Electronic Supplementary Material (ESI) for Molecular Omics.

Repurposing drugs against main protease of SARS-CoV-2: mechanism based insights supported by available laboratory and clinical data

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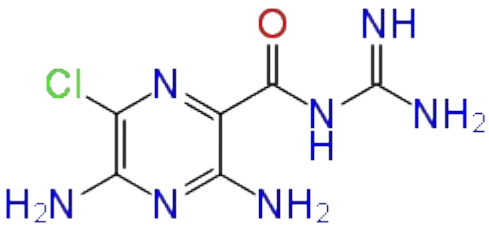
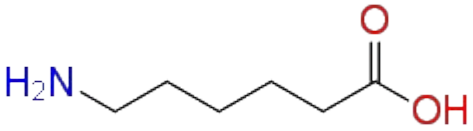
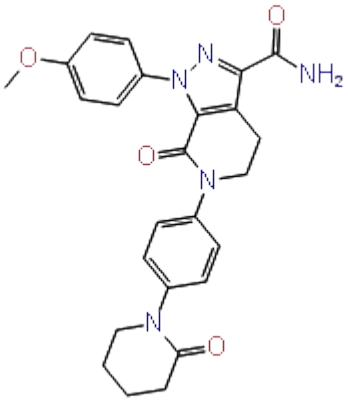
Supplementary Information:

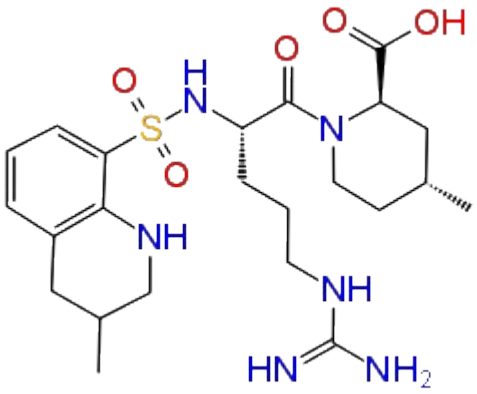
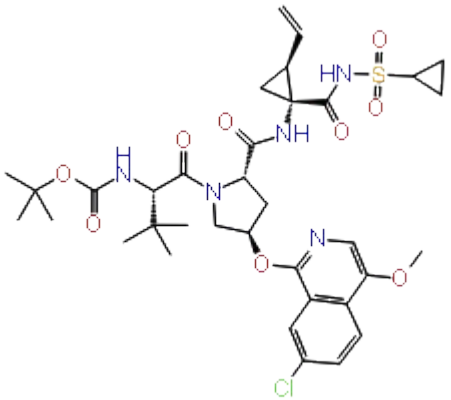
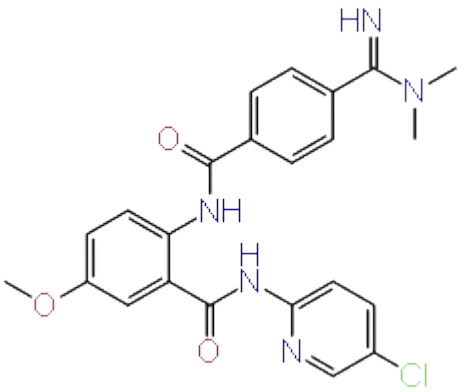
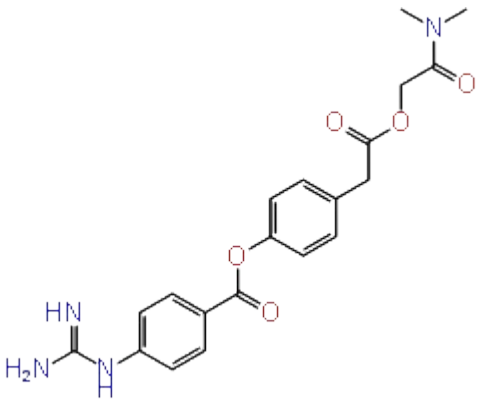
I. 2D chemical structures of molecules considered for docking in workflow-I (the images of the structures have been generated using Maestro GUI (Schrödinger, LLC) freely available for academic usage).

