID 143897349	(1 <i>S</i> ,4 <i>R</i> ,6 <i>R</i> ,14 <i>S</i> ,18 <i>R</i>)-14-anilino- <i>N</i> -cyclopropylsulfonyl-18-isoquinolin-1-yloxy-2,15-dioxo-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadecane-4-carboxamide
CID 87474442	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>E</i> ,14 <i>S</i> ,18 <i>R</i>)-14-amino- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 123706840	<i>N</i> -cyclopropylsulfonyl-5-methylidene-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 123764424	<i>N</i> -cyclopropylsulfonyl-15-[(5-methylpyrazine-2-carbonyl)amino]-2,16-dioxo-19-phenanthridin-6-yloxy-3,17-diazatricyclo[15.3.0.0 ^{4,7}]icos-8-ene-4-carboxamide
CID 144881773	<i>N</i> -[(1 <i>S</i> ,4 <i>R</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)-18-(7,8-dihydrophenanthridin-6-yloxy)-2,15-dioxo-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-en-14-yl]-5-methylpyrazine-2-carboxamide
CID 44180178	<i>N</i> -[(2 <i>S</i>)-1-[(2 <i>S</i> ,4 <i>R</i>)-2-[[1 <i>R</i> ,2 <i>S</i>)-1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(7-methoxy-2-phenylquinolin-4-yl)oxypyrrolidin-1-yl]-3-[methyl(prop-2-enoyl)amino]-1-oxopropan-2-yl]pyrazine-2-carboxamide
CID 131982843	(1 <i>S</i> ,4 <i>R</i> ,8 <i>Z</i> ,15 <i>S</i> ,19 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-15-[(5-methylpyrazine-2-carbonyl)amino]-2,16-dioxo-19-phenanthridin-6-yloxy-3,17-diazatricyclo[15.3.0.0 ^{4,7}]icos-8-ene-4-carboxamide
CID 73211765	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide;hydrate
CID 89997539	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,18 <i>R</i>)-1-[6-(cyclopropylsulfonylcarbamoyl)-3-methylpyrazin-2-yl]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 123658396	<i>N</i> -cyclopropylsulfonyl-12-ethyl-3-[(5-methylpyrazine-2-carbonyl)amino]-2,14-dioxo-17-phenanthridin-6-yloxy-1,13-diazabicyclo[13.3.0]octadec-9-ene-12-carboxamide

CID 16075882	<i>tert</i> -butyl <i>N</i> -[(2 <i>S</i>)-1-[(2 <i>S</i> ,4 <i>R</i>)-2-[[1-(1 <i>R</i> ,2 <i>S</i>)-1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(3-pyrazin-2-ylisoquinolin-1-yl)oxypyrrolidin-1-yl]-3,3-dimethyl-1-oxobutan-2-yl]carbamate
CID 23595603	<i>tert</i> -butyl <i>N</i> -[1-[2-[[1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(3-pyrazin-2-ylisoquinolin-1-yl)oxypyrrolidin-1-yl]-3,3-dimethyl-1-oxobutan-2-yl]carbamate
CID 123202053	<i>N</i> -[2-ethenyl-1-[(1-methylcyclopropyl)sulfonylcarbamoyl]cyclopropyl]-22,25-dioxo-11-pyridin-4-yl-2,21-dioxa-4,23,26-triazapentacyclo[24.2.1.0 ^{3,12} .0 ^{5,10} .0 ^{18,20}]nonacos-3,5,7,9,11-pentaene-27-carboxamide
CID 87476180	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>E</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-14-(pyrazine-2-carbonylamino)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 87475090	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>E</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 117625846	(1 <i>R</i> ,18 <i>R</i> ,20 <i>R</i> ,24 <i>S</i> ,27 <i>S</i>)-24-cyclohexyl- <i>N</i> -[(3 <i>S</i>)-3-ethyl-1-[(1-methylcyclopropyl)sulfonylamino]-1-oxopent-4-en-2-yl]-22,25-dioxo-11-pyridin-4-yl-2,21-dioxa-4,23,26-triazapentacyclo[24.2.1.0 ^{3,12} .0 ^{5,10} .0 ^{18,20}]nonacos-3,5,7,9,11-pentaene-27-carboxamide
CID 87471819	<i>N</i> -ethylethanamine;(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>E</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylic acid
CID 87473750	3- <i>O</i> - <i>tert</i> -butyl 4- <i>O</i> -ethyl (1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>E</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-3,4-dicarboxylate
CID 23595490	<i>N</i> -[1-[2-[[1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(6-methoxyisoquinolin-1-yl)oxypyrrolidin-1-yl]-3,3-dimethyl-1-oxobutan-2-yl]pyrazine-2-carboxamide

