

## Supplementary data

**Table S1.** Results of the docking of DrugBank compounds onto GRP78 (NBD) (only molecules with lower docking scores than control ATP are presented).

Molecule name	Final docking score S (kcal/mol)
Imatinib	-9.26206
FK-614	-8.9803
Selonsertib	-8.85865
Sorafenib	-8.841712
CID 5288250	-8.6442
Pemetrexed	-8.6247129
4SC-203	-8.61179
Zafirlukast	-8.59865
(2S)-2-[[4-[2-[(6S)-2-Amino-4-oxo-5,6,7,8-tetrahydro-3H-pyrido[2,3-d]pyrimidin-6-yl]ethyl]benzoyl]amino]pentanedioic acid	-8.58657
Icariin	-8.46474
Raltegravir	-8.44994
4-[(5-[[4-(3-Chlorophenyl)-3-oxopiperazin-1-yl]methyl]-1H-imidazol-1-yl)methyl]benzotrile	-8.44899
Dacomitinib	-8.4483
[(1S)-1-Cyclohexyloxycarbonyloxyethyl] 2-ethoxy-3-[[4-[2-(2H-tetrazol-5-yl)phenyl]phenyl]methyl]benzimidazole-4-carboxylate	-8.43484
Darexaban	-8.4267
Tenofovir disoproxil	-8.4124937
Neratinib	-8.39573
Ponatinib	-8.38035
6-(3-(Dimethylcarbamoyl)phenylsulfonyl)-4-(3-methoxyphenylamino)-8-methylquinoline-3-carboxamide	-8.32773
2'-Deoxy-N-(naphthalen-1-ylmethyl)guanosine 5'-(dihydrogen phosphate)	-8.31957
3-(5-[[4-(Aminomethyl)piperidin-1-yl]methyl]-1h-Indol-2-yl)quinolin-2(1h)-One	-8.30333
(2R)-N-[2-[4-[5-[4-[(4-Acetamidophenyl)methoxy]-2,3-dichlorophenyl]-2-methylpyrazol-3-yl]piperidin-1-yl]-2-oxoethyl]-2-(diaminomethylideneamino)-4-methylpentanamide	-8.2941
Butafenacil	-8.29337
Nilotinib	-8.28767
Gedatolisib	-8.27715
N-(Sulfanylacetyl)tyrosylprolylmethioninamide	-8.27166
Leucovorin	-8.2563314
Asp3026	-8.24956
Methyl (1R,2S)-2-(hydroxycarbamoyl)-1-[[4-[(2-methylquinolin-4-yl)methoxy]phenyl]methyl]cyclopropane-1-carboxylate	-8.2435
GW-493838	-8.1977
2-({4-[4-(Pyridin-4-ylmethyl)-1H-pyrazol-3-yl]phenoxy}methyl)quinoline	-8.18944
2-({4-[(5-Chloro-1H-indol-2-yl)sulfonyl]piperazin-1-yl}carbonyl)thieno[3,2-B]pyridine 4-oxide	-8.17951
Travoprost	-8.162818

Hexamidine	-8.14578
4-(1,3-Benzodioxol-5-Yloxy)-2-[4-(1h-Imidazol-1-Yl)phenoxy]pyrimidine	-8.14297
Sjg-136	-8.12716
(2S,3R,6S)-4-Oxo-6-[4-[(2-phenylquinolin-4-yl)methoxy]phenyl]-5-azaspiro[2.4]heptane-2-carboxylic acid	-8.10969
ORG-25435	-8.10411
Squalene	-8.10209
6,7-Dimethoxy-4-[(3r)-3-(2-Naphthyloxy)pyrrolidin-1-Yl]quinazoline	-8.10006
(5S)-5-[[4-[2-(5-Methyl-2-phenyl-1,3-oxazol-4-yl)ethoxy]-1-benzothiophen-7-yl]methyl]-1,3-thiazolidine-2,4-dione	-8.09299
Asp-4058	-8.08662
(5S)-5-[[4-[3-(5-Methyl-2-phenyl-1,3-oxazol-4-yl)propanoyl]phenyl]methyl]-1,3-thiazolidine-2,4-dione	-8.02981
Uridylyl-2'-5'-phospho-adenosine	-8.02227
HKI-357	-8.02173
n-[4-[[Glutamic acid]-carbonyl]-benzene-sulfonyl-d-prolinyl]-3-amino-propanoic acid	-8.02126
Grapiprant	-8.00985
Dirlotapide	-8.00538
AMG-131	-7.98479
Flumatinib	-7.9804
Siponimod	-7.97261
Bafetinib	-7.97087
1-((2-Hydroxyethoxy)methyl)-5-(3-(benzyloxy)benzyl)-6-hydroxypyrimidine-2,4(1H,3H)-dione	-7.96472
(1-Hydroxy-1-phosphono-2-[1,1';4',1'']terphenyl-3-yl-ethyl)-phosphonic acid	-7.95892
Toreforant	-7.95254
Ceftriaxone	-7.94988
Atecegatran metoxil	-7.94223
N-(5-[(2s)-4-Amino-2-(3-Chlorophenyl)butanoyl]amino)-1h-Indazol-3-Yl)benzamide	-7.93776
Lumacaftor	-7.91532
Alvelestat	-7.89843
Aldose reductase-IN-1	-7.89767
Guanosine 5'-diphosphate 2':3'-cyclic monophosphate	-7.8961
5'-Guanosine-diphosphate-monothiophosphate	-7.89037
6-(12-Hydroxydodecyl)-2,3-dimethoxy-5-methyl-1,4-benzoquinone	-7.88111
Dihydrofolic acid	-7.88086
Danusertib	-7.87696
Unii-642PS51324	-7.87616
Dasatinib	-7.87318
[(3S)-3-(Dimethylamino)pyrrolidin-1-yl]-[4-[[5-fluoro-4-(2-methyl-3-propan-2-ylimidazol-4-yl)pyrimidin-2-yl]amino]phenyl]methanone	-7.83605
Raltitrexed	-7.83305
Glesatinib	-7.82904
N,4-Dimethyl-3-[(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)amino]benzamide	-7.82707
2,6-Dimethyl-1-(3-[3-methyl-5-isoxazolyl]-propanyl)-4-[2n-methyl-2h-tetrazol-5-yl]-phenol	-7.82541
Tivozanib	-7.825
Trifluorofurnesyl diphosphate	-7.82168

