Table S1. SARS-CoV2 M^{pro} ligand binding Sites

Serial No	PDB Entry	Ligand	Binding Site	Bonding	DOI
1	7KYU	XC4: 1-[(1H-indole-5-carbonyl)oxy]-1H-benzotriazole (Cys145-1H-indole-5-carboxylate)	A	Covalent	To be published
2	6XHM	V2M: N-[(2S)-1-({(2S,3S)-3,4-dihydroxy-1-[(3S)-2-oxopyrrolidin-3-yl]butan-2-yl}amino)-4-methyl-1-oxopentan-2-yl]-4-methoxy-1H-indole-2-carboxamide (4-methoxy-N-[(2S)-4-methyl-1-oxo-1-({(2S)-3-oxo-1-[(3S)-2-oxopyrrolidin-3-yl]butan-2-yl}amino)pentan-2-yl]-1H-indole-2-carboxamide)	A	Covalent	10.1021/acs.jmedchem.0c01063
3	7K6D	SV6: (1S,3aR,6aS)-2-[(2S)-2-({(2S)-2-cyclohexyl-2-[(pyrazin-2-ylcarbonyl)amino]acetyl}amino)-3,3-dimethylbutanoyl]-N-[(2R,3S)-1-(cyclopropyla2mino)-2-hydroxy-1-oxohexan-3-yl]octahydrocyclopenta[c]pyrrole-1-carboxamide	A	Covalent	To be published
4	7AY7	S8T: 9-fluoranyl-3-propan-2-yl-5,6-dihydrobenzo[b][1]benzothiepine (Isofloxythepin)	A	Covalent	10.1126/science.abf7945
5	7D1M	K36: (1S,2S)-2-({N-[(benzyloxy)carbonyl]-L-leucyl}amino)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (GC376)	A	Covalent	10.1038/s41467-020-18233-x
6	6XBH	Inhibitor UAW247: P6S1+PHE2+ELL3	A	Covalent	10.1126/sciadv.abe0751
7	6XMK	QYS: (1S,2S)-2-[(N-{[(4,4-difluorocyclohexyl)methoxy]carbonyl}-L-leucyl)amino]-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (inhibitor 7j)	A	Covalent	10.1126/scitranslmed.abc5332
8	6WNP	U5G: Boceprevir (bound form)	A	Covalent	To be published
9	6LZE	FHR: ~{N}-[(2~{S})-3-cyclohexyl-1-oxidanylidene-1-[[(2~{S})-1-oxidanylidene-3-[(3~{S})-2-oxidanylidenepyrrolidin-3-yl]propan-2-yl]amino]propan-2-yl]-1~{H}-indole-2-carboxamide (inhibitor 11a)	A	Covalent	10.1126/science.abb4489
10	7JKV	V7G: N-[(2S)-1-({(1S,2S)-1-(1,3-benzothiazol-2-yl)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}amino)-4-methyl-1-oxopentan-2-yl]-4-methoxy-1H-indole-2-carboxamide (inhibitor GRL-2420)	A	Covalent	10.1038/s41467-021-20900-6
11	6XR3	V7G: N-[(2S)-1-({(1S,2S)-1-(1,3-benzothiazol-2-yl)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}amino)-4-methyl-1-oxopentan-2-yl]-4-methoxy-1H-indole-2-carboxamide (GRL-024-20)	A	Covalent	To be published
12	6XBI	Inhibitor UAW248: UZ1 5 + UZ4 4 + LEU 3 + LEU 2 + UZ7 1	A	Covalent	10.1126/sciadv.abe0751
13	7K0F	VR4: N-{(2S,3R)-4-(benzylamino)-3-hydroxy-4-oxo-1-[(3S)-2-oxopyrrolidin-3-yl]butan-2-yl}-N~2~-[(benzyloxy)carbonyl]-L-leucinamide (a deuterated GC376 alpha-ketoamide analog (compound 5))	A	Covalent	To be published
14	6XA4	Inhibitor UAW241: UXS 4 + LEU 3 + LEU 2 + ACE 1	A	Covalent	10.1126/sciadv.abe0751
15	7D3I	GQU: (3~{S},3~{a}~{S},6~{a}~{R})-2-[3-[3,5-bis(fluoranyl)phenyl]propanoyl]-~{N}-[(2~{S})-1-oxidanylidene-3-[(3~{S})-2-	A	Covalent	10.1126/science.abf1611

		oxidanylidenepyrrolidin-3-yl]propan-2-yl]-3,3~{a},4,5,6,6~{a}-hexahydro-1~{H}-cyclopenta[c]pyrrole-3-carboxamide (MI-23)			
16	7C6S	U5G: Boceprevir (bound form)	A	Covalent	10.1038/s41467-020-18233-x
17	7K40	U5G: Boceprevir (bound form)	A	Covalent	To be published
18	6Z2E	Q5T: (4~{S})-4-[[(2~{S})-2-[[(2~{S})-2-[[(2~{S})-2-[3-[2-[2-[2-[2-[5-[(3~{a}~{S},4~{R},6~{a}~{R})-2-oxidanylidene-3,3~{a},4,6~{a}-tetrahydro-1~{H}-thieno[3,4-d]imidazol-4-yl]pentanoylamino]ethoxy]ethoxy]ethoxy]propanoylamino]butanoyl]amino]-3,3-dimethyl-butanoyl]amino]-4-methyl-pentanoyl]amino]-6-methylsulfonyl-hexanamide (biotin-PEG(4)-Abu-Tle-Leu-Gln-vinylsulfone)	A	Covalent	To be published
19	6M0K	FJC: ~{N}-[(2~{S})-3-(3-fluorophenyl)-1-oxidanylidene-1-[[(2~{S})-1-oxidanylidene-3-[(3~{S})-2-oxidanylidenepyrrolidin-3-yl]propan-2-yl]amino]propan-2-yl]-1~{H}-indole-2-carboxamide (inhibitor 11b)	A	Covalent	10.1126/science.abb4489
20	7L5D	XNJ: N-(4-methyl-3-{[4-(pyridin-3-yl)-1,3-thiazol-2-yl]amino}phenyl)-4-[(piperazin-1-yl)methyl]benzamide (demethylated analog of masitinib)	A	Non-covalent	To be published
21	6XBG	UAW246: P6S 1 + LEU 2 + UZ4 3 + UZ1 4	A	Covalent	10.1126/sciadv.abe0751
22	7B3E	MYC: 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-4h-chromen-4-one (myricetin)	A	Covalent	To be published
23	6XFN	UAW243: UZ7 1 + LEU 2 + V1V 3 + APY 4	A	Non-covalent	10.1126/sciadv.abe0751
24	5RGW	UGM: 2-(5-cyanopyridin-3-yl)-N-(pyridin-3-yl)acetamide (Z4444621910 (Mpro-x2569))	A	Non-covalent	To be published
25	5RHB	USD: (E)-1-(pyrimidin-2-yl)methanimine (Cov_HetLib030 (Mpro-x2097)	A	Covalent	10.1038/s41467-020-18709-w
26	6XQS	SV6: (1S,3aR,6aS)-2-[(2S)-2-({(2S)-2-cyclohexyl-2-[(pyrazin-2-ylcarbonyl)amino]acetyl}amino)-3,3-dimethylbutanoyl]-N-[(2R,3S)-1-(cyclopropylamino)-2-hydroxy-1-oxohexan-3-yl]octahydrocyclopenta[c]pyrrole-1-carboxamide (Telaprevir)	A	Covalent	10.1016/j.str.2020.10.007
27	7AHA	SIN: Succinic acid (Maleate)	A	Covalent	10.1126/science.abf7945
28	6ZRU	U5G: Boceprevir (bound form)	A	Covalent	10.1039/D0MD00367K
29	5RHE	UPD: 1-acetyl-N-(6-methoxypyridin-3-yl)piperidine-4-carboxamide (PG-COV-42 (Mpro-x2052))	A	Covalent	10.1038/s41467-020-18709-w
30	7BRP	U5G: boceprevir (bound form)	A	Covalent	10.1038/s41467-020-18233-x
31	5RL5	VEY: N-(4-tert-butylphenyl)-N-[(1R)-2-(ethylamino)-2-oxo-1-(pyridin-3-yl)ethyl]propanamide (LON-WEI-adc59df6-30 (Mpro-x3359))	A	Covalent	To be published
32	7JU7	G65: Masitinib	A	Non-covalent	To be published
33	6ZRT	SV6: (1S,3aR,6aS)-2-[(2S)-2-({(2S)-2-cyclohexyl-2-[(pyrazin-2-ylcarbonyl)amino]acetyl}amino)-3,3-dimethylbutanoyl]-N-[(2R,3S)-1-(cyclopropylamino)-2-hydroxy-1-oxohexan-3-yl]octahydrocyclopenta[c]pyrrole-1-carboxamide (inhibitor Telaprevir)	A	Covalent	10.1039/D0MD00367K