CID 16075909	<i>N</i> -[(2 <i>S</i>)-1-[(2 <i>S</i> ,4 <i>R</i>)-2-[[<i>(1R</i> ,2 <i>S</i>)-1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(6-methoxyisoquinolin-1-yl)oxypyrrolidin-1-yl]-3,3-dimethyl-1-oxobutan-2-yl]pyrazine-2-carboxamide
CID 58594019	<i>tert</i> -butyl (2 <i>S</i> ,4 <i>R</i>)-2-[[<i>(1R</i> ,2 <i>S</i>)-1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(3-pyridin-4-ylisoquinolin-1-yl)oxypyrrolidine-1-carboxylate
CID 68500752	(1 <i>R</i> ,2 <i>S</i>)-2-ethenyl-2-ethyl-1-[(2-methylpropan-2-yl)oxycarbonyl]-[(2 <i>S</i> ,4 <i>R</i>)-1-[2-[(5-methylpyrazine-2-carbonyl)amino]non-8-enoyl]-4-phenanthridin-6-yloxy]pyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylic acid
CID 67296958	(1 <i>R</i> ,2 <i>S</i>)-2-ethenyl-2-ethyl-1-[(2-methylpropan-2-yl)oxycarbonyl]-[(2 <i>S</i> ,4 <i>R</i>)-1-[(2 <i>S</i>)-2-[(5-methylpyrazine-2-carbonyl)amino]non-8-enoyl]-4-phenanthridin-6-yloxy]pyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylic acid
CID 129900715	<i>N</i> -[2-[(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>R</i> ,18 <i>R</i>)-4-(2-cyclopropylsulfonylacetyl)-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-en-14-yl]acetyl]-5-methylpyrazine-2-carboxamide
CID 23595731	<i>tert</i> -butyl 2-[[1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(3-pyridin-4-ylisoquinolin-1-yl)oxypyrrolidine-1-carboxylate
CID 68498890	3- <i>O</i> - <i>tert</i> -butyl 4- <i>O</i> -ethyl (1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-3,4-dicarboxylate
CID 67983962	ethyl (1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylate
CID 87471820	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>E</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylic acid
CID 58594100	<i>N</i> -[(2 <i>S</i>)-1-[(2 <i>S</i>)-2-[[<i>(1R</i> ,2 <i>S</i>)-1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(6-methoxyisoquinolin-1-yl)oxypyrrolidin-1-yl]-3,3-dimethyl-1-oxobutan-2-yl]pyrazine-2-carboxamide