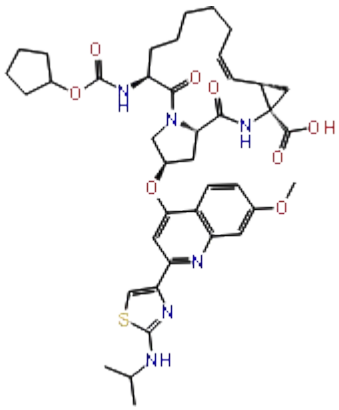
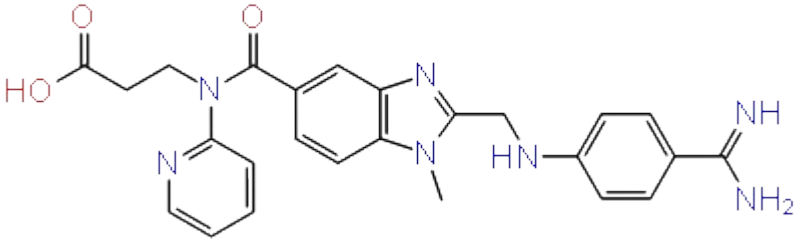
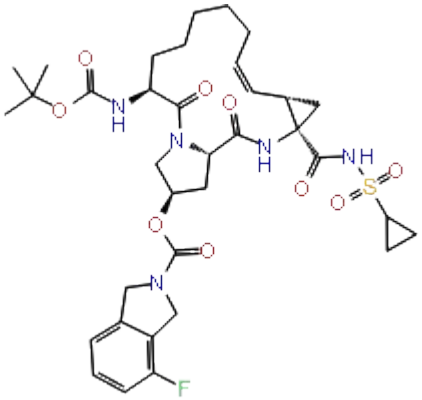
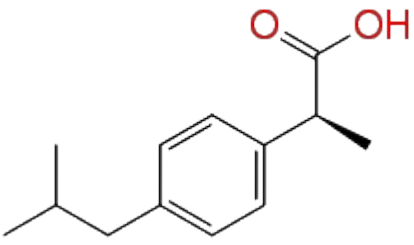
II. 2D chemical structures of molecules considered for docking in workflow-II (the images of the structures have been generated using Maestro GUI (Schrödinger, LLC) freely available for academic usage).

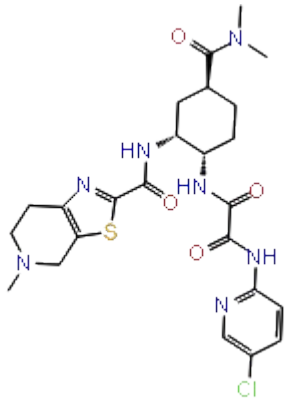
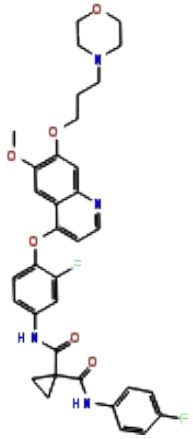
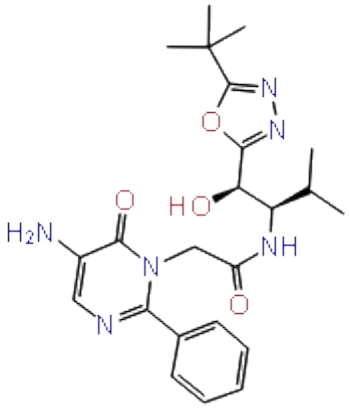
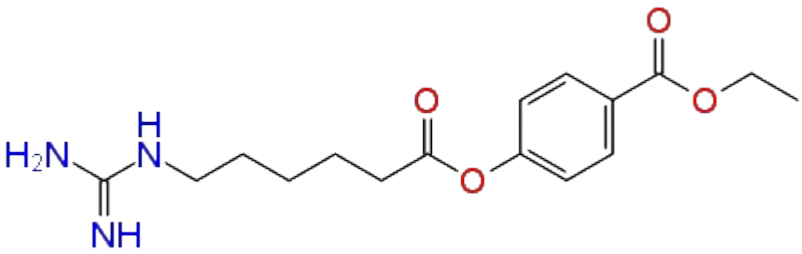
III. List of references to support anti-viral and/specifically anti-coronavirus property of indicated molecules in Table S4.

