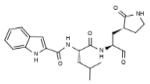
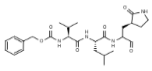
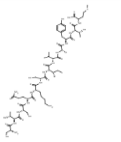
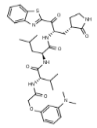
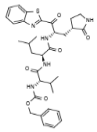
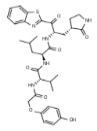
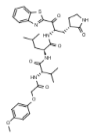
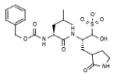
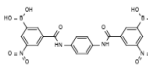
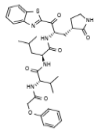
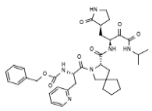
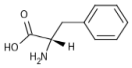
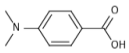
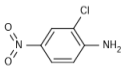
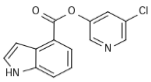
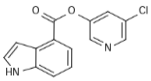
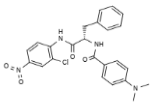
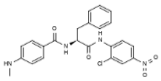
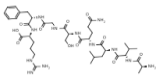
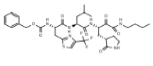
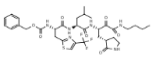
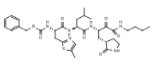
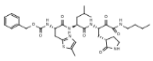
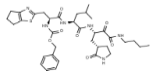
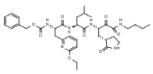
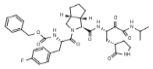
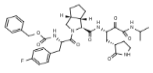
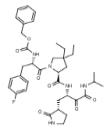
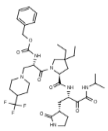
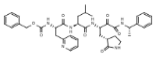
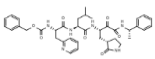
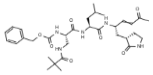
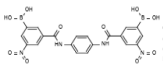
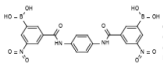
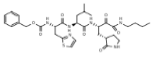
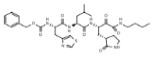
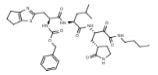
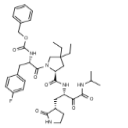
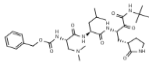
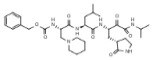
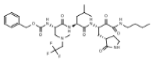
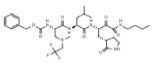
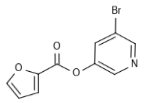
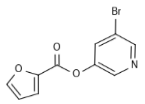
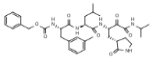
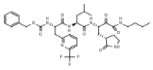
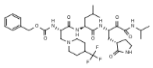
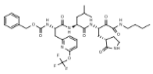
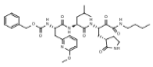
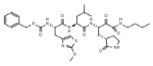
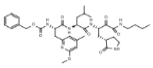
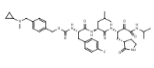
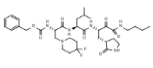
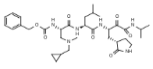
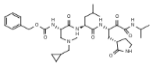
Reaxys® Medicinal Chemistry

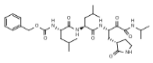
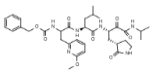
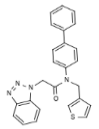
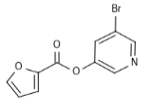
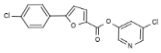
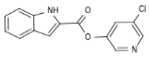
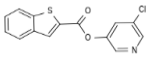
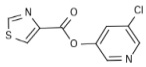
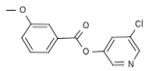
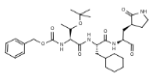
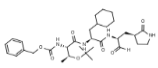
Structure	SMILES	Reaxys Registry Number	Link to Reaxys	pX	CAS Registry Number	Chemical Name	Molecular Formula	Molecular Weight	InChI Key	LogP	Lipinski Number	Veber Number	Target Name	Target Species	Substance Action on Target	Bioassay Details	Measured Parameter	Unit	Qualitative value	Quantitative value
	CC(C)C[C@H](NC(=O)C1=CC2=CC=CC=C2N1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	1.3E+07	1.3E+07	10.7		N-((S)-1-((S)-1-formyl-2-((S)-2-oxopyrrolidin-3-yl)ethylcarbamoyl)-3-methylbutyl)-1H-indole-2-carboxamide	C22H28N4O	412.489	HXJZYYCIU	2.331	4	1	Sars Cov 3C-Like Protease [Coronaviridae]	Coronavirdae	Inhibitor	Inhibitory a	IC50	nM	=	0.02
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)NC(C[C@@H]1CCNC1=O)C=O	1.5E+07	1.5E+07	10.2		N-[(benzyloxy)carbonyl]-L-valyl-N1-(1-formyl-2-[(3S)-2-oxopyrrolidin-3-yl]ethyl)-L-leucinamide	C26H38N4O	502.611	RUHYGYHI	2.682	3	0	Sars Cov 3C-Like Protease [Coronaviridae]	Coronavirdae	Inhibitor	Inhibitory a	IC50	nM	=	0.06
	CC[C@H](C)[C@H](NC(=O)[C@H](CO)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCC(N)=O)NC(=O)[C@H](CO)NC(=O)[C@@H](NC(=O)[C@@H](NC(O)[C@@H](C)O)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](CC1=CC=C(O)C=C1)C(=O)N[C@@H](([C@@H](C)O)C(=O)N[C@@H](CCSC)C(O)=O	2.5E+07	2.5E+07	8.73			C56H94N14	1315.51	RBLTWUZI	-8.375	1	0	Spike glycoprotein [SARS coronavirus]	SARS coronavirus	Inhibitor	Concentrat	IC50	nM	=	1.88
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	8.52	1417704-35-8		C35H46N6O	678.853	CALSXGHS	3.516	2	0	3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]	SARS coronavirus			Ki (inhibitio	muM		0.003
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	8.39	1359941-93-7		C33H41N5O	635.784	KSCRVOKC	3.789	2	0	3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]	SARS coronavirus			Ki (inhibitio	muM		0.0041
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	7.96	1359941-94-8		C33H41N5O	651.784	ORLPJQUZ	2.901	3	0	3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]	SARS coronavirus			Ki (inhibitio	muM		0.011
	COC1=CC=C(OCC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)C2=NC3=CC=CC=C3S2)C=C1	2.3E+07	2.3E+07	7.85	1383922-80-2		C34H43N5O	665.811	DYFSDLME	3.222	3	0	3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]	SARS coronavirus			Ki (inhibitio	muM		0.014
	[Na+].CC(C)C[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC1CCNC1=O)C(O)S([O-])(=O)=O	2.3E+07	2.3E+07	7.7	1416992-39-0	sodium (2S)-2-((S)-2-(((benzyloxy)carbonyl)amino)-4-methylpentanamido)-1-hydroxy-3-(2-oxopyrrolidin-3-yl)propane-1-sulfonate	C21H30N3O	507.54	BSPJDKCM	0.325	2	0	3C-like protease [Coronavirinae]	Coronavirinae	Inhibitor		EC50	muM		0.02 - 0.05
	OB(O)C1=CC(=CC(=C1)N(=O)=O)C(=O)NC1=CC=C(NC(=O)C2=CC(=CC(=C2)B(O)O)N(=O)=O)C=C1	1.9E+07	1.9E+07	7.66	693235-40-4		C20H16B2N	493.99	JBHJLTFEE	1.798	3	1	3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]	SARS coronavirus			Ki (inhibitio	muM		0.022
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	7.66	1383922-52-8		C33H41N5O	635.784	APIXGBAH	3.307	3	0	3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]	SARS coronavirus			Ki (inhibitio	muM		0.022
	CC(C)NC(=O)C(=O)[C@H](C[C@@H](1CCNC1=O)N(C(=O)[C@@H](1CCC2(CCC2)CN1C(=O)[C@H](CC1=NC=CC=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	7.6		benzyl N-[(2S)-1-oxo-1-[(3S)-3-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]-2-azaspiro[4.4]nonan-2-yl]-3-(pyridin-2-yl)propan-2-yl]carbamate	C36H46N6O	674.797	BYAQBIUK	2.502	2	0	3CL protease [Human coronavirus 229E]	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.6

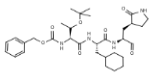
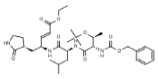
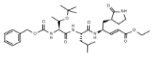
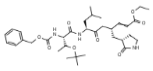
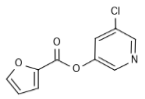
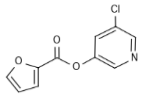
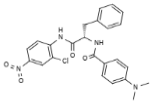
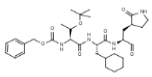
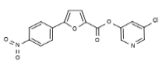
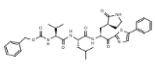
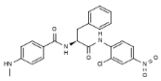
	[H][C@](N)([H])CC1=CC=CC=C1)C(O)=O	1910408	1910408	**7.52**	63-91-2	L-phenylalanine	C9H11NO2	165.192	COLNVLDH	0.84	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/	In vitro bin	Ki (inhibitio	muM	=	0.03
	CN(C)C1=CC=C(C=C1)C(O)=O	386867	386867	**7.52**	619-84-1	p-N,N-dimethylaminobenzoic acid; 4-(Dimethylamino)benzoic acid	C9H11NO2	165.192	YDIYEOMD	1.846	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/	In vitro bin	Ki (inhibitio	muM	=	0.03
	NC1=C(Cl)C=C(C=C1)N(=O)=O	638657	638657	**7.52**	121-87-9	2-Chloro-4-nitroaniline	C6H5ClN2O2	172.571	LOCWBQJV	1.719	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/	In vitro bin	Ki (inhibitio	muM	=	0.03
	ClC1=CN=CC(OC(=O)C2=C3C=CNC3=CC=C2)=C1	1.9E+07	1.9E+07	**7.52**	1087243-14-5		C14H9ClN2O	272.691	BOSZJNSIC	3.047	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus		Inhibitory c	IC50	nM		30
	ClC1=CN=CC(OC(=O)C2=C3C=CNC3=CC=C2)=C1	1.9E+07	1.9E+07	**7.52**	1087243-14-5		C14H9ClN2O	272.691	BOSZJNSIC	3.047	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c	IC50	nM	=	30
	CN(C)C1=CC=C(C=C1)C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O	1E+07	1E+07	**7.52**			C24H23ClN4	466.924	NBBWJEW	4.859	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			Ki (inhibitio	muM		0.03
	CNC1=CC=C(C=C1)C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)NC1=CC=C(C=C1Cl)N(=O)=O	2.6E+07	2.6E+07	**7.52**			C23H21ClN4	452.897	FQYWZML	4.296	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibition c	Ki (inhibitio	muM	=	0.03
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)N)C(C)C)C(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CO)C(=O)NCC(=O)N[C@@H](CC1=CC=CC=C1)C(=O)N[C@@H](CCCNC(N)=N)C(O)=O	2.6E+07	2.6E+07	**7.51**	608531-54-0		C39H64N12	877.011	MTHIRMPI	-4.414	1	0	**Sars Cov 3C-Like Protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c	IC50	muM	=	0.031
	CCCCNC(=O)C(=O)[C@H](C)C[C@@H](1CCNC1=O)N(C(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(=CS1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.5**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[4-(trifluoromethyl)-1,3-thiazol-2-yl]ethyl]carbamate	C33H43F3N	724.802	SQARSOUI	3.306	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.5
	CCCCNC(=O)C(=O)[C@H](C)C[C@@H](1CCNC1=O)N(C(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(=CS1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.5**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[4-(trifluoromethyl)-1,3-thiazol-2-yl]ethyl]carbamate	C33H43F3N	724.802	SQARSOUI	3.306	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.5
	CCCCNC(=O)C(=O)[C@H](C)C[C@@H](1CCNC1=O)N(C(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(=CS1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.5**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(5-methyl-1,3-thiazol-2-yl)ethyl]carbamate	C33H46N6O	670.83	GKSGNHPI	1.908	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.5

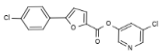
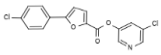
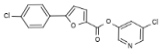
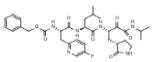
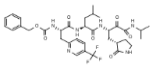
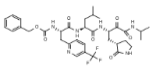
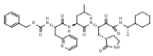
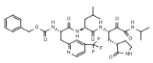
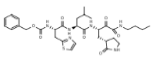
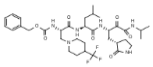
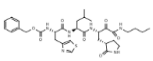
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC=C(S1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.5**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(5-methyl-1,3-thiazol-2-yl)ethyl]carbamate	C33H46N6O	670.83	GKSGNHPI	1.908	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.5
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC=C(CCC2)S1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.5**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(4H,5H,6H-cyclopenta[d][1,3]thiazol-2-yl)ethyl]carbamate	C35H48N6O	696.868	JOVXDSIHI	2.266	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.5
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(OCCC)=CC=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.5**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(6-ethoxypyridin-2-yl)ethyl]carbamate	C36H50N6O	694.828	JMSOJCLYI	3.755	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.5
	[H][C@@]12CCC[C@]1([H])[C@H](N[C2(C(=O)[C@H](CC1=CC=C(F)C=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.5**		benzyl N-[(2S)-1-[(1S,3aR,6aS)-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]octahydrocyclopenta[c]pyrrol-2-yl]-3-(4-fluorophenyl)-1-oxopropan-2-yl]carbamate	C36H44FN5	677.773	GCSPVCXS	3.159	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.5
	[H][C@@]12CCC[C@]1([H])[C@H](N[C2(C(=O)[C@H](CC1=CC=C(F)C=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.5**		benzyl N-[(2S)-1-[(1S,3aR,6aS)-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]octahydrocyclopenta[c]pyrrol-2-yl]-3-(4-fluorophenyl)-1-oxopropan-2-yl]carbamate	C36H44FN5	677.773	GCSPVCXS	3.159	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.5
	CCC1(CC)C[C@H](N(C1)C(=O)[C@H](CC1=CC=C(F)C=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.5**		benzyl N-[(2S)-1-[(2S)-4,4-diethyl-2-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]pyrrolidin-1-yl]-3-(4-fluorophenyl)-1-oxopropan-2-yl]carbamate	C37H48FN5	693.816	AFQMPDIC	4.166	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.5
	CCC1(CC)C[C@H](N(C1)C(=O)[C@H](CN1CCC(C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.5**		benzyl N-[(2S)-1-[(2S)-4,4-diethyl-2-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]pyrrolidin-1-yl]-1-oxo-3-[4-(trifluoromethyl)piperidin-1-yl]propan-2-yl]carbamate	C37H53F3N	750.859	MXYZABAJ	4.153	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.5
	CC(C)C[C@H](NC(=O)[C@H](CC1=NC=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H](C)CC1=O)C(=O)N[C@@H](C)C1=CC=CC=C1	3.3E+07	3.3E+07	**7.5**		benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[[(1S)-1-phenylethyl]carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-(pyridin-2-yl)ethyl]carbamate	C38H46N6O	698.819	NADDXCJM	3.575	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.5
	CC(C)C[C@H](NC(=O)[C@H](CC1=NC=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H](C)CC1=O)C(=O)N[C@@H](C)C1=CC=CC=C1	3.3E+07	3.3E+07	**7.5**		benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[[(1S)-1-phenylethyl]carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-(pyridin-2-yl)ethyl]carbamate	C38H46N6O	698.819	NADDXCJM	3.575	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.5
	CC(C)C[C@H](NC(=O)[C@H](CNC(=O)C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=CC(C)=O	2.5E+07	2.5E+07	**7.42**		TG-0204998	C32H47N5O	613.754	YJBNUBPV	2.304	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	muM	0.038
	OB(O)C1=CC(=CC(=C1)N(=O)=O)C(=O)NC1=CC=C(N(C(=O)C2=CC(=CC(=C2)B(O)O)N(=O)=O)C=C1	1.9E+07	1.9E+07	**7.4**	693235-40-4		C20H16B2N	493.99	JBHJLTFEE	1.798	3	1	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Radioligand (/ Inhibition c	Ki (inhibitio	muM	0.04

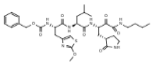
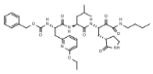
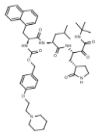
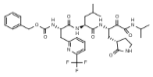
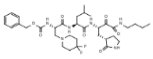
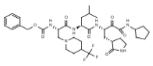
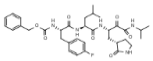
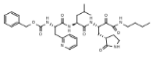
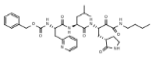
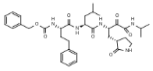
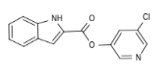
	OB(O)C1=CC(=CC(=C1)N(=O)=O)C(=O)NC1=CC=C(NC(=O)C2=CC(=CC(=C2)B(O)O)N(=O)=O)C=C1	1.9E+07	1.9E+07	**7.4**	693235-40-4		C20H16B2N	493.99	JBHJLTFEE	1.798	3	1	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/	In vitro bin	Ki (inhibitio	muM	=	0.04
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC=CS1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.4**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(1,3-thiazol-2-yl)ethyl]carbamate	C32H44N6O	656.803	SUIHQODL	2.057	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.4
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=CSC=N1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.4**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(1,3-thiazol-4-yl)ethyl]carbamate	C32H44N6O	656.803	CFEMQHZI	2.756	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.4
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC2=C(CCC2)S1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.4**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(4H,5H,6H-cyclopenta[d][1,3]thiazol-2-yl)ethyl]carbamate	C35H48N6O	696.868	JOVXDSIHI	2.266	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.4
	CCC1(CC)C[C@H](N(C1)C(=O)[C@H](CC1=CC=C(F)C=CC=C1)C(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.4**		benzyl N-[(2S)-1-[(2S)-4,4-diethyl-2-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]pyrrolidin-1-yl]-3-(4-fluorophenyl)-1-oxopropan-2-yl]carbamate	C37H48FN5	693.816	AFQMPDIC	4.166	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.4
	CC(C)C[C@H](NC(=O)[C@H](CN(C)C)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.4**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(dimethylamino)ethyl]carbamate	C31H48N6O	616.758	RBXUCWG	1.787	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.4
	CC(C)C[C@H](NC(=O)[C@H](CN1CCCCC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.4**		benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-(piperidin-1-yl)ethyl]carbamate	C33H50N6O	642.796	YAPXNEGF	2.234	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.4
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CN(C)CC(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.4**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[methyl(2,2,2-trifluoroethyl)amino]ethyl]carbamate	C32H47F3N	684.756	DYBMFWII	3.262	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.4
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CN(C)CC(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.4**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[methyl(2,2,2-trifluoroethyl)amino]ethyl]carbamate	C32H47F3N	684.756	DYBMFWII	3.262	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.4
	BrC1=CC[OC(=O)C2=CC=CO2]=CN=C1	1.1E+07	1.1E+07	**7.3**	936371-58-3		C10H6BrNO	268.067	HMICIXHT	1.77	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	nM		50
	BrC1=CC[OC(=O)C2=CC=CO2]=CN=C1	1.1E+07	1.1E+07	**7.3**	936371-58-3		C10H6BrNO	268.067	HMICIXHT	1.77	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c	IC50	nM	=	50