34	5RHA	T8M: 1-{4-[(thiophen-2-yl)methyl]piperazin-1-yl}ethan-1-one (Z147647874 (Mpro-x2779))	A	Covalent	To be published
35	5RFE	JGG: N-[(4-cyanophenyl)methyl]morpholine-4-carboxamide (Z509756472)	A	Non-covalent	10.1038/s41467-020-18709-w
36	5RL3	VEP: N-(4-tert-butylphenyl)-N-[(1R)-2-[(oxan-4-yl)amino]-2-oxo-1-(pyridin-3-yl)ethyl]propanamide (LON-WEI-adc59df6-39 (Mpro-x3117))	A	Covalent	To be published
37	5RFV	T8J: 1-[4-(thiophene-2-carbonyl)piperazin-1-yl]ethan-1-one (PCM-0102306)	A	Covalent	10.1038/s41467-020-18709-w
38	5RF2	HVB: 1-azanylpropylideneazanium (Z1741969146)	A	Non-covalent	10.1038/s41467-020-18709-w
39	5RHD	US7: 1-[4-(methylsulfonyl)phenyl]piperazine (SF013 (Mpro-x2193))	A	Non-covalent	10.1038/s41467-020-18709-w
40	5RGV	UGG: 2-(isoquinolin-4-yl)-N-phenylacetamide (Z4444622066 (Mpro-x2563))	A	Non-covalent	To be published
41	7A1U	FUA: Fusidic acid	A	Non-covalent	10.1126/science.abf7945
42	5RHC	USA: (E)-1-(1H-imidazol-2-yl)methanimine (Cov_HetLib053 (Mpro-x2119))	A	Covalent	10.1038/s41467-020-18709-w
43	5RGZ	UH1: 2-(3-cyanophenyl)-N-(pyridin-3-yl)acetamide (Z1343543528 (Mpro-x2600))	A	Non-covalent	To be published
44	5RH6	UHY: N-[(1R)-2-[(2-ethyl-6-methylphenyl)amino]-2-oxo-1-(pyridin-3-yl)ethyl]-N-[6-(propan-2-yl)pyridin-3-yl]propanamide (Z4439011588 (Mpro-x2703))	A	Covalent	To be published
45	7ANS	RNW: 2-[(diphenylmethyl)-oxidanyl-$l^{3}-sulfanyl]-~{N}-oxidanyl-ethanamide (Adrafinil)	A	Non-covalent	10.1126/science.abf7945
46	5RF3	T5V: pyrimidin-5-amine (Z1741970824)	A	Non-covalent	10.1038/s41467-020-18709-w
47	5RF7	T67: 1-(4-methylpiperazin-1-yl)-2-(1H-pyrrolo[2,3-b]pyridin-3-yl)ethan-1-one (Z316425948_minor)	A	Non-covalent	10.1038/s41467-020-18709-w
48	5RL2	VEM: N-(4-tert-butylphenyl)-N-[(1R)-2-[(2-methoxyethyl)amino]-2-oxo-1-(pyridin-3-yl)ethyl]propanamide (LON-WEI-adc59df6-26 (Mpro-x3115))	A	Covalent	To be published
49	5RL0	VEG: ethyl N-[(2R)-2-[(4-tert-butylphenyl)(propanoyl)amino]-2-(pyridin-3-yl)acetyl]-beta-alaninate (LON-WEI-adc59df6-2 (Mpro-x3110))	A	Covalent	To be published
50	5RGK	U0V: 2-fluoro-N-[2-(pyridin-4-yl)ethyl]benzamide (Z1310876699 (Mpro-x0426))	A	Non-covalent	10.1038/s41467-020-18709-w
51	5RGX	UGP: 2-(3-cyanophenyl)-N-(4-methylpyridin-3-yl)acetamide (Z1344037997 (Mpro-x2572))	A	Non-covalent	To be published
52	6XQU	U5G: Boceprevir (bound form)	A	Covalent	10.1016/j.str.2020.10.007
53	7ADW	R7Q: 2-methyl-1-(4-methylphenyl)propan-1-one (2,4'-Dimethylpropiophenone)	A	Covalent	10.1126/science.abf7945

54	5RFU	T8D: 1-{4-[(5-chlorothiophen-2-yl)sulfonyl]piperazin-1-yl}ethan-1-one (PCM-0102121)	A	Covalent	10.1038/s41467-020-18709-w
55	5RH7	UJ1: N-(5-tert-butyl-1H-pyrazol-3-yl)-N-[(1R)-2-[(2-ethyl-6-methylphenyl)amino]-2-oxo-1-(pyridin-3-yl)ethyl]propanamide (Z4439011584 (Mpro-x2705))	A	Covalent	To be published
56	5RL4	VEV: N-(4-tert-butylphenyl)-N-[(1R)-2-(methylamino)-2-oxo-1-(pyridin-3-yl)ethyl]propanamide (LON-WEI-adc59df6-3 (Mpro-x3124))	A	Covalent	To be published
57	5RGI	U0P: N'-cyclopropyl-N-methyl-N-[(5-methyl-1,2-oxazol-3-yl)methyl]urea (Z369936976 (Mpro-x0397))	A	Non-covalent	10.1038/s41467-020-18709-w
58	7AWS	S8E: 5-[[(2-bromoethylamino)-(ethylamino)phosphoryl]oxymethyl]-1-methyl-~{N},~{N}-bis(oxidanyl)imidazol-2-amine (TH-302)	A	Non-covalent	10.1126/science.abf7945
59	7AWU	S8B: ~{N}-propan-2-yl-5-(2-pyridin-4-ylethynyl)pyridine-2-carboxamide (LSN2463359)	A	Non-covalent	10.1126/science.abf7945
60	7BUY	JRY: Hexylcarbamic acid (carmofur)	A	Covalent	10.1038/s41594-020-0440-6
61	6XCH	Leupeptin: ACE 1 + LEU 2 + LEU 3 + AR7 4	A	Covalent	10.1016/j.str.2020.10.007
62	5RFX	T8P: 1-[4-(4-methoxyphenyl)piperazin-1-yl]ethan-1-one (PCM-0102254)	A	Covalent	10.1038/s41467-020-18709-w
63	5R83	K0G: N-phenyl-N'-pyridin-3-ylurea (Z44592329)	A	Non-covalent	10.1038/s41467-020-18709-w
64	5RES	T3V: 1-{4-[(2-fluorophenyl)sulfonyl]piperazin-1-yl}ethan-1-one (PCM-0102281)	A	Covalent	10.1038/s41467-020-18709-w
65	5RGL	U0Y: 1-[4-(4-methylbenzene-1-carbonyl)piperazin-1-yl]ethan-1-one (PCM-0102962 (Mpro-x0705))	A	Covalent	10.1038/s41467-020-18709-w
66	6LU7	N3 (prd_002214): N-[(5-methylisoxazol-3-yl)carbonyl]alanyl-l-valyl-n~1~-((1r,2z)-4-(benzyloxy)-4-oxo-1-{[(3r)-2-oxopyrrolidin-3-yl]methyl}but-2-enyl)-l-leucinamide (inhibitor N3)	A	Covalent	10.1038/s41586-020-2223-y
67	5RFY	T8S: 1-acetyl-N-methyl-N-(propan-2-yl)piperidine-4-carboxamide (PCM-0102974)	A	Covalent	10.1038/s41467-020-18709-w
68	5RH3	UHA: (2R)-2-(3-chlorophenyl)-N-(4-methylpyridin-3-yl)propanamide (Z1264525706 (Mpro-x2649))	A	Non-covalent	To be published
69	5REL	T2G: 1-{4-[(3-methylphenyl)methyl]piperazin-1-yl}ethan-1-one (PCM-0102340)	A	Covalent	10.1038/s41467-020-18709-w
70	7K6E	SV6: (1S,3aR,6aS)-2-[(2S)-2-({(2S)-2-cyclohexyl-2-[(pyrazin-2-ylcarbonyl)amino]acetyl}amino)-3,3-dimethylbutanoyl]-N-[(2R,3S)-1-(cyclopropylamino)-2-hydroxy-1-oxohexan-3-yl]octahydrocyclopenta[c]pyrrole-1-carboxamide	A	Covalent	To be published
71	5REV	T4J: N-[3-(thiomorpholine-4-carbonyl)phenyl]acetamide (PCM-0103072)	A	Covalent	10.1038/s41467-020-18709-w
72	5RFT	T8A:	A	Covalent	10.1038/s41467-

		1-[(4S)-4-phenyl-3,4-dihydroisoquinolin-2(1H)-yl]ethan-1-one (PCM-0102432)			020-18709-w
73	5RF6	NTG: 5-(1,4-oxazepan-4-yl)pyridine-2-carbonitrile (Z1348371854)	A	Non-covalent	10.1038/s41467-020-18709-w
74	5RFL	T7G: 1-acetyl-N-(2-hydroxyphenyl)piperidine-4-carboxamide (PCM-0102389)	A	Covalent	10.1038/s41467-020-18709-w
75	5RH5	UHV: N-(5-tert-butyl-1,2-oxazol-3-yl)-N-[(1R)-2-[(4-methoxy-2-methylphenyl)amino]-2-oxo-1-(pyridin-3-yl)ethyl]propanamide (Z4439011520 (Mpro-x2694))	A	Covalent	To be published
76	5REK	T1Y: 1-{4-[(3-fluorophenyl)sulfonyl]piperazin-1-yl}ethan-1-one (PCM-0102327)	A	Covalent	10.1038/s41467-020-18709-w
77	5RFZ	T8V: N-(2-chloropyridin-3-yl)acetamide (PCM-0102274)	A	Covalent	10.1038/s41467-020-18709-w
78	5RFQ	T7Y: N-[3-(2-oxopyrrolidin-1-yl)phenyl]acetamide (PCM-0102179)	A	Covalent	10.1038/s41467-020-18709-w
79	5RGH	U0M: 5-fluoro-1-[(5-methyl-1,3,4-thiadiazol-2-yl)methyl]-1,2,3,6-tetrahydropyridine (Z1619978933 (Mpro-x0395))	A	Non-covalent	10.1038/s41467-020-18709-w
80	5REW	T4M: N-[(1R)-1-(naphthalen-1-yl)ethyl]acetamide (PCM-0102275)	A	Covalent	10.1038/s41467-020-18709-w
81	5REP	T3G: 1-{4-[(2,6-difluorophenyl)sulfonyl]piperazin-1-yl}ethan-1-one (PCM-0102201)	A	Covalent	10.1038/s41467-020-18709-w
82	5RG1	T9J: Nalpha-acetyl-N-(3-bromoprop-2-yn-1-yl)-L-tyrosinamide (NCL-00024905)	A	Non-covalent	10.1038/s41467-020-18709-w
83	5REU	T4D: 2-[(4-acetylpiperazin-1-yl)sulfonyl]benzonitrile (PCM-0102395)	A	Covalent	10.1038/s41467-020-18709-w
84	5R82	RZS: 6-(ethylamino)pyridine-3-carbonitrile (Z219104216)	A	Non-covalent	10.1038/s41467-020-18709-w
85	5R7Z	HWH: ~{N}-[2-(5-fluoranyl-1~{H}-indol-3-yl)ethyl]ethanamide (Z1220452176)	A	Non-covalent	10.1038/s41467-020-18709-w
86	7AP6	RQN: 4-(4-ethyl-5-fluoranyl-2-oxidanyl-phenoxy)-3-fluoranyl-benzamide (MUT056399)	A	Non-covalent	10.1126/science.abf7945
87	5RGO	U1G: 1-[4-(furan-2-carbonyl)piperazin-1-yl]ethan-1-one (PCM-0102248 (Mpro-x0736))	A	Covalent	10.1038/s41467-020-18709-w
88	5RHF	UPJ: 1-acetyl-N-methyl-N-phenylpiperidine-4-carboxamide (PG-COV-34 (Mpro-x2754))	A	Covalent	10.1038/s41467-020-18709-w
89	5RG3	T9P: N~2~-acetyl-N~1~-prop-2-en-1-yl-L-aspartamide (NCL-00025412)	A	Covalent	10.1038/s41467-020-18709-w
90	5RGY	UGS: N-(4-methoxypyridin-2-yl)-2-(naphthalen-2-yl)acetamide (Z1535580916 (Mpro-x2581))	A	Non-covalent	To be published
91	7C6U	K36: (1S,2S)-2-({N-[(benzyloxy)carbonyl]-L-leucyl}amino)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-	A	Covalent	10.1038/s41467-020-18233-x