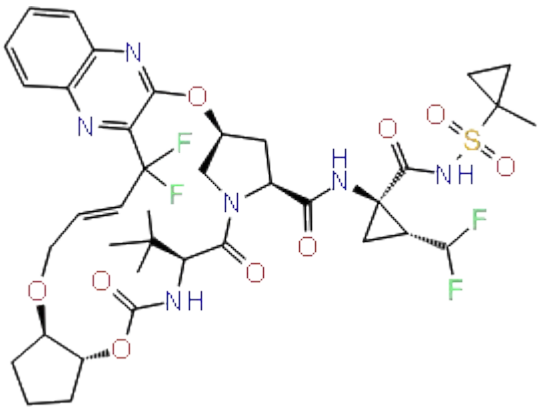
I. 2D chemical structures of molecules considered for docking in workflow-I

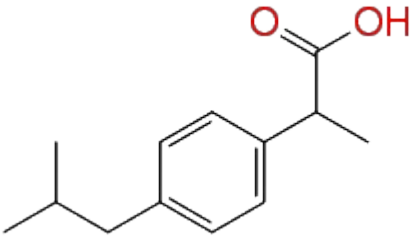
Sl. No.	Chemical structure	Name of the molecule
1		Amiloride
2		Aminocarpoic acid
3		Apixaban

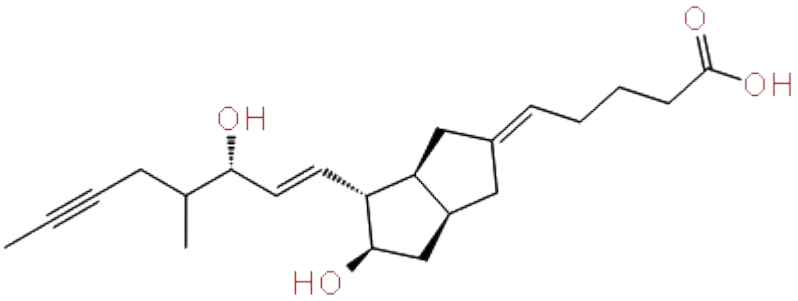
4		Argatroban
5		Asunapreir
6		Betrixaban
7		Camostat

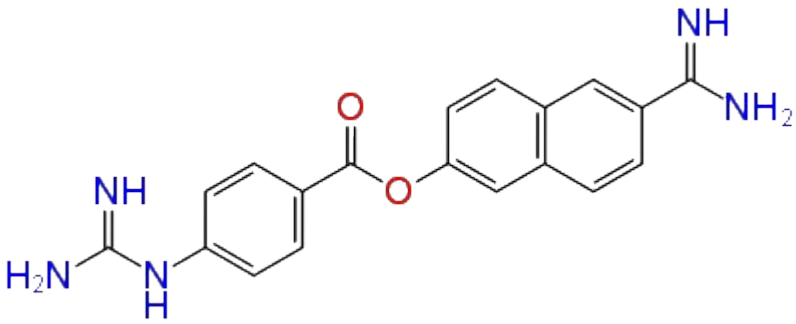
8		Ciluprevir
9		Dabigatran
10		Danoprevir
11		Dexibuprofen