5-(7-(5-Hydro-4-methyl-2-oxazolyl)phenoxy)heptyl)-3-methyl isoxazole	-7.81605
Norbixin	-7.81135
Aminoquinuride	-7.80693
Entinostat	-7.80107
Pyrotinib	-7.79242
4-[[1-Methyl-5-(2-methyl-benzoimidazol-1-ylmethyl)-1H-benzoimidazol-2-ylmethyl]-amino]-benzamidine	-7.78962
3-[[3-Fluoro-2-(methylsulfamoylamino)pyridin-4-yl]methyl]-4-methyl-7-pyrimidin-2-yloxychromen-2-one	-7.77858
Troriluzole	-7.77349
Olaparib	-7.76574
1,3-Dimethyl-7-[2-[[[(2R)-1-phenylpropan-2-yl]amino]ethyl]purine-2,6-dione	-7.76025
Axitinib	-7.72446
5-[2-Fluoro-5-[3-(3-hydroxy-2-methoxycarbonyl-phenoxy)-propenyl]-phenyl]-isoxazole-3-carboxylic acid	-7.72172
Atevirdine	-7.71884
N-{3-[4-(3-Amino-propyl)-piperazin-1-YL]-propyl}-3-nitro-5-(galactopyranosyl)-beta-benzamide	-7.71813
Flufenoxuron	-7.71614
4-Amino-8-(2-fluoro-6-methoxyphenyl)-N-propylcinnoline-3-carboxamide	-7.71045
Teneligliptin	-7.70647
Pexidartinib	-7.70575
Cerdulatinib	-7.70386
Phthalylsulfathiazole	-7.69539
N-(4-Phenoxyphenyl)-2-[(Pyridin-4-Ylmethyl)amino]nicotinamide	-7.68645
PTP1B Inhibitor	-7.68611
Novobiocin	-7.68053
HT-0712	-7.67965
(9E)-15-(2-Pyrrolidin-1-ylethoxy)-7,12,26-trioxa-19,21,24-triazatetracyclo[18.3.1.12,5.114,18]hexacosa-1(24),2,4,9,14,16,18(25),20,22-nonaene	-7.67722
N-Cyclopropyl-4-methyl-3-[1-(2-methylphenyl)phthalazin-6-yl]benzamide	-7.67502
Penamecillin	-7.66775
Carboxyamidotriazole	-7.66609
3-[2,6,8-Trioxo-9-[(2S,3S,4R)-2,3,4,5-tetrahydroxypentyl]-3H-purin-7-yl]propyl dihydrogen phosphate	-7.66503
(7R)-7-Phenyl-7-(2,4,5-trimethyl-3,6-dioxocyclohexa-1,4-dien-1-yl)heptanoic acid	-7.66483
Losmapimod	-7.65774
Alamifovir	-7.6565
HG_7_85_01	-7.65557
5-[3-(2-Methoxyphenyl)-1h-Pyrrolo[2,3-B]pyridin-5-yl]-n,n-dimethylpyridine-3-carboxamide	-7.65465
Olmutinib	-7.65387
5-(4-Morpholin-4-YL-phenylsulfanyl)-2,4-quinazolinediamine	-7.6527
CID 6914621	-7.65228
1-(5-Chloro-6-(2-methylpropoxy)-3-pyridinyl)-3-methyl-N-(methylsulfonyl)-1H-indazole-5-carboxamide	-7.64941
s-Benzyl-glutathione	-7.64403
Simfibrate	-7.63094
Etofamide	-7.62563