		3-yl]propane-1-sulfonic acid (GC376)			
92	5RGP	U1M: 1-{4-[(2,4-dimethylphenyl)sulfonyl]piperazin-1-yl}ethan-1-one (PCM-0102628 (Mpro-x0771))	A	Covalent	10.1038/s41467-020-18709-w
93	5RFW	T8M: 1-{4-[(thiophen-2-yl)methyl]piperazin-1-yl}ethan-1-one (PCM-0102243)	A	Covalent	10.1038/s41467-020-18709-w
94	7C8U	K36: (1S,2S)-2-({N-[(benzyloxy)carbonyl]-L-leucyl}amino)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (GC376)	A	Covalent	To be published
95	5RFI	T71: 1-{4-[(2,5-dimethylphenyl)sulfonyl]piperazin-1-yl}ethan-1-one (PCM-0102353)	A	Covalent	10.1038/s41467-020-18709-w
96	7JPZ	GHX: (phenylmethyl) N-[(2S)-1-oxidanylidene-1-[[(2S)-1-oxidanyl-3-[(3S)-2-oxidanylidenepyrrolidin-3-yl]propan-2-yl]amino]-3-phenyl-propan-2-yl]carbamate (inhibitor MPI1)	A	Covalent	10.1002/cmdc.202000924
97	5REB	T0Y: 1-[(thiophen-3-yl)methyl]piperidin-4-ol (Z2856434899)	A	Non-covalent	10.1038/s41467-020-18709-w
98	5RFK	T7D: N-(1-acetylpiperidin-4-yl)benzamide (PCM-0102575)	A	Covalent	10.1038/s41467-020-18709-w
99	5RG2	T9M: N~2~-acetyl-N-prop-2-en-1-yl-D-allothreoninamide (NCL-00025058)	A	Covalent	10.1038/s41467-020-18709-w
100	5RFN	T7P: N-[(3R)-1,1-dioxo-2,3-dihydro-1H-1lambda~6~-thiophen-3-yl]-N-(4-fluorophenyl)acetamide (PCM-0102868)	A	Covalent	10.1038/s41467-020-18709-w
101	5REJ	T1V: 1-{4-[(thiophen-2-yl)sulfonyl]piperazin-1-yl}ethan-1-one (PCM-0102241)	A	Covalent	10.1038/s41467-020-18709-w
102	5RF1	T5G: 4-bromobenzene-1-sulfonamide (NCL-00023830)	A	Non-covalent	10.1038/s41467-020-18709-w
103	5RGN	U1A: 1-{4-[(4-methylphenyl)sulfonyl]piperazin-1-yl}ethan-1-one (PCM-0102759 (Mpro-x0731))	A	Covalent	10.1038/s41467-020-18709-w
104	5RET	T47: 1-{4-[(3-chlorophenyl)methyl]piperazin-1-yl}ethan-1-one (PCM-0102269)	A	Covalent	10.1038/s41467-020-18709-w
105	5RH2	UH7: 2-(3-chlorophenyl)-N-(4-methylpyridin-3-yl)acetamide (Z1129289650 (Mpro-x2646))	A	Non-covalent	To be published
106	5RH8	UHM: 2-(cyanomethoxy)-N-[(1,2-thiazol-4-yl)methyl]benzamide (Z4444621965 (Mpro-x2764))	A	Non-covalent	To be published
107	7D1O	NNA: (1R,2S,5S)-3-[N-({1-[(tert-butylsulfonyl)methyl]cyclohexyl}carbamoyl)-3-methyl-L-valyl]-N-{(1S)-1-[(1R)-2-(cyclopropylamino)-1-hydroxy-2-oxoethyl]pentyl}-6,6-dimethyl-3-azabicyclo[3.1.0]hexane-2-carboxamide (narlaprevir)	A	Covalent	10.1038/s41392-021-00468-9
108	7JYC	NNA: (1R,2S,5S)-3-[N-({1-[(tert-butylsulfonyl)methyl]cyclohexyl}carbamoyl)-3-methyl-L-valyl]-N-{(1S)-1-[(1R)-2-(cyclopropylamino)-1-hydroxy-2-oxoethyl]pentyl}-6,6-dimethyl-3-azabicyclo[3.1.0]hexane-2-carboxamide	A	Covalent	To be published

		(Inhibitor Narlaprevir)			
109	5RG0	T8Y: 1,1'-(piperazine-1,4-diyl)di(ethan-1-one) (PCM-0102535)	A	Covalent	10.1038/s41467-020-18709-w
110	7AQJ	S7H: (Left) 1-[(2~{R})-2-oxidanylpropyl]-3-[[(2~{R})-oxiran-2-yl]methyl]-5-[[(2~{S})-oxiran-2-yl]methyl]-1,3,5-triazinane-2,4,6-trione RV8: (Right) Triglycidyl isocyanurate	A	Covalent	10.1126/science.abf7945
111	5REO	T2Y: N-[(2H-1,3-benzodioxol-5-yl)methyl]acetamide (PCM-0102578)	A	Covalent	10.1038/s41467-020-18709-w
112	5RFR	T81: 1-{4-[(5-bromothiophen-2-yl)methyl]piperazin-1-yl}ethan-1-one (PCM-0102169)	A	Covalent	10.1038/s41467-020-18709-w
113	5RH1	UGV: 2-(5-chlorothiophen-2-yl)-N-(pyridin-3-yl)acetamide (Z2010253653 (Mpro-x2643))	A	Non-covalent	To be published
114	7LB7	SV6: (1S,3aR,6aS)-2-[(2S)-2-({(2S)-2-cyclohexyl-2-[(pyrazin-2-ylcarbonyl)amino]acetyl}amino)-3,3-dimethylbutanoyl]-N-[(2R,3S)-1-(cyclopropylamino)-2-hydroxy-1-oxohexan-3-yl]octahydrocyclopenta[c]pyrrole-1-carboxamide (Telaprevir)	A	Covalent	10.1021/acs.jmedchem.1c00058
115	7AVD	S1W: 3-[[5-[3-(dimethylamino)phenoxy]pyrimidin-2-yl]amino]phenol (SEN1269 ligand)	A	Non-covalent	10.1126/science.abf7945
116	7CX9	GKF: 3-iodanyl-1~{H}-indazole-7-carbaldehyde (INZ-1)	A	Covalent	To be published
117	5R7Y	JFM: N-(2-phenylethyl)methanesulfonamide (Z45617795)	A	Non-covalent	10.1038/s41467-020-18709-w
118	5RFJ	T7A: N-(4-methoxy-1,3-benzothiazol-2-yl)acetamide (PCM-0103067)	A	Covalent	10.1038/s41467-020-18709-w
119	7JQ2	VHM: N-(3-{[(2R)-4-oxoazetidin-2-yl]oxy}phenyl)-2-(pyrimidin-5-yl)acetamide (inhibitor MPI5)	A	Covalent	10.1002/cmdc.202000924
120	5RGU	UGD: N-(3-{[(2R)-4-oxoazetidin-2-yl]oxy}phenyl)-2-(pyrimidin-5-yl)acetamide (Z4444622180 (Mpro-x2562))	A	Non-covalent	To be published
121	5RER	T3J: 1-[(2R)-2-(4-fluorophenyl)morpholin-4-yl]ethan-1-one (PCM-0102615)	A	Covalent	10.1038/s41467-020-18709-w
122	6XQT	NNA: (1R,2S,5S)-3-[N-({1-[(tert-butylsulfonyl)methyl]cyclohexyl}carbamoyl)-3-methyl-L-valyl]-N-{(1S)-1-[(1R)-2-(cyclopropylamino)-1-hydroxy-2-oxoethyl]pentyl}-6,6-dimethyl-3-azabicyclo[3.1.0]hexane-2-carboxamide (Narlaprevir)	A	Covalent	10.1016/j.str.2020.10.007
123	5REY	T4Y: 1-{4-[(2-methylphenyl)methyl]-1,4-diazepan-1-yl}ethan-1-one (PCM-0102911)	A	Covalent	10.1038/s41467-020-18709-w
124	5RL1	VEJ: N-(4-tert-butylphenyl)-N-[(1R)-2-[(3-methoxypropyl)amino]-2-oxo-1-(pyridin-3-yl)ethyl]propanamide (LON-WEI-adc59df6-27 (Mpro-x3113))	A	Covalent	To be published
125	7COM	U5G: Boceprevir (bound form) (Boceprevir (space group P212121))	A	Covalent	10.1126/science.abf1611
126	5RH0	UH4:	A	Non-	To be published