CID 87472503	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>E</i> ,14 <i>S</i> ,18 <i>R</i>)- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-14-(pyridazine-4-carbonylamino)-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide
CID 68496037	ethyl (1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylate;hydrochloride
CID 87472307	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>E</i> ,14 <i>S</i> ,18 <i>R</i>)-19-ethyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylic acid
CID 67296951	ethyl (1 <i>R</i> ,2 <i>S</i>)-2-ethenyl-1-[(2-methylpropan-2-yl)oxycarbonyl]-[(2 <i>S</i> ,4 <i>R</i>)-1-[(2 <i>S</i>)-2-[(5-methylpyrazine-2-carbonyl)amino]non-8-enoyl]-4-phenanthridin-6-yloxypyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylate
CID 141228784	ethyl (2 <i>S</i>)-2-ethenyl-1-[(2-methylpropan-2-yl)oxycarbonyl]-[(2 <i>S</i> ,4 <i>R</i>)-1-[2-[(5-methylpyrazine-2-carbonyl)amino]non-8-enoyl]-4-phenanthridin-6-yloxypyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylate
CID 67296803	2-ethenyl-1-[[[(2 <i>S</i>)-2-[(5-methylpyrazine-2-carbonyl)amino]non-8-enoyl]-[(2 <i>S</i> ,4 <i>R</i>)-4-phenanthridin-6-yloxypyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylic acid
CID 58594022	(2 <i>S</i> ,4 <i>R</i>)- <i>N</i> -[(1 <i>R</i> ,2 <i>S</i>)-1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]-4-(3-pyrazin-2-yloxyquinolin-1-yl)oxypyrrolidine-2-carboxamide
CID 58593964	<i>tert</i> -butyl (2 <i>S</i> ,4 <i>R</i>)-2-[[[(1 <i>R</i> ,2 <i>S</i>)-1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(3-pyrazin-2-yloxyquinolin-1-yl)oxypyrrolidine-1-carboxylate
CID 67296808	2-ethenyl-1-[[[(2 <i>S</i> ,4 <i>R</i>)-1-[(2 <i>S</i>)-2-[(5-methylpyrazine-2-carbonyl)amino]non-8-enoyl]-4-phenanthridin-6-yloxypyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylic acid
CID 68494544	(1 <i>S</i> ,4 <i>R</i> ,6 <i>S</i> ,7 <i>Z</i> ,14 <i>S</i> ,18 <i>R</i>)-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylic acid

CID 68496262	2-ethenyl-1-[[<i>(2S,4R)</i> -1-[2-[(5-methylpyrazine-2-carbonyl)amino]non-8-enoyl]-4-phenanthridin-6-yloxy]pyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylic acid
CID 135001966	ethyl (<i>1R,2S</i>)-2-ethenyl-1-[[<i>(2S,4R)</i> -1-[(<i>2S</i>)-2-[(2-methylpropan-2-yl)oxycarbonyl-(5-methylpyrazine-2-carbonyl)amino]non-8-enoyl]-4-phenanthridin-6-yloxy]pyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylate
CID 23595521	<i>N</i> -[1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]-4-(3-pyrazin-2-ylisoquinolin-1-yl)oxypyrrolidine-2-carboxamide
CID 23595734	<i>tert</i> -butyl 2-[[1-(cyclopropylsulfonylcarbamoyl)-2-ethenylcyclopropyl]carbamoyl]-4-(3-pyrazin-2-ylisoquinolin-1-yl)oxypyrrolidine-1-carboxylate
CID 86660471	ethyl (<i>1R,2S</i>)-2-ethenyl-1-[[<i>(2S,4R)</i> -1-[(<i>2S</i>)-2-[(5-methylpyrazine-2-carbonyl)amino]non-8-enoyl]-4-phenanthridin-6-yloxy]pyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylate
CID 117804962	<i>N</i> -[(<i>Z,2S</i>)-1-[(<i>2S,4R</i>)-2-carbamoyl-4-phenanthridin-6-yloxy]pyrrolidin-1-yl]-9-[(<i>1S,2S</i>)-2-(cyclopropylsulfonylcarbamoyl)cyclopropyl]-1-oxonon-8-en-2-yl]-5-methylpyrazine-2-carboxamide
CID 144881772	<i>N</i> -cyclopropylsulfonylacetamide; <i>N</i> -[(<i>1S,4R,7Z,14S,18R</i>)-18-(7,8-dihydrophenanthridin-6-yloxy)-2,15-dioxo-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-en-14-yl]-5-methylpyrazine-2-carboxamide
CID 68499875	(<i>1S,4R,6S,7Z,14S,18R</i>)-14-amino- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide;hydrochloride
CID 87472306	(<i>1S,4R,6S,7E,14S,18R</i>)-19-ethyl-14-[(5-methylpyrazine-2-carbonyl)amino]-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxylic acid;hydrochloride
CID 87474441	(<i>1S,4R,6S,7E,14S,18R</i>)-14-amino- <i>N</i> -cyclopropylsulfonyl-2,15-dioxo-18-phenanthridin-6-yloxy-3,16-diazatricyclo[14.3.0.0 ^{4,6}]nonadec-7-ene-4-carboxamide;hydrochloride

Table S3. Molecular Docking Result of Protease Inhibitors with Binding Energy.