Verdinexor	-7.62995
5-[[6-[2,4-Bis(trifluoromethyl)phenyl]pyridazin-3-yl]methyl]-2-(2-fluorophenyl)-1h-imidazo[4,5-c]pyridine	-7.62547
S-23	-7.62451
N-[4-(2-Chlorophenyl)-1,3-dioxo-1,2,3,6-tetrahydropyrrolo[3,4-c]carbazol-9-yl]formamide	-7.61237
Unii-XH93U6nije	-7.60956
2-[3-[(2S)-4,4-Difluoro-2-(pyrrolidine-1-carbonyl)pyrrolidin-1-yl]-3-oxopropyl]isoindole-1,3-dione	-7.60441
N6-Isopentenyl-adenosine-5'-monophosphate	-7.60094
Sonedenoson	-7.59855
Lintitript	-7.59544
2-Hydroxy-5-((1-[(2-naphthyloxy)methyl]-3-oxoprop-1-enyl)amino)tyrosine	-7.59333
ATP*	-7.59121
Honokiol*	-6.99529
hkh40a*	-6.66791
VER-155008*	-6.81304
Isoliquiritigenin*	-6.19445
Epigallocatechin gallate*	-4.94584

\*positive controls.

**Table 2S.** Results of the docking of DrugBank compounds onto GRP78 (SBD) (only molecules with lower docking scores than control region IV (C480-C488) from SARS-CoV-2 spike are presented).

<b>Molecule name</b>	<b>Final docking score S (kcal/mol)</b>
Zilucoplan	-13.534038
Obinepitide	-13.276237
Corticotropin ovine triflutate	-13.069051
CID 131704298	-12.854046
N-[(3E)-1-Oxo-3-hexenyl]Somatoliberin	-12.760726
Tifuvirtide	-12.726995
Cotadutide	-12.652015
Semaglutide	-12.464309
CID 118984461	-12.390542
Taspoglutide	-11.908224
Adrenocorticotrophic hormone 1-24	-11.165439
Adenosine-5'-ditungstate	-11.0066
CID 16139342	-10.820189
Brimapitide	-10.814741
CID 145994601	-10.75272
Albuvirtide	-10.431156



oxopropan-2-yl]amino]-2-oxoethyl]amino]-3-methyl-1-oxobutan-2-yl]amino]-1-oxopropan-2-yl]amino]-3-(1H-indol-3-yl)-1-oxopropan-2-yl]amino]-1,5-dioxopentan-2-yl]amino]-1,4-dioxobutan-2-yl]amino]-2-oxoethyl]amino]-4-methyl-1-oxopentan-2-yl]amino]-5-carbamimidamido-1-oxopentan-2-yl]-2-[[2S)-5-oxopyrrolidine-2-carbonyl]amino]pentanediamide	-9.1110048
(2R)-6-Amino-2-[[2R)-2-[[2R)-2-[[2R)-2-[[2R)-2-[[2R)-2-[[2R)-2-[[2R)-1-[[2R)-2-[[2R)-2-[[2R)-2-[[2R)-2-[[2R)-2-[[2R)-2-amino-3-(1H-indol-3-yl)propanoyl]amino]-3-(1H-indol-3-yl)propanoyl]amino]-3-hydroxybutanoyl]amino]-3-phenylpropanoyl]amino]-3-phenylpropanoyl]amino]-4-methylpentanoyl]pyrrolidine-2-carbonyl]amino]-3-hydroxypropanoyl]amino]-3-hydroxybutanoyl]amino]-4-methylpentanoyl]amino]-3-(1H-indol-3-yl)propanoyl]amino]-4-carboxybutanoyl]amino]-5-carbamimidamidopentanoyl]amino]hexanoic acid	-8.9104519
Omiganan	-8.7780027
Ganirelix	-8.5557013
Triptorelin	-8.5525694
Ozarelix	-8.5197821
Melanotan-1	-8.4410248
Gramicidin D	-8.3783236
4F-Benzoyl-TN14003	-8.3450165
Compstatin analog peptide CP40	-8.3361301
Degarelix	-8.2986946
[(3R)-1-[(2R,3R,4R,5S,6R)-2-[[2R,3S,4R,5R,6R)-3-Hydroxy-4-[(3R)-3-hydroxydecoxy]-5-(3-oxotetradecanoylamino)-6-phosphonoxyoxan-2-yl]methoxy]-6-(methoxymethyl)-3-(3-oxotetradecanoylamino)-5-phosphonoxyoxan-4-yl]oxydecan-3-yl] (Z)-dodec-5-enoate	-8.2736235
(2S)-2-[[4-[(2-Amino-4-oxo-3H-pteridin-6-yl)methylamino]benzoyl]amino]-3-[4-[2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)indol-1-ium-2-yl]ethenyl]-6-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)indol-2-ylidene]ethylidene]cyclohexen-1-yl]oxyphenyl]propanoic acid	-8.1998796
Fondaparinux	-8.1666164
Immther	-8.0779819
Abarelix	-7.9749308
3-Nitro-N-[3-[4-[3-[[2-[3-[4-[3-[[3-nitro-5-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzoyl]amino]propyl]piperazin-1-yl]propylamino]-3,4-dioxocyclobuten-1-yl]amino]propyl]piperazin-1-yl]propyl]-5-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzamide	-7.9554586
Daptomicina	-7.8939037
Ceruletide	-7.8754039
L-Phenylalaninamide, N2-(1-oxohexadecyl)-L-lysyl-L-lysyl-L-seryl-L-arginyl-L-alanyl-L-leucyl-	-7.8446903
Somatostatin	-7.7792234
Fertagyl	-7.7791991
Tetradecanoyl-CoA	-7.741888
2-(4-Amino-4,6-dimethyl-5-oxooxan-2-yl)oxy-22-(2-amino-2-oxoethyl)-5,15-dichloro-18,32,35,37-tetrahydroxy-19-[[4-methyl-2-(methylamino)pentanoyl]amino]-20,23,26,42,44-pentaoxo-48-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-7,13-dioxa-21,24,27,41,43-pentazaocyclo[26.14.2.23,6.214,17.18,12.129,33.010,25.034,39]pentaconta-3,5,8,10,12(48),14,16,29(45),30,32,34(39),35,37,46,49-pentadecaene-40-carboxylic acid	