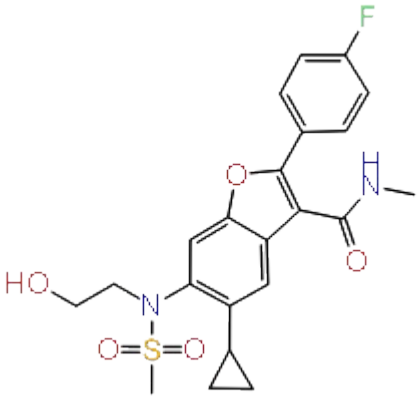
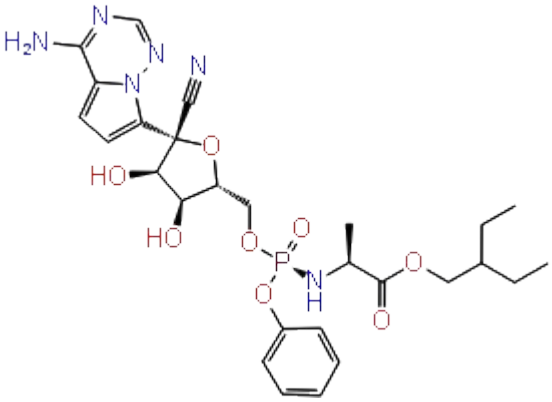
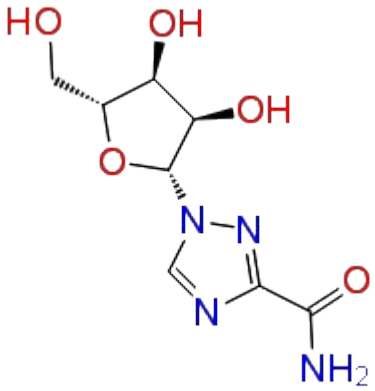
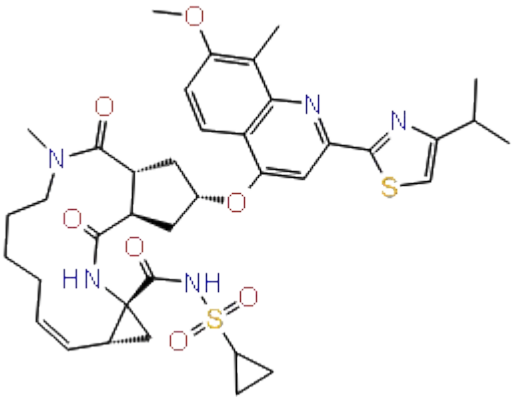
12		Edoaxaban
13		Foretinib
14		Freselestat
15		Gabexate