		N-(5-methylthiophen-2-yl)-N'-pyridin-3-ylurea (Z1286870272 (Mpro-x2608))		covalent	
127	5REM	T2J: 1 1-(4-(2-nitrophenyl)piperazin-1-yl)ethan-1-one (PCM-0103016)	A	Covalent	10.1038/s41467-020-18709-w
128	6YNQ	P6N: (2~{S})-2-methyl-3,4-dihydro-2~{H}-naphthalen-1-one (2-Methyl-1-tetralone)	A	Covalent	10.1126/science.abf7945
129	7C7P	SV6: (Chain A) (1S,3aR,6aS)-2-[(2S)-2-({(2S)-2-cyclohexyl-2-[(pyrazin-2-ylcarbonyl)amino]acetyl}amino)-3,3-dimethylbutanoyl]-N-[(2R,3S)-1-(cyclopropylamino)-2-hydroxy-1-oxohexan-3-yl]octahydrocyclopenta[c]pyrrole-1-carboxamide FK3: (Chain B) (3~{S},3~{a}~{S},6~{a}~{R})-~{N}-[(2~{R},3~{S})-1-(cyclopropylamino)-2-oxidanyl-1-oxidanylidene-hexan-3-yl]-2-methanoyl-3,3~{a},4,5,6,6~{a}-hexahydro-1~{H}-cyclopenta[c]pyrrole-3-carboxamide (Telaprevir)	A	Covalent	10.1126/science.abf1611
130	5RE4	SZY: N-(4-methylpyridin-3-yl)acetamide (Z1129283193)	A	Non-covalent	10.1038/s41467-020-18709-w
131	5RGT	UHS: N-[(1R)-2-(tert-butylamino)-2-oxo-1-(pyridin-3-yl)ethyl]-N-(5-tert-butyl-1,2-oxazol-3-yl)propanamide (Z4439011607 (Mpro-x2540))	A	Covalent	To be published
131	5R81	RZJ: 1-methyl-3,4-dihydro-2~{H}-quinoline-7-sulfonamide (Z1367324110)	A	Non-covalent	10.1038/s41467-020-18709-w
132	5RGM	U1D: N'-acetyl-4,5,6,7-tetrahydro-1-benzothiophene-2-carbohydrazide (PCM-0102142 (Mpro-x0708))	A	Covalent	10.1038/s41467-020-18709-w
133	6Y2G	O6K: ~{tert}-butyl ~{N}-[1-[(2~{S})-3-cyclopropyl-1-oxidanylidene-1-[[(2~{S},3~{R})-3-oxidanyl-4-oxidanylidene-1-[(3~{S})-2-oxidanylidenepyrrolidin-3-yl]-4-[(phenylmethyl)amino]butan-2-yl]amino]propan-2-yl]-2-oxidanylidene-pyridin-3-yl]carbamate (tert-butyl(1-((S)-1-(((S)-4-(benzylamino)-3,4-dioxo-1-((S)-2-oxopyrrolidin-3-yl)butan-2-yl)amino)-3-cyclopropyl-1-oxopropan-2-yl)-2-oxo-1,2-dihydropyridin-3-yl)carbamate (alpha-ketoamide 13b))	A	Covalent	10.1126/science.abb3405
134	5REZ	T54: (1R,2S)-2-(thiophen-3-yl)cyclopentane-1-carboxamide (POB0129)	A	Non-covalent	10.1038/s41467-020-18709-w
135	6W63	X77: N-(4-tert-butylphenyl)-N-[(1R)-2-(cyclohexylamino)-2-oxo-1-(pyridin-3-yl)ethyl]-1H-imidazole-4-carboxamide (inhibitor X77)	A	Non-covalent	To be published
136	7JQ0	VHV: N-[(benzyloxy)carbonyl]-L-valyl-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-L-leucinamide (inhibitor MPI3)	A	Covalent	10.1002/cmdc.202000924
137	7JQ1	VHJ: N-[(benzyloxy)carbonyl]-L-valyl-N-{(2S)-1-hydroxy-3-[(3R)-2-oxo-3,4-dihydro-2H-pyrrol-3-yl]propan-2-yl}-L-phenylalaninamide	A	Covalent	10.1002/cmdc.202000924
138	5RFH	T6Y: 1-{4-[(5-chlorothiophen-2-yl)methyl]piperazin-1-yl}ethan-1-one (PCM-0102277)	A	Covalent	10.1038/s41467-020-18709-w
139	6WTT	K36: (1S,2S)-2-({N-[(benzyloxy)carbonyl]-L-	A	Covalent	10.1101/2020.04.20.051581

		leucyl}amino)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (inhibitor GC-376)			
140	6Y2F	O6K: ~{tert}-butyl ~{N}-[1-[(2~{S})-3-cyclopropyl-1-oxidanylidene-1-[[(2~{S},3~{R})-3-oxidanyl-4-oxidanylidene-1-[(3~{S})-2-oxidanylidenepyrrolidin-3-yl]-4-[(phenylmethyl)amino]butan-2-yl]amino]propan-2-yl]-2-oxidanylidene-pyridin-3-yl]carbamate (tert-butyl(1-((S)-1-(((S)-4-(benzylamino)-3,4-dioxo-1-((S)-2-oxopyrrolidin-3-yl)butan-2-yl)amino)-3-cyclopropyl-1-oxopropan-2-yl)-2-oxo-1,2-dihydropyridin-3-yl)carbamate(alpha-ketoamide 13b))	A	Covalent	10.1126/science.abb3405
141	5RFM	T7J: N-[(3R)-1,1-dioxo-2,3-dihydro-1H-1lambda~6~-thiophen-3-yl]-N-(4-methylphenyl)acetamide (PCM-0102539)	A	Covalent	10.1038/s41467-020-18709-w
142	5RFF	T6M: 1-{4-[(4-chlorophenyl)sulfonyl]piperazin-1-yl}ethan-1-one (PCM-0102704)	A	Covalent	10.1038/s41467-020-18709-w
143	5RFO	T7S: 1-[4-(piperidine-1-carbonyl)piperidin-1-yl]ethan-1-one (PCM-0102972)	A	Covalent	10.1038/s41467-020-18709-w
144	5RH9	UJ4: N-{4-[(1S)-1-methoxyethyl]phenyl}-N-[(1R)-2-[(4-methoxy-2-methylphenyl)amino]-2-oxo-1-(pyridin-3-yl)ethyl]propanamide (Z4438424255 (Mpro-x2776))	A	Covalent	To be published
145	7C8B	Z-VAD(OMe)-FMK	A	Covalent	To be published
146	6M2N	3WL: 5,6,7-trihydroxy-2-phenyl-4H-chromen-4-one	A	Non-covalent	10.1038/s41401-020-0483-6
147	5RE9	LPZ: 2-(4-methylphenoxy)-1-(4-methylpiperazin-4-ium-1-yl)ethanone (Z2856434836)	A	Non-covalent	10.1038/s41467-020-18709-w
148	5RFG	T6V: N-[(3S)-1,1-dioxo-2,3-dihydro-1H-1lambda~6~-thiophen-3-yl]-N-phenylacetamide (PCM-0102372)	A	Covalent	10.1038/s41467-020-18709-w
149	5REH	AWP: 1-cyclohexyl-3-(2-pyridin-4-ylethyl)urea (Z111507846)	A	Non-covalent	10.1038/s41467-020-18709-w
150	5REX	T4V: 1-{4-[(naphthalen-1-yl)methyl]piperazin-1-yl}ethan-1-one (PCM-0102287)	A	Covalent	10.1038/s41467-020-18709-w
151	6WTJ	K36: (1S,2S)-2-({N-[(benzyloxy)carbonyl]-L-leucyl}amino)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid	A	Covalent	10.1038/s41467-020-18096-2
152	7JQ3	VHP: N-[(benzyloxy)carbonyl]-O-tert-butyl-L-threonyl-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-L-leucinamide (inhibitor MPI6)	A	Covalent	10.1002/cmdc.202000924
156	7JQ4	XM2: N-[(benzyloxy)carbonyl]-O-tert-butyl-L-threonyl-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-L-phenylalaninamide (inhibitor MPI7)	A	Covalent	10.1002/cmdc.202000924
157	5R84	GWS: 2-cyclohexyl-~{N}-pyridin-3-yl-ethanamide (Z31792168)	A	Non-covalent	10.1038/s41467-020-18709-w
158	6WTK	UED: N~2~-[(benzyloxy)carbonyl]-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-L-leucinamide	A	Covalent	10.1038/s41467-020-18096-2
159	7KX5	X7V: N-([1,1'-biphenyl]-4-yl)-N-[(1R)-2-oxo-2-{[(1S)-1-phenylethyl]amino}-1-(pyridin-3-	A	Non-covalent	To be published