Sincalide	-7.729105
Bradykinin	-7.6730123
Rimiducid	-7.6237817
Unii-YI2S0guq2C	-7.618494
Coenzyme Q10	-7.6177607
Delparantag	-7.6103325
(4S)-4-[[[(2S)-2-[[[(2S)-2-[[[(2S)-2-Acetamido-3-hydroxypropanoyl]amino]-3-(4-hydroxyphenyl)propanoyl]amino]-3-hydroxypropanoyl]amino]-4-methylsulfanylbutanoyl]amino]-5-[[1-[[[(2S)-1-[[[(2S)-1-[[[(2S)-1-[[2-[[[(2S)-6-amino-1-[(2S)-2-[[[(2S)-1-amino-3-methyl-1-oxobutan-2-yl]carbamoyl]pyrrolidin-1-yl]-1-oxohexan-2-yl]amino]-2-oxoethyl]amino]-3-(1H-indol-3-yl)-1-oxopropan-2-yl]amino]-5-carbamimidamido-1-oxopentan-2-yl]amino]-1-oxo-3-phenylpropan-2-yl]amino]-3-(1H-imidazol-5-yl)-1-oxopropan-2-yl]amino]-5-oxopentanoic acid	-7.6015368
Suramin	-7.5867271
Antarelix	-7.5620089
Bepecin	-7.5540962
Sinapoyl coenzyme A	-7.5208478
Triolein	-7.5046391
Dotatate	-7.4802132
Abt-510	-7.4741888
Bhsar-SP	-7.4709034
Angiotensin II	-7.4678698
Oncopore	-7.4600463
Bambermycins	-7.4599528
Ala-geninthiocin	-7.4431362
alpha-GalCer	-7.4146681
Palmitoyl tetrapeptide-7	-7.3767581
3-[(1R,6R,9S,12S,15S,21S,24S,27S,30S,33R,36S,39S,45S,48S,53R)-53-[(2-Aminoacetyl)amino]-30-(2-amino-2-oxoethyl)-9-[(2S)-butan-2-yl]-36-(3-carbamimidamidopropyl)-6-carbamoyl-24,45-bis(carboxymethyl)-48-(hydroxymethyl)-27-[(4-hydroxyphenyl)methyl]-21-(1H-imidazol-5-ylmethyl)-8,11,14,20,23,26,29,32,35,38,44,47,50,52-tetradeca-3,4,5,5,5,5-tetrathia-7,10,13,19,22,25,28,31,34,37,43,46,49,51-tetradecazatetracyclo[31.17.7.015,19.039,43]heptapentacontan-12-yl]propanoic acid	-7.3716264
Deslorelin	-7.3678479
Etelcalcetide	-7.3659992
Uproleselan	-7.3155847
Leuprorelin	-7.3120184
(2R,3R,4S,5S,6R)-2-[(2R,3S,4R,5R,6S)-6-[(1R,4S,5S,6R)-4-[[[(2R,3S,4S,5R,6R)-6-[[[(2R,3S,4R,5R,6R)-4,5-Dihydroxy-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxan-3-yl]oxy-4,5-dihydroxy-2-methyloxan-3-yl]amino]-5,6-dihydroxy-2-(hydroxymethyl)cyclohex-2-en-1-yl]oxy-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol	-7.2878718
Bremelanotide	-7.2748389
D-Glucopyranose, pentakis[3,4-dihydroxy-5-[(3,4,5-trihydroxybenzoyl)oxy]benzoate]	-7.2686925
Mivacurium	-7.2632093