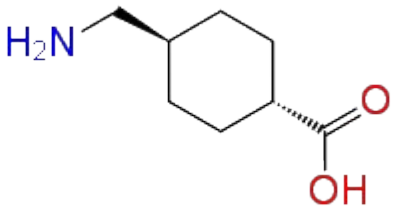
16  Glecaprevir

17  Ibuprofen

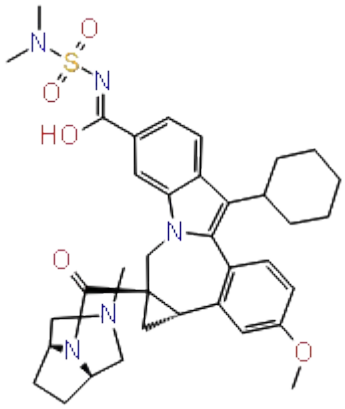
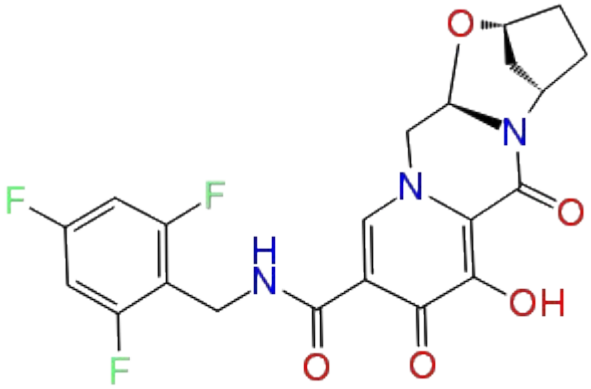
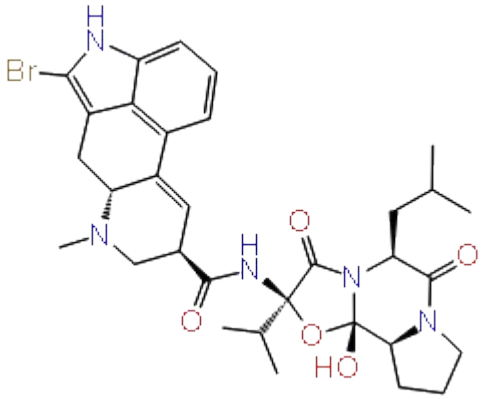
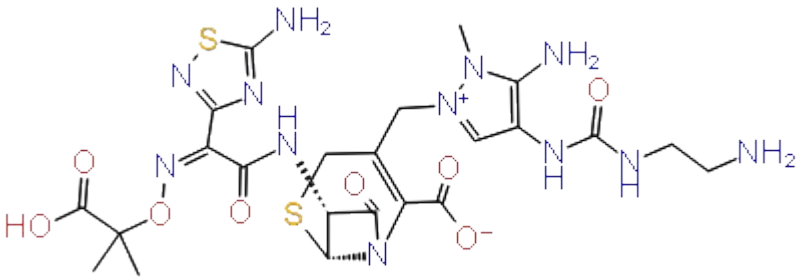
18  Iloprost

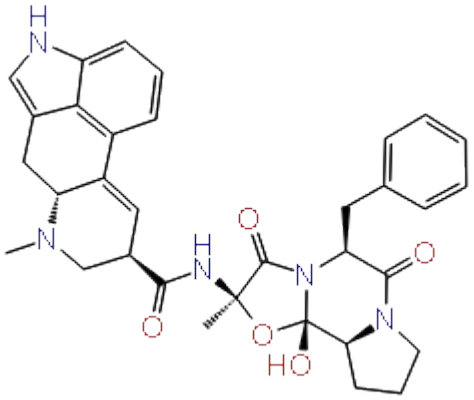
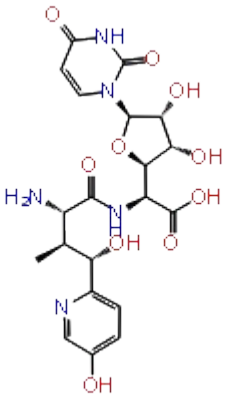
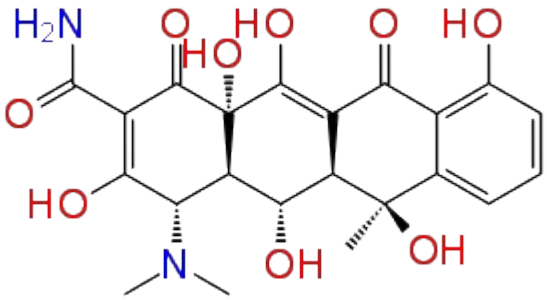
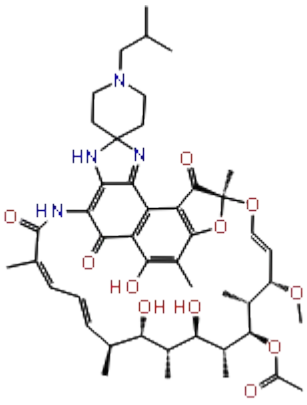
19  Nafamostat