		yl)ethyl]furan-2-carboxamide (inhibitor Jun8-76-3A)			
160	5R80	RZG: methyl 4-sulfamoylbenzoate (Z18197050)	A	Non-covalent	10.1038/s41467-020-18709-w
161	5RFP	T7V: N-[(1S)-1-(3-chlorophenyl)ethyl]acetamide (PCM-0102190)	A	Covalent	10.1038/s41467-020-18709-w
162	5REN	T2V: 1-[(3R)-3-(1,3-benzothiazol-2-yl)piperidin-1-yl]ethan-1-one (PCM-0102425)	A	Covalent	10.1038/s41467-020-18709-w
163	7C8T	NOL: n-[(benzyloxy)carbonyl]-o-(tert-butyl)-l-threonyl-3-cyclohexyl-n-[(1s)-2-hydroxy-1-{[(3s)-2-oxopyrrolidin-3-yl]methyl}ethyl]-l-alaninamide (TG-0205221)	A	Covalent	To be published
164	7C8R	TG3: ethyl (4R)-4-[[(2S)-4-methyl-2-[[(2S,3R)-3-[(2-methylpropan-2-yl)oxy]-2-(phenylmethoxycarbonylamino)butanoyl]amino]pentanoyl]amino]-5-[(3S)-2-oxidanylidenepyrrolidin-3-yl]pentanoate (TG-0203770)	A	Covalent	To be published
165	7JQ5	NOL: n-[(benzyloxy)carbonyl]-o-(tert-butyl)-l-threonyl-3-cyclohexyl-n-[(1s)-2-hydroxy-1-{[(3s)-2-oxopyrrolidin-3-yl]methyl}ethyl]-l-alaninamide (inhibitor MPI8)	A	Covalent	10.1002/cmdc.202000924
166	5RFS	T84: 1-{4-[(thiophen-3-yl)methyl]piperzin-1-yl}ethan-1-one (PCM-0102739)	A	Covalent	10.1038/s41467-020-18709-w
167	7CBT	K36: (1S,2S)-2-({N-[(benzyloxy)carbonyl]-L-leucyl}amino)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (GC376)	A	Covalent	To be published
168	7AK4	Tretazicar: 5-(aziridin-1-yl)-2,4-dinitrobenzamide	A	Non-Covalent	10.1126/science.abf7945
169	7AKU	RN2: Calpeptin	A	Covalent	10.1126/science.abf7945
170	6XB2	NEN: 1-ethyl-pyrrolidine-2,5-dione	A	Covalent	10.1107/S2052252520012634
171	7BQY	N-[(5-methylisoxazol-3-yl)carbonyl]alanyl-l-valyl-n~1~-((1r,2z)-4-(benzyloxy)-4-oxo-1-{[(3r)-2-oxopyrrolidin-3-yl]methyl}but-2-enyl)-l-leucinamide	A	Covalent	10.1038/s41586-020-2223-y
172	7LFE	XWS: (2R,4R)-1-phenylhexahydropyrimidine-2,4-diol	A	Non-covalent	To be published
173	7L11	XF1: 2-[3-(3-chloro-5-propoxyphenyl)-2-oxo[2H-[1,3'-bipyridine]]-5-yl]benzonitrile (COMPOUND 5)	A	Non-covalent	10.1021/acscentsci.1c00039
174	7L12	XF4: (5S)-5-{3-[3-(benzyloxy)-5-chlorophenyl]-2-oxo[2H-[1,3'-bipyridine]]-5-yl}pyrimidine-2,4(3H,5H)-dione (COMPOUND 14)	A	Non-Covalent	10.1021/acscentsci.1c00039
175	7L13	XF7: (5S)-5-(3-{3-chloro-5-[(2chlorophenyl)methoxy]phenyl}-2-oxo[2H-[1,3'-bipyridine]]-5-yl)pyrimidine-2,4(3H,5H)-dione (COMPOUND 21)	A	Non-covalent	10.1021/acscentsci.1c00039
176	7L14	XFD: 2-{3-[3-chloro-5-(cyclopropylmethoxy)phenyl]-2-oxo[2H-[1,3'-bipyridine]]-5-yl}benzonitrile	A	Non-covalent	10.1021/acscentsci.1c00039

		(COMPOUND 26)			
177	7LTJ	YD1: 6-[4-(3,4-dichlorophenyl)piperazin-1-yl]carbonyl-1~{H}-pyrimidine-2,4-dione (Inhibitor Mcule-5948770040)	A	Non-covalent	10.1021/acscentsci.1c00039
178	7BE7	ALD: N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-1-hydroxy-4-methylpentan-2-yl]-L-leucinamide (MG-132)	A	COVALENT	To be published
179	7NBY	U88(406): 5-nitro-1,3-thiazole SU3327 (halicin)	A	Covalent	To be published.
180	7NBR	U5G: (boceprevir (bound form)) (HCV NS3/4A inhibitor boceprevir)	A	Covalent	To be published
181	7NBS	SV6: 1S,3aR,6aS)-2-[(2S)-2-({(2S)-2-cyclohexyl-2-[(pyrazin-2-ylcarbonyl)amino]acetyl}amino)-3,3-dimethylbutanoyl]-N-[(2R,3S)-1-(cyclopropylamino)-2-hydroxy-1-oxohexan-3-yl]octahydrocyclopenta[c]pyrrole-1-carboxamide (HCV NS3/4A inhibitor telaprevir)	A	Covalent	To be published
182	7AQE	RV5: N-1,2,3-Benzothiadiazol-6-yl-N'-[2-oxo-2-(1-piperidinyl)ethyl]urea also called unc-2327 (UNC-2327)	A	Non-Covalent	10.1126/science.abf7945
183	7BGP	PRD_001210 (ALD): PHQ-Leu-Leu-Leu-aldehyde MG-132, bound form (MG-132)	A	Covalent	To be published
184	7BFB	9JT: {N}-phenyl-2-selanyl-benzamide (Ebselen)	A	Non-Covalent	To be published
185	7L10	XEY: 2-[3-(3,5-dichlorophenyl)-2-oxo[2H-[1,3'-bipyridine]]-5-yl]benzonitrile (COMPOUND 4)	A	Non-Covalent	10.1021/acscentsci.1c00039
186	7NEV	PRD_000216 (Leupeptin)	A	Covalent	10.1126/science.abf7945
187	5RFC	K1Y: methyl (2-methyl-4-phenyl-1,3-thiazol-5-yl)carbamate (Z979145504)	B	Non-covalent	10.1038/s41467-020-18709-w
188	5RH4	UHG: (2R)-2-(6-chloro-9H-carbazol-2-yl)propanoic acid (Z1530425063 (Mpro-x2659))	B	Non-covalent	To be published
189	5RE5	T0J: N~1~-phenylpiperidine-1,4-dicarboxamide (Z33545544)	B	Non-covalent	10.1038/s41467-020-18709-w
190	6YVF	A82: 2-[[(1R)-1-(7-methyl-2-morpholin-4-yl-4-oxidanylidene-pyrido[1,2-a]pyrimidin-9-yl)ethyl]amino]benzoic acid (AZD6482)	B	Non-covalent	10.1126/science.abf7945
191	5RGG	NZD: 4-methyl-N-phenylpiperazine-1-carboxamide (Z2856434890 (Mpro-x0165))	B	Non-covalent	10.1038/s41467-020-18709-w
192	5RFB	K3S: N-[(1-methyl-1H-1,2,3-triazol-4-yl)methyl]ethanamine (Z1271660837)	C	Non-covalent	10.1038/s41467-020-18709-w
193	5RE6	O0S: N-{4-[(pyrimidin-2-yl)oxy]phenyl}acetamide (Z54571979)	C	Non-covalent	10.1038/s41467-020-18709-w
194	5RF8	SFY: 4-amino-N-(pyridin-2-yl)benzenesulfonamide	D	Non-covalent	10.1038/s41467-020-18709-w

		(Z271004858)			
195	5RGR	K1G: N,1-dimethyl-N-(propan-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine (Z328695024(Mpro-x1101))	E	Non-covalent	10.1038/s41467-020-18709-w
196	5RF5	HV2: 1,1-bis(oxidanylidene)thietan-3-ol (Z3241250482)	E	Non-covalent	10.1038/s41467-020-18709-w
197	5RED	JJG: 4-[2-(phenylsulfanyl)ethyl]morpholine (Z2856434865)	E	Non-covalent	10.1038/s41467-020-18709-w
198	5REI	T1S: 4-[(3-chlorophenyl)methyl]morpholine (Z2856434856)	E	Non-covalent	10.1038/s41467-020-18709-w
199	5REG	LWA: (2~{S})-~{N}-(4-aminocarbonylphenyl)oxolane-2-carboxamide (Z1545313172)	F	Non-covalent	10.1038/s41467-020-18709-w
200	5RF0	T5D: [1-(pyridin-2-yl)cyclopentyl]methanol (POB0073)	G	Non-covalent	10.1038/s41467-020-18709-w
201	5RGS	S7V: [(2~{R})-4-(phenylmethyl)morpholin-2-yl]methanol (Z1259086950(Mpro-x1163))	H	Non-covalent	10.1038/s41467-020-18709-w
202	5REC	T1J: 2-{[(1H-benzimidazol-2-yl)amino]methyl}phenol (Z1587220559)	H	Non-covalent	10.1038/s41467-020-18709-w
203	5REE	T1M: (2R,3R)-1-benzyl-2-methylpiperidin-3-ol (Z2217052426)	H	Non-covalent	10.1038/s41467-020-18709-w
204	7LDX	R9V: (3-endo)-8-benzyl-8-azabicyclo[3.2.1]octan-3-ol	H	Non-covalent	To be published
205	5RGR	K1G: N,1-dimethyl-N-(propan-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine(Z328695024 (Mpro-x1101))	I	Non-covalent	10.1038/s41467-020-18709-w
206	5RE7	T0S: N-[(4-sulfamoylphenyl)methyl]acetamide (Z30932204)	J	Non-covalent	10.1038/s41467-020-18709-w
207	5RFD	T6J: 2-[(methylsulfonyl)methyl]-1H-benzimidazole (Z126932614)	K	Non-covalent	10.1038/s41467-020-18709-w
208	5RF4	T5Y: pyridin-2-ol (Z1741982125)	K	Non-covalent	10.1038/s41467-020-18709-w
209	7AWW	CLU: 2,6-dichloro-n-imidazolidin-2-ylideneaniline (Clonidine)	K	Non-covalent	10.1126/science.abf7945
210	5RF9	S7D: 1-[(2~{S})-2-methylmorpholin-4-yl]-2-pyrazol-1-yl-ethanone (Z217038356)	L	Non-covalent	10.1038/s41467-020-18709-w
211	5RGJ	U0S: (5S)-7-(pyrazin-2-yl)-2-oxa-7-azaspiro[4.4]nonane (Z1401276297 (Mpro-x0425))	L	Non-covalent	10.1038/s41467-020-18709-w
212	5RE8	T0V: 1-(3-fluorophenyl)-N-[(furan-2-yl)methyl]methanamine (Z2737076969)	L	Non-covalent	10.1038/s41467-020-18709-w
213	5RFA	JGY: 1-methyl-N-{[(2S)-oxolan-2-yl]methyl}-1H-pyrazole-3-carboxamide (Z2643472210)	M	Non-covalent	10.1038/s41467-020-18709-w
214	5RGQ	U1V: 1-(4-fluoro-2-methylphenyl)methanesulfonamide (Z1849009686 (Mpro-x1086))	M	Non-covalent	10.1038/s41467-020-18709-w
215	7AGA	LZE: 4-{[(2,6-dichlorophenyl)carbonyl]amino}-N-	N	Covalent	10.1126/