Colistin sodium methanesulfonate	-7.2589989
Cibinetide	-7.2571716
Goserelin	-7.2503462
Vapreotide	-7.2494888
Glutathionylspermidine disulfide	-7.2469893
Tat-BP	-7.2457705
[2-Amino-3-[3-[4-[3-[[3-nitro-5-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzoyl]amino]propyl]piperazin-1-yl]propyl]carbamoyloxy]propyl] N-[3-[4-[3-[[3-nitro-5-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzoyl]amino]propyl]piperazin-1-yl]propyl]carbamate	-7.2409163
Setmelanotide	-7.2327309
CID 17753951	-7.2154012
Depreotide	-7.2144785
Nafarelin	-7.2102528
1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol	-7.2046738
Eritoran	-7.1976666
Lanreotide acetate	-7.1871324
Bacitracin A	-7.1833935
CoA-S-acetyl 5-bromotryptamine	-7.1813159
Semapimod	-7.1751194
Terlipressin	-7.1704521
Notomycin A1	-7.1515746
(2R)-N-[(2S)-6-Amino-1-anilino-1-oxohexan-2-yl]-2-[[2-[(2S)-2-[(2S)-6-amino-1-anilino-1-oxohexan-2-yl]carbamoyl]hexyl]hydrazinyl]methyl]hexanamide	-7.1362066
(R)-3-Hydroxydecanoyl-CoA	-7.1291924
Arylomycin A2	-7.1237774
Inhibitor bea409	-7.123332
Reidispongiolide A	-7.115509
Lauroyl-CoA	-7.1137977
Trierucin	-7.1008019
Labradimil	-7.1003852
C24:1 Sulfatide	-7.0981321
Ubiquinol-10	-7.0977497
Unii-rwy5U5kzv3	-7.0745702
Brilacidin	-7.074276
Etarfolatide	-7.062871
Doxacurium	-7.0600328
Colistina	-7.0597138
(3S,6S,12S,15S,18S,21S,24R,27S)-3,6-Dibenzyl-12-[(2R)-butan-2-yl]-4,16,22-trimethyl-24-[(2R)-3-methylbutan-2-yl]-18-(2-methylpropyl)-9,15,21-tri(propan-2-yl)-13-oxa-1,4,7,10,16,19,22,25-octazabicyclo[25.3.0]triacontane-2,5,8,11,14,17,20,23,26-nonone	-7.0276241
Venetoclax	-7.0154495
Candicidin D	-6.9966493
Telavancin	-6.9900298
Triglu-5-formyl-tetrahydrofolate	-6.9813905
Ethylhexyl triazone	-6.9788446
L-Carnitiny-CoA	-6.9501667
Dipalmitoylphosphatidylglycerol	-6.9480577
Sulfogalactoceramide	-6.9408188