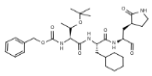
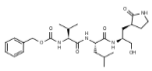
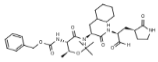
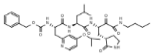
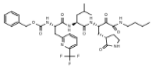
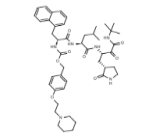
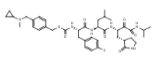
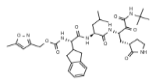
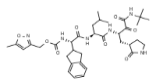
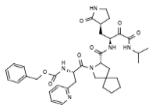
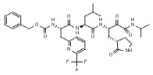
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC(C)=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.3**	benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-(3-methylphenyl)ethyl]carbamate	C35H47N5O	649.787	PVFWUOR	3.822	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	CCCCN(C(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=CC=C(C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.3**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[6-(trifluoromethyl)pyridin-2-yl]ethyl]carbamate	C35H45F3N	718.774	HOPNWLC	3.703	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	CC(C)C[C@H](NC(=O)[C@H](CN1CCC(CC1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.3**	benzyl ((S)-1-(((S)-1-(((S)-4-(isopropylamino)-3,4-dioxo-1-[(S)-2-oxopyrrolidin-3-yl)butan-2-yl)amino)-4-methyl-1-oxopentan-2-yl)amino)-1-oxo-3-(4-(trifluoromethyl)piperidin-1-yl)propan-2-yl)carbamate; benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-	C34H49F3N	710.794	SACDDFO\	3.533	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	CCCCN(C(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(OC(F)(F)F)=CC=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.3**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[6-(trifluoromethoxy)pyridin-2-yl]ethyl]carbamate	C35H45F3N	734.773	BRFLNKOD	4.584	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	CCCCN(C(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(OC)=CC=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.3**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(6-methoxypyridin-2-yl)ethyl]carbamate	C35H48N6O	680.802	KDOSPHR\	3.332	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	CCCCN(C(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=CSC(OC)=N1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.3**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(2-methoxy-1,3-thiazol-4-yl)ethyl]carbamate	C33H46N6O	686.83	JYGUFLM\	2.663	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	CCCCN(C(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(OC)=CC(C)=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.3**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(6-methoxy-4-methylpyridin-2-yl)ethyl]carbamate	C36H50N6O	694.828	LLWOBJFC	3.769	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=C(F)C=C1)NC(=O)OCC1=CC=C(CN(C)C2CC2)C=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.3**	(4-([cyclopropyl(methyl)amino]methyl)phenyl)methyl N-[(1S)-2-(4-fluorophenyl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C39H53FN6	736.884	MEQYIGW	3.84	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.3
	CCCCN(C(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=CC(F)(F)F)CC1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.3**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(4,4-difluoropiperidin-1-yl)ethyl]carbamate	C34H50F2N	692.804	ISOPIEXEA	3.224	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	CC(C)C[C@H](NC(=O)[C@H](CN(C)CC1CC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.3**	benzyl N-[(1S)-2-[(cyclopropylmethyl)(methyl)amino]-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C33H50N6O	642.796	KEVALLZB	2.108	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	CC(C)C[C@H](NC(=O)[C@H](CN(C)CC1CC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.3**	benzyl N-[(1S)-2-[(cyclopropylmethyl)(methyl)amino]-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C33H50N6O	642.796	KEVALLZB	2.108	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.3

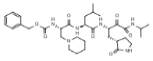
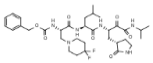
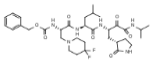
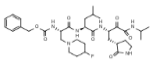
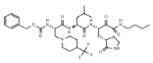
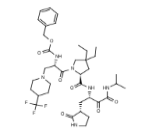
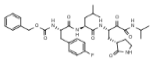
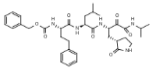
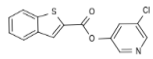
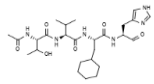
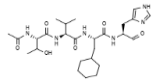
	CC(C)C[C@H](NC(=O)OC1=CC=CC=C1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)N(C)C(C)C	3.3E+07	3.3E+07	**7.3**		benzyl N-[(1S)-3-methyl-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-{(3S)-2-oxopyrrolidin-3-yl}-1-{(propan-2-yl)carbamoyl}propan-2-yl]carbamoyl}butyl]carbamoyl}butyl]carbamate	C31H47N5O	601.743	HEVXFSPU	3.375	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.3
	COC1=CC=CC(CC(NC(=O)OCC2=CC=CC=C2)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)C(=O)NC(C)C)=N1	3.3E+07	3.3E+07	**7.3**		benzyl N-[2-(6-methoxypyridin-2-yl)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-{(3S)-2-oxopyrrolidin-3-yl}-1-{(propan-2-yl)carbamoyl}propan-2-yl]carbamoyl}butyl]carbamoyl}ethyl]carbamate	C34H46N6O	666.775	QNSIYJPYC	2.865	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.3
	O=C(CN1N=NC2=C1C=CC=C2)N(CC1=CSC=C1)C1=CC=C(C=C1)C1=CC=CC=C1	2.4E+07	2.4E+07	**7.29**			C25H20N4O	424.526	BRLBTOJQ	4.926	4	2	**3CLpro (3-chymotrypsin-like protease) [SARS coronavirus]**	SARS coronavirus		IC50	muM	0.051
	BrC1=CC(OC(=O)C2=CC=CO2)=CN=C1	1.1E+07	1.1E+07	**7.28**	936371-58-3		C10H6BrNO	268.067	HMICIXHT	1.77	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		inhibition ra	%	98
	ClC1=CC=C(C=C1)C1=CC=C(O1)C(=O)OC1=CC(Cl)=CN=C1	1.1E+07	1.1E+07	**7.28**			C16H9Cl2NO	334.158	UICFGOSR	4.169	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		inhibition ra	%	98
	ClC1=CN=CC(OC(=O)C2=CC3=CC=CC=C3N2)=C1	1.1E+07	1.1E+07	**7.28**			C14H9ClN2O	272.691	LJTINUKM	3.06	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		inhibition ra	%	99
	ClC1=CN=CC(OC(=O)C2=CC3=CC=CC=C3S2)=C1	1.1E+07	1.1E+07	**7.28**			C14H8ClNO	289.742	MNUHXGJ	3.294	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		inhibition ra	%	96
	ClC1=CN=CC(OC(=O)C2=CSC=N2)=C1	1.1E+07	1.1E+07	**7.28**			C9H5ClN2O	240.67	CSEAAOW	1.798	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		inhibition ra	%	98
	COC1=CC(=CC=C1)C(=O)OC1=CC(Cl)=CN=C1	1.1E+07	1.1E+07	**7.28**			C13H10ClNO	263.68	UIXQHURF	2.809	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		inhibition ra	%	97
	CC(OC(C)(C)C)[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@@H](CC[C@@H]1CCNC1=O)C=O	2.4E+07	2.4E+07	**7.28**		TG-0205221	C32H48N4O	600.756					**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	muM	0.053
	[H]C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC1CCCCC1)NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)[C@H](C)OC(C)(C)C	2.5E+07	2.5E+07	**7.28**			C32H48N4O	600.756	YFUZVOLE	4.541	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [Coronaviridae]**	Coronaviridae	Radioligand (/ In vitro bin	Ki (inhibitio	muM	= 0.053

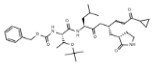
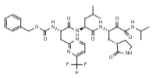
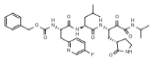
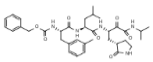
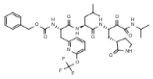
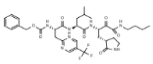
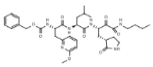
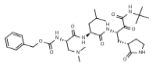
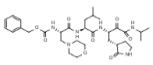
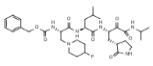
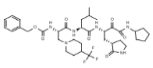
	CC(OC(C)(C)C)[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@@H](C(C@@H]1CCNC1=O)C=O	2.4E+07	2.4E+07	**7.27**	TG-0205221	C32H48N4O	600.756				**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			Ki (inhibitio	muM		0.054
	CCOC(=O)/C=C\/C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)[C@H](C)OC(C)(C)C	2.5E+07	2.5E+07	**7.24**		C33H50N4O	630.782	PWBQMVI	4.109	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [Coronaviridae]**	Coronaviridae	Radioligand (/	In vitro bin	Ki (inhibitio	muM	=	0.058
	CCOC(=O)/C=C\/C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)OC(C)(C)C	2.4E+07	2.4E+07	**7.24**		C33H50N4O	630.782				**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			Ki (inhibitio	muM		0.058
	CCOC(=O)C=C[C@H](C[C@@H]1CCNC1=O)CC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)OC(C)(C)C	2.5E+07	2.5E+07	**7.24**	TG-0203770	C34H51N3O	629.794	JGQOJHCA	4.339	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			Ki (inhibitio	muM		0.058
	ClC1=CC(OC(=O)C2=CC=CO2)=CN=C1	1.1E+07	1.1E+07	**7.22**	353257-73-5	C10H6ClNO	223.616	DWJOEJDC	1.594	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	nM		60
	ClC1=CC(OC(=O)C2=CC=CO2)=CN=C1	1.1E+07	1.1E+07	**7.22**	353257-73-5	C10H6ClNO	223.616	DWJOEJDC	1.594	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory	IC50	nM	=	60
	CN(C)C1=CC=C(C=C1)C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O	1E+07	1E+07	**7.22**		C24H23ClN4	466.924	NBBWJEW	4.859	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.06
	CC(OC(C)(C)C)[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@@H](C(C@@H]1CCNC1=O)C=O	1.4E+07	1.4E+07	**7.22**		C32H48N4O	600.756	YFUZVOLE	4.541	2	0	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus		Inhibition c	Ki (inhibitio	nM	~	60
	ClC1=CC(OC(=O)C2=CC=C(O2)C2=CC=C(C=C2)N(=O)=O)=CN=C1	1.6E+07	1.6E+07	**7.22**	1007551-98-5	C16H9ClN2O	344.711	KVPGYJGIF	3.439	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	nM		60
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N[C@@H](C(C@@H]1CCNC1=O)C(=O)C1=NC=C(S1)C1=CC=CC=C1	2.5E+07	2.5E+07	**7.22**		C35H43N5O	661.822	PJDLIABG	4.017	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			Ki (inhibitio	muM		0.06
	CNC1=CC=C(C=C1)C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)NC1=CC=C(C=C1Cl)N(=O)=O	2.6E+07	2.6E+07	**7.22**		C23H21ClN4	452.897	FQYWZML	4.296	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory a	IC50	muM	=	0.06

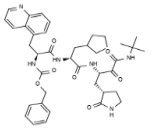
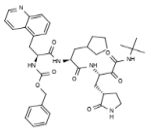
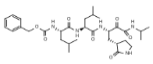
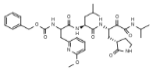
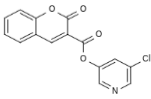
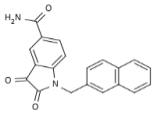
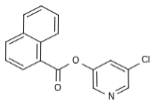
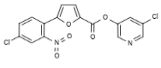
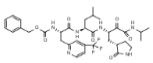
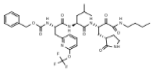
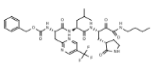
	ClC1=CC=C(C=C1)C1=CC=C(O1)C(=O)OC1=CC(Cl)=CN=C1	1.1E+07	1.1E+07	**7.2**		C16H9Cl2NO	334.158	UICFGOSR	4.169	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM		63
	ClC1=CC=C(C=C1)C1=CC=C(O1)C(=O)OC1=CC(Cl)=CN=C1	1.1E+07	1.1E+07	**7.2**		C16H9Cl2NO	334.158	UICFGOSR	4.169	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM		63
	ClC1=CC=C(C=C1)C1=CC=C(O1)C(=O)OC1=CC(Cl)=CN=C1	1.1E+07	1.1E+07	**7.2**		C16H9Cl2NO	334.158	UICFGOSR	4.169	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c IC50	nM	=	63
	CC(C)C(C@H)NC(=O)(C@H)(CC1=NC=C(F)C=C1)NC(=O)OCC1=CC=CC=C1C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-2-(5-fluoropyridin-2-yl)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl}ethyl]carbamate	C33H43FN6	654.739	PYRJSQGX	2.383	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit		7.2
	CC(C)C(C@H)NC(=O)(C@H)(CC1=NC=C(C=C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl}-2-[5-(trifluoromethyl)pyridin-2-yl]ethyl]carbamate	C34H43F3N	704.747	PVEAZVRG	3.147	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit		7.2
	CC(C)C(C@H)NC(=O)(C@H)(CC1=NC=C(C=C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl}-2-[5-(trifluoromethyl)pyridin-2-yl]ethyl]carbamate	C34H43F3N	704.747	PVEAZVRG	3.147	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit		7.2
	CC(C)C(C@H)NC(=O)(C@H)(CC1=NC=CC=C1)C(=O)OCC1=CC=CC=C1)C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)N(C@@H)(C)C1CCCCC1	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-{[(1S)-1-cyclohexylethyl]carbamoyl}-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-(pyridin-2-yl)ethyl]carbamate	C38H52N6O	704.867	KIPIKDUHE	4.244	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit		7.2
	CC(C)C(C@H)NC(=O)(C@H)(CC1=NC=CC(=C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl}-2-[4-(trifluoromethyl)pyridin-2-yl]ethyl]carbamate	C34H43F3N	704.747	SUGDGIXB	3.147	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit		7.2
	CCCCNC(=O)C(=O)(C@H)(C@@H)(CCNC1=O)NC(=O)(C@H)(CC(C)C)NC(=O)(C@H)(CC1=NC=CS1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-{butylcarbamoyl}-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-(1,3-thiazol-2-yl)ethyl]carbamate	C32H44N6O	656.803	SUIHQODL	2.057	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit		7.2
	CC(C)C(C@H)NC(=O)(C@H)(CN1CCC(CC1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.2**	benzyl (S)-1-(((S)-1-(((S)-4-(isopropylamino)-3,4-dioxo-1-[(S)-2-oxopyrrolidin-3-yl]butan-2-yl)amino)-4-methyl-1-oxopentan-2-yl)amino)-1-oxo-3-(4-(trifluoromethyl)piperidin-1-yl)propan-2-yl)carbamate; benzyl N-[(1S)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-	C34H49F3N	710.794	SACDDFOV	3.533	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit		7.2
	CCCCNC(=O)C(=O)(C@H)(C@@H)(CCNC1=O)NC(=O)(C@H)(CC(C)C)NC(=O)(C@H)(CC1=CSC=N1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-{butylcarbamoyl}-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-(1,3-thiazol-4-yl)ethyl]carbamate	C32H44N6O	656.803	CFEMQHZI	2.756	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit		7.2

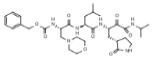
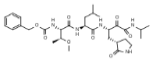
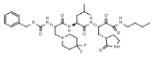
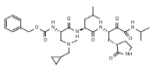
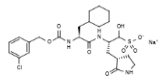
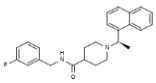
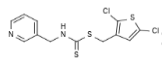
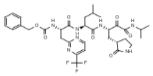
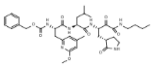
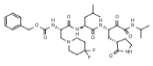
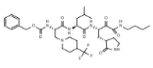
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=CSC(OC)=N1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(2-methoxy-1,3-thiazol-4-yl)ethyl]carbamate	C33H46N6O	686.83	JYGUFLMV	2.663	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.2
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(OCC)=CC=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(6-ethoxypyridin-2-yl)ethyl]carbamate	C36H50N6O	694.828	JMSOJCLYI	3.755	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.2
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=CC2=CC=CC=C12)N(C=O)OCC1=CC=C(OCCN2CCCCC2)C=C1)C(=O)N[C@@H](C[C@@H](C)CCN(C=O)C(=O)C(C)C)C	3.3E+07	3.3E+07	**7.2**	{4-[2-(piperidin-1-yl)ethoxy]phenyl}methyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(naphthalen-1-yl)ethyl]carbamate	C46H62N6O	827.034	SLCZPZZD	5.7	1	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.2
	CC(C)C[C@H](NC(=O)[C@H](CC1=NC(=CC=C1)C(F)(F)F)N(C=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H](CCN(C=O)C(=O)C(C)C)C(=O)C(=O)NC)C(C	3.3E+07	3.3E+07	**7.2**	benzyl ((S)-1-(((S)-1-(((S)-4-(isopropylamino)-3,4-dioxo-1-[(S)-2-oxopyrrolidin-3-yl)butan-2-yl)amino)-4-methyl-1-oxopentan-2-yl)amino)-1-oxo-3-(6-(trifluoromethyl)pyridin-2-yl)propan-2-yl)carbamate; benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-	C34H43F3N	704.747	DQTFXZMI	3.236	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.2
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CN1CCC(F)(F)C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(4,4-difluoropiperidin-1-yl)ethyl]carbamate	C34H50F2N	692.804	ISOPIEXEA	3.224	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.2
	CC(C)C[C@H](NC(=O)[C@H](CN1CCC(CC1)C(F)(F)F)N(C=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC1CCCC1	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(cyclopentylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[4-(trifluoromethyl)piperidin-1-yl]ethyl]carbamate	C36H51F3N	736.832	OWNQCYI	3.909	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.2
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=C(F)C=C1)N(C=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-2-(4-fluorophenyl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C34H44FN5	653.751	ZUZMPCW	3.546	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.2
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=CC=CC=C1)N(C=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(pyridin-2-yl)ethyl]carbamate	C34H46N6O	650.775	DAVBQPJS	2.689	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.2
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC=CC=C1)N(C=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(pyridin-2-yl)ethyl]carbamate	C34H46N6O	650.775	DAVBQPJS	2.689	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7.2
	CC(C)C[C@H](NC(=O)[C@H](CCC1=CC=CC=C1)N(C=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.2**	benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-3-phenylpropyl]carbamate	C35H47N5O	649.787	MHOCJTN	3.743	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7.2
	ClC1=CN=CC(OC(=O)C2=CC3=CC=CC=C3N2)=C1	1.1E+07	1.1E+07	**7.19**	C14H9ClN2O	272.691	LJTINUKM	3.06	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM	65

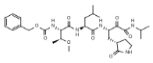
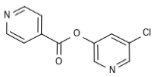
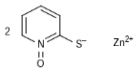
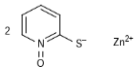
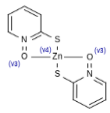
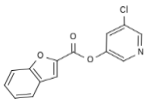
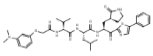
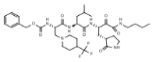
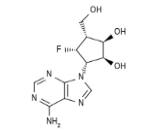
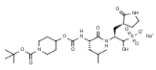
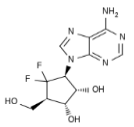
	CC(OC(C)(C)C)[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@@H](C[C@@H](CCN1C1=O)C=O	2.4E+07	2.4E+07	**7.17**		TG-0205221	C32H48N4O	600.756				**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [Human coronavirus 229E]**	Human coronavirus 229E		Ki (inhibitio	muM	=	0.068
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N[C@@H](CO)C[C@@H]1CCNC1=O	1.5E+07	1.5E+07	**7.17**	890648-83-6	N-[(benzyloxy)carbonyl]-L-valyl-N1-((1S)-2-hydroxy-1-{[(3S)-2-oxopyrrolidin-3-yl]methyl}ethyl)-L-leucinamide	C26H40N4O	504.627	GLZAWCK(	2.111	3	0	**Sars Cov 3C-Like Protease [Coronaviridae]**	Coronaviridae	Inhibitor	Inhibitory a	IC50	nM	=	68
	[H]C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](C[C@@H](NC(=O)OCC1=CC=CC=C1)(C[C@H](C)OC(C)(C)C)C	2.5E+07	2.5E+07	**7.17**			C32H48N4O	600.756	YFUZVOLE	4.541	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [Coronaviridae]**	Coronaviridae	Radioligand (/	In vitro bin	Ki (inhibitio	muM	=	0.068
	CCCCCN(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC=CC(OC(C)C)=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.1**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-[4-(propan-2-yloxy)pyridin-2-yl]ethyl]carbamate	C37H52N6O	708.855	QQYAQVN	3.487	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.1
	CCCCCN(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC=CC=C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.1**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-[6-(trifluoromethyl)pyridin-2-yl]ethyl]carbamate	C35H45F3N	718.774	HOPNWLC	3.703	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=C2=CC=CC=C12)N(C)=O)OCC1=CC=C(CN(C)OCCN2CCCCC2)C=C1)C(=O)N(C)[C@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C(C)C	3.3E+07	3.3E+07	**7.1**		{4-[2-(piperidin-1-yl)ethoxy]phenyl}methyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-(naphthalen-1-yl)ethyl]carbamate	C46H62N6O	827.034	SLCZPZZD	5.7	1	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=C(F)C=C1)N(C=O)OCC1=CC=C(CN(C)C2CC2)C=C1)C(=O)N(C)[C@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.1**		(4-{[cyclopropyl(methyl)amino]methyl}phenyl)methyl N-[(1S)-2-(4-fluorophenyl)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl}butyl]carbamoyl}ethyl]carbamate	C39H53FN6	736.884	MEQYIGW	3.84	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=NOC(C)=C1)C1CC2=CC=CC=C2C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C)C	3.3E+07	3.3E+07	**7.1**		(5-methyl-1,2-oxazol-3-yl)methyl N-[(S)-{[(1S)-1-{[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}(2,3-dihydro-1H-inden-2-yl)methyl]carbamate	C35H48N6O	680.802	BETCAOZC	2.793	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=NOC(C)=C1)C1CC2=CC=CC=C2C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C)C	3.3E+07	3.3E+07	**7.1**		(5-methyl-1,2-oxazol-3-yl)methyl N-[(S)-{[(1S)-1-{[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}(2,3-dihydro-1H-inden-2-yl)methyl]carbamate	C35H48N6O	680.802	BETCAOZC	2.793	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.1
	CC(C)NC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@@H]1CC2(CCCC2)CN1C(=O)[C@H](C[C@@H](CC1=NC=CC=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.1**		benzyl N-[(2S)-1-oxo-1-[(3S)-3-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl}-2-azaspiro[4.4]nonan-2-yl]-3-(pyridin-2-yl)propan-2-yl]carbamate	C36H46N6O	674.797	BYAQBIUK	2.502	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)CC1=CC=CC=C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.1**		benzyl (S)-1-(((S)-1-(((S)-4-(isopropylamino)-3,4-dioxo-1-[(S)-2-oxopyrrolidin-3-yl]butan-2-yl)amino)-4-methyl-1-oxopentan-2-yl)amino)-1-oxo-3-(6-(trifluoromethyl)pyridin-2-yl)propan-2-yl)carbamate; benzyl N-[(1S)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-	C34H43F3N	704.747	DQTFXZMI	3.236	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.1