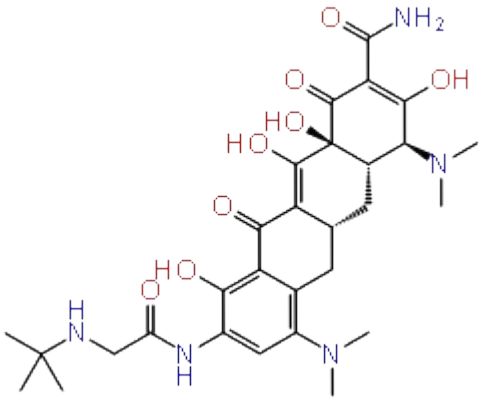
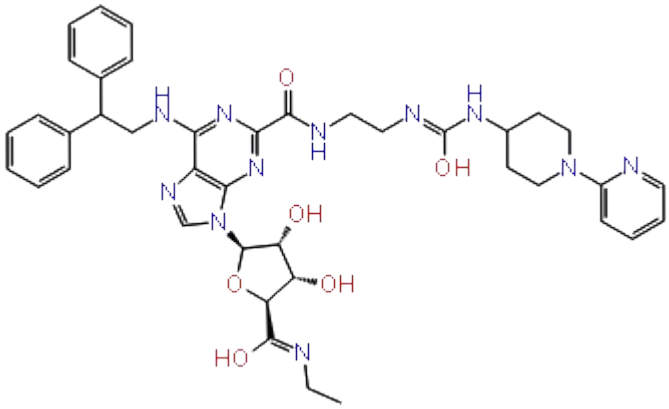
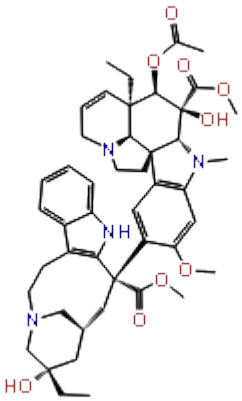
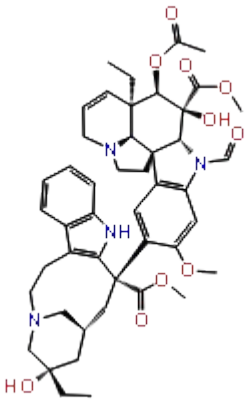
20		Nesbuvir
21		Remdesivir
22		Ribavirin
23		Simeprevir

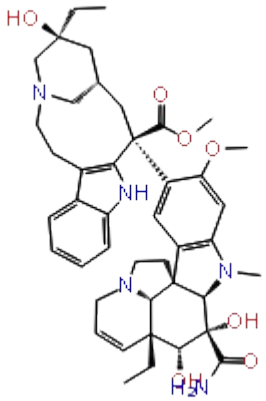
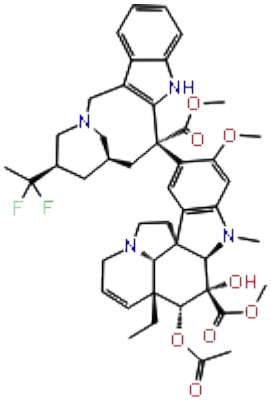
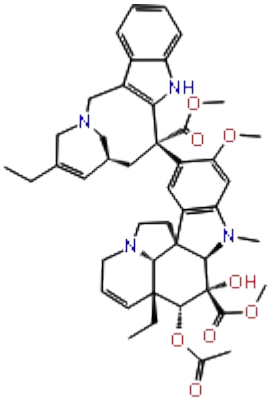
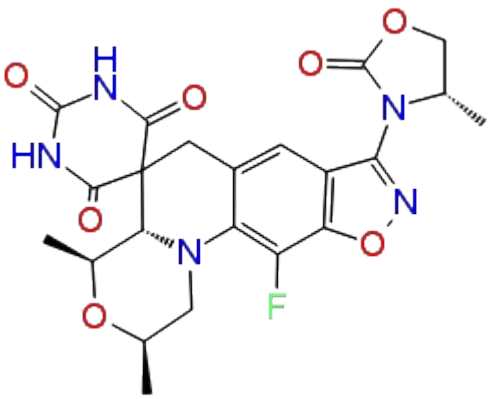
24  Tranexamic acid