Dimyristoylphosphatidylglycerol	-6.9336691
Octreotide acetate	-6.9301686
Tenapanor	-6.9041467
2-[[[(4S)-4-[[[(4S)-4-[[4-[2-(2-Amino-4-oxo-3,7-dihydropyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]amino]-4-carboxybutanoyl]amino]-4-carboxybutanoyl]amino]-4-carboxybutanoyl]amino]pentanedioic acid	-6.9035096
2-[[[(2R)-2,3-Bis[[[(9Z,12Z)-octadeca-9,12-dienoyl]oxy]propoxy]-hydroxyphosphoryl]oxyethyl-trimethylazanium	-6.9006743
Angiotensin (1-7)	-6.8859501
Nona-arginine	-6.881742
DSPC;L-beta,gamma-Distearoyl-alpha-lecithin	-6.8807964
Demoxytocin	-6.8710155
5-Mercaptoethanol-2-decenoyl-coenzyme A	-6.8692455
1,2-Dioleoyl-sn-glycero-3-phosphocholine(1+)	-6.8565731
Velpatasvir	-6.852726
Voclosporin	-6.844852
Proglumetacin	-6.8427505
Unii-J1J4P3pqzd	-6.832921
Sugammadex	-6.8125958
Selepressin	-6.8108587
(3S)-4-[[[(3S,6R,12S,15S,18S,21R,24S,28S,30R)-18-(4-Aminobutyl)-6-(1-carboxyethyl)-15-[carboxy(hydroxy)methyl]-12-(carboxymethyl)-25,30-dimethyl-2,5,8,11,14,17,20,23,27-nonaoxo-3,21-di(propan-2-yl)-1,4,7,10,13,16,19,22,26-nonazabicyclo[26.3.0]hentriacontan-24-yl]amino]-2-methyl-3-[[[(2E,4Z)-8-methyldeca-2,4-dienoyl]amino]-4-oxobutanoic acid	-6.8007655
2-[[4-[[[(2S)-3-Methyl-1-oxo-1-[(2S)-2-[[[(3S)-1,1,1-trifluoro-4-methyl-2-oxopentan-3-yl]carbamoyl]pyrrolidin-1-yl]butan-2-yl]carbamoyl]benzoyl]amino]acetic acid	-6.8007655
Aclerastide	-6.7991471
5-Hydroxyferuloyl-CoA	-6.79245
Ipamorelin	-6.7911024
Friulimycin B	-6.7760978
CID 5289562	-6.7739582
Anatibant	-6.76813
Angiotensinamide	-6.7556543
Carfilzomib	-6.7467966
Murepavadin	-6.7444425
2-[4-[(2S)-2-Acetamido-3-oxo-3-[[[(3S)-2-oxo-1-[(4-phenylphenyl)methyl]azepan-3-yl]amino]propyl]-2-methoxycarbonylphenyl]-2-fluoropropanedioic acid	-6.7250972
N-(2-Hydroxyoctadecanoyl)-4R-hydroxysphinganine	-6.7219591
Cetrorelix	-6.7210383
Reactive Red 6 hapten	-6.719985
Alisporivir	-6.7160454
Ddavp	-6.7113504
3-Thiaoctanoyl-coenzyme A	-6.710319
Bis(gamma-glutamyl-cysteinyl-glycyl)spermidine	-6.7033076
Soblidotin	-6.6945066
Nicotinamide-Adenine-Dinucleotide	-6.6828265
Dadle	-6.6812816

[4-[(2S)-2-Acetamido-3-[[5S)-3-carbamoyl-2-(cyclohexylmethoxy)-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-yl]amino]-3-oxopropyl]-2-phosphonophenyl]phosphonic acid	-6.6811619
Pibrentasvir	-6.67345
Lodenafil carbonate	-6.6667376
Valspodar	-6.6489363
(2S)-N-[(2R)-1-[(2S)-1-Amino-6-(diaminomethylideneamino)-1-oxohexan-2-yl]amino]-3-(4-hydroxyphenyl)-1-oxopropan-2-yl]-1-[(2R)-3-cyclohexyl-2-[[4-[(diaminomethylideneamino)methyl]cyclohexanecarbonyl]amino]propanoyl]azetidine-2-carboxamide	-6.648747
Pasireotide	-6.6476345
Flavin adenine dinucleotide	-6.6392889
(3S)-4-[[3S,6R,12S,15S,18S,21R,24S,28S,30R)-18-(4-Aminobutyl)-6-(1-carboxyethyl)-15-[carboxy(hydroxy)methyl]-12-(carboxymethyl)-25,30-dimethyl-2,5,8,11,14,17,20,23,27-nona-3,21-di(propan-2-yl)-1,4,7,10,13,16,19,22,26-nonazabicyclo[26.3.0]hentriacontan-24-yl]amino]-2-methyl-3-[(2E,4Z)-8-methylnona-2,4-dienoyl]amino]-4-oxobutanoic acid	-6.6375017
Temsirolimus	-6.6330647
Crocin	-6.6299481
Iscotrizinol	-6.6291451
Cobicistat	-6.6274652
Monogalactosyl-diacylglycerol	-6.6216884
4-[[2S)-2-[(2R)-2-[(2R)-3-(1-Benzothiophen-3-yl)-2-(piperidine-4-carboxylamino)propanoyl]amino]-3-(1H-indol-3-yl)propanoyl]amino]-3-phenylpropanoyl]amino]piperidine-4-carboxamide	-6.6209373
DI-Stearoyl-3-SN-phosphatidylcholine	-6.6160131
Folate-FITC	-6.608109
Boc-gamma-D-glu-L-lys(cbz)-D-boroala	-6.6065769
DMPC;L-beta,gamma-Dimyristoyl-alpha-lecithin	-6.60566
Ioglycamic Acid	-6.6030331
(2S)-2-[[2S)-2-[[2S)-2-[[2S,3R)-2-[[2S)-2-[[2S)-2-[[2S)-2-[[2S)-2-[[2S)-2-(2-Acetamidoacetyl)amino]propanoyl]amino]-5-amino-5-oxopentanoyl]amino]-3-phenylpropanoyl]amino]-3-hydroxypropanoyl]amino]-6-aminohexanoyl]amino]-3-hydroxybutanoyl]amino]propanoyl]amino]propanoyl]amino]-6-aminohexanoic acid	-6.5977979
Ombitasvir	-6.5924101
adenylate-3'-phosphate-[[2'-deoxy-uridine-5'-phosphate]-3'-phosphate]	-6.57637
4-[4-Carboxybutyl-[2-[(18S,25S,35S)-35-[(S)-hydroxy(phenyl)methyl]-28-(methoxymethyl)-21-methyl-18-[2-(methylamino)-2-oxoethyl]-16,23,30,33-tetraoxo-25-propan-2-yl-3,13,20,27,37-pentathia-7,17,24,31,34,39,40,41,42,43-decazaheptacyclo[34.2.1.12,5.112,15.119,22.126,29.06,11]tritetraconta-1(38),2(43),4,6(11),7,9,12(42),14,19(41),21,26(40),28,36(39)-tridecaen-8-yl]-1,3-thiazol-4-yl]carbamoyl]oxycyclohexane-1-carboxylic acid	-6.5604935
Hexapeptide 3	-6.5602956
Anidulafungin	-6.5572481
Methacrylyl-CoA	-6.5532589
4-amino-n-{4-[2-(2,6-dimethyl-phenoxy)-acetylamino]-3-hydroxy-1-isobutyl-5-phenyl-pentyl}-benzamide	-6.5443