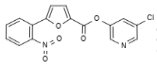
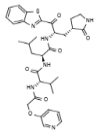
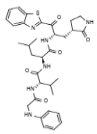
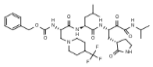
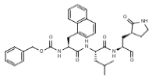
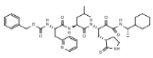
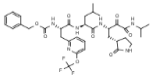
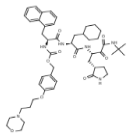
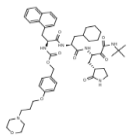
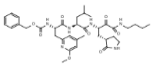
	CC(C)C[C@H](NC(=O)[C@H](CN1CCCCC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.1**	benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-(piperidin-1-yl)ethyl]carbamate	C33H50N6O	642.796	YAPXNEGF	2.234	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@H](CN1CCC(F)(F)CC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.1**	benzyl N-[(1S)-2-(4,4-difluoropiperidin-1-yl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C33H48F2N	678.777	FCTXOXQV	2.757	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@H](CN1CCC(F)(F)CC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.1**	benzyl N-[(1S)-2-(4,4-difluoropiperidin-1-yl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C33H48F2N	678.777	FCTXOXQV	2.757	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@H](CN1CCC(F)(F)CC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.1**	benzyl N-[(1S)-2-(4-fluoropiperidin-1-yl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C33H49FN6	660.786	HLWOHQI	2.378	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.1
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CCC)C(N)C(=O)[C@H](CN1CCC(C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7.1**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[4-(trifluoromethyl)piperidin-1-yl]ethyl]carbamate	C35H51F3N	724.821	ZHJLTDNP	4	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.1
	CCC1(CC)C[C@H](N(C1)C(=O)[C@H](CN1CCC(C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N(C)[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.1**	benzyl N-[(2S)-1-[(2S)-4,4-diethyl-2-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]pyrrolidin-1-yl]-1-oxo-3-[4-(trifluoromethyl)piperidin-1-yl]propan-2-yl]carbamate	C37H53F3N	750.859	MXYZABAJ	4.153	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=C(F)C=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.1**	benzyl N-[(1S)-2-(4-fluorophenyl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C34H44FN5	653.751	ZUZMPCW	3.546	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.1
	CC(C)C[C@H](NC(=O)[C@H](CCC1=CC=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7.1**	benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-3-phenylpropyl]carbamate	C35H47N5O	649.787	MHOCJTN	3.743	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		7.1
	ClC1=CN=CC(OC(=O)C2=CC3=CC=CC=C3S2)=C1	1.1E+07	1.1E+07	**7.02**		C14H8ClNO	289.742	MNUHXGJ	3.294	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	nM		95
	CC(C)[C@H](NC(=O)[C@@H](NC(C)=O)C(C)O)C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@@H](C[C@@H]1CC1=CNC=N1)C=O	2.4E+07	2.4E+07	**7.01**		C26H42N6O	534.656	ZECWIGXE	1.62	1	0	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c	IC50	nM	=	98
	CC(C)[C@H](NC(=O)[C@@H](NC(C)=O)C(C)O)C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@@H](C[C@@H]1CC1=CNC=N1)C=O	2.4E+07	2.4E+07	**7.01**		C26H42N6O	534.656	ZECWIGXE	1.62	1	0	**SARS-CoV 3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor		IC50	muM		0.098

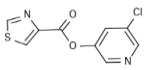
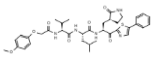
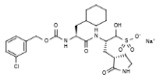
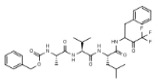
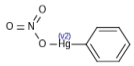
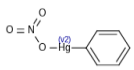
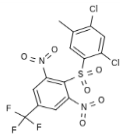
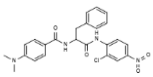
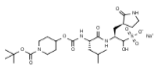
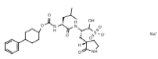
	CC(C)C[C@H](NC(=O)(C@@H](NC(=O)OCC1=CC=CC=C1)C(C)OC(C)(C)C)C1=O)C[C@@H](C[C@@H]1CCNC1=O)C=CC(=O)C1CC1	2.5E+07	2.5E+07	**7**	TG-0205486	C35H51N3O	625.806	CPRMAAC	4.063	3	1	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Ki (inhibitio	muM	0.099
	CC(C)C[C@H](NC(=O)(C@H](CC1=NC(=CC=N1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C)C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-[4-(trifluoromethyl)pyrimidin-2-yl]ethyl]carbamate	C33H42F3N	705.734	FSEJHJVN(	2.195	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7
	CC(C)C[C@H](NC(=O)(C@H](CC1=NC=C(F)C=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-2-(5-fluoropyridin-2-yl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C33H43FN6	654.739	PYRJSQGX	2.383	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7
	CC(C)C[C@H](NC(=O)(C@H](CC1=CC()C=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-(3-methylphenyl)ethyl]carbamate	C35H47N5O	649.787	PVFWUOR	3.822	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7
	CC(C)C[C@H](NC(=O)(C@H](CC1=NC(OC(F)(F)F)=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-[6-(trifluoromethoxy)pyridin-2-yl]ethyl]carbamate	C34H43F3N	720.746	SDGSGHDI	4.117	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC=C(C=N1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[5-(trifluoromethyl)pyrimidin-2-yl]ethyl]carbamate	C34H44F3N	719.761	ICROBMCI	2.573	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(OC)=CC=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(6-methoxypyridin-2-yl)ethyl]carbamate	C35H48N6O	680.802	KDOSPHR\	3.332	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7
	CC(C)C[C@H](NC(=O)(C@H](CN(C)C)NC(=O)OC(C)(C)C)C[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)(C)C	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(dimethylamino)ethyl]carbamate	C31H48N6O	616.758	RBXUCWG	1.787	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7
	CC(C)C[C@H](NC(=O)(C@H](CN1CCOCC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-(morpholin-4-yl)ethyl]carbamate	C32H48N6O	644.769	QPWPPKQ	0.97	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7
	CC(C)C[C@H](NC(=O)(C@H](CN1CCC(F)CC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-2-(4-fluoropiperidin-1-yl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C33H49FN6	660.786	HLWOHQI	2.378	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7
	CC(C)C[C@H](NC(=O)(C@H](CN1CCC(CC1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC1CCCC1	3.3E+07	3.3E+07	**7**	benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(cyclopentylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[4-(trifluoromethyl)piperidin-1-yl]ethyl]carbamate	C36H51F3N	736.832	OWNQCY	3.909	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7

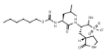
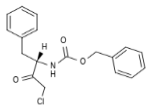
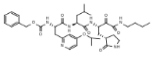
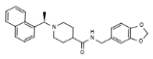
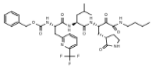
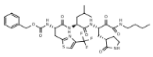
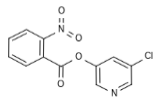
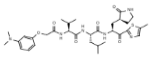
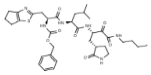
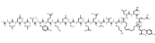
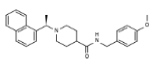
	CC(C)C[N@@H]1CCNC1=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)[C@@H](CC1=CC=CC=C1)NC(=O)OC1=CC=CC=C1	3.3E+07	3.3E+07	**7**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-2-cyclopentylethyl]carbamoyl}-2-(quinolin-5-yl)ethyl]carbamate	C40H50N6O	726.873	VCUZBAJG	4.703	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7
	CC(C)C[N@@H]1CCNC1=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)[C@@H](CC1=CC=CC=C1)NC(=O)OC1=CC=CC=C1	3.3E+07	3.3E+07	**7**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-2-cyclopentylethyl]carbamoyl}-2-(quinolin-5-yl)ethyl]carbamate	C40H50N6O	726.873	VCUZBAJG	4.703	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7
	CC(C)C[C@@H](NC(=O)OC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**7**		benzyl N-[(1S)-3-methyl-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-{(3S)-2-oxopyrrolidin-3-yl}-1-{(propan-2-yl)carbamoyl}propan-2-yl}carbamoyl}propan-2-yl}carbamoyl}butyl]carbamate	C31H47N5O	601.743	HEVXFSPU	3.375	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	7
	COC1=CC=CC(CC)NC(=O)OC2=CC=CC=C2)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)C(=O)NC(C)C)=N1	3.3E+07	3.3E+07	**7**		benzyl N-[2-(6-methoxypyridin-2-yl)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-{(3S)-2-oxopyrrolidin-3-yl}-1-{(propan-2-yl)carbamoyl}propan-2-yl}carbamoyl}butyl]carbamoyl}ethyl]carbamate	C34H46N6O	666.775	QNSIYJPY	2.865	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	7
	ClC1=CN=CC(OC(=O)C2=CC3=CC=CC=C3OC2=O)=C1	8492554	8492554	**6.97**		5-chloro-3-pyridyl 2-oxo-2H-1-benzopyran-3-carboxylate	C15H8ClNO	301.686	SGHKVFYA	2.564	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM	108
	NC(=O)C1=CC=C2N(CC3=CC4=C(C=CC=C4)C=C3)C(=O)C(=O)C2=C1	7597721	7597721	**6.92**			C20H14N2O	330.343	NTNYHMJ	2.59	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	M	1.20E-07
	ClC1=CC(OC(=O)C2=C3C=CC=CC3=CC=C2)=CN=C1	1.6E+07	1.6E+07	**6.91**	1007552-07-9		C16H10ClNO	283.714	MBLPTPFV	4.16	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM	124
	ClC1=CC(C=C(C=C1)C1=CC=C(O1)C(=O)OC1=CN=CC(Cl)=C1)N(=O)=O	1.6E+07	1.6E+07	**6.91**	1007551-99-6		C16H8Cl2N2	379.156	YEGHZGNC	4.061	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM	122
	CC(C)C[C@@H](NC(=O)OC1=CC=CC=C1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)[C@@H](CC1=NC=C(C=CC=C1)C(F)(F)F)NC(=O)[C@@H](C[C@@H]1CCNC1=O)NC(C)C	3.3E+07	3.3E+07	**6.9**		benzyl N-[(1S)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-{(3S)-2-oxopyrrolidin-3-yl}-1-{(propan-2-yl)carbamoyl}propan-2-yl}carbamoyl}butyl]carbamoyl}-2-[4-(trifluoromethyl)pyridin-2-yl]ethyl]carbamate	C34H43F3N6	704.747	SUGDGIXB	3.147	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	6.9
	CCCCNC(=O)C(=O)[C@@H](C[C@@H]1CCNC1=O)NC(=O)[C@@H](CC(C)C)NC(=O)[C@@H](CC1=NC=C(C=N1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.9**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-[6-(trifluoromethoxy)pyridin-2-yl]ethyl]carbamate	C35H45F3N6	734.773	BRFLNKOC	4.584	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	6.9
	CCCCNC(=O)C(=O)[C@@H](C[C@@H]1CCNC1=O)NC(=O)[C@@H](CC(C)C)NC(=O)[C@@H](CC1=NC=C(C=N1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.9**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-[5-(trifluoromethyl)pyrimidin-2-yl]ethyl]carbamate	C34H44F3N7	719.761	ICROBMCE	2.573	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	6.9

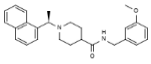
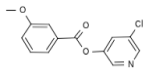
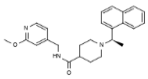
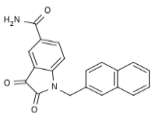
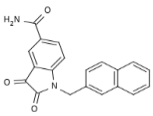
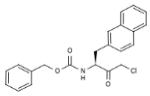
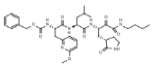
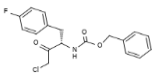
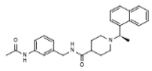
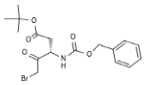
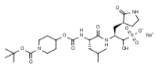
	CC(C)C[C@H](NC(=O)[C@H](CN1CCOCC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.9**		benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-(morpholin-4-yl)ethyl]carbamate	C32H48N6O	644.769	QPWPPKQ	0.97	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		6.9
	CO[C@@H](C)[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.9**		benzyl N-[(1S,2S)-2-methoxy-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]propyl]carbamate	C30H45N5O	603.716	LYNTYGQC	1.787	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		6.9
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CN1CCC(F)(F)C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.87**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(4,4-difluoropiperidin-1-yl)ethyl]carbamate	C34H50F2N	692.804	ISOPIEXEA	3.224	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor		pIC50	no unit		6.87
	CC(C)C[C@H](NC(=O)[C@H](CN(C)CC1CC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.84**		benzyl N-[(1S)-2-[(cyclopropylmethyl)(methyl)amino]-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C33H50N6O	642.796	KEVALLZBI	2.108	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor		pIC50	no unit		6.84
	[Na+].OC(=O)[C@H](C[C@@H]1CCNC1=O)N[C(=O)[C@H](CC1CCCCC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)[O-]).[Na+]	3.2E+07	3.2E+07	**6.82**			C24H33ClN3	582.05	QBZITZQG	2.314	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor		IC50	muM		0.15
	C[C@@H](N1CCC(CC1)C(=O)NCC1=CC(F)=CC=C1)C1=CC=CC2=CC=CC=C12	2.7E+07	2.7E+07	**6.82**	1581755-45-4	(R)-N-(3-fluorobenzyl)-1-(1-naphthalen-1-yl)ethyl)-piperidine-4-carboxamide	C25H27FN2O	390.501	XJTWGMH	5.142	3	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.15
	C1C1=CC(CSC(=S)NCC2=CC=CN=C2)=C(Cl)S1	1.4E+07	1.4E+07	**6.8**	370065-68-2	(Pyridin-3-ylmethyl)dithiocarbamic acid 2,5-dichloro-thiophen-3-ylmethyl ester	C12H10Cl2N	349.329	DGYDYUNI	2.528	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c	IC50	muM	=	0.16
	CC(C)C[C@H](NC(=O)[C@H](CC1=NC(=CC=N1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.8**		benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-[4-(trifluoromethyl)pyrimidin-2-yl]ethyl]carbamate	C33H42F3N	705.734	FSEJHJVN	2.195	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		6.8
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(OC)=CC(C)=C1)N(C)=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.8**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(6-methoxy-4-methylpyridin-2-yl)ethyl]carbamate	C36H50N6O	694.828	LLWOBJFC	3.769	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		6.8
	CC(C)C[C@H](NC(=O)[C@H](CN1CCC(F)(F)CC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.8**		benzyl N-[(1S)-2-(4,4-difluoropiperidin-1-yl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]ethyl]carbamate	C33H48F2N	678.777	FCTXOXQV	2.757	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor		pIC50	no unit		6.8
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CN1CCC(CC1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.8**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[4-(trifluoromethyl)piperidin-1-yl]ethyl]carbamate	C35H51F3N	724.821	ZHJLTDNP	4	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor		pIC50	no unit		6.8

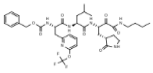
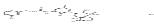
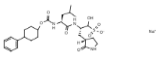
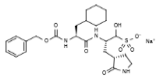
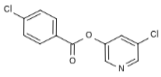
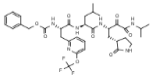
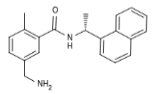
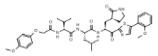
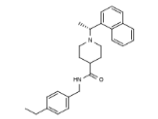
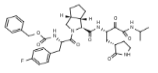
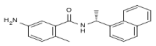
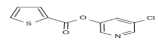
	CO[C@@H](C)[C@H](N C(=O)OCC1=CC=CC=C1) C(=O)N[C@@H](CC(C)C) C(=O)N[C@@H](C[C@@ H]1CCN1C=O)C(=O)C(= O)NC(C)C	3.3E+07	3.3E+07	**6.8**		benzyl N-[(1S,2S)-2-methoxy-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]propyl]carbamate	C30H45N5O	603.716	LYNTYGQC	1.787	2	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	6.8
	ClC1=CC(OC(=O)C2=CC= NC=C2)=CN=C1	1.6E+07	1.6E+07	**6.79**	1007552-02-4		C11H7ClN2O	234.642	DPPNJVAV	1.642	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM	164
	[Zn++].[S-]C1=N(=O)C=CC=C1	1.1E+07	1.1E+07	**6.77**	13463-41-7	zinc pyrithione; 1-hydroxypyridine-2-thione, Zn(II) complex; bis(N-oxopyridine-2-thionato) zinc(II); 1-hydroxypyridine-2-thione zinc salt; zinc 2-mercaptopyridine N-oxide; pyrithione zinc; zinc-pyrithion	2C5H4NOS*	317.708	PURMLSM	1.645	4	2	**Sars Cov 3C-Like Protease [SARS coronavirus]**	SARS coronavirus	Radioligand (/	Binding aff Ki (inhibitio	muM	=	0.17
	[Zn++].[S-]C1=N(=O)C=CC=C1	1.1E+07	1.1E+07	**6.77**	13463-41-7	zinc pyrithione; 1-hydroxypyridine-2-thione, Zn(II) complex; bis(N-oxopyridine-2-thionato) zinc(II); 1-hydroxypyridine-2-thione zinc salt; zinc 2-mercaptopyridine N-oxide; pyrithione zinc; zinc-pyrithion	2C5H4NOS*	317.708	PURMLSM	1.645	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/	In vitro bin Ki (inhibitio	muM	=	0.17
	S1C2=CC=CC=N2=[O][Zn]11SC2=N(C=CC=C2)=[O]1	1.1E+07	1.1E+07	**6.77**		pyrithione zinc; 2-pyridylthiol-1-oxide zinc; Pyrithione zinc; 1-hydroxypyridine-2-thione zinc salt; bis(2-pyridylthio)zinc 1,1'-dioxide; 1-hydroxypyridine-2-thione zinc; bis(2-pyridylthio-1-oxide)zinc	C10H8N2O2	317.708	OTPSWLR2		3	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibition c Ki (inhibitio	muM	=	0.17
	ClC1=CC(OC(=O)C2=CC3 =C(O2)C=CC=C3)=CN=C 1	1.1E+07	1.1E+07	**6.77**			C14H8ClNO3	273.675	QHBWMD	2.95	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM	170
	CC(C)C[C@H](NC(=O)[C @@H](NC(=O)COC1=CC =CC=C1)N[C@](C)(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C1=N C=C(S1)C1=CC=CC=C1	2.5E+07	2.5E+07	**6.77**			C37H48N6O	704.891	SAUDUBF2	3.744	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	muM		0.17
	CCCCNC(=O)C(=O)[C@H](C[C@@H](1CCNC1=O) N[C(=O)[C@@H](CC(C)C)N C(=O)[C@H](CN1CCC(C C1)C(F)(F)F)NC(=O)OCC 1=CC=CC=C1	3.3E+07	3.3E+07	**6.71**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[4-(trifluoromethyl)piperidin-1-yl]ethyl]carbamate	C35H51F3N	724.821	ZHJLTDNP	4	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.71
	NC1=NC=NC2=C1N=CN 2[C@H](1[C@H](O)[C@H](O)[C@@H](CO)[C@H] 1F	1E+07	1E+07	**6.7**		(1R,2S,3S,4R,5R)-3-(6-amino-9H-purin-9-yl)-4-fluoro-5-(hydroxymethyl)cyclopentane-1,2-diol; (-)-6?-beta-fluoro-aristeromycin; 6'-beta-fluoroaristeromycin	C11H14FN5	283.262	LFSGVDMI	-0.667	4	2	**RNA dependent RNA polymerase [Middle East respiratory syndrome coronavirus]; Adenosylhomocysteinase [human]**	Middle East respiratory syndrome coronavirus; human	Inhibitor	EC50	muM	0.2
	[Na+].CC(C)C[C@H](NC(=O)OC1CCN(CC1)C(=O) OC(C)(C)C)C(=O)N[C@@ H](C[C@@H]1CCNC1=O)C(O)S(O-])(=O)=O	3.2E+07	3.2E+07	**6.7**		sodium (2S)-2-((S)-2-[({[1-(tert-butoxycarbonyl)piperidin-4-yl]oxy} carbonyl)amino]-4-methylpentanamido)-1-hydroxy-3-[(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C24H41N4O	600.666	MVNGOUI	0.271	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM	0.2
	NC1=C2N=CN[C@H](C[C@H](O)[C@H](O)[C@@ H](CO)C3(F)F)C2=NC=N 1	3.5E+07	3.5E+07	**6.7**		(1R,2S,3S,5R)-3-(6-amino-9H-purin-9-yl)-4,4-difluoro-5-(hydroxymethyl)cyclopentane-1,2-diol; 6',6'-difluoroaristeromycin	C11H13F2N	301.253	XSXKATM	-0.288	4	2	**RNA dependent RNA polymerase [Middle East respiratory syndrome coronavirus]; Adenosylhomocysteinase [human]**	Middle East respiratory syndrome coronavirus; human	Inhibitor	EC50	muM	0.2