		piperidin-4-yl-1H-pyrazole-3-carboxamide (AT7519)			science.abf7945
216	5REF	6SU: 3-(methylsulfonylamino)benzoate (Z24758179)	N	Covalent	10.1038/s41467-020-18709-w
217	5REA	JGP: (azepan-1-yl)(2H-1,3-benzodioxol-5-yl)methanone (Z31432226)	O	Non-covalent	10.1038/s41467-020-18709-w
218	7AXO	QCP: AR-42	P	Non-covalent	10.1126/science.abf7945
219	7AF0	R9W: 2,3,5,6,7,8-hexahydro-1~{H}-cyclopenta[b]quinolin-9-amine (Ipidacrine)	P	Non-covalent	10.1126/science.abf7945
220	7AXM	93J: (2E)-N-{4-[(3-chloro-4-fluorophenyl)amino]-3-cyano-7-ethoxyquinolin-6-yl}-4-(dimethylamino)but-2-enamide (Pelitinib)	Q	Non-covalent	10.1126/science.abf7945
221	7ABU	R6Q: 1'-[2-[4-(trifluoromethyl)phenyl]ethyl]spiro[1~{H}-3,1-benzoxazine-4,4'-piperidine]-2-one (RS102895)	Q	Non-covalent	10.1126/science.abf7945
222	7AQI	QEL: 4-[(1R,2S)-2-(4-benzylpiperidin-1-yl)-1-hydroxypropyl]phenol (Ifenprodil)	Q	Non-covalent	10.1126/science.abf7945
223	7APH	RT2: Tofogliflozin	Q	Non-covalent	10.1126/science.abf7945
224	7AMJ	RMZ: (3~{S})-3-[2-[4-(3,4-dimethylphenyl)piperazin-1-yl]ethyl]-2,3-dihydroisoindol-1-one (PD 168568)	Q	Non-covalent	10.1126/science.abf7945
225	7ARF	RVW: (2~{S},3~{R},4~{R},5~{S},6~{S})-2-(hydroxymethyl)-6-sulfanyl-oxane-3,4,5-triol (thioglucose)	R	Covalent	10.1126/science.abf7945
226	7BFB	9JT: {N}-phenyl-2-selanyl-benzamide (Ebselen)	R	Covalent	To be published
227	7NBY	U88(406): 5-nitro-1,3-thiazole SU3327 (halicin)	R	covalent	To be published
228	6XB1	NEN: 1-ethyl-pyrrolidine-2,5-dione	R	covalent	10.1107/S2052252520012634
229	6XB2	NEN: 1-ethyl-pyrrolidine-2,5-dione	R	covalent	10.1107/S2052252520012634
230	7AX6	S8H: (2~{S})-2-azanyl-5-oxidanylidene-5-[[(2~{S})-1-oxidanylidene-1-[(2-oxidanylidene-2-propan-2-yloxy-ethyl)amino]-3-sulfanyl-propan-2-yl]amino]pentanoic acid (Glutathione isopropyl ester)	R, S	Non-covalent	10.1126/science.abf7945
231	7AWR	S7W: Tegafur	S	Non-covalent	10.1126/science.abf7945
232	7KVL	X4P: 2-chloropyridine-4-carboxamide	T	Non-covalent	To be published
233	7KVR	X4V: N~4~,N~4~-dimethylpyridine-2,4-diamine	U	Non-covalent	To be published
234	7LFP	XY4: N-phenyl-N'-propan-2-ylurea	V	Non-covalent	To be published

Table S2. SARS-CoV2 M^{pro} structure summary

Binding site	PDB ID
No ligands	7ALH, 6M2Q, 7ALI, 7AR5, 6XB0, 7JR4, 6XHU, 7JR3, 7K3T, 6XKH, 6YB7, 5R8T, 7AR6, 6WQF, 7KPH, 6Y84, 6M03, 7JFQ, 7KFI, 7JPY, 6Y2E, 7BRO, 6WTM, 7CWB, 7JP1, 6XKF, 7C2Y, 7C2Q, 6XOA, 7KVG, 7JUN, 7JOY, 7KHP, 7JOX, 7CWC, 7JVZ, 7JST, 7BB2
A	7KYU, 6XHM, 7K6D, 7AY7, 7D1M, 6XBH, 6XMK, 6WNP, 6LZE, 7JKV, 6XR3, 6XBI, 7K0F, 6XA4, 7D3I, 7C6S, 7K40, 6Z2E, 6M0K, 7I5D, 6XBG, 7B3E, 6XFN, 5RGW, 5RHB, 6XQS, 7AHA, 6ZRU, 5RHE, 7BRP, 5RL5, 7JU7, 6ZRT, 5RHA, 5RFE, 5RL3, 5RFV, 5RF2, 5RHD, 5RGV, 7A1U, 5RHC, 5RGZ, 5RH6, 7ANS, 5RF3, 5RF7, 5RL2, 5RL0, 5RGK, 5RGX, 6XQU, 7ADW, 5RFU, 5RH7, 5RL4, 5RGI, 7AWS, 7AWU, 7BUY, 6XCH, 5RFX, 5R83, 5RES, 5RGL, 6LU7, 5RFY, 5RH3, 5REL, 7K6E, 5REV, 5RFT, 5RF6, 5RFL, 5RH5, 5REK, 5RFZ, 5RFQ, 5RGH, 5REW, 5REP, 5RG1, 5REU, 5R82, 5R7Z, 7AP6, 5RGO, 5RHF, 5RG3, 5RGY, 7C6U, 5RGP, 5RFW, 7C8U, 5RFI, 7JPZ, 5REB, 5RFK, 5RG2, 5RFN, 5REJ, 5RF1, 5RGN, 5RET, 5RH2, 5RH8, 7D1O, 7JYC, 5RG0, 7AQJ, 5REO, 5RFR, 5RH1, 7IB7, 7AVD, 7CX9, 5R7Y, 5RFJ, 7JQ2, 5RGU, 5RER, 6XQT, 5REY, 5RL1, 7COM, 5RH0, 5REM, 6YNQ, 7C7P, 5RE4, 5RGT, 5R81, 5R81, 5RGM, 6Y2G, 5REZ, 6W63, 7JQ0, 5RFH, 6WTT, 6Y2F, 5RFM, 5RFF, 5RFO, 5RH9, 7C8B, 6M2N, 5RE9, 5RFG, 5REH, 5REX, 6WTJ, 7JQ3, 7JQ4, 5R84, 6WTK, 7KX5, 5R80, 5RFP, 5REN, 7C8T, 7C8R, 7JQ5, 7CBT, 7AKU, 7AK4, 5RFS, 7BQY, 6XB2, 7LFE, 7L11, 7L12, 7L13, 7L14, 7LTJ, 7BE7, 7NBR, 7NBY, 7NBS, 7AQE, 7BGP, 7BFB, 7l10, 7NEV
B	5RFC, 6YVF, 5RGG, 5RE5, 5RH4
C	5RE6, 5RFB
D	5RF8
E	5RGR, 5RF5, 5RED, 5REI
F	5REG
G	5RF0
H	5RGS, 5REC, 5REE, 7LDX
I	5RGR
J	5RE7
K	5RFD, 5RF4, 7AWW
L	5RF9, 5RGJ, 5RE8
M	5RFA, 5RGQ
N	7AGA, 5REF
O	5REA
P	7AXO, 7AF0
Q	7AXM, 7ABU, 7AQI, 7APH, 7AMJ
R	7ARF, 7AX6, 6XB1, 6XB2, 7BFB, 7NBY
S	7AWR, 7AX6
T	7KVL
U	7KVR
V	7LFP