8-[4-(2-Butoxyethoxy)phenyl]-1-(2-methylpropyl)-N-[4-[(3-propylimidazol-4-yl)methylsulfinyl]phenyl]-3,4-dihydro-2H-1-benzazocine-5-carboxamide	-6.5426102
Micafungin	-6.534081
Deslanoside	-6.5284748
Saralasin	-6.5260315
Rilapladib	-6.5220246
2-[2-[[2-[[[(2R)-1-[[[(4R,7S,10S,13R,16S,19R)-10-(4-Aminobutyl)-16-benzyl-4-[[[(2R,3R)-1,3-dihydroxybutan-2-yl]carbamoyl]-7-[(1R)-1-hydroxyethyl]-13-(1H-indol-3-ylmethyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentazacycloicos-19-yl]amino]-1-oxo-3-phenylpropan-2-yl]amino]-2-oxoethyl]- (carboxymethyl)amino]ethyl-2-[bis(carboxymethyl)amino]ethyl]amino]acetic acid	-6.5151515
[(2S)-2-[(Z)-Hexadec-9-enoyl]oxy-3-[hydroxy(2-hydroxyethoxy)phosphoryl]oxypropyl] (Z)-octadec-9-enoate	-6.5102944
DI-Stearoyl-3-SN-phosphatidylethanolamine	-6.5082421
gliquidone	-6.50701
Unii-19ztz9YC4O	-6.5061979
Unii-5l2g5Z2Q	-6.5046973
Zeaxanthin	-6.5043249
4SC-203	-6.50353
Priftin	-6.4999089
Neladenoson bialanate	-6.4957514
2-Octaprenylphenol	-6.4947829
Elamipretide	-6.492218
CoA-s-acetyl tryptamine	-6.4837537
(E)-N-[4-[3-Chloro-4-[(3-fluorophenyl)methoxy]anilino]-3-cyano-7-ethoxyquinolin-6-yl]-4-(dimethylamino)but-2-enamide	-6.4814477
3-Hydroxybutyryl-coenzyme A	-6.4812236
N-Acetyl-N-[1-(1,1'-biphenyl-4-ylmethyl)-2-oxoazepan-3-yl]-3-formyl-O-phosphonotyrosinamide	-6.4790406
Unii-qmh3V8vspb	-6.4690313
2-[[2-Hexadecanoyloxy-3-[(Z)-octadec-9-enoyl]oxypropoxy]-hydroxyphosphoryl]oxyethyl-trimethylazanium	-6.4652758
Merotocin	-6.4613204
Clorobiocin	-6.4612813
Itacitinib	-6.46057
Vancomycin	-6.4546638
Uridyl-2'-5'-phospho-adenosine	-6.4519858
[[[(2R,3S,4R,5R)-3,4-Dihydroxy-5-(6-iminopurin-9-ium-9-yl)oxolan-2-yl]methoxy-hydroxyphosphoryl] [(2R,3S,4S)-5-[7,8-dimethyl-5-(2-methylpropanoyl)-2,4-dioxo-1H-benzo[g]pteridin-10-yl]-2,3,4-trihydroxypentyl] hydrogen phosphate	-6.4514418
2-Ethoxyethyl (2s,3s)-4-((s)-2-benzyl-3-oxo-4-((3ar,8r,8as)-2-oxo-3,3a,8,8a-tetrahydro-2h-indeno[1,2-d]oxazol-8-yl)-2,3-dihydro-1h-pyrrol-2-yl)-3-hydroxy-1-phenylbutan-2-ylcarbamate	-6.45052
Larazotide	-6.4498482
Valinomicin	-6.4474573
2-(L-Phenylalanine)-8-L-lysinevasopressin	-6.4396729
Odalasvir	-6.4347672
Timcodar	-6.4333954