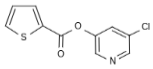
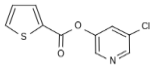
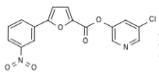
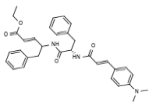
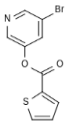
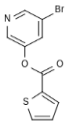
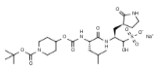
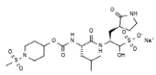
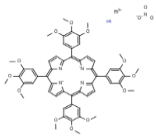
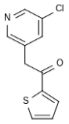
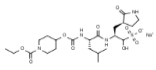
	ClC1=CC(OC(=O)C2=CC=C(O2)C2=C(C=CC=C2)N(=O)=O)=CN=C1	1.6E+07	1.6E+07	**6.68**	1007552-00-2		C16H9ClN2O	344.711	OGRUFOQ	3.439	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	IC50	nM	208
	CC(C)C(C@H)NC(=O)(C@@H)(NC(=O)COC1=CC=CN=C1)C(C)C)C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)C1=NC2=CC=CC=C251	2.3E+07	2.3E+07	**6.66**	1383922-92-6		C32H40N6O	636.772	VOKLNKGF	2.055	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Ki (inhibitio	muM	0.22
	CC(C)C(C@H)NC(=O)(C@@H)(NC(=O)CNC1=CC=CC=C1)C(C)C)C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)C1=NC2=CC=CC=C251	2.3E+07	2.3E+07	**6.66**	1383922-55-1		C33H42N6O	634.8	PPHLPUPC	3.038	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Ki (inhibitio	muM	0.22
	CC(C)C(C@H)NC(=O)(C@H)(CN1CCC(CC1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.66**		benzyl ((S)-1-(((S)-1-(((S)-4-(isopropylamino)-3,4-dioxo-1-((S)-2-oxopyrrolidin-3-yl)butan-2-yl)amino)-4-methyl-1-oxopentan-2-yl)amino)-1-oxo-3-(4-(trifluoromethyl)piperidin-1-yl)propan-2-yl)carbamate; benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-	C34H49F3N	710.794	SACDDFO\	3.533	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.66
	CC(C)C(C@H)NC(=O)(C@H)(CC1=CC=CC2=C1C=CC=C2)N(C=O)OCC1=CC=CC=C1)C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C=O	2.4E+07	2.4E+07	**6.64**		(1-{3-methyl-1-[2-oxo-1-(2-oxo-pyrrolidin-3-ylmethyl)ethylcarbamoyl]butylcarbamoyl}-2-naphthalen-1-yl-ethyl)carbamic acid benzyl ester	C34H40N4O	600.715	UULYLRNR	4.738	3	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	IC50	muM	0.23
	CC(C)C(C@H)NC(=O)(C@H)(CC1=NC=CC=C1)N(C(=O)OCC1=CC=CC=C1)C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)N(C@@H)(C)C1CCCCC1	3.3E+07	3.3E+07	**6.6**		benzyl N-[(1S)-1-[[(1S)-1-{[(2S)-1-{[(1S)-1-cyclohexylethyl]carbamoyl}-1-oxo-3-{(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-(pyridin-2-yl)ethyl]carbamate	C38H52N6O	704.867	KIPIKDUHE	4.244	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	6.6
	CC(C)C(C@H)NC(=O)(C@H)(CC1=NC(OC(F)(F)F)=CC=C1)N(C(=O)OCC1=CC=CC=C1)C(=O)N(C@@H)(C(C@@H)1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.6**		benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-{(propan-2-yl)carbamoyl}propan-2-yl]carbamoyl}butyl]carbamoyl}-2-[6-(trifluoromethoxy)pyridin-2-yl]ethyl]carbamate	C34H43F3N	720.746	SDGSGHDI	4.117	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	6.6
	CC(C)(C)NC(=O)C(=O)(C@H)(C(C@@H)1CCNC1=O)N(C(=O)(C@H)(CCC(C)(C)NC(=O)(C@H)(CC1=NC(OC1=CC=CC2=CC=CC=C12)NC(=O)OCC1=CC=C(OCCCN2CCOCC2)C=C1	3.3E+07	3.3E+07	**6.6**		{4-[3-(morpholin-4-yl)propoxy]phenyl}methyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-{(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}carbamoyl}-2-cyclohexylethyl]carbamoyl}-2-(naphthalen-1-yl)ethyl]carbamate	C49H66N6O	883.098	RKUQPVSF	6.161	1	0	**3CL protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	pIC50	no unit	6.6
	CC(C)(C)NC(=O)C(=O)(C@H)(C(C@@H)1CCNC1=O)N(C(=O)(C@H)(CC1=NC(OC1=CC=CC2=CC=CC=C12)NC(=O)OCC1=CC=C(OCCCN2CCOCC2)C=C1	3.3E+07	3.3E+07	**6.6**		{4-[3-(morpholin-4-yl)propoxy]phenyl}methyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(tert-butylcarbamoyl)-1-oxo-3-{(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}carbamoyl}-2-cyclohexylethyl]carbamoyl}-2-(naphthalen-1-yl)ethyl]carbamate	C49H66N6O	883.098	RKUQPVSF	6.161	1	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	6.6
	CCCCNC(=O)C(=O)(C@H)(C(C@@H)1CCNC1=O)N(C(=O)(C@H)(CCC(C)(C)NC(=O)(C@H)(CC1=N(C(=O)=CC(C)=C1)N(C(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.59**		benzyl N-[(1S)-1-[[(1S)-1-{[(2S)-1-(butylcarbamoyl)-1-oxo-3-{(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}carbamoyl}-3-methylbutyl]carbamoyl}-2-(6-methoxy-4-methylpyridin-2-yl)ethyl]carbamate	C36H50N6O	694.828	LLWOBJFC	3.769	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.59
	C5CC(C@H)(NC(=O)(C@H)(CCC(O)=O)NC(=O)(C@H)(CC1=CC=C(O)C=C1)NC(=O)(C@@H)(NC(=O)(C@H)(CC(C)C)NC(=O)(C@H)(CCC(O)=O)NC(=O)(C@H)(CC(C)C)NC(C)=O)(C@@H)(C)C)C(=O)N)C@@H)(CC(C)C)C(=O)N(C@@H)(CCC(N)=O)C(=O)N(C@@)1(C)CCCC=CCCCC@)(C)NC(=O)(C@@H)(CCCCN)NC(=O)(C@@H)(N C(=O)(C@@H)(NC1=O)C	3.3E+07	3.3E+07	**6.59**			C118H189N	2550.01	XJXOKQDA	0.598	1	0	**spike protein [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM	0.26

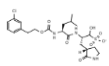
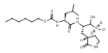
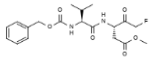
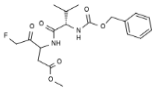
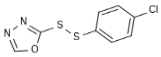
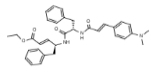
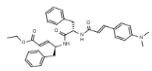
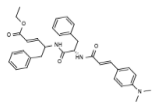
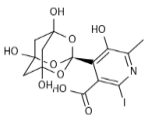
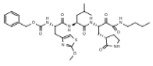
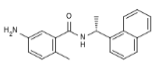
	ClC1=CN=CC(OC(=O)C2=CSC=N2)=C1	1.1E+07	1.1E+07	**6.57**			C9H5ClN2O	240.67	CSEAAOW	1.798	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM		270
	COC1=CC=C(OCC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)C2=NC=C(S)C2=CC=CC=C2)C=C1	2.5E+07	2.5E+07	**6.57**			C36H45N5O	691.849	WEJYZSSF	3.45	3	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	muM		0.27
	[Na+].OC(=[C@H](C[C@@H]1CCN(C1=O)N(C(=O)[C@H](CC1CCCCC1)NC(=O)OCC1=CC(Cl)=CC=C1)S([O-])(=O)=O	3.2E+07	3.2E+07	**6.54**			C24H33ClN3	582.05	QBZITZQG	2.314	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	IC50	muM		0.29
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)NC(CC1=CC=CC=C1)C(=O)C(F)(F)F	1.9E+07	1.9E+07	**6.54**	1034140-83-4		C32H41F3N4	634.696	PDLFIYNG	5.092	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/ Binding aff	Ki (inhibitio	muM	=	0.29
No Structure		2.5E+07	2.5E+07	**6.54**		Benzyloxycarbonyl-AVLF(D/L)-Trifluoromethyl							**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	muM		0.29
	O=N(=O)O[Hg]C1=CC=CC=C1	3770377	3770377	**6.52**	55-68-5	Phenylmercuric nitrate; phenylmercury (1+); nitrate; Phenylquecksilber(1+); Nitrat; phenylmercury nitrate; phenyl mercuric nitrate; phenyl mercury nitrate; Phenylmercurinitrat	C6H5HgNO3	339.701	PDTFCHSE	2.466	4	2	**Sars Cov 3C-Like Protease [SARS coronavirus]**	SARS coronavirus	Radioligand (/ Binding aff	Ki (inhibitio	muM	=	0.3
	O=N(=O)O[Hg]C1=CC=CC=C1	3770377	3770377	**6.52**	55-68-5	Phenylmercuric nitrate; phenylmercury (1+); nitrate; Phenylquecksilber(1+); Nitrat; phenylmercury nitrate; phenyl mercuric nitrate; phenyl mercury nitrate; Phenylmercurinitrat	C6H5HgNO3	339.701	PDTFCHSE	2.466	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/ In vitro bin	Ki (inhibitio	muM	=	0.3
	CC1=C(Cl)C=C(Cl)C(=C1)S(=O)(=O)C1=C(C=C(C=C1N(=O)=O)C(F)(F)F)N(=O)=O	1.1E+07	1.1E+07	**6.52**		2-[(2,4-dichloro-5-methylphenyl)sulfonyl]-1,3-dinitro-5-(trifluoromethyl)benzene	C14H7Cl2F3	459.187	INAZPZCJ	5.175	3	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.3
	CN(C)C1=CC=C(C=C1)C(=O)N(C)(CC1=CC=CC=C1)C(=O)NC1=CC=C(C=C1Cl)N(=O)=O	2.5E+07	2.5E+07	**6.52**			C24H23ClN4	466.924	NBBWJEW	4.859	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/ In vitro bin	Ki (inhibitio	muM	=	0.3
	[Na+].CC(C)C[C@H](NC(=O)OC1CCN(CC1)C(=O)OC(C)(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(O-])(=O)=O	3.2E+07	3.2E+07	**6.52**		sodium (2S)-2-[(S)-2-[({[1-(tert-butoxycarbonyl)piperidin-4-yl]oxy} carbonyl)amino]-4-methylpentanamido]-1-hydroxy-3-[(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C24H41N4O	600.666	MVNGOUI	0.271	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	IC50	muM		0.3
	[Na+].[H][C@@]1(C[C@H](NC(=O)[C@H](CC(C)C)NC(=O)OC2CCC(CC2)C2=CC=CC=C2)C(O)S(O-])(=O)=O)CCNC1=O	3.3E+07	3.3E+07	**6.52**			C26H38N3O	575.659	OOMCVQ	1.823	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM		0.3

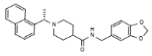
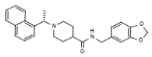
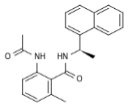
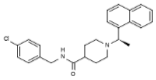
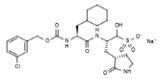
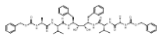
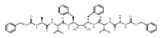
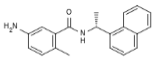
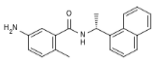
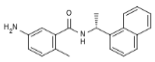
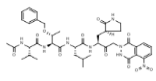
	[Na+].[H][C@@]1(C[C@H][NC(=O)[C@H][CC(C)C]N(C(=O)OCCCCCCC)O)S(=O)(=O)CCNC1=O	3.3E+07	3.3E+07	**6.52**			C20H36N3O	501.577	PNIWTLYN	1.103	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM	0.3
	[H][C@@](CC1=CC=CC=C1)(NC(=O)OCC1=CC=CC=C1)C(=O)CCl	4264876	4264876	**6.51**	26049-94-5	(S)-benzyl (4-chloro-3-oxo-1-phenylbutan-2-yl)carbamate; (S)-(1-benzyl-3-chloro-2-oxopropyl)carbamic acid benzyl ester; (3S)-1-chloro-2-oxo-3-N-benzyloxycarbonylamino-4-phenylbutane; N-carbobenzyloxy-L-phenylalanyl chloromethyl ketone: (3S)-3-	C18H18ClN	331.799	OYHLRJGD	3.446	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	nM	306
	CCCCNC(=O)C(=O)[C@H][C@@H]1CCNC1=O)NC(=O)[C@H][CC(C)C]N(=O)[C@H][CC1=NC=CC(OC(C)C)=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.5**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[4-(propan-2-yloxy)pyridin-2-yl]ethyl]carbamate	C37H52N6O	708.855	QQYAQVN	3.487	2	0	**3CL protease [Human coronavirus 229E]**	Human coronavirus 229E	Inhibitor	pIC50	no unit	6.5
	C[C@@H](N1CCC[CC1)C(=O)NCC1=CC2=C(OCO2)C=C1)C1=C2C=CC=CC2=CC=C1	2.1E+07	2.1E+07	**6.49**	1234195-91-5	1-[(R)-1-(1-naphthyl)ethyl]-4-[3,4-(methylenedioxy)benzylamino]carbonylpiperidine; GRL-0667S	C26H28N2O	416.52	IVXBCFLW	4.47	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM	0.32
	CCCCNC(=O)C(=O)[C@H][C@@H]1CCNC1=O)NC(=O)[C@H][CC(C)C]N(=O)[C@H][CC1=NC(=CC=C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.49**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[6-(trifluoromethyl)pyridin-2-yl]ethyl]carbamate	C35H45F3N	718.774	HOPNWLC	3.703	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.49
	CCCCNC(=O)C(=O)[C@H][C@@H]1CCNC1=O)NC(=O)[C@H][CC(C)C]N(=O)[C@H][CC1=NC(=CS1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.49**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[4-(trifluoromethyl)-1,3-thiazol-2-yl]ethyl]carbamate	C33H43F3N	724.802	SQARSOUI	3.306	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.49
	O[C1=CC(OC(=O)C2=C(C=CC=C2)N(=O)=O)=CN=C1	1.6E+07	1.6E+07	**6.48**	1007552-05-7		C12H7ClN2O	278.652	BWJAVTA\	2.786	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM	333
	CC(C)C[C@H]]NC(=O)[C@@H][NC(=O)COC1=CC(=CC=C1)N(C)C)C)C)C(=O)N[C@@H](C[C@@H][C@H](C)NC(=O)C1=NC=C(C)S1	2.5E+07	2.5E+07	**6.48**			C32H46N6O	642.82	CEZLCCHF	2.03	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	muM	0.33
	CCCCNC(=O)C(=O)[C@H]]CC[C@@H][CCNC1=O)NC(=O)[C@H][CC(C)C]N(=O)[C@H][CC1=NC2=C(CCC2)S1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.48**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(4H,5H,6H-cyclopenta[d][1,3]thiazol-2-yl)ethyl]carbamate	C35H48N6O	696.868	JOVXDSIH	2.266	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.48
	CSCC[C@H]]NC(=O)[C@H][CC(O)=O)NC(=O)[C@@H][CC1=CC=C(O)C=C1)NC(=O)[C@@H]]NC(=O)[C@H][CC(C)C]NC(=O)[C@H][CC(O)=O)N(C=O)[C@H][CC(C)C]NC(C=O)[C@@H]](C)O)C(=O)N]C@@H]][CC(C)C](=O)N[C@@H]][CC(C)C](=O)N[C@@H]][CCC(N)=O)C(=O)N[C@@H]][CC(C)C](=O)N[C@@H]][CC(C)C](=O)N[C@@H]][CCCCN)C(=O)	3.3E+07	3.3E+07	**6.48**			C120H192N	2591.06	ZEXNMYV(	0.906	1	0	**spike protein [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM	0.33
	COC1=CC=C(CNC(=O)C2CCN(CC2)[C@H](C)C)C2=CC=CC3=C2C=CC=C3)C=C1	2.1E+07	2.1E+07	**6.47**	1233939-86-4	1-[(R)-1-(1-naphthyl)ethyl]-4-(4-methoxybenzylamino)carbonylpiperidine	C26H30N2O	402.536	NTMTVRC	4.896	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM	0.34