<i>Main Protease Protein Inhibitors</i>	<i>Molecular Binding Affinity with SARS-COV-2 (kcal/mol)</i>
Paritaprevir	-10.9
Glecaprevir	-9.3
Nelfinavir	-8.7
Simeprevir	-8.6
Lopinavir	-8.4
Ritonavir	-8.4
Telaprevir	-8.3
Grazoprevir	-8.3
Indinavir	-8.2
Amprenavir	-7.9
Atazanavir	-7.9
Darunavir	-7.9
Fosamprenavir	-7.9
Saquinavir	-7.9
Asunaprevir	-7.4
Boceprevir	-7.1

Table S4. Molecular Docking Result of Paritaprevir derivatives.

<i>Derivatives of Paritaprevir</i>	<i>Molecular Binding Affinity with SARS-COV-2 (kcal/mol)</i>	<i>Derivatives of Paritaprevir</i>	<i>Molecular Binding Affinity with SARS-COV-2 (kcal/mol)</i>	<i>Derivatives of Paritaprevir</i>	<i>Molecular Binding Affinity with SARS-COV-2 (kcal/mol)</i>
CID 131982844	-16.3	CID132207185	-14.4	CID117625846	-12.8
CID 117860584	-16.1	CID 123457581	-14.4	CID87471819	-12.7
CID 144881776	-16.1	CID68494543	-14.3	CID87473750	-12.7
CID 144881777	-16	CID68494548	-14.3	CID 23595490	-12.7
CID 89997958	-15.5	CID140642415	-14.3	CID16075909	-12.6
CID 90479564	-15.2	CID144411760	-14.3	CID58594019	-12.6
CID 117930281	-15.2	CID144411796	-14.3	CID68500752	-12.6
CID 126760198	-15.2	CID 123172379	-14.3	CID67296958	-12.5
CID 130368695	-15.2	CID58001490	-14.2	CID129900715	-12.5
CID 129606829	-15.2	CID123747270	-14.2	CID 23595731	-12.5
CID 134503655	-15.2	CID139598190	-14.2	CID68498890	-12.4
CID 91971755	-15.2	CID 77506125	-14.2	CID 67983962	-12.4
CID129190351	-15.1	CID87473268	-14.1	CID 87471820	-12.4
CID134689630	-15.1	CID133548468	-14.1	CID68499875	-12.1
CID 76528926	-15.1	CID123942813	-14	CID58594100	-12
CID57415626	-14.9	CID 68499876	-13.9	CID87472503	-12
CID132247343	-14.9	CID143897349	-13.8	CID68496037	-11.7
CID 123539122	-14.9	CID 87474442	-13.8	CID 87472307	-11.6
CID68500653	-14.8	CID123706840	-13.7	CID67296951	-11.5
CID139266795	-14.8	CID123764424	-13.7	CID141228784	-11.5
CID140642412	-14.8	CID144881773	-13.7	CID 67296803	-11.4
CID 75093025	-14.8	CID44180178	-13.6	CID58594022	-11.2
CID 123207199	-14.8	CID131982843	-13.6	CID58593964	-11.1
CID45110641	-14.7	CID 73211765	-13.5	CID67296808	-11.1
CID126970090	-14.7	CID 89997539	-13.5	CID 68494544	-11.1
CID134693118	-14.7	CID 123658396	-13.4	CID68496262	-11
CID145142292	-14.7	CID16075882	-13.3	CID135001966	-10.8
CID134322927	-14.7	CID 23595603	-13.3	CID 23595521	-10.8
CID 67985746	-14.7	CID 123202053	-13.2	CID 23595734	-10.4
CID 68496388	-14.7	CID87472306	-13.2	CID86660471	-10.1
CID45110639	-14.6	CID87476180	-13	CID 117804962	-8.7
CID144678769	-14.6	CID87474441	-12.9	CID144881772	-5.6
CID68498031	-14.4	CID87475090	-12.8		

Table S5. ADME analysis of top ten Paritaprevir derivatives by using SwissADME.