Table S3. SARS M^{pro} ligand binding Sites

Serial No	PDB entry	Ligand	Binding Site	Bonding	DOI
1	6W79	X77: N-(4-Tert-Butylphenyl)-N-[(1R)-2-(Cyclohexylamino)-2-Oxo-1-(Pyridin-3-Yl)Ethyl]-1H-Imidazole-4-Carboxamide (Inhibitor X77)	A	Non-covalent	To be published
2	5N19	D03: (S)-N-Benzyl-3-((S)-2-Cinnamamido-3-Phenylpropanamido)-2-Oxo-4-((S)-2-Oxopyrrolidin-3-Yl)Butanamide (Alpha-ketoamide(S)-N-benzyl-3-((S)-2-cinnamamido-3-phenylpropanamido)-2-oxo-4-((S)-2-oxopyrrolidin-3-yl)butanamide)	A	Covalent	To be published
3	3TNT	G85: N-[(Benzyloxy)Carbonyl]-O-Tert-Butyl-L-Seryl-N-{(2R)-5-Ethoxy-5-Oxo-1-[(3S)-2-Oxopyrrolidin-3-Yl]Pentan-2-Yl}-L-Phenylalaninamide (Alpha, beta-unsaturated ethyl ester inhibitor SG85)	A	Covalent	To be published
4	3SZN	G75: Ethyl (4r)-4-({N-[(Benzyloxy)Carbonyl]-L-Phenylalanyl}Amino)-5-[(3s)-2-Oxopyrrolidin-3-Yl]Pentanoate (Alpha, beta- unsaturated ethyl ester inhibitor SG75)	A	Covalent	To be published
5	6LNQ	EJF: N-[(2S)-3-Methyl-1-[[(2S)-4-Methyl-1-Oxidanylidene-1-[[(2S)-1-Oxidanylidene-3-[(3S)-2-Oxidanylidenepyrrolidin-3-Yl]Propan-2-Yl]Amino]Pentan-2-Yl]Amino]-1-Oxidanylidene-Butan-2-Yl]-1H-Indole-2-Carboxamide (Aldehyde inhibitor M7)	A	Covalent	10.1021/acscatal.0c00110
6	6WCO	X47: N-(4-Tert-Butylphenyl)-N-[(1R)-2-(Cyclopentylamino)-2-Oxo-1-(Pyridin-3-Yl)Ethyl]-1H-Imidazole-4-Carboxamide (Inhibitor X47)	A	Non-covalent	To be published
7	3TNS	G83: Ethyl (5s,8s,11r)-8-Benzyl-5-(2-Tert-Butoxy-2-Oxoethyl)-3,6,9-Trioxo-11-{[(3s)-2-Oxopyrrolidin-3-Yl]Methyl}-1-Phenyl-2-Oxa-4,7,10-Triazatetradecan-14-Oate (Alpha, beta-unsaturated ethyl ester inhibitor SG83)	A	Covalent	To be published
8	5C5O	SDJ: (2S)-3-(1H-Imidazol-5-Yl)-2-({[(3S,4ar,8as)-2-(N-Phenyl-Beta-Alanyl)Decahydroisoquinolin-3-Yl]Methyl}Amino)Propanal (Phenyl-beta-alanyl(S,R)-N-decalin type inhibitor)	A	Covalent	To be published
9	3TIT	G81: Ethyl (4r)-4-{[N-(Tert-Butoxycarbonyl)-L-Phenylalanyl]Amino}-5-[(3s)-2-Oxopyrrolidin-3-Yl]Pentanoate (Alpha, beta-unsaturated ethyl ester SG81)	A	Covalent	To be published
10	5N5O	8O5: (2~{R},3~{S})-3-[[(2~{S})-3-Cyclopropyl-2-[[(~{E})-3-Phenylprop-2-Enoyl]Amino]Propanoyl]Amino]-2-Oxidanyl-4-[(3~{S})-2-Oxidanylidenepyrrolidin-3-Yl]-~{N}-(Phenylmethyl)Butanamide (Alpha-ketoamide (S)-N-benzyl-3-((S)-2-cinnamamido-3-cyclopropylpropanamido)-2-oxo-4-((S)-2-oxopyrrolidin-3-yl)butanamide	A	Covalent	To be published

Serial No	PDB entry	Ligand	Binding Site	Bonding	DOI
		(Cinnamoyl-cyclopropylalanine-GlnLactam-CO-CO-NH-benzyl))			
11	2ZU5	ZU5: N-[(Benzyloxy)Carbonyl]-O-Tert-Butyl-L-Threonyl-N-[(1R)-4-Cyclopropyl-4-Oxo-1-{[(3S)-2-Oxopyrrolidin-3-Yl]Methyl}Butyl]-L-Leucinamide (TG-0205486)	A	Covalent	10.1074/jbc.M807947200
12	2HOB	Prd_002214: N-[(5-Methylisoxazol-3-Yl)Carbonyl]Alanyl-L-Valyl-N~1~-((1r,2z)-4-(Benzyloxy)-4-Oxo-1-{[(3r)-2-Oxopyrrolidin-3-Yl]Methyl}But-2-Enyl)-L-Leucinamide (Michael acceptor N3)	A	Covalent	10.1016/j.jmb.2006.11.073
13	2GX4	Nol: N-[(Benzyloxy)Carbonyl]-O-(Tert-Butyl)-L-Threonyl-3-Cyclohexyl-N-[(1s)-2-Hydroxy-1-{[(3s)-2-Oxopyrrolidin-3-Yl]Methyl}Ethyl]-L-Alaninamide	A	Covalent	10.1021/jm0603926
14	4TWY	3BL: (2S)-2-({[(3S,4ar,8as)-2-(Biphenyl-4-Ylcarbonyl)Decahydroisoquinolin-3-Yl]Methyl}Amino)-3-(1H-Imidazol-5-Yl)Propanal (Phenylbenzoyl(S,R)-N-decalin type inhibitor)	A	Covalent	10.1016/j.bmc.2014.12.028
15	3TIU	G82: Ethyl (5s,8s,11r)-8-Benzyl-5-(3-Tert-Butoxy-3-Oxopropyl)-3,6,9-Trioxo-11-{[(3s)-2-Oxopyrrolidin-3-Yl]Methyl}-1-Phenyl-2-Oxa-4,7,10-Triazatetradecan-14-Oate (Alpha,beta-unsaturated ethyl ester inhibitor SG82)	A	Covalent	To be published
16	2OP9	Wr1: Nalpha-[(Benzyloxy)Carbonyl]-N-[(1r)-4-Hydroxy-1-Methyl-2-Oxobutyl]-L-Phenylalaninamide	A	Non-covalent	10.1021/bi0621415
17	2Z94	TLD: 4-Methylbenzene-1,2-Dithiol (TDT)	A	Non-covalent	10.1016/j.febslet.2007.10.048
18	3SND	Ac-ESTLQ-H	A	Covalent	10.1016/j.antiviral.2011.08.001
19	2Z3C	PRD_000250: N-Acetyl-L-Valyl-O-Benzyl-L-Threonyl-N-[(1R,2R)-2-Hydroxy-1-{[(3R)-2-Oxopyrrolidin-3-Yl]Methyl}Propyl]-L-Leucinamide	A	Covalent	10.1016/j.jmb.2007.06.001
20	2GZ8	F3f: S-[5-(Trifluoromethyl)-4h-1,2,4-Triazol-3-Yl] 5-(Phenylethynyl)Furan-2-Carbothioate	A	Non-covalent	10.1021/jm060207o
21	2GZ7	D3f: 2-[(2,4-Dichloro-5-Methylphenyl)Sulfonyl]-1,3-Dinitro-5-(Trifluoromethyl)Benzene	A	Non-covalent	10.1021/jm060207o
22	4WY3	3X5: (2S)-2-({[(3R,4as,8ar)-2-(Biphenyl-4-Ylcarbonyl)Decahydroisoquinolin-3-Yl]Methyl}Amino)-3-(1H-Imidazol-5-Yl)Propanal (Phenylbenzoyl(R,S)-N-decalin type inhibitor)	A	Non-covalent	10.1016/j.bmc.2014.12.028
23	5C5N	SLH: (2S)-3-(1H-Imidazol-5-Yl)-2-({[(3R,4as,8ar)-2-(N-Phenyl-Beta-Alanyl)Decahydroisoquinolin-3-Yl]Methyl}Amino)Propanal (Phenyl-beta-alanyl(R,S)-N-decalin type inhibitor)	A	Covalent	To be published
24	2AMD	9in: N-(3-Furoyl)-D-Valyl-L-Valyl-N~1~-	A	Covalent	

Serial No	PDB entry	Ligand	Binding Site	Bonding	DOI
		((1r,2z)-4-Ethoxy-4-Oxo-1-{[(3s)-2-Oxopyrrolidin-3-Yl]Methyl}But-2-Enyl)-D-Leucinamide (Inhibitor N9)			10.1371/journal.pbio.0030324
25	1WOF	I12: N-[(5-Methylisoxazol-3-Yl)Carbonyl]-L-Alanyl-L-Valyl-N~1~-((1s)-4-Ethoxy-4-Oxo-1-{[(3s)-2-Oxopyrrolidin-3-Yl]Methyl}But-2-Enyl)-L-Leucinamide (Inhibitor N1)	A	Covalent	10.1371/journal.pbio.0030324
26	2Z3D	PRD_000235: N-Acetyl-L-Leucyl-L-Alanyl-N-[(1R,2R)-2-Hydroxy-1-{[(3S)-2-Oxopyrrolidin-3-Yl]Methyl}Propyl]-L-Alaninamide	A	Covalent	10.1016/j.jmb.2007.06.001
27	2QIQ	Cyv: Ethyl (4r)-4-{[(2r,5s)-5-{[N-(Tert-Butoxycarbonyl)-L-Seryl]Amino}-6-Methyl-2-(3-Methylbut-2-En-1-Yl)-4-Oxoheptanoyl]Amino}-5-[(3r)-2-Oxopyrrolidin-3-Yl]Pentanoate	A	Non-covalent	10.1016/j.bmcl.2007.08.031
28	2ZU4	ZU3: N-[(Benzyloxy)Carbonyl]-3-[(2,2-Dimethylpropanoyl)Amino]-L-Alanyl-N-[(1R)-4-Oxo-1-{[(3S)-2-Oxopyrrolidin-3-Yl]Methyl}Pentyl]-L-Leucinamide (TG-0204998)	A	Covalent	10.1074/jbc.M807947200
29	3SNB	Ac-DSFDQ-H	A	Covalent	10.1016/j.antiviral.2011.08.001
30	4TWW	3A7: (2S)-2-({[(3S,4ar,8as)-2-(4-Bromobenzoyl)Decahydroisoquinolin-3-Yl]Methyl}Amino)-3-(1H-Imidazol-5-Yl)Propanal (Bromobenzoyl(S,R)-N-decalin type inhibitor)	A	Non-covalent	10.1016/j.bmc.2014.12.028
31	2VJ1	Xp1: 4-(Dimethylamino)Benzoic Acid	A	Covalent	10.1016/J.Chembiol.2008.04.011
32	2Z3E	PRD_000250: N-Acetyl-L-Valyl-O-Benzyl-L-Threonyl-N-[(1R,2R)-2-Hydroxy-1-{[(3R)-2-Oxopyrrolidin-3-Yl]Methyl}Propyl]-L-Leucinamide	A	Covalent	10.1016/j.jmb.2007.06.001
33	2AMQ	Prd_002214: N-[(5-Methylisoxazol-3-Yl)Carbonyl]Alanyl-L-Valyl-N~1~-((1r,2z)-4-(Benzyloxy)-4-Oxo-1-{[(3r)-2-Oxopyrrolidin-3-Yl]Methyl}But-2-Enyl)-L-Leucinamide (Inhibitor N3)	A	Covalent	10.1371/journal.pbio.0030324
34	2GTB	Azp: (5s,8s,14r)-Ethyl 11-(3-Amino-3-Oxopropyl)-8-Benzyl-14-Hydroxy-5-Isobutyl-3,6,9,12-Tetraoxo-1-Phenyl-2-Oxa-4,7,10,11-Tetraazapentadecan-15-Oate (Aza-peptide epoxide inhibitor in the space group P43212)	A	Covalent	10.1016/j.jmb.2006.11.078
35	2A5I	Azp: (5s,8s,14r)-Ethyl 11-(3-Amino-3-Oxopropyl)-8-Benzyl-14-Hydroxy-5-Isobutyl-3,6,9,12-Tetraoxo-1-Phenyl-2-Oxa-4,7,10,11-Tetraazapentadecan-15-Oate (Aza-peptide epoxide inhibitor in the space group C2)	A	Covalent	10.1016/j.jmb.2005.09.004