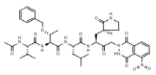
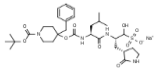
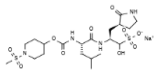
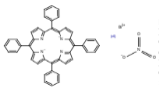
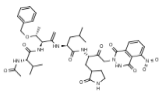
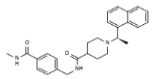
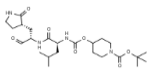
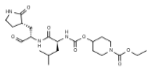
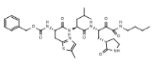
	COC1=CC(CNC(=O)C2CC N(CC2)[C@H])[C]C2=CC= CC3=C2C=CC=C3)=CC=C 1	2.1E+07	2.1E+07	**6.47**	1233939-85-5	1-[(R)-1-(1-naphthyl)ethyl]-4-(3-methoxybenzylamino)carbonylpiperidine	C26H30N2O	402.536	QKYBTDRN	4.896	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.34
	COC1=CC(=CC=C1)C(=O) OC1=CC(Cl)=CN=C1	1.1E+07	1.1E+07	**6.47**			C13H10ClN(	263.68	UIXQHURF	2.809	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM		340
	COC1=NC=CC(CNC(=O)C 2CCN(CC2)[C@H])[C]C2= CC=CC3=CC=CC=C23)=C 1	2.7E+07	2.7E+07	**6.46**	1581755-52-3	(R)-N-((2-methoxypyridin-4-yl)methyl)-1-(1-(naphthalen-1-yl)ethyl)piperidine-4-carboxamide	C25H29N3O	403.524	MMIABLSF	4.372	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.35
	NC(=O)C1=CC=C2N(CC3 =CC4=C(C=CC=C4)C=C3) C(=O)C(=O)C2=C1	7597721	7597721	**6.43**			C20H14N2O	330.343	NTNYHMJ	2.59	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.37
	NC(=O)C1=CC=C2N(CC3 =CC4=C(C=CC=C4)C=C3) C(=O)C(=O)C2=C1	7597721	7597721	**6.43**			C20H14N2O	330.343	NTNYHMJ	2.59	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c IC50	muM	=	0.37
	C(CC(=O))[C@H])[CC1=CC 2=CC=CC=C2C=C1)N C(=O)OCC1=CC=CC=C1	1.2E+07	1.2E+07	**6.43**		benzyl [3-chloro-1(S)-[(2-naphthyl)methyl]-2-oxopropyl] carbamate	C22H20ClN(	381.859	BMGGQJB	4.712	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	nM		371
	CCCCNC(=O)C(=O)[C@H][C]C@@H])1CCNC1=O) NC(=O)[C@H])[CC]C]CN C(=O)[C@H])[CC1=NC(O C)=CC=C1)NC(=O)OCC1 =CC=CC=C1	3.3E+07	3.3E+07	**6.43**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-(6-methoxypyridin-2-yl)ethyl]carbamate	C35H48N6O	680.802	KDOSPHR\	3.332	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit		6.43
	FC1=CC=C(C[C@H])NC(= O)OCC2=CC=CC=C2)C(= O)CC)C=C1	9935262	9935262	**6.42**	400771-48-4	(3S)-3-benzyloxycarbonylamino-1-chloro-4-(p-fluorophenyl)-2-butanone; [N-(benzyloxycarbonyl)-3-(4-fluorophenyl)-DL-alanyl]methyl chloride	C18H17ClFN	349.789	SSXSAFSL\	3.607	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	nM		380
	C[C@@H])N1CCC(CC1)C (=O)NCC1=CC(NC)C]=O) =CC=C1)C1=CC=CC2=CC =CC=C12	2.7E+07	2.7E+07	**6.41**	1581755-39-6	(R)-N-(3-acetamidobenzyl)-1-(1-(naphthalen-1-yl)ethyl)-piperidine-4-carboxamide	C27H31N3O	429.562	YQRGVYYF	4.235	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.39
	CC(C)(C)OC(=O)C[C@H])[NC(=O)OCC1=CC=CC=C 1)C(=O)CBr	6820432	6820432	**6.4**	153088-76-7	(S)-3-benzyloxycarbonylamino-5-bromo-4-oxo-pentanoic acid tert-butyl ester; (3S)-3-(N-benzyloxycarbonyl)amino-5-bromo-4-oxopentanoic acid tert-butyl ester; (S)-3-benzyloxycarbonylamino-5-bromo-4-oxopentanoic acid tert-butyl ester; (S)-tert-butyl 3-	C17H22BrN(	400.269	PBVFTOAY	3.077	4	1	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	nM		400
	[N+].CC(C)C[C@H])[NC(=O)OC1CCN(CC1)C(=O) OC]C)C)C(=O)N)[C@@ H])[C]C@@H])1CCNC1=O)C]O)S(O-])(=O)=O	3.2E+07	3.2E+07	**6.4**		sodium (2S)-2-[(S)-2-[([(1-(tert-butoxycarbonyl)piperidin-4-yl]oxy) carbonyl)amino]-4-methylpentanamido]-1-hydroxy-3-[(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C24H41N4O	600.666	MVNGOUF	0.271	2	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	IC50	muM		0.4

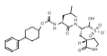
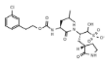
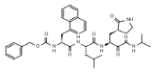
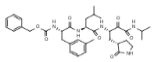
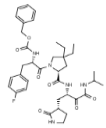
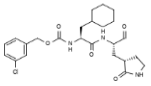
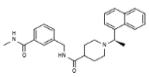
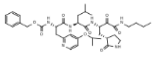
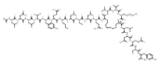
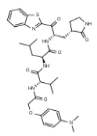
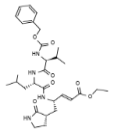
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC1=NC(CC(F)(F)F)=CC=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.4**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl]-3-methylbutyl]carbamoyl]-2-[6-(trifluoromethoxy)pyridin-2-yl]ethyl]carbamate	C35H45F3N	734.773	BRFLNKOD	4.584	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.4
	[Na+].[H][C@@]1(C[C@H](NC(=O)[C@H](CCC(C)C)NC(=O)OCC2=CC(Cl)=CC=C2)C(O)S(O-])(=O)=O)CCNC1=O	3.3E+07	3.3E+07	**6.4**			C21H29ClN2	541.985	QERRPHDI	0.947	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	EC50	muM	0.4
	[Na+].[H][C@@]1(C[C@H](NC(=O)[C@H](CCC(C)C)NC(=O)OC2CCCC(C2)C2=CC=CC=C2)C(O)S(O-])(=O)=O)CCNC1=O	3.3E+07	3.3E+07	**6.4**			C26H38N3O	575.659	OOMCVQ\	1.823	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	EC50	muM	0.4
	[Na+].OC(]C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC1CCCCC1)NC(=O)OCC1=CC=CC=C1)S(O-])(=O)=O	3.2E+07	3.2E+07	**6.38**			C24H34N3O	547.605	QJIXTKHVL	1.692	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	IC50	muM	0.42
	ClC1=CC=C(C=C1)C(=O)OC1=CN=CC(Cl)=C1	1.6E+07	1.6E+07	**6.36**	1007552-04-8		C12H7Cl2NO	268.099	KLXHMZDA	3.516	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	nM	434
	CC(C)C[C@H](NC(=O)[C@H](CC1=NC(OC(F)(F)F)=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.36**		benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl]-2-[6-(trifluoromethoxy)pyridin-2-yl]ethyl]carbamate	C34H43F3N	720.746	SDGSGHDI	4.117	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.36
	C[C@@H](NC(=O)C1=C(C)C=CC(N)=C1)C1=CC=CC2=CC=CC=C12	2E+07	2E+07	**6.34**	1184301-69-6	5-methylamino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide	C21H22N2O	318.418	BIKTWHW	4.488	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM	0.46
	COC1=CC=C(OCC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)C2=NC=C(S2)C2=C(OC)C=CC=C2)C=C1	2.5E+07	2.5E+07	**6.33**			C37H47N5O	721.875	BWUPIUXI	3.365	3	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	muM	0.47
	CCC1=CC=C(CNC(=O)C2CCN(CC2)[C@H](C)C2=CC=CC3=C2C=CC=C3)C=C1	2.7E+07	2.7E+07	**6.33**	1581755-35-3	(R)-N-(4-ethylbenzyl)-1-(1-(naphthalen-1-yl)ethyl)-piperidine-4-carboxamide	C27H32N2O	400.564	XPZZHYRW	5.882	3	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM	0.47
	[H][C@@]12CCC[C@]1([H])[C@H](N[C2](C=O))[C@H](CC1=CC=C(F)C=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.33**		benzyl N-[(2S)-1-[(1S,3aR,6aS)-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]octahydrocyclopenta[c]pyrrol-2-yl]-3-(4-fluorophenyl)-1-oxopropan-2-yl]carbamate	C36H44FN5	677.773	GCSPVCXS	3.159	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.33
	C[C@@H](NC(=O)C1=C(C)C=CC(N)=C1)C1=C2C=CC=CC2=CC=C1	2E+07	2E+07	**6.31**	1093070-16-4	5-amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide; GRL-0617S; 5-Amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide	C20H20N2O	304.392	UVERBUNI	4.549	4	2	**Papain-like protease [Coronaviridae]**	Coronavirinae	Biodistribu	Ki (inhibitio	muM	=	0.49
	C[C@@H](N1CCC(CC1)C(=O)NCC1=CC=C(F)C=C1)C1=CC=CC2=CC=CC=C12	2.7E+07	2.7E+07	**6.31**	1581755-44-3	(R)-N-(4-fluorobenzyl)-1-(1-(naphthalen-1-yl)ethyl)-piperidine-4-carboxamide	C25H27FN2	390.501	VTAUBQM	5.142	3	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM	0.49
$Hg(_{2+})$	[Hg]	3587187	3587187	**6.3**		mercury ion; Mercury; mercury(II) chloride; mercury(II) cation; mercury(II) ion; mercury(II)(2+); mercury(II)-ion	Hg	200.59	QSHDDOU	0	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/ In vitro bin	Ki (inhibitio	muM	=	0.5
	ClC1=CC(OC(=O)C2=CC=CS2)=CN=C1	1.9E+07	1.9E+07	**6.3**	219929-01-8		C10H6ClNO	239.682	PAVJYVVZ	1.956	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [Coronaviridae]**	Coronavirinae	Inhibitory (	IC50	muM	=	0.5

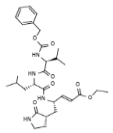
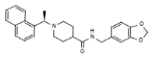
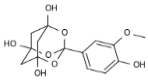
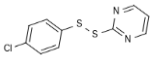
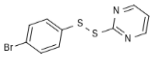
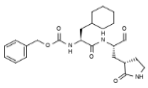
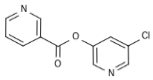
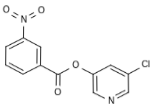
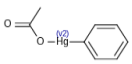
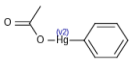
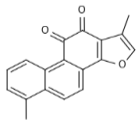
	ClC1=CC(OC(=O)C2=CC=CS2)=CN=C1	1.9E+07	1.9E+07	**6.3**	219929-01-8		C10H6ClNO:	239.682	PAVJYVVZI	1.956	4	2	**Sars Cov 3C-Like Protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory (	IC50	muM	=	0.5
	ClC1=CC(OC(=O)C2=CC=CS2)=CN=C1	1.9E+07	1.9E+07	**6.3**	219929-01-8		C10H6ClNO:	239.682	PAVJYVVZI	1.956	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Inhibitor	In vitro inh	IC50	muM	=	0.5
	ClC1=CC(OC(=O)C2=CC=C(O2)C2=CC(=CC=C2)N(=O)=O)=CN=C1	1.6E+07	1.6E+07	**6.3**	1007552-01-3		C16H9ClN2(	344.711	FFZBRNPL\	3.439	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	nM		500
	CCOC(=O)\C=C\C(CC1=CC=CC=C1)NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)\C=C\C1=CC=C(C=C1)N(C)C	2.6E+07	2.6E+07	**6.3**			C33H37N3O	539.674	JWPLKCW'	5.753	2	1	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/	In vitro bin	Ki (inhibitio	muM	=	0.5
	BrC1=CC(OC(=O)C2=CC=CS2)=CN=C1	2.6E+07	2.6E+07	**6.3**			C10H6BrNO	284.133	DBZLJJMK	2.132	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus		Inhibitory (	IC50	muM		0.5
	BrC1=CC(OC(=O)C2=CC=CS2)=CN=C1	2.6E+07	2.6E+07	**6.3**			C10H6BrNO	284.133	DBZLJJMK	2.132	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory (	IC50	muM	=	0.5
	[Na+].CC(C)C[C@H](NC(=O)OC1CCN(CC1)C(=O)OC(C)(C)C)C(=O)N[C@@H](C[C@@H](CCNC1=O)C(O)S(O-])(=O)=O	3.2E+07	3.2E+07	**6.3**		sodium (2S)-2-{(S)-2-{({[1-(tert-butoxycarbonyl)piperidin-4-yl]oxy} carbonyl)amino}-4-methylpentanamido}-1-hydroxy-3-{(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C24H41N4O	600.666	MVNGOUI	0.271	2	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor		EC50	muM		0.5
	[Na+].CC(C)C[C@H](NC(=O)OC1CCN(CC1)S(C)(=O)=O)C(=O)N[C@@H](C[C@@H](CCNC1=O)C(O)S(O-])(=O)=O	3.2E+07	3.2E+07	**6.3**		sodium (2S)-1-hydroxy-2-{(S)-4-methyl-2-{({[1-(methylsulfonyl)piperidin-4-yl]oxy}carbonyl)amino]pentanamido}-3-{(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C20H35N4O	578.64	OXYUFTID	-1.395	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor		IC50	muM		0.5
	[Bi+3].[O-]N(=O)=O.COC1=CC(=CC(OC)=C1OC)C1=C2)N-]C1(C=C/2)=C(/C2=N/C(/C=C2)=C1)C2=CC=C2)N-]2)/C(=C2/C=CC\1=N/2)C1=CC(OC)=C(OC)(OC)=C1)C1=CC(OC)=C(OC)C(OC)=C1)C1=CC(OC)=C(OC)C(OC)=C1	1.6E+07	1.6E+07	**6.3**			Bi*C56H52N	1244.03	GUVHQKN		1	0	**helicase [SARS coronavirus]**	SARS coronavirus		Effect : enz	IC50	muM		0.5
	ClC1=CC(CC(=O)C2=CC=CS2)=CN=C1	2.6E+07	2.6E+07	**6.3**	1222829-75-5		C11H8ClNO:	237.71	HKMXTOF	1.86	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Inhibitor	In vitro inh	IC50	muM	=	0.5
	[Na+].CCOC(=O)N1CCC(CC1)OC(=O)N[C@@H](CC[C@@H](CCNC1=O)C(O)S(O-])(=O)=O	3.2E+07	3.2E+07	**6.3**		sodium (2S)-2-{(S)-2-{({[1-(ethoxycarbonyl)piperidin-4-yl]oxy}carbonyl)amino}-4-methylpentanamido}-1-hydroxy-3-{(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C22H37N4O	572.612	FTLUCMW	-0.606	2	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor		IC50	muM		0.5

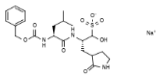
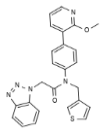
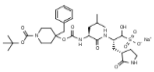
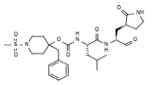
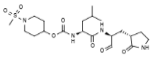
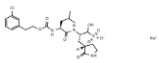
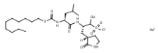
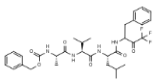
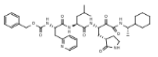
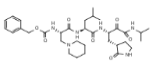
	[Na+].[H][C@@]1([C[C@H][N(C[=O])[C@H][CC(C)C)NC(=O)OCCC2=CC=CC(C)=C2)C(O)S(][O-])(=O)=O)CCNC1=O	3.3E+07	3.3E+07	**6.3**			C22H31ClN3	556.012	ZIVZAVLW	1.105	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor		EC50	muM		0.5
	[Na+].[H][C@@]1([C[C@H][N(C[=O])[C@H][CC(C)C)NC(=O)OCCCCCC)C(O)S(][O-])(=O)=O)CCNC1=O	3.3E+07	3.3E+07	**6.3**			C20H36N3O	501.577	PNIWTLYN	1.103	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor		EC50	muM		0.5
	COC(=O)C[C@H][NC(=O)[C@@H][NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)CF	2.5E+07	2.5E+07	**6.29**			C19H25FN2	396.416					**Protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	Equilibriun	Ki (inhibitio	nM	=	512
	COC(=O)CC[NC(=O)][C@@H][NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)CF	9654802	9654802	**6.29**		benzyloxycarbonyl-L-Val-DL-Asp(OMe)-fluoromethylketone; Z-Val-DL-Asp(OMe)-fluoromethylketone	C19H25FN2	396.416	DPHACENJ	1.655	4	1	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			Ki (inhibitio	nM		512
	ClC1=CC=C[SSC2=NN=CO2]C=C1	3.1E+07	3.1E+07	**6.29**		2-[(4-chlorophenyl)disulfanyl]-1,3,4-oxadiazole	C8H5ClN2O	244.725	YANPJRMI	4.021	4	2	**Main proteinase (Mpro) [SARS coronavirus]**	SARS coronavirus	Inhibitor		IC50	muM		0.516
	CCOC(=O)[C=C\C(C@H)[C1=CC=CC=C1)NC(=O)[C@H)[CC1=CC=CC=C1)NC(=O)[C=C\C1=CC=C[C=C1)N(C)C	1.1E+07	1.1E+07	**6.28**			C33H37N3O	539.674	JWPLKCW'	5.753	2	1	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			Ki (inhibitio	muM		0.52
	CCOC(=O)[C=C\C(C@H)[C1=CC=CC=C1)NC(=O)[C@H)[CC1=CC=CC=C1)NC(=O)[C=C\C1=CC=C[C=C1)N(C)C	1.1E+07	1.1E+07	**6.28**			C33H37N3O	539.674	JWPLKCW'	5.753	2	1	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Radioligand (/	Inhibition c	Ki (inhibitio	muM		0.52
	CCOC(=O)[C=C\C(CC1=CC=CC=C1)NC(=O)[C@H)[CC1=CC=CC=C1)NC(=O)\C=C\C1=CC=C[C=C1)N(C)C	2.6E+07	2.6E+07	**6.28**			C33H37N3O	539.674	JWPLKCW'	5.753	2	1	**Sars Cov 3C-Like Protease [SARS coronavirus]**	SARS coronavirus	Radioligand (/	Binding aff	Ki (inhibitio	muM	=	0.52
	CC1=NC(I)=C(C(O)=O)C(=C1O)[C@@]12OC3(O)C(O)(C(,O)(C3)O1)O2	2.5E+07	2.5E+07	**6.27**			C14H14INO	467.171	HCDBOXM	-0.336	4	1	**helicase [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibition c	IC50	muM	=	0.54
	CCCCNC(=O)C(=O)[C@H][C(C@@H][CCNC1=O)N(C(=O)[C@H][CC(C)C]CN C(=O)[C@H][CC1=CSC(OC)=N1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.26**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-(2-methoxy-1,3-thiazol-4-yl)ethyl]carbamate	C33H46N6O	686.83	JYGUFLMV	2.663	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor		pIC50	no unit		6.26
	C[C@@H][NC(=O)C1=C(C)C=CC(N)=C1)C1=C2C=CC=CC2=CC=C1	2E+07	2E+07	**6.25**	1093070-16-(	5-amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide; GRL-0617S; 5-Amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide	C20H20N2O	304.392	UVERBUNI	4.549	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.56