Parameter		PubChem ID of Paritaprevir derivatives									
		CID 131982844	CID 117860584	CID 144881776	CID 144881777	CID 89997958	CID 90479564	CID 117930281	CID 126760198	CID 130368695	CID 129606829
Physico-chemical parameters	Formula	C40H45N7O7S	C39H41F2N7O7S	C41H45N7O7S	C41H45N7O7S	C39H41N7O7S	C40H47N7O9S	C40H43N7O7S	C40H43N7O7S	C40H43N7O7S	C40H43N7O7S
	Molecular weight	767.89 g/mol	789.85 g/mol	779.90 g/mol	779.90 g/mol	751.85 g/mol	801.91 g/mol	765.88 g/mol	765.88 g/mol	765.88 g/mol	765.88 g/mol
	Molar Refractivity	214.07	208.36	216.76	216.76	206.99	218.05	211.96	211.96	211.96	211.96
	TPSA	198.03 Å ²	190.07 Å ²	198.03 Å ²	198.03 Å ²	198.03 Å ²	216.49 Å ²	198.03 Å ²	198.03 Å ²	198.03 Å ²	198.03 Å ²
Lipophilicity	Log P _{o/w} (iLOGP)	3.82	3.54	2.97	4.04	2.37	3.37	2.33	3.12	5.53	3.22
	Log P _{o/w} (XLOGP3)	5.1	4.57	4.67	4.67	4.25	3.7	4.65	4.65	4.65	4.65
	Log P _{o/w} (WLOGP)	4.28	4.65	4.43	4.43	3.58	3.76	3.89	3.89	3.89	3.89
	Log P _{o/w} (MLOGP)	0.88	2.26	1.05	1.05	0.71	-0.59	0.88	0.88	0.88	0.88
	Log P _{o/w} (SILICOS-IT)	2.59	2.18	2.91	2.91	1.74	2.28	2.28	2.28	2.28	2.28
	Consensus Log P _{o/w}	3.33	3.44	3.2	3.42	2.53	2.51	2.81	2.96	3.45	2.98
Pharmacokinetics Water	GI absorption	Low	Low	Low	Low	Low	Low	Low	Low	Low	Low
	BBB permeant	No	No	No	No	No	No	No	No	No	No
	P-gp substrate	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
	CYP1A2 inhibitor	No	No	No	No	No	No	No	No	No	No
	CYP2C19 inhibitor	No	No	No	No	No	No	No	No	No	No
	CYP2C9 inhibitor	No	No	No	No	Yes	No	No	No	No	No
	CYP2D6 inhibitor	No	No	No	No	No	No	No	No	No	No
	CYP3A4 inhibitor	Yes	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
	Log K _p (skin permeation)	-7.36 cm/s	-7.87 cm/s	-7.74 cm/s	-7.74 cm/s	-7.87 cm/s	-8.56 cm/s	-7.67 cm/s	-7.67 cm/s	-7.67 cm/s	-7.67 cm/s
	Log S (SILICOS-IT)	-10.09	-9.02	-10.45	-10.45	-9.38	-9.74	-9.74	-9.74	-9.74	-9.74
Water Solubility	Solubility	6.30e-08 mg/ml ; 8.20e-11 mol/l	7.53e-07 mg/ml ; 9.53e-10 mol/l	2.77e-08 mg/ml ; 3.56e-11 mol/l	2.77e-08 mg/ml ; 3.56e-11 mol/l	3.15e-07 mg/ml ; 4.19e-10 mol/l	1.45e-07 mg/ml ; 1.81e-10 mol/l	1.38e-07 mg/ml ; 1.81e-10 mol/l	1.38e-07 mg/ml ; 1.81e-10 mol/l	1.38e-07 mg/ml ; 1.81e-10 mol/l	1.38e-07 mg/ml ; 1.81e-10 mol/l

pdb | 5RH9 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RH8 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RH7 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RH6 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RH5 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RH4 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RH3 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RH2 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RH1 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RH0 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RGZ | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RGY | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RGX | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RGW | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RGV | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RGU | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RGT | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6WQF | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RHF | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5RHE | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6W63 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5R84 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5R82 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5R81 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 5R7Y | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6YZ6 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6XCH | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6YT8 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6YNQ | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6YVF | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6WTK | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6WTJ | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 6XB2 | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 7C8U | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 7BRR | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 7BRP | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR
pdb | 7BRO | YEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVR

pdb | 6WTT | QCSGVTHHHHHH
pdb | 6XG2 | QCSGVTFQ----
pdb | 6XB1 | QCSGVTFQ----
pdb | 6XB0 | QCSGVTFQ----
pdb | 6XBI | QCSGVTFQ----
pdb | 6XBG | QCSGVTFQ----
pdb | 6XBH | QCSGVTFQ----
pdb | 6XFN | QCSGVTFQ----
pdb | 6XA4 | QCSGVTFQ----
pdb | 6M0K | QCSGVT-----
pdb | 6LZE | QCSGV-----
pdb | 6M2N | QCSGVTFQ----
pdb | 6Y2G | QCSGVTFQ----
pdb | 6WTM | QCSGVTFQ----
pdb | 7BUY | QCSGVTFQ----
pdb | 6Y2F | QCSGVTFQ----
pdb | 6Y2E | QCSGVTFQ----
pdb | 7BQY | QCSGVTFQ----

pdb 6LU7	QCSGVTFQ-----
pdb 5RGS	QCSGVTFQ-----
pdb 5RGR	QCSGVTFQ-----
pdb 5RGQ	QCSGVTFQ-----
pdb 5RGP	QCSGVTFQ-----
pdb 5RGO	QCSGVTFQ-----
pdb 5RGN	QCSGVTFQ-----
pdb 5RGM	QCSGVTFQ-----
pdb 5RGL	QCSGVTFQ-----
pdb 5RGK	QCSGVTFQ-----
pdb 5RGJ	QCSGVTFQ-----
pdb 5RGI	QCSGVTFQ-----
pdb 5RGH	QCSGVTFQ-----
pdb 5RGG	QCSGVTFQ-----
pdb 5RG3	QCSGVTFQ-----
pdb 5RG2	QCSGVTFQ-----
pdb 5RG1	QCSGVTFQ-----
pdb 6M2Q	QCSGVTFQ-----
pdb 6WNP	QCSGVTFQ-----
pdb 5R83	QCSGVTFQ-----
pdb 5R80	QCSGVTFQ-----
pdb 5R7Z	QCSGVTFQ-----
pdb 6YB7	QCSGVTFQ-----
pdb 5R8T	QCSGVTFQ-----
pdb 5RG0	QCSGVTFQ-----
pdb 5RFZ	QCSGVTFQ-----
pdb 5RFY	QCSGVTFQ-----
pdb 5RFX	QCSGVTFQ-----
pdb 5RFW	QCSGVTFQ-----
pdb 5RFV	QCSGVTFQ-----
pdb 5RFU	QCSGVTFQ-----
pdb 5RFT	QCSGVTFQ-----
pdb 5RFS	QCSGVTFQ-----
pdb 5RFR	QCSGVTFQ-----
pdb 5RFQ	QCSGVTFQ-----
pdb 5RFP	QCSGVTFQ-----
pdb 5RFO	QCSGVTFQ-----
pdb 5RFN	QCSGVTFQ-----
pdb 5RFM	QCSGVTFQ-----
pdb 5RFL	QCSGVTFQ-----
pdb 5RFK	QCSGVTFQ-----
pdb 5RFJ	QCSGVTFQ-----
pdb 5RFI	QCSGVTFQ-----
pdb 5RFH	QCSGVTFQ-----
pdb 5RFG	QCSGVTFQ-----
pdb 5RFF	QCSGVTFQ-----
pdb 5RFB	QCSGVTFQ-----
pdb 5RFE	QCSGVTFQ-----
pdb 5RFD	QCSGVTFQ-----
pdb 5RFC	QCSGVTFQ-----
pdb 5RFA	QCSGVTFQ-----
pdb 5RF9	QCSGVTFQ-----
pdb 5RF8	QCSGVTFQ-----
pdb 5RF7	QCSGVTFQ-----
pdb 5RF6	QCSGVTFQ-----
pdb 5RF5	QCSGVTFQ-----
pdb 5RF0	QCSGVTFQ-----