II. 2D chemical structures of molecules considered for docking in workflow-II

Sl. No.	Chemical structure	Name of the molecule
1		Beclabuvir
2		Bictegravir
3		Bromocriptine
4		Ceftolozane

5		Ergotamine
6		Nikkomycin Z
7		Oxytetracycline
8		Rifabutin

9		Tigecycline
10		UK-432,097
11		Vinblastine
12		Vincristine

13		Vindesine
14		Vinflunine
15		Vinorelbine
16		Zoliflodacin

III. List of references to support anti-viral and/specifically anti-coronavirus property of indicated molecules in Table S4.

Sl. No. as per table S4	Drug_Name [Ref.]
1	Benzyl (2-oxopropyl)carbamate [1]
2	2-[(2,4-dichloro-5-methylphenyl)sulfonyl]-1,3-dinitro-5-(trifluoromethyl)benzene [2]
3	S-[5-(trifluoromethyl)-4h-1,2,4-triazol-3-yl] 5-(phenylethynyl)furan-2-carbothioate [2]
4	5-amino-2-methyl-N-[(1R)-1-naphthalen-1-ylethyl]benzamide [3]
5	Nalpha-[(benzyloxy)carbonyl]-n-[(1r)-4-hydroxy-1-methyl-2-oxobutyl]-l-phenylalaninamide [4]
6	4-(Dimethylamino)benzoic acid [5]
8	Ethyl (4R)-4-{[(2R,5S)-2-(4-fluorobenzyl)-6-methyl-5-{[(5-methyl-1,2-oxazol-3-yl)carbonyl]amino}-4-oxoheptanoyl]amino}-5-[(3S)-2-oxo-3-pyrrolidinyl]pentanoate [6–8]
9	Phenylalanine boronic acid [9–11]
29	{1-[2-(1-formyl-propyl)-3-methanesulfonylamino-pyrrolidine-1-carbonyl]-2-methyl-propyl}-carbamic acid tert-butyl ester [12]
30	Nesbuvir [13]
31	Asunaprevir [14]
32	(2z)-2-(Benzoylamino)-3-[4-(2-Bromophenoxy)Phenyl]-2-Propenoic Acid [15]
33	Ciluprevir [16]
34	Danoprevir [17]
35	N-[(2R,3S)-1-((2S)-2-{[(cyclopentylamino)carbonyl]amino}-3-methylbutanoyl)-2-(1-formyl-1-cyclobutyl)pyrrolidinyl]cyclopropanecarboxamide [18]
36	Simeprevir [19]
37	Glecaprevir [20]
38	(3R)-3-[3,5-Bis(trifluoromethyl)anilino]-2-cyano-3-sulfanylpropanamide [21]
39	2-{[N-(2-acetyl-5-chloro-4-fluorophenyl)glycyl]amino}benzoic acid [22]
40	2-{[(4-chlorophenoxy)acetyl]amino}benzoic acid [22]
41	1-[(2-amino-4-chloro-5-methylphenyl)sulfonyl]-l-proline [23]
42	3-(1,1-dioxido-4H-1,2,4-benzothiadiazin-3-yl)-4-hydroxy-1-(3-methylbutyl)quinolin-2(1H)-one [24]
43	5-(4-cyanophenyl)-3-{[(2-methylphenyl)sulfonyl]amino}thiophene-2-carboxylic acid [25]
44	5-(4-fluorophenyl)-3-{[(4-methylphenyl)sulfonyl]amino}thiophene-2-carboxylic acid [25]
45	5'-acetyl-4-{[(2,4-dimethylphenyl)sulfonyl]amino}-2,2'-bithiophene-5-carboxylic acid [25]
71	N-Benzyloxycarbonyl-l-serine-betalactone [26,27]
72	Phenylalanylamide [26]
113	Bictegravir [28,29]
129	Ruzasvir [30]
132	Setrobuvir [31]

136	Beclabuvir [32]
148	GS-9256 [33]

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