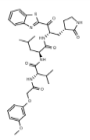
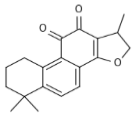
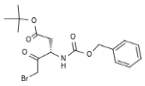
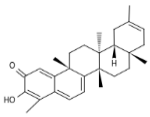
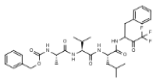
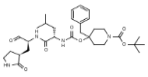
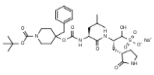
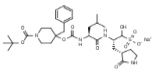
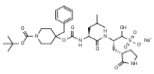
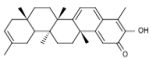
	C[C@H](N1CCC(CC1)C(=O)NCC1=CC2=C(OCO2)C=C1)C1=C2C=CC=CC2=CC=C1	2.1E+07	2.1E+07	**6.25**	1233939-90-(	1-[(S)-1-(1-naphthyl)ethyl]-4-[3,4-(methylenedioxy)benzylamino]carbonylpiperidine; GRL-0737S	C26H28N2O	416.52	IVXBCFLW	4.47	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.56
	C[C@H](N1CCC(CC1)C(=O)NCC1=CC2=C(OCO2)C=C1)C1=C2C=CC=CC2=CC=C1	2.1E+07	2.1E+07	**6.25**	1233939-90-(	1-[(S)-1-(1-naphthyl)ethyl]-4-[3,4-(methylenedioxy)benzylamino]carbonylpiperidine; GRL-0737S	C26H28N2O	416.52	IVXBCFLW	4.47	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c IC50	muM	=	0.56
	C[C@H](NC(=O)C1=C(C)C=CC=C1NC(C)=O)C1=CC=CC2=CC=CC=C12	2.5E+07	2.5E+07	**6.25**			C22H22N2O	346.429	OQBMJEFI	5.049	3	2	**Papain-like protease [Coronaviridae]**	Coronaviridae	Inhibitor	Inhibitory c IC50	muM	=	0.56
	C[C@H](N1CCC(CC1)C(=O)NCC1=CC=C(C)C=C1)C1=CC=CC2=CC=CC=C12	2.7E+07	2.7E+07	**6.24**	1581755-42-:	(R)-N-(4-chlorobenzyl)-1-(1-(naphthalen-1-yl)ethyl)-piperidine-4-carboxamide	C25H27ClN2	406.955	WYSVTAF(	5.603	3	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.58
	[Na+].OC(C[C@H](C[C@@H]1CCNC1=O)N(C(=O)[C@H](CC1CCCCC1)NC(=O)OCC1=CC(Cl)=C=C1)S([O-])(=O)=O	3.2E+07	3.2E+07	**6.23**			C24H33ClN2	582.05	QBZITZQG	2.314	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	IC50	muM		0.59
	CC(C)[C@H](NC(=O)[C@H](C)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C1=CC=CC=C1)[C@@H](O)[C@H](O)[C@H](CC1=CC=CC=C1)NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCC1=CC=CC=C1)C(C)C	8250026	8250026	**6.22**	204907-85-7	phenylmethyl N-[(2S)-1-[[(2S)-1-[[(2S,3R,4R,5S)-3,4-dihydroxy-5-[[(2S)-3-methyl-2-[[(2S)-2-(phenylmethoxycarbonylamino)propanoyl]amino]butanoyl]amino]-1,6-di(phenyl)hexan-2-yl]amino]-3-methyl-1-oxobutan-2-yl]amino]-1-oxopropan-2-yl]carbamate; TL3; TL-3	C50H64N6O	909.092	BJJPNOGN	5.54	0	0	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Radioligand (/	Inhibition c Ki (inhibitio	muM	=	0.6
	CC(C)[C@H](NC(=O)[C@H](C)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C1=CC=CC=C1)[C@@H](O)[C@H](O)[C@H](CC1=CC=CC=C1)NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCC1=CC=CC=C1)C(C)C	8250026	8250026	**6.22**	204907-85-7	phenylmethyl N-[(2S)-1-[[(2S)-1-[[(2S,3R,4R,5S)-3,4-dihydroxy-5-[[(2S)-3-methyl-2-[[(2S)-2-(phenylmethoxycarbonylamino)propanoyl]amino]butanoyl]amino]-1,6-di(phenyl)hexan-2-yl]amino]-3-methyl-1-oxobutan-2-yl]amino]-1-oxopropan-2-yl]carbamate; TL3; TL-3	C50H64N6O	909.092	BJJPNOGN	5.54	0	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/	In vitro bin Ki (inhibitio	muM	=	0.6
	C[C@@H](NC(=O)C1=C(C)C=CC(N)=C1)C1=C2C=CC=CC2=CC=C1	2E+07	2E+07	**6.22**	1093070-16-(	5-amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide; GRL-0617S; 5-Amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide	C20H20N2O	304.392	UVERBUNI	4.549	4	2	**Papain-like protease [Coronaviridae]**	Coronaviridae		Minimum i IC50	muM	=	0.6
	C[C@@H](NC(=O)C1=C(C)C=CC(N)=C1)C1=C2C=CC=CC2=CC=C1	2E+07	2E+07	**6.22**	1093070-16-(	5-amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide; GRL-0617S; 5-Amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide	C20H20N2O	304.392	UVERBUNI	4.549	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus		Inhibitory c IC50	nM		600
	C[C@@H](NC(=O)C1=C(C)C=CC(N)=C1)C1=C2C=CC=CC2=CC=C1	2E+07	2E+07	**6.22**	1093070-16-(	5-amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide; GRL-0617S; 5-Amino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide	C20H20N2O	304.392	UVERBUNI	4.549	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c IC50	muM	=	0.6
	[H][C@@]1(C[C@H](NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(C)=O)C(C)C)[C@@H](C)OCC2=CC=CC=C2)C(=O)CN2N(C(=O)C3=C(C=CC=C3N)N(=O)=O)C2=O)CCNC1=O	9892814	9892814	**6.22**			C40H52N8O	820.9	TYWILPQK	3.013	1	0	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory a IC50	muM	=	0.6

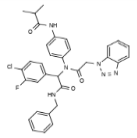
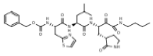
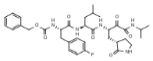
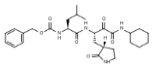
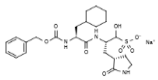
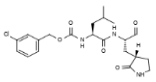
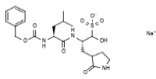
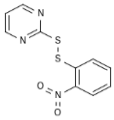
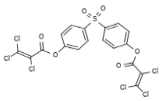
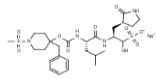
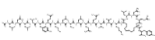
	[H][C@@]1(C[C@H](NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C(C)(C)[C@@H](C)OCC2=CC=CC=C2)C(=O)CN2N(C(=O)C3=C(C=CC=C3N(=O)=O)C2=O)CCNC1=O	9892814	9892814	**6.22**			C40H52N8O	820.9	TYWILPQK	3.013	1	0	**Sars Cov 3C-Like Protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory (	IC50	muM	=	0.6
	[Na+].CC(C)C[C@H](NC(=O)OC1(CC2=CC=CC=C2)CN(CC1)C(=O)OC(C)(C)C)C[C@](=O)N[C@@H](C)C[C@@H](1CCNC1=O)C(O)S(=(O-))(=O)=O	3.2E+07	3.2E+07	**6.22**		sodium (2S)-2-{(S)-2-{({[4-benzyl-1-(tert-butoxycarbonyl)piperidin-4-yl]oxy}carbonyl)amino]-4-methylpentanamido}-1-hydroxy-3-{(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C31H47N4O	690.791	GODLXHBI	2.133	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor		IC50	muM		0.6
	[Na+].CC(C)C[C@H](NC(=O)OC1CCN(CC1)S(C)(=O)=O)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(=(O-))(=O)=O	3.2E+07	3.2E+07	**6.22**		sodium (2S)-1-hydroxy-2-{(S)-4-methyl-2-{({[1-(methylsulfonyl)piperidin-4-yl]oxy}carbonyl)amino]pentanamido}-3-{(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C20H35N4O	578.64	OXYUFTID	-1.395	2	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor		IC50	muM		0.6
	[Bi+3].[O-]N(=O)=O.[N-]1C2=CC=C1C(C1=CC=CC=C1)=C1\C=CC(=N\1)/C(C1=CC=CC=C1)=C1[N-]C(/C=C\1)=C(\C1=N)C(\C=C1)=C/2C1=CC=CC=C1)C1=CC=CC=C1	1.6E+07	1.6E+07	**6.22**			Bi*C44H28N	883.718	ZUMUQSX		2	2	**helicase [SARS coronavirus]**	SARS coronavirus		Effect : enz	IC50	muM		0.6
No Structure		2.4E+07	2.4E+07	**6.22**		Acetyl-VT(O-(Benzyl))LA(3-((S)-2-oxopyrrolidin-3-yl))-(1,4-dioxo-2,3-dihydro-5-nitro-phthalazine-2-yl)methyl							**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.6
No Structure		2.5E+07	2.5E+07	**6.22**		Acetyl-VS(O-(Benzyl))LA(3-((R)-2-oxo-3-pyrrolidyl))-(1,4-dioxo-2,3-dihydro-5-nitro-phthalazine-2-yl)methyl							**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.6
	CC(C)C[C@H](NC(=C)[C@@H](NC(=O)[C@@H](NC(C)=O)C(C)C)[C@@H](OCC1=CC=CC=C1)C(=O)N[C@@H](CC1CCNC1=O)C(=O)CN1NC(=O)C2=C(C=CC=C2N(=O)=O)C1=O	2.6E+07	2.6E+07	**6.22**	1350215-80-3		C41H54N8O	818.927	SJIZFTYKK	4.094	1	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Inhibitor	In vitro inh	IC50	muM	=	0.6
	CN(C)=O)C1=CC=C(CNC(=O)C2CCN(CC2)[C@H](C)C2=CC=CC3=CC=CC=C23)C=C1	2.7E+07	2.7E+07	**6.22**	1581755-36-3	(R)-N-(4-(methylcarbamoyl)benzyl)-1-(1-(naphthalen-1-yl)-ethyl)piperidine-4-carboxamide	C27H31N3O	429.562	CLOQJEW	4.386	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.6
	CC(C)C[C@H](NC(=O)OC1CCN(CC1)C(=O)OC(C)(C)C)C(=O)N[C@@H](C)C[C@@H]1CCNC1=O)C=O	3.2E+07	3.2E+07	**6.22**		tert-butyl 4-({[(S)-4-methyl-1-oxo-1-{((S)-1-oxo-3-[(S)-2-oxopyrrolidin-3-yl]propan-2-yl)amino)pentan-2-yl]carbamoyl}oxy)piperidine-1-carboxylate	C24H40N4O	496.604	SBHUNCJS	2.275	3	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor		IC50	muM		0.6
	CCOC(=O)N1CCC(CC1)OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	3.2E+07	3.2E+07	**6.22**		ethyl 4-({[(S)-4-methyl-1-oxo-1-{((S)-1-oxo-3-[(S)-2-oxopyrrolidin-3-yl]propan-2-yl)amino]pentan-2-yl]carbamoyl}oxy)piperidine-1-carboxylate	C22H36N4O	468.55	YYTRYFVB	1.398	3	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor		IC50	muM		0.6
	CCCCNC(=O)C(=O)[C@H](C[C@@H](1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](CC1=NC=C(CS1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.22**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-(5-methyl-1,3-thiazol-2-yl)ethyl]carbamate	C33H46N6O	670.83	GKSGNHPI	1.908	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor		pIC50	no unit		6.22

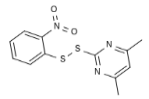
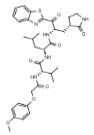
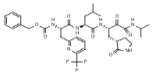
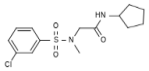
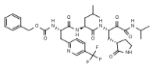
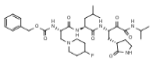
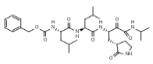
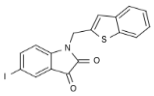
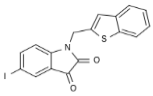
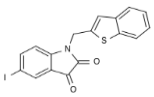
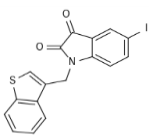
	[N+].[H][C@@]1(C[C@H][N(C(=O)[C@H](CC(C)C)NC(=O)OC2CCC(CC2)C2=CC=CC=C2)C(O)S)[O-])(=O)=O)CCNC1=O	3.3E+07	3.3E+07	**6.22**			C26H38N3O	575.659	OOMCVQ\	1.823	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	IC50	muM	0.6
	[N+].[H][C@@]1(C[C@H][N(C(=O)[C@H](CC(C)C)NC(=O)OCCC2=CC=CC(C)=C2)C(O)S)[O-])(=O)=O)CCNC1=O	3.3E+07	3.3E+07	**6.22**			C22H31ClN2	556.012	ZIVZAVLW	1.105	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	EC50	muM	0.6
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=CC2=C1C=CC=C2)N(C(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	2.4E+07	2.4E+07	**6.21**			C38H47N5O	685.82	GCYUVLW	4.651	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	muM	0.61
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC[C]=CC=C1)N(C=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.21**		benzyl N-[(1S)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl}-2-(3-methylphenyl)ethyl]carbamate	C35H47N5O	649.787	PVFWUOR	3.822	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.21
	CCC1(CC)C[C@H](N(C1)C(=O)[C@H](CC1=CC=C(F)C=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.21**		benzyl N-[(2S)-1-[(2S)-4,4-diethyl-2-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl}pyrrolidin-1-yl]-3-(4-fluorophenyl)-1-oxopropan-2-yl]carbamate	C37H48FN5	693.816	AFQMPDK	4.166	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.21
	ClC1=CC=CC(COC(=O)N[C@@H](C2CCCCC2)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C=O)=C1	3.2E+07	3.2E+07	**6.2**			C24H32ClN3	477.988	FXHORQM	4.318	4	1	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	IC50	muM	0.63
	CNC(=O)C1=CC=CC(CNC(=O)[C@H]1CCN(C=O)[C@H](C)C2=CC=CC3=CC=CC=C23)=C1	2.7E+07	2.7E+07	**6.2**	1581755-37-4	(R)-N-(3-(methylcarbamoyl)benzyl)-1-(1-(naphthalen-1-yl)-ethyl)piperidine-4-carboxamide	C27H31N3O	429.562	SCVNWDH	4.386	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus		IC50	muM	0.63
	CCCCNC(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC1=NC=CC(=O)C(OC(C)C)=C1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.2**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-{butylcarbamoyl}-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-[4-(propan-2-yloxy)pyridin-2-yl]ethyl]carbamate	C37H52N6O	708.855	QQYAQVN	3.487	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.2
	L.L.L.L.L.L@H](NL(+L)L)L@H](CC(O)=O)NC(=O)[C@H](CC1=CC=C(O)C=C1)NC(=O)[C@@H](NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC(O)=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](CC(C)C)C(=O)NC(C@@H)(CC(C)C)C(=O)NC(C@@H)(CC(C)C)C(=O)NC(C@@H)(CCC(N)=O)C(=O)NC(C@@)1(C)CCCC=CCCC(C@)(C)NC(=O)[C@H](CCCCN)NC(=O)[C@@H](NC(=O)[C@@H](NC1=O)C	3.3E+07	3.3E+07	**6.2**			C119H191N	2531.97	FTNDXEAV	1.123	1	0	**spike protein [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM	0.63
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)COC1=CC=CC=C1)NC(C)C)C(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	**6.19**	1383923-00-9		C35H46N6O	678.853	VEMALIBH	3.516	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	muM	0.65
	CCOC(=O)/C=C\C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C	1.1E+07	1.1E+07	**6.18**			C30H44N4O	572.702	WDMSWV	3.617	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [Coronaviridae]**	Coronaviridae	Radioligand (/	In vitro bin Ki (inhibitio	muM	= 0.66

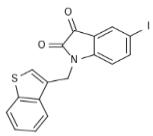
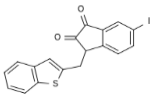
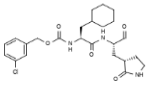
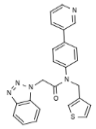
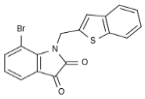
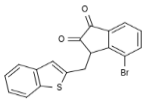
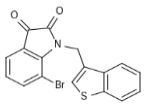
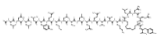
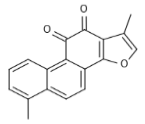
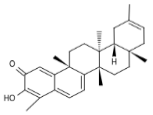
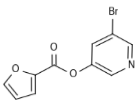
	CCOC(=O)[C@H](C=C\[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C	2.4E+07	2.4E+07	**6.18**			C30H44N4O	572.702				**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			Ki (inhibitio	muM		0.66
	C[C@@H](N1CCC(CC1)C(=O)NCC1=CC2=C(OCO2)C=C1)C1=CZC=CC=CC2=CC=C1	2.1E+07	2.1E+07	**6.17**	1234195-91-5	1-[(R)-1-(1-naphthyl)ethyl]-4-[3,4-(methylenedioxy)benzylamino]carbonylpiperidine; GRL-0667S	C26H28N2O	416.52	IVXBCFLW	4.47	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.67
	COC1=CC(=CC=C1O)C12OC3(O)CC(O)(CC(O)(C3)O1)O2	2.5E+07	2.5E+07	**6.17**			C14H16O8	312.276	HEBOXBAV	-0.524	4	2	**helicase [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibition c	IC50	muM	=	0.68
	ClC1=CC=C[SSC2=NC=CC=N2]C=C1	3.1E+07	3.1E+07	**6.16**		2-((4-chlorophenyl)disulfanyl)pyrimidine	C10H7ClN2S	254.764	SPHGDOQ	2.89	4	2	**Main proteinase (Mpro) [SARS coronavirus]**	SARS coronavirus	Inhibitor		IC50	muM		0.684
	BrC1=CC=C[SSC2=NC=CC=N2]C=C1	3.1E+07	3.1E+07	**6.16**		2-((4-bromophenyl)disulfanyl)pyrimidine	C10H7BrN2S	299.215	OAGXVFKK	3.066	4	2	**Main proteinase (Mpro) [SARS coronavirus]**	SARS coronavirus	Inhibitor		IC50	muM		0.697
	O=C[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC1CCCCC1)NC(=O)OCC1=CC=CC=C1	3.2E+07	3.2E+07	**6.16**			C24H33N3O	443.543	YDHLZYPC	3.696	4	1	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor		IC50	muM		0.69
	ClC1=CC(OC(=O)C2=CN=CC=C2)=CN=C1	1.6E+07	1.6E+07	**6.16**	1007552-03-5		C11H7ClN2O	234.642	ARSVVAZB	1.642	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	nM		697
	ClC1=CC(OC(=O)C2=CC(=CC=C2)N(=O)=O)=CN=C1	1.6E+07	1.6E+07	**6.16**	1007552-06-8		C12H7ClN2O	278.652	GDFHBGYI	2.786	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	nM		684
	CC(=O)O[Hg]C1=CC=CC=C1	3662930	3662930	**6.15**	62-38-4	phenylmercuric acetate; phenylmercury(II) acetate; phenyl mercuric acetate; phenyl-mercuric acetate; phenylmercury acetate; phenylmercuriacetate; PMA	C8H8HgO2	336.74	XEBWQGV	2.254	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibition c	Ki (inhibitio	muM	=	0.7
	CC(=O)O[Hg]C1=CC=CC=C1	3662930	3662930	**6.15**	62-38-4	phenylmercuric acetate; phenylmercury(II) acetate; phenyl mercuric acetate; phenyl-mercuric acetate; phenylmercury acetate; phenylmercuriacetate; PMA	C8H8HgO2	336.74	XEBWQGV	2.254	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/	In vitro bin	Ki (inhibitio	muM	=	0.7
	CC1=COC2=C1C(=O)C(=O)C1=C3C=CC=C(C)C3=CC=C21	237369	237369	**6.15**	568-73-0	Tanshinone I; 1,6-dimethyl-phenanthreno[1,2-b]furan-10,11-diketone; 1,6-dimethylnaphtho[1,2-g][1]benzofuran-10,11-dione; 1,6-dimethylphenanthro[1,2-b]furan-10,11-dione; tanshinone IIA; tanshinone I; tanshinone-1	C18H12O3	276.291	AIGAZQPH	3.769	4	2	**Papain-like protease [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.7