pdb 5RF1	QCSGVTFQ-----
pdb 5RF2	QCSGVTFQ-----
pdb 5RF3	QCSGVTFQ-----
pdb 5RF4	QCSGVTFQ-----
pdb 5REZ	QCSGVTFQ-----
pdb 5REY	QCSGVTFQ-----
pdb 5REX	QCSGVTFQ-----
pdb 5REW	QCSGVTFQ-----
pdb 5REV	QCSGVTFQ-----
pdb 5REU	QCSGVTFQ-----
pdb 5RET	QCSGVTFQ-----
pdb 5RES	QCSGVTFQ-----
pdb 5RER	QCSGVTFQ-----
pdb 5REP	QCSGVTFQ-----
pdb 5REO	QCSGVTFQ-----
pdb 5REN	QCSGVTFQ-----
pdb 5REM	QCSGVTFQ-----
pdb 5REL	QCSGVTFQ-----
pdb 5REK	QCSGVTFQ-----
pdb 5REJ	QCSGVTFQ-----
pdb 5REI	QCSGVTFQ-----
pdb 5REH	QCSGVTFQ-----
pdb 5REG	QCSGVTFQ-----
pdb 5REF	QCSGVTFQ-----
pdb 5REE	QCSGVTFQ-----
pdb 5RED	QCSGVTFQ-----
pdb 5REC	QCSGVTFQ-----
pdb 5REB	QCSGVTFQ-----
pdb 5REA	QCSGVTFQ-----
pdb 5RE9	QCSGVTFQ-----
pdb 5RE8	QCSGVTFQ-----
pdb 5RE7	QCSGVTFQ-----
pdb 5RE6	QCSGVTFQ-----
pdb 5RE5	QCSGVTFQ-----
pdb 5RE4	QCSGVTFQ-----
pdb 6Y84	QCSGVTFQ-----
pdb 6M03	QCSGVTFQ-----
pdb 5RHD	QCSGVTFQ-----
pdb 5RHC	QCSGVTFQ-----
pdb 5RHB	QCSGVTFQ-----
pdb 5RHA	QCSGVTFQ-----
pdb 5RH9	QCSGVTFQ-----
pdb 5RH8	QCSGVTFQ-----
pdb 5RH7	QCSGVTFQ-----
pdb 5RH6	QCSGVTFQ-----
pdb 5RH5	QCSGVTFQ-----
pdb 5RH4	QCSGVTFQ-----
pdb 5RH3	QCSGVTFQ-----
pdb 5RH2	QCSGVTFQ-----
pdb 5RH1	QCSGVTFQ-----
pdb 5RH0	QCSGVTFQ-----
pdb 5RGZ	QCSGVTFQ-----
pdb 5RGY	QCSGVTFQ-----
pdb 5RGX	QCSGVTFQ-----
pdb 5RGW	QCSGVTFQ-----
pdb 5RGV	QCSGVTFQ-----
pdb 5RGU	QCSGVTFQ-----

pdb 5RGT	QCSGVTFQ-----
pdb 6WQF	QCSGVTFQ-----
pdb 5RHF	QCSGVTFQ-----
pdb 5RHE	QCSGVTFQ-----
pdb 6W63	QCSGVTFQ-----
pdb 5R84	QCSGVTFQ-----
pdb 5R82	QCSGVTFQ-----
pdb 5R81	QCSGVTFQ-----
pdb 5R7Y	QCSGVTFQ-----
pdb 6YZ6	QCSGVTFQ-----
pdb 6XCH	QCSGVTFQ-----
pdb 6YT8	QCSGVTFQ-----
pdb 6YNQ	QCSGVTFQ-----
pdb 6YVF	QCSGVTFQ-----
pdb 6WTK	QCSGVTFQ-----
pdb 6WTJ	QCSGVTFQ-----
pdb 6XB2	QCSGVTFQ-----
pdb 7C8U	QCSGVTFQ-----
pdb 7BRR	QCSGVTFQ-----
pdb 7BRP	QCSGVTFQ-----
pdb 7BRO	QCSGVTFQ-----