Serial No	PDB entry	Ligand	Binding Site	Bonding	DOI
36	2ALV	Cy6: N-((3s,6r)-6-((S,E)-4-Ethoxycarbonyl-1-((S)-2-Oxopyrrolidin-3-Yl)But-3-En-2-Ylcarbamoyl)-2,9-Dimethyl-4-Oxodec-8-En-3-Yl)-5-Methylisoxazole-3-Carboxamide (Designed Anti-viral inhibitors)	A	Covalent	10.1021/jm050548m
37	3SNE	Ac-ESTLQ-H (Peptide aldehyde inhibitor)	A	Covalent	10.1016/ j.antiviral.2011.08.001
38	2A5K	Azp: (5s,8s,14r)-Ethyl 11-(3-Amino-3-Oxopropyl)-8-Benzyl-14-Hydroxy-5-Isobutyl-3,6,9,12-Tetraoxo-1-Phenyl-2-Oxa-4,7,10,11-Tetraazapentadecan-15-Oate (Aza-peptide epoxide inhibitor in space group P212121)	A	Covalent	10.1016/j.jmb.2005.09.004
39	1UK4	5-Mer Peptide Inhibitor	A	Covalent	10.1073/pnas.1835675100
40	3SNC	Ac-NSTSQ-H	A	Covalent	10.1016/ j.antiviral.2011.08.001
41	2D2D	Enb: Ethyl (2e,4s)-4-[((2r)-2-{[N-(Tert-Butoxycarbonyl)-L-Valyl]Amino}-2-Phenylethanoyl)Amino]-5-[(3s)-2-Oxopyrrolidin-3-Yl]Pent-2-Enoate (Inhibitor I2)	A	Covalent	10.1371/ journal.pbio.0030324
42	3D62	959: Benzyl (2-Oxopropyl)Carbamate (Broad-Spectrum Halomethyl Ketone Inhibitors)	A	Covalent	10.1111/j.1747-0285.2008.00679.x
43	3IWM	Prd_002214: N-[(5-Methylisoxazol-3-Yl)Carbonyl]Alanyl-L-Valyl-N~1~-((1r,2z)-4-(Benzyloxy)-4-Oxo-1-{[(3r)-2-Oxopyrrolidin-3-Yl]Methyl}But-2-Enyl)-L-Leucinamide	A	Non-Covalent	10.1007/s13238-010-0044-8
44	2V6N	Axp: 4-(dimethylamino)benzoic Acid Mes: 2-(N-Morpholino)-Ethanesulfonic Acid	A F	Non-covalent	10.1016/ j.chembiol.2008.04.011
45	2GT7	Mes: 2-(N-Morpholino)-Ethanesulfonic Acid	Pseudo-binding site	Non-covalent	10.1016/j.jmb.2006.11.078

Table S4. SARS-CoV M^{pro} structure summary

Binding site	PDB ID
No ligands	2H2Z, 2Z9G, 4ZUH, 2QCY, 2Q6G, 2DUC, 3EA8, 3EBN, 2Z9K, 5B6O, 2GT8, 2Z9J, 2GZ9, 3M3S, 2C3S, 1UJ1, 2BX3, 2Z9L, 2BX3, 3E91, 3EA9, 2A5A, 3EA7, 1UK2, 3EAJ, 1UK3, 2BX4, 2PWX, 3M3T, 1Z1J, 3M3V, 2QC2, 1Z1I, 2K7X
A	6W79, 5N19, 3TNT, 3SZN, 6LNQ, 6WCO, 3TNS, 5C5O, 3TIT, 5N5O, 2ZU5, 2HOB, 2GX4, 4TWY, 3TIU, 2OP9, 2Z94, 3SND, 2Z3C, 2GZ8, 2GZ7, 4WY3, 5C5N, 2AMD, 1WOF, 2Z3D, 2QIQ, 2ZU4, 3SNB, 4TWW, 2VJ1, 2Z3E, 2AMQ, 2GTB, 2A5I, 2ALV, 3SNE, 2A5K, 1UK4, 3SNC, 2D2D, 3D62, 3IWM, 2V6N
F	2V6N
Pseudo-binding site	2GT7

Table S5. MERS-CoV M^{pro} ligand binding Sites

Serial No	PDB ID	Ligand	Binding Site	Bonding	DOI
1	5WKJ	B1S: (1R,2S)-2-({N-[(benzyloxy)carbonyl]-L-leucyl}amino)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid K36: (1S,2S)-2-({N-[(benzyloxy)carbonyl]-L-leucyl}amino)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (Inhibitor GC376)	A	Covalent	10.1016/ j.ejmech.2018.03.004
2	5WKL	AVY: (1R,2S)-2-{[N-({[4-benzyl-1-(tert-butoxycarbonyl)piperidin-4-yl]oxy}carbonyl)-L-leucyl]amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid B3J: (1S,2S)-2-{[N-({[4-benzyl-1-(tert-butoxycarbonyl)piperidin-4-yl]oxy}carbonyl)-L-leucyl]amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (Piperidine-based peptidomimetic inhibitor 17)	A	Covalent	10.1016/ j.ejmech.2018.03.004
3	5WKK	AW4: (1S,2S)-2-[(N-{[2-(3-chlorophenyl)ethoxy]carbonyl}-L-leucyl)amino]-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid B3G: (1R,2S)-2-[(N-{[2-(3-chlorophenyl)ethoxy]carbonyl}-L-leucyl)amino]-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (Inhibitor GC813)	A	Covalent	10.1016/ j.ejmech.2018.03.004
4	5WKM	N02: (1S,2S)-2-{[N-({[1-(tert-butoxycarbonyl)-4-ethylpiperidin-4-yl]oxy}carbonyl)-L-leucyl]amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid B6Y: (1R,2S)-2-{[N-({[1-(tert-butoxycarbonyl)-4-ethylpiperidin-4-yl]oxy}carbonyl)-L-leucyl]amino}-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (Piperidine-based peptidomimetic inhibitor 21)	A	Covalent	10.1016/ j.ejmech.2018.03.004
5	6VGZ	QZG: N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-N~2~-({[trans-4-(propan-2-yl)cyclohexyl]oxy}carbonyl)-L-leucinamide (Inhibitor 6d)	A	Covalent	10.1126/ scitranslmed.abc5332
6	6VGY	QZJ: N~2~-{[(trans-4-ethylcyclohexyl)oxy]carbonyl}-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-L-leucinamide (Inhibitor 6b)	A	Covalent	10.1126/ scitranslmed.abc5332
7	6VH1	QZ7: N~2~-{[(4,4-difluorocyclohexyl)oxy]carbonyl}-N-{(2S)-1-hydroxy-3-[(3S)-2-	A	Covalent	10.1126/ scitranslmed.abc5332

Serial No	PDB ID	Ligand	Binding Site	Bonding	DOI
		oxopyrrolidin-3-yl]propan-2-yl}-L-leucinamide (Inhibitor 6h)			
8	6VH0	QZD: N~2~-{[(5-ethyl-1,3-dioxan-5-yl)oxy]carbonyl}-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-L-leucinamide (Inhibitor 6g)	A	Covalent	10.1126/scitranslmed.abc5332
9	6VH3	QYS: (1S,2S)-2-[(N-{[(4,4-difluorocyclohexyl)methoxy]carbonyl}-L-leucyl)amino]-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid	A	Covalent	10.1126/scitranslmed.abc5332
10	6VH2	QZ4: 4,4-difluorocyclohexyl [(2S)-3-cyclohexyl-1-({(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}amino)-1-oxopropan-2-yl]carbamate (Inhibitor 7i)	A	Covalent	10.1126/scitranslmed.abc5332
11	4YLU	R30: N-{4-[(1H-benzotriazol-1-ylacetyl)(thiophen-3-ylmethyl)amino]phenyl}propanamide	A	Non-Covalent	10.1074/jbc.M115.651463

Table S6. MERS-CoV M^{pro} structure summary

Binding site	PDB ID
No ligands	5C3N, 4WMD, 4WME, 4WMF
A	5WKJ, 5WKL, 5WKK, 5WKM, 6VGZ, 6VGY, 6VH1, 6VH0, 6VH3, 6VH2, 4YLU