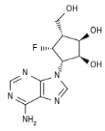
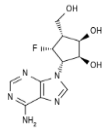
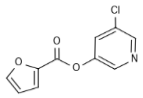
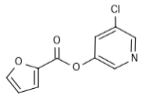
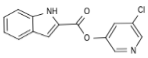
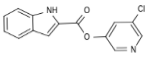
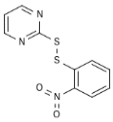
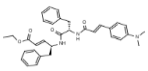
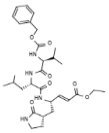
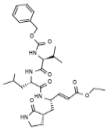
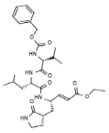
	[Na+].CC(C)C[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC1CCNC1=O)C(O)S(O-])(=O)=O	2.3E+07	2.3E+07	**6.15**	1416992-39-(	sodium (2S)-2-((S)-2-(((benzyloxy)carbonyl)amino)-4-methylpentanamido)-1-hydroxy-3-(2-oxopyrrolidin-3-yl)propane-1-sulfonate	C21H30N3O	507.54	BSPJDKCM	0.325	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	IC50	muM	0.7
	COC1=NC=CC=C1C1=CC=C(C=C1)N(CC1=CSC=C1)C(=O)N(C@@H](CC1CCNC1=O)=NC2=C1C=CC=C2	2.4E+07	2.4E+07	**6.15**			C25H21N5O	455.54	NGIZLVDU	4.317	4	2	**3CLpro (3-chymotrypsin-like protease) [SARS coronavirus]**	SARS coronavirus	Inhibitor	IC50	muM	0.7
	[Na+].CC(C)C[C@H](NC(=O)OC1(CC2=CC=CC=C2)CCN(CC1)S(=O)=O)C(=O)N[C@@H](CC1CCNC1=O)C(O)S(O-])(=O)=O	3.2E+07	3.2E+07	**6.15**		sodium (2S)-2-[(S)-2-{({[4-benzyl-1-(tert-butoxycarbonyl)piperidin-4-yl]oxy}carbonyl)amino]-4-methylpentanamido}-1-hydroxy-3-[(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C31H47N4O	690.791	GODLXHBI	2.133	2	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	IC50	muM	0.7
	CC(C)C[C@H](NC(=O)OC1(CC2=CC=CC=C2)CCN(CC1)S(C)(=O)=O)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	3.2E+07	3.2E+07	**6.15**		4-benzyl-1-(methylsulfonyl)piperidin-4-yl {(S)-4-methyl-1-oxo-1-[{(S)-1-oxo-3-[(S)-2-oxopyrrolidin-3-yl]propan-2-yl}amino]pentan-2-yl}carbamate	C27H40N4O	564.703	ZLOZUJAXI	2.471	2	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	IC50	muM	0.7
	CC(C)C[C@H](NC(=O)OC1CCN(S(C)(=O)=O)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	3.2E+07	3.2E+07	**6.15**		1-(methylsulfonyl)piperidin-4-yl {(S)-4-methyl-1-oxo-1-[{(S)-1-oxo-3-[(S)-2-oxopyrrolidin-3-yl]propan-2-yl}amino]pentan-2-yl}carbamate	C20H34N4O	474.579	POHZAMN	0.609	3	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	IC50	muM	0.7
	[Na+].[H][C@@]1(C[C@H](NC(=O)[C@H](CC(C)C)NC(=O)OCCCC2=CC=CC(=C)=C2)C[O]S[O-])(=O)=O)CCNC1=O	3.3E+07	3.3E+07	**6.15**			C22H31ClN3	556.012	ZIVZAVLW	1.105	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	IC50	muM	0.7
	[Na+].[H][C@@]1(C[C@H](NC(=O)[C@H](CC(C)C)NC(=O)OCCCCCCCCCC)C[O]S[O-])(=O)=O)CCNC1=O	3.3E+07	3.3E+07	**6.15**			C24H44N3O	557.684	HHNLARZI	3.379	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM	0.7
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N(CCC1=CC=CC=C1)C(=O)C(F)(F)F	1.9E+07	1.9E+07	**6.14**	1034140-83-(		C32H41F3N4	634.696	PDLFIYNG(	5.092	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/ Binding aff	Ki (inhibitio	muM	= 0.73
No Structure		2.5E+07	2.5E+07	**6.14**		Benzyloxycarbonyl-AVLF(D/L)-Trifluoromethyl							**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	muM	0.73
	CC(C)C[C@H](NC(=O)[C@H](CC1=NC=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)N(C[C@@H](C)C1CCCCC1	3.3E+07	3.3E+07	**6.13**		benzyl N-[(1S)-1-[[(1S)-1-[[(2S)-1-[((1S)-1-cyclohexylethyl]carbamoyl}-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl]-2-(pyridin-2-yl)ethyl]carbamate	C38H52N6O	704.867	KIPIKDUH	4.244	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.13
	CC(C)C[C@H](NC(=O)[C@H](CN1CCCCC1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)N(C)C)C	3.3E+07	3.3E+07	**6.13**		benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl}-2-(piperidin-1-yl)ethyl]carbamate	C33H50N6O	642.796	YAPXNEGF	2.234	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.13

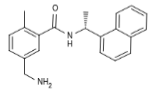
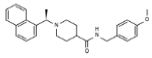
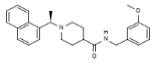
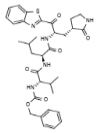
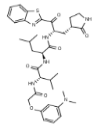
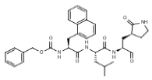
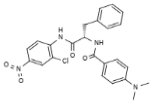
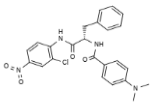
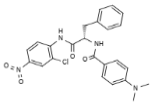
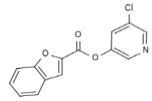
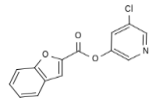
	COC1=CC=CC(OCC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C(C@@H](2CCN C2=O)C(=O)C2=NC3=CC=CC=C3S2)=C1	2.3E+07	2.3E+07	**6.12**	1383922-88-(		C34H43N5O	665.811	IWZSFDOR	3.222	3	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.75
	CC1COC2=C1C(=O)C(=O)C1=C3CCCC(C)(C)C3=CC=C21	288778	288778	**6.1**	17545-07-2;	(+/-)-cryptotanshinone; (+/-)-chryptotanshinone; cryptotanshinone; crytotanshinone; 1,6,6-trimethyl-1,2,6,7,8,9-hexahydro-phenanthro[1,2-b]furan-10,11-dione; 1,6,6-trimethyl-1,2,6,7,8,9-hexahydro-phenanthro[1,2-b]furan-10,11-quinone; 1,6,6-Trimethyl-1,2,6,7,8,9-hexahydro-phenanthro[1,2-(S)-3-	C19H20O3	296.366	GVKKJJON	4.152	4	2	**PIpro [SARS coronavirus]**	SARS coronavirus	Inhibitory (	IC50	muM	=	0.8
	CC(C)(C)OC(=O)C(C@H)(NC(=O)OCC1=CC=CC=C1)C(=O)CBr	6820432	6820432	**6.1**	153088-76-7	benzyloxycarbonylamino-5-bromo-4-oxo-pentanoic acid tert-butyl ester; (3S)-3-(N-benzyloxycarbonyl)amino-5-bromo-4-oxopentanoic acid tert-butyl ester; (S)-3-benzyloxycarbonylamino-5-bromo-4-oxopentanoic acid tert-butyl ester; (S)-tert-butyl 3-	C17H22BrN	400.269	PBVFTOAY	3.077	4	1	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Radioligand (/	Kd (dissocia	nM		800
	[H][C@@]12CC(C)=CC(C@]3([C)CC(C@]1(C)C3=CC=C4C(C)=C(O)C(=O)C=C4)C@]3(C)CC(C@@]21C	2184039	2184039	**6.1**	53527-47-2	Iguesterin; iguesterin; iguestrin; Iguestresin	C28H36O2	404.593	FLMDVQJV	8.906	3	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		Ki (inhibitio	muM		0.8
	CC(C)C(C@H)(NC(=O)(C@@H](NC(=O)[C@H](C)NC(=O)OCC1=CC=CC=C1)C)C(=O)NC(CC1=CC=CC=C1)C(=O)C(F)(F)F	1.9E+07	1.9E+07	**6.1**	1034140-83-4		C32H41F3N4	634.696	PDLFIYNG(	5.092	2	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory (	IC50	muM	=	0.8
	CC(C)C(C@H)(NC(=O)OC1(CC2=CC=CC=C2)CCN(CC1)C(=O)OC(C)(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	3.2E+07	3.2E+07	**6.1**		tert-butyl 4-benzyl-4-(((((S)-4-methyl-1-oxo-1-[(((S)-1-oxo-3-((S)-2-oxopyrrolidin-3-yl]propan-2-yl]amino]pentan-2-yl)carbamoyl]oxy)piperidine-1-carboxylate	C31H46N4O	586.729	UGEDYCZH	4.137	2	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	IC50	muM		0.8
	[Na+].CC(C)C[C@H](NC(=O)OC1(CC2=CC=CC=C2)CCN(CC1)C(=O)OC(C)(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(([O-])(=O)=O	3.2E+07	3.2E+07	**6.1**		sodium (2S)-2-[(S)-2-[(([(4-benzyl-1-(tert-butoxycarbonyl)piperidin-4-yl]oxy)carbonyl)amino]-4-methylpentanamido)-1-hydroxy-3-[(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C31H47N4O	690.791	GODLXHBI	2.133	2	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM		0.8
	[Na+].CC(C)C[C@H](NC(=O)OC1(CC2=CC=CC=C2)CCN(CC1)C(=O)OC(C)(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(([O-])(=O)=O	3.2E+07	3.2E+07	**6.1**		sodium (2S)-2-[(S)-2-[(([(4-benzyl-1-(tert-butoxycarbonyl)piperidin-4-yl]oxy)carbonyl)amino]-4-methylpentanamido)-1-hydroxy-3-[(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C31H47N4O	690.791	GODLXHBI	2.133	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM		0.8
	[Na+].CC(C)C[C@H](NC(=O)OC1(CC2=CC=CC=C2)CCN(CC1)C(=O)OC(C)(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S(([O-])(=O)=O	3.2E+07	3.2E+07	**6.1**		sodium (2S)-2-[(S)-2-[(([(4-benzyl-1-(tert-butoxycarbonyl)piperidin-4-yl]oxy)carbonyl)amino]-4-methylpentanamido)-1-hydroxy-3-[(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C31H47N4O	690.791	GODLXHBI	2.133	2	0	**3C-like proteinase [Coronavirinae]**	Coronavirinae	Inhibitor	EC50	muM		0.8
No Structure		2.5E+07	2.5E+07	**6.1**		Benzyloxycarbonyl-AVLF(D/L)-Trifluoromethyl							**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.8
	CC1=CC(C@]2(C)CC(C@]3(C)C4=CC=CSC(C)=C(O)C(=O)C=CS(C@]4(C)CC(C@@]3(C)C2C1	2.6E+07	2.6E+07	**6.1**			C28H36O2	404.593	FLMDVQJV	8.906	3	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [Coronaviridae]**	Coronaviridae	Inhibitor	Inhibition (	Ki (inhibitio	muM	=	0.8

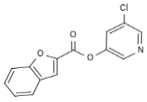
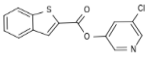
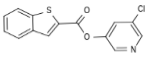
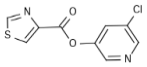
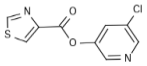
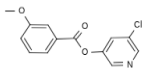
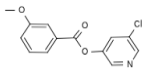
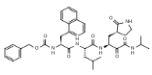
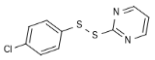
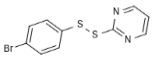
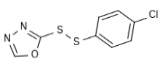
	CC(C)C(=O)NC1=CC=C(C=C1)N(C)C(=O)NCC1=CC=CC=C1)C=CC=C(C)C)C(F)=C1)C(=O)CN1N=NC2=CC=CC=C12	3.2E+07	3.2E+07	**6.1**		N-(4-{2-{1H-benzo[d][1,2,3]triazol-1-yl}-N-{2-[benzylamino]-1-(4-chloro-3-fluorophenyl)-2-oxoethyl}acetamido)phenyl)isobutyramide	C33H30ClFN	613.091	ISHXMYLD	4.924	3	1	**3C-like protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	IC50	muM	0.8
	CCCCN(=O)C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)N(C)=O)[C@H](CC1=NC=CS1)NC(=O)OCC1=CC=CC=C1	3.3E+07	3.3E+07	**6.1**		benzyl N-[(1S)-1-{[(1S)-1-{[(2S)-1-(butylcarbamoyl)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl}-3-methylbutyl]carbamoyl}-2-(1,3-thiazol-2-yl)ethyl]carbamate	C32H44N6O	656.803	SUIHQODL	2.057	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.1
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=C(F)C=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	3.3E+07	3.3E+07	**6.09**		benzyl N-[(1S)-2-(4-fluorophenyl)-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl}butyl]carbamoyl}ethyl]carbamate	C34H44FN5	653.751	ZUZMPCW	3.546	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor	pIC50	no unit	6.09
	[H][C@@]1(C[C@H](NC(=O)[C@H](CC(C)C)NC(=O)OCC2=CC=CC=C2)C(=O)C(=O)NC2CCCCC2)CCNC1=O	3.4E+07	3.4E+07	**6.08**			C28H40N4O	528.649	XOIKFGSU	3.187	3	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	IC50	muM	0.83
	[Na+].OC(=[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC1CCCCC1)NC(=O)OCC1=CC=CC=C1)S([O-])(=O)=O	3.2E+07	3.2E+07	**6.07**			C24H34N3O	547.605	QIIXTKHVL	1.692	2	0	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	IC50	muM	0.86
	[H][C@@](1C(C[C@H](NC(=O)[C@H](CC(C)C)NC(=O)OCC2=CC=CC(Cl)=C2)C=O)CCNC1=O	3.4E+07	3.4E+07	**6.06**			C21H28ClN3	437.923	ORVJRZJF	2.951	4	1	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	IC50	muM	0.88
	[Na+].CC(C)C[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC1CCNC1=O)C(O)S([O-])(=O)=O	2.3E+07	2.3E+07	**6.05**	1416992-39-(	sodium (2S)-2-((S)-2-(((benzyloxy)carbonyl)amino)-4-methylpentanamido)-1-hydroxy-3-(2-oxopyrrolidin-3-yl)propane-1-sulfonate	C21H30N3O	507.54	BSPJDKCM	0.325	2	0	**3C-like protease [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM	0.9
	O=N(=O)C1=CSSC2=NC=CC=N2)C=CC=C1	804680	804680	**6.05**		2-((2-nitrophenyl)disulfanyl)pyrimidine; 2-(2-nitro-phenyldisulfanyl)-pyrimidine; 2-(2'-Nitrophenyldithio)-pyrimidin	C10H7N3O2	265.316	ADRGABK(	2.16	4	2	**Main proteinase (Mpro) [SARS coronavirus]**	SARS coronavirus	Inhibitor	IC50	muM	0.883
	Cl\C(Cl)=C/(Cl)C(=O)OC1=CC=C(C=C1)S(=O)(=O)C1=CC=C(OC(=O)C(\Cl)=C(/Cl)Cl)C=C1	1.1E+07	1.1E+07	**6.05**			C18H8Cl6O6	565.042	HXYPMMA	6.49	2	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Inhibitor	IC50	muM	0.9
	[Na+].CC(C)C[C@H](NC(=O)OC1C2=CC=CC=C2CCNC1)S(C)(=O)=O)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(O)S([O-])(=O)=O	3.2E+07	3.2E+07	**6.05**		sodium (2S)-2-((S)-2-[(([4-benzyl-1-(methylsulfonyl)piperidin-4-yl]oxy)carbonyl)amino]-4-methylpentanamido)-1-hydroxy-3-[(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C27H41N4O	668.765	PVFOFJYH	0.467	2	0	**Replicase polyprotein 1ab [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	IC50	muM	0.9
	CSCC(C@H](NC(=O)[C@H](CCC(O)=O)NC(=O)[C@H](CC1=CC=C(O)C=C1)NC(=O)[C@@H](NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC(O)=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CCC(O)=O)NC(=O)[C@@H](CCCCN)C(=O)	3.3E+07	3.3E+07	**6.05**			C120H192N	2591.06	ZEXNMYV(	0.906	1	0	**spike protein [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM	0.89

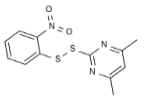
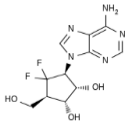
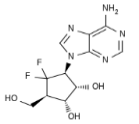
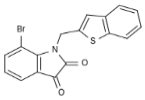
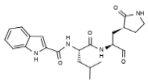
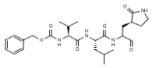
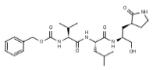
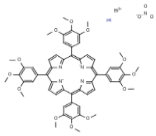
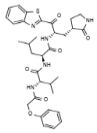
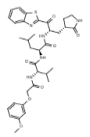
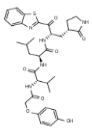
	CC1=CC(C)=NC(SSC2=CC=CC=C2N(=O)=O)=N1	3.1E+07	3.1E+07	**6.04**		4,6-dimethyl-2-((2-nitrophenyl)disulfanyl)pyrimidine	C12H11N3O	293.37	OXOOBQV	2.79	4	2	**Main proteinase (Mpro) [SARS coronavirus]**	SARS coronavirus	Inhibitor		IC50	muM		0.921
	COC1=CC=C(OCC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)[C@@H]2CCN(C2=O)C(=O)C2=NC3=CC=CC=C352)C=C1	2.3E+07	2.3E+07	**6.04**	1383922-80-:		C34H43N5O	665.811	DYFSDLME	3.222	3	0	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.92
	CC(C)C[C@H](NC(=O)[C@H](CC1=NC(=CC=C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C)C@@H](1CCN(C1=O)C(=O)C(=O)NC)C)C	3.3E+07	3.3E+07	**6.04**		benzyl ((5)-1-(((S)-1-(((S)-4-(isopropylamino)-3,4-dioxo-1-((S)-2-oxopyrrolidin-3-yl)butan-2-yl)amino)-4-methyl-1-oxopentan-2-yl)amino)-1-oxo-3-(6-(trifluoromethyl)pyridin-2-yl)propan-2-yl)carbamate; benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-	C34H43F3N	704.747	DQTFXZM	3.236	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor		pIC50	no unit		6.04
	CN(CC(=O)NC1CCCC1)S(=O)(=O)C1=CC(Cl)=CC=C1	2.7E+07	2.7E+07	**6.03**	853595-74-1		C14H19ClN2	330.835					**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c	IC50	muM	=	0.94
	CC(C)C[C@H](NC(=O)[C@H](CC1=NC=C(C=C1)C(F)(F)F)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C)C@@H](1CCN(C1=O)C(=O)C(=O)NC)C)C	3.3E+07	3.3E+07	**6.03**		benzyl N-[(1S)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl}-2-[5-(trifluoromethyl)pyridin-2-yl]ethyl]carbamate	C34H43F3N	704.747	PVEAZVRG	3.147	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor		pIC50	no unit		6.03
	CC(C)C[C@H](NC(=O)[C@H](CN1CCC(F)(F)C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C)C@@H](1CCNC1=O)C(=O)C(=O)NC)C)C	3.3E+07	3.3E+07	**6.03**		benzyl N-[(1S)-2-(4-fluoropiperidin-1-yl)-1-[[(1S)-3-methyl-1-[[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl]butyl]carbamoyl}ethyl]carbamate	C33H49FN6	660.786	HLWOHQI	2.378	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor		pIC50	no unit		6.03
	CC(C)C[C@H](NC(=O)OC C1=CC=CC=C1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C)C@@H](1CCN(C1=O)C(=O)C(=O)NC)C)C	3.3E+07	3.3E+07	**6.03**		benzyl N-[(1S)-3-methyl-1-{[(1S)-3-methyl-1-{[(2S)-1-oxo-3-[(3S)-2-oxopyrrolidin-3-yl]-1-[(propan-2-yl)carbamoyl]propan-2-yl]carbamoyl}butyl]carbamoyl}butyl]carbamate	C31H47N5O	601.743	HEVXFSPU	3.375	2	0	**3CL protease [Coronavirinae]**	Coronavirinae	Inhibitor		pIC50	no unit		6.03
	IC1=CC=C2N(CC3=CC4=CC=CC=C453)C(=O)C(=O)C2=C1	7594653	7594653	**6.02**	861216-06-0		C17H10INO2	419.242	MAYSJMB	3.905	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus			IC50	muM		0.95
	IC1=CC=C2N(CC3=CC4=CC=CC=C453)C(=O)C(=O)C2=C1	7594653	7594653	**6.02**	861216-06-0		C17H10INO2	419.242	MAYSJMB	3.905	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus	Inhibitor	In vitro inh	IC50	muM	=	0.95
	IC1=CC=C2N(CC3=CC4=CC=CC=C453)C(=O)C(=O)C2=C1	7594653	7594653	**6.02**	861216-06-0		C17H10INO2	419.242	MAYSJMB	3.905	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c	IC50	muM	=	0.95
	IC1=CC=C2N(CC3=CSC4=C3C=CC=C4)C(=O)C(=O)C2=C1	2.5E+07	2.5E+07	**6.02**			C17H10INO2	419.242	BQVHRIFP	4.235	4	2	**Sars Cov 3C-Like Protease [SARS coronavirus]**	SARS coronavirus	Inhibitor	Inhibitory c	IC50	muM	=	0.95

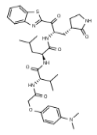
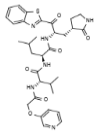
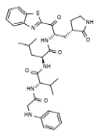
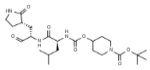
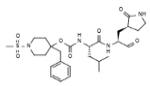
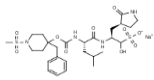
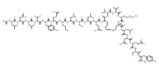
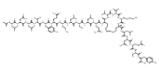
	IC1=CC=C2N(CC3=CSC4=C3C=CC=C4)C(=O)C(=O)C2=C1	2.5E+07	2.5E+07	**6.02**			C17H10INO	419.242	BQVHRIFP	4.235	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitory	IC50	muM		0.95
	IC1=CC=C2C(CC3=CC4=C(S3)C=CC=C4)C(=O)C(=O)C2=C1	2.6E+07	2.6E+07	**6.02**			C18H11IO2S	418.255	CWBDSMS	4.147	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor Inhibitory	IC50	muM	=	0.95
	ClC1=CC=CC(COC(=O)N[C@@H](CC2CCCCC2)C(=O)N[C@@H](C[C@@H](C[C@@H]2CCNC2=O)C=O)=C1	3.2E+07	3.2E+07	**6.01**			C24H32ClN3	477.988	FXHORQM	4.318	4	1	**3C-like protease [Coronavirinae]**	Coronavirinae	Inhibitor	IC50	muM		0.98
	O=C(CN1N=NC2=C1C=CC=C2)N(CC1=CSC=C1)C1=CC=C(C=C1)C1=CC=CN=C1	2.4E+07	2.4E+07	**6.01**			C24H19N5O	425.514	LHBIUOYH	3.674	4	2	**3CLpro (3-chymotrypsin-like protease) [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.97
	BrC1=CC=CC2=C1N(CC1=CC3=C(S1)C=CC=C3)C(=O)C2=O	1E+07	1E+07	**6.01**			C17H10BrN	372.242	UFOWXDL	3.635	4	2	**3C-like proteinase (cleavage product of Replicase polyprotein 1ab) [SARS coronavirus]**	SARS coronavirus		IC50	muM		0.98
	BrC1=C2C(CC3=CC4=C(S3)C=CC=C4)C(=O)C(=O)C2=CC=C1	2.6E+07	2.6E+07	**6.01**			C18H11BrO	371.254	XDCJGGHI	3.877	4	2	**Severe Acute Respiratory Syndrome-Cov 3Clpro [SARS coronavirus]**	SARS coronavirus	Inhibitor Inhibitory	IC50	muM	=	0.98
	BrC1=CC=CC2=C1N(CC1=CSC3=C1C=CC=C3)C(=O)C2=O	2.6E+07	2.6E+07	**6.01**	1347890-63-		C17H10BrN	372.242	GSJXYXKS	3.965	4	2	**Sars Cov 3C-Like Protease [SARS coronavirus]**	SARS coronavirus	Inhibitor Inhibitory	IC50	muM	=	0.98
	CSCC[C@H](NC(=O)[C@H](CCC(O)=O)NC(=O)[C@H](CC1=CC=C(O)C=C1)NC(=O)[C@@H](NC(=O)[C@@H](CC(C)C)NC(=O)[C@H](CC(O)=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](C)O)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCCCN)C(=O)	3.3E+07	3.3E+07	**6.01**			C120H192N	2591.06	ZEXNMYV(	0.906	1	0	**spike protein [Middle East respiratory syndrome coronavirus]**	Middle East respiratory syndrome coronavirus	Inhibitor	EC50	muM		0.97
	CC1=COC2=C1C(=O)C(=O)C1=C3=CC=C(C)C3=CC=C21	237369	237369		568-73-0	Tanshinone I; 1,6-dimethyl-phenanthreno[1,2-b]furan-10,11-diketone; 1,6-dimethylnaphtho[1,2-g][1]benzofuran-10,11-dione; 1,6-dimethylphenanthro[1,2-b]furan-10,11-dione; tanshinone IIA; tanshinone I; tanshinone-1	C18H12O3	276.291	AIGAZQPH	3.769	4	2							
	[H][C@@]12CC(C)=CC[C@]3([C]CC[C@]3(C)K3=CC=C4C(C)=C(O)C(=O)C=C4)C@]3([C]CC[C@@]21C	2184039	2184039		53527-47-2	Iguesterin; iguesterin; iguestrin; Iguestresin	C28H36O2	404.593	FLMDVQJV	8.906	3	2							
	BrC1=CC[OC(=O)C2=CC=CO2]=CN=C1	1.1E+07	1.1E+07		936371-58-3		C10H6BrNO	268.067	HMICIXHT	1.77	4	2							

	NC1=NC=NC2=C1N=CN2[C@H]1[C@H](O)[C@H](O)[C@H]1F	1E+07	1E+07		(1R,2S,3S,4R,5R)-3-(6-amino-9H-purin-9-yl)-4-fluoro-5-(hydroxymethyl)cyclopentane-1,2-diol; (-)-6?-beta-fluoro-aristeromycin; 6'-beta-fluoroaristeromycin	C11H14FN5	283.262	LFSGVDMI	-0.667	4	2
	NC1=NC=NC2=C1N=CN2[C@H]1[C@H](O)[C@H](O)[C@H]1F	1E+07	1E+07		(1R,2S,3S,4R,5R)-3-(6-amino-9H-purin-9-yl)-4-fluoro-5-(hydroxymethyl)cyclopentane-1,2-diol; (-)-6?-beta-fluoro-aristeromycin; 6'-beta-fluoroaristeromycin	C11H14FN5	283.262	LFSGVDMI	-0.667	4	2
	ClC1=CC(OC(=O)C2=CC=CO2)=CN=C1	1.1E+07	1.1E+07	353257-73-5		C10H6ClNO	223.616	DWJOEJD	1.594	4	2
	ClC1=CC(OC(=O)C2=CC=CO2)=CN=C1	1.1E+07	1.1E+07	353257-73-5		C10H6ClNO	223.616	DWJOEJD	1.594	4	2
	ClC1=CN=CC(OC(=O)C2=CC3=CC=CC=C3N2)=C1	1.1E+07	1.1E+07			C14H9ClN2	272.691	LJTINUKM	3.06	4	2
	ClC1=CN=CC(OC(=O)C2=CC3=CC=CC=C3N2)=C1	1.1E+07	1.1E+07			C14H9ClN2	272.691	LJTINUKM	3.06	4	2
	O=N(=O)C1=CSSC2=NC=CC=N2)C=CC=C1	804680	804680		2-((2-nitrophenyl)disulfanyl)pyrimidine; 2-(2-nitro-phenyldisulfanyl)-pyrimidine; 2-(2'-Nitrophenyldithio)-pyrimidin	C10H7N3O2	265.316	ADRGABK	2.16	4	2
	CCOC(=O)/C=C\C@H](C1=CC=CC=C1)NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)/C=C\C1=CC=C(C=C1)N(C)C	1.1E+07	1.1E+07			C33H37N3O	539.674	JWPLKCW	5.753	2	1
	CCOC(=O)/C=C\C@H](C[C@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H]1NC(=O)CCC1=CC=CC=C1)C(C)C	1.1E+07	1.1E+07			C30H44N4O	572.702	WDMSWV	3.617	2	0
	CCOC(=O)/C=C\C@H](C[C@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H]1NC(=O)CCC1=CC=CC=C1)C(C)C	1.1E+07	1.1E+07			C30H44N4O	572.702	WDMSWV	3.617	2	0
	CCOC(=O)/C=C\C@H](C[C@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H]1NC(=O)CCC1=CC=CC=C1)C(C)C	1.1E+07	1.1E+07			C30H44N4O	572.702	WDMSWV	3.617	2	0

	C[C@@H](NC(=O)C1=C(C)C=CC(CN)=C1)C1=CC=CC2=CC=CC=C12	2E+07	2E+07	1184301-69-(	5-methylamino-2-methyl-N-[(R)-1-(1-naphthyl)ethyl]benzamide	C21H22N2O	318.418	BIKTWHW	4.488	4	2
	COC1=CC=C(CNC(=O)C2CCN(CC2)[C@H](C)C2=CC=CC3=C2C=CC=C3)C=C1	2.1E+07	2.1E+07	1233939-86-(	1-[(R)-1-(1-naphthyl)ethyl]-4-(4-methoxybenzylamino)carbonylpiperidine	C26H30N2O	402.536	NTMTVRC	4.896	4	2
	COC1=CC(CNC(=O)C2CCN(CC2)[C@H](C)C2=CC=CC3=C2C=CC=C3)=CC=C1	2.1E+07	2.1E+07	1233939-85-(	1-[(R)-1-(1-naphthyl)ethyl]-4-(3-methoxybenzylamino)carbonylpiperidine	C26H30N2O	402.536	QKYBTDRN	4.896	4	2
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N[C@@H](C[C@@H](C)CNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	1359941-93-1		C33H41N5O	635.784	KSCRVOKC	3.789	2	0
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)N(C)C)C(=O)N[C@@H](C[C@@H](C)C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	1417704-35-8		C35H46N6O	678.853	CALSXGHS	3.516	2	0
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=CC2=C1C=CC=C2)N(C)=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	2.4E+07	2.4E+07		(1-{3-methyl-1-[2-oxo-1-(2-oxo-pyrrolidin-3-ylmethyl)ethylcarbamoyl]butylcarbamoyl}-2-naphthalen-1-yl-ethyl)carbamic acid benzyl ester	C34H40N4O	600.715	UULYLRNR	4.738	3	0
	CN(C)C1=CC=C(C=C1)C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O	1E+07	1E+07			C24H23ClN4	466.924	NBBWJEW	4.859	4	2
	CN(C)C1=CC=C(C=C1)C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O	1E+07	1E+07			C24H23ClN4	466.924	NBBWJEW	4.859	4	2
	CN(C)C1=CC=C(C=C1)C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O	1E+07	1E+07			C24H23ClN4	466.924	NBBWJEW	4.859	4	2
	ClC1=CC(OC(=O)C2=CC3=C(O2)C=CC=C3)=CN=C1	1.1E+07	1.1E+07			C14H8ClNO3	273.675	QHBWMD	2.95	4	2
	ClC1=CC(OC(=O)C2=CC3=C(O2)C=CC=C3)=CN=C1	1.1E+07	1.1E+07			C14H8ClNO3	273.675	QHBWMD	2.95	4	2

	ClC1=CC(OC(=O)C2=CC3=C(O2)C=CC=C3)=CN=C1	1.1E+07	1.1E+07		C14H8ClNO:	273.675	QHBWMD	2.95	4	2
	ClC1=CN=CC(OC(=O)C2=CC3=CC=CC=C3S2)=C1	1.1E+07	1.1E+07		C14H8ClNO:	289.742	MNUHXGJ	3.294	4	2
	ClC1=CN=CC(OC(=O)C2=CC3=CC=CC=C3S2)=C1	1.1E+07	1.1E+07		C14H8ClNO:	289.742	MNUHXGJ	3.294	4	2
	ClC1=CN=CC(OC(=O)C2=CSC=N2)=C1	1.1E+07	1.1E+07		C9H5ClN2O:	240.67	CSEAAOW	1.798	4	2
	ClC1=CN=CC(OC(=O)C2=CSC=N2)=C1	1.1E+07	1.1E+07		C9H5ClN2O:	240.67	CSEAAOW	1.798	4	2
	COC1=CC(=CC=C1)C(=O)OC1=CC(Cl)=CN=C1	1.1E+07	1.1E+07		C13H10ClN(	263.68	UIXQHURF	2.809	4	2
	COC1=CC(=CC=C1)C(=O)OC1=CC(Cl)=CN=C1	1.1E+07	1.1E+07		C13H10ClN(	263.68	UIXQHURF	2.809	4	2
	CC(C)C[C@H](NC(=O)[C@H](CC1=CC=CC2=C1C=CC=C2)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NC(C)C	2.4E+07	2.4E+07		C38H47N5O	685.82	GCYUVLW	4.651	2	0
	ClC1=CC=C[SSC2=NC=CC=N2]C=C1	3.1E+07	3.1E+07	2-[(4-chlorophenyl)disulfanyl]pyrimidine	C10H7ClN2S	254.764	SPHGDOQ	2.89	4	2
	BrC1=CC=C[SSC2=NC=CC=N2]C=C1	3.1E+07	3.1E+07	2-[(4-bromophenyl)disulfanyl]pyrimidine	C10H7BrN2S	299.215	OAGXVFKI	3.066	4	2
	ClC1=CC=C[SSC2=NN=CO2]C=C1	3.1E+07	3.1E+07	2-[(4-chlorophenyl)disulfanyl]-1,3,4-oxadiazole	C8H5ClN2OS	244.725	YANPJRMI	4.021	4	2

	CC1=CC(C)=NC(SSC2=CC=CC=C2N(=O)=O)=N1	3.1E+07	3.1E+07		4,6-dimethyl-2-((2-nitrophenyl)disulfanyl)pyrimidine	C12H11N3O	293.37	OXOOBQV	2.79	4	2
	NC1=C2N=CN([C@H]3[C@H](O)[C@H](O)[C@@H](CO)C3(F)F)C2=NC=N1	3.5E+07	3.5E+07		(1R,2S,3S,5R)-3-(6-amino-9H-purin-9-yl)-4,4-difluoro-5-(hydroxymethyl)cyclopentane-1,2-diol; 6',6'-difluoroaristeromycin	C11H13F2N	301.253	XSXKATM	-0.288	4	2
	NC1=C2N=CN([C@H]3[C@H](O)[C@H](O)[C@@H](CO)C3(F)F)C2=NC=N1	3.5E+07	3.5E+07		(1R,2S,3S,5R)-3-(6-amino-9H-purin-9-yl)-4,4-difluoro-5-(hydroxymethyl)cyclopentane-1,2-diol; 6',6'-difluoroaristeromycin	C11H13F2N	301.253	XSXKATM	-0.288	4	2
	BrC1=CC=CC2=C1N(CC1=CC3=C(S1)C=CC=C3)C(=O)C2=O	1E+07	1E+07			C17H10BrN	372.242	UFOWXDL	3.635	4	2
	CC(C)C[C@H](NC(=O)C1=CC2=CC=CC=C2N1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	1.3E+07	1.3E+07		N-((S)-1-((S)-1-formyl-2-((S)-2-oxopyrrolidin-3-yl)ethylcarbamoyl)-3-methylbutyl)-1H-indole-2-carboxamide	C22H28N4O	412.489	HXJZYYCIL	2.331	4	1
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N(C[C@@H]1CCNC1=O)C=O	1.5E+07	1.5E+07		N-[(benzyloxy)carbonyl]-L-valyl-N1-{1-formyl-2-[(3S)-2-oxopyrrolidin-3-yl]ethyl}-L-leucinamide	C26H38N4O	502.611	RUHYGYHI	2.682	3	0
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N(C[C@@H](CO)[C@@H]1CCNC1=O	1.5E+07	1.5E+07	890648-83-6	N-[(benzyloxy)carbonyl]-L-valyl-N1-((1S)-2-hydroxy-1-{[(3S)-2-oxopyrrolidin-3-yl]methyl}ethyl)-L-leucinamide	C26H40N4O	504.627	GLZAWCK	2.111	3	0
	[Bi+3].[O-]N(=O)=O.COC1=CC(=CC(OC)=C1OC)C1=C2[N-]C(C=C/2)=C(/C2=N/C(/C=C2)=C(C2=CC=C2)[N-]2)/C(=C2/C=CC\1=N/2)C1=CC(OC)=C(OC)C(OC)=C1)C1=CC(OC)=C(OC)C(OC)=C1)C1=CC(OC)=C(OC)C(OC)=C1	1.6E+07	1.6E+07		Bi*C56H52N	1244.03	GUVHQKN		1	0
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)COC1=CC=CC=C1)C(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	1383922-52-8		C33H41N5O	635.784	APIXGBAH	3.307	3	0
	COC1=CC=CC(OCC(=O)N[C@@H](C[C@C]C(=O)N[C@@H](C[C@C]C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)C2=NC3=CC=CC=C3S2)=C1	2.3E+07	2.3E+07	1383922-88-0		C34H43N5O	665.811	IWZSFDOR	3.222	3	0
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)COC1=CC=C(OC)C=C1)C(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	1359941-94-8		C33H41N5O	651.784	ORLPJQUZ	2.901	3	0

	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)COC1=CC=C(C=C1)N(C)C)C)C)C(=O)N[C@@H](C)C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	1383923-00-9		C35H46N6O	678.853	VEMALIBH	3.516	2	0
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)COC1=CC=CN=C1)C)C)C)C(=O)N[C@@H](C)C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	1383922-92-8		C32H40N6O	636.772	VOKLNKGF	2.055	2	0
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)CNC1=CC=CC=C1)C)C)C)C(=O)N[C@@H](C)C[C@@H]1CCNC1=O)C(=O)C1=NC2=CC=CC=C2S1	2.3E+07	2.3E+07	1383922-55-1		C33H42N6O	634.8	PPHLPUPC	3.038	2	0
	CC(C)C[C@H](NC(=O)OC1CCN(CC1)C(=O)OC(C)(C)C)C(=O)N[C@@H](C)C[C@@H]1CCNC1=O)C=O	3.2E+07	3.2E+07		tert-butyl 4-(([(S)-4-methyl-1-oxo-1-[((S)-1-oxo-3-[(S)-2-oxopyrrolidin-3-yl]propan-2-yl]carbamoyl)oxy)piperidine-1-carboxylate	C24H40N4O	496.604	SBHUNCJS	2.275	3	0
	CC(C)C[C@H](NC(=O)OC1(CC2=CC=CC=C2)CCN(CC1)S(C)(=O)=O)C(=O)N[C@@H](C)C[C@@H]1CCNC1=O)C=O	3.2E+07	3.2E+07		4-benzyl-1-(methylsulfonyl)piperidin-4-yl ((S)-4-methyl-1-oxo-1-[((S)-1-oxo-3-[(S)-2-oxopyrrolidin-3-yl]propan-2-yl)amino]pentan-2-yl)carbamate	C27H40N4O	564.703	ZLOZUJAXI	2.471	2	0
	[Na+].CC(C)C[C@H](NC(=O)OC1(CC2=CC=CC=C2)CCN(CC1)S(C)(=O)=O)C(=O)N[C@@H](C)C[C@@H]1CCNC1=O)C(O)S([O-])(=O)=O	3.2E+07	3.2E+07		sodium (2S)-2-{(S)-2-{({[4-benzyl-1-(methylsulfonyl)piperidin-4-yl]oxy}carbonyl)amino}-4-methylpentanamido}-1-hydroxy-3-[(S)-2-oxopyrrolidin-3-yl]propane-1-sulfonate	C27H41N4O	668.765	PVFOFJYH	0.467	2	0
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@@H](CCC(O)=O)NC(=O)[C@@H](CC1=CC=C(O)C=C1)NC(=O)[C@@H](NC(=O)[C@@H](CC(C)C)NC(=O)[C@@H](CC(O)=O)NC(=O)[C@@H](CCC(C)NC(=O)[C@@H](C)O)C(=O)N)C@@H](CC(C)C)C(=O)N)C@@H](CC(O)=O)N)C@@H](CCC(N)=O)C(=O)N[C@@]1(C)CCCC=CCCC[C@@](C)NC(=O)[C@@H](CCCCN)NC(=O)[C@@H])NC(=O)[C@@H](NC1=O)CCSCC[C@@H](NC(=O)[C@@H](CCC(O)=O)NC(=O)[C@@H](CC1=CC=C(O)C=C1)NC(=O)[C@@H](NC(=O)[C@@H](CC(C)C)NC(=O)[C@@H](CC(O)=O)NC(=O)[C@@H](CCC(C)NC(=O)[C@@H](C)O)C(=O)N)C@@H](CC(C)C)C(=O)N)C@@H](CCC(O)=O)N)C@@H](CCC(N)=O)C(=O)N[C@@]1(C)CCCC=CCCC[C@@](C)NC(=O)[C@@H](CCCCN)NC(=O)[C@@H])NC(=O)[C@@H](NC1=O)C	3.3E+07	3.3E+07		C119H191N	2531.97	FTNDXEAV	1.123	1	0
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@@H](CCC(O)=O)NC(=O)[C@@H](CC1=CC=C(O)C=C1)NC(=O)[C@@H](NC(=O)[C@@H](CC(C)C)NC(=O)[C@@H](CC(O)=O)NC(=O)[C@@H](CCC(C)NC(=O)[C@@H](C)O)C(=O)N)C@@H](CC(C)C)C(=O)N)C@@H](CC(O)=O)N)C@@H](CCC(N)=O)C(=O)N[C@@]1(C)CCCC=CCCC[C@@](C)NC(=O)[C@@H](CCCCN)NC(=O)[C@@H])NC(=O)[C@@H](NC1=O)C	3.3E+07	3.3E+07		C118H189N	2550.01	XJXOKQDA	0.598	1	0

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