Fasitibant	-6.4295049
Trypan Blue free acid	-6.4288964
4-(N,N-Dimethylamino)cinnamoyl-CoA	-6.4194269
3,8-Diamino-6-phenyl-5-[6-[1-[2-[(1,2,3,4-tetrahydro-9-acridinyl)amino]ethyl]-1h-1,2,3-triazol-4-yl]hexyl]-phenanthridinium	-6.41461
Denufosol	-6.4072843
4-[(6S,9S,9aS)-1-(Benzylcarbamoyl)-2,9-dimethyl-4,7-dioxo-8-(8-quinolinylmethyl)octahydro-2H-pyrazino[2,1-c][1,2,4]triazin-6-yl]methyl}phenyl dihydrogen phosphate	-6.40557
Efonidipine	-6.405437
Fozivudine tidoxil	-6.4046016
Difelikefalin	-6.398294
N,N-[2,5-O-Dibenzyl-glucaryl]-DI-[valinyl-aminomethanyl-pyridine]	-6.3966646
CID 131704254	-6.3933682
[(3E,5E,8R,9S,10R,11R,14S,15E,18R,20R,21E,24S)-24-[(E,2S,3S,4S,7R,8S,9R,10R)-9-Acetyloxy-7-[(2S)-2-(dimethylamino)propanoyl]oxy-12-[formyl(methyl)amino]-3-hydroxy-4,8,10-trimethyldodec-11-en-2-yl]-10-hydroxy-14,20-dimethoxy-9,11,15,18-tetramethyl-2-oxo-1-oxacyclotetracos-3,5,15,21-tetraen-8-yl] (2S)-2-(dimethylamino)-3-methoxypropanoate	-6.3907189
Ibodutant	-6.390193
Telmisartan	-6.3899698
Talactoferrin alpha	-6.3838325
CID 131704228	-6.3835149
Menaquinone-7	-6.3804426
Brostallicin	-6.3760753
Foxy-5	-6.3707175
N-(Ethylsulfonyl)-5-propoxy-L-tryptophyl-N~1~-{4-[amino(imino)methyl]benzyl}-L-glutamamide	-6.3693395
1-[(2R,3R,4S,5R)-5-[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-dihydroxy-tetrahydrofuran-2-yl]methoxy-hydroxy-phosphoryl]oxy-hydroxy-phosphoryl]oxymethyl]-3,4-dihydroxy-tetrahydrofuran-2-yl]pyridin-1-ium-3-carboxylic acid	-6.36784
Olcegepant	-6.3647766
6-Phenyl-5-[6-[1-[2-(1,2,3,4-tetrahydroacridin-9-ylamino)ethyl]triazol-4-yl]hexyl]phenanthridin-5-ium-3,8-diamine	-6.3647103
[2,4,6-Triisopropyl-phenylsulfonyl-1-[3-amidino-phenylalaninyl]]-n'-β-alaninyl-piperazine	-6.35334
Reversin 121	-6.3508687
Manidipine	-6.3480783
Selatogrel	-6.3477368
Astaxanthin	-6.34728
Cellulose hydroxyethylate	-6.340929
1,2-Dipalmitoyl-sn-glycero-3-phosphoethanolamine	-6.3409286
Adamantane-1-carboxylic acid-5-dimethylamino-naphthalene-1-sulfonylamino-octyl-amide	-6.3398166
2-[4-[(2S)-3-[4-(3-Hydroxy-2-methoxycarbonylphenoxy)butylamino]-3-oxo-2-(prop-2-enoxycarbonylamino)propyl]-N-oxaloanilino]benzoic acid	-6.3295193
Bietaserpine	-6.3292842
Granotapide	-6.3289695

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(2R)-N-[2-[4-[5-[4-[(4-Acetamidophenyl)methoxy]-2,3-dichlorophenyl]-2-methylpyrazol-3-yl]piperidin-1-yl]-2-oxoethyl]-2-(diaminomethylideneamino)-4-methylpentanamide	-6.3274131
1-Palmitoyl-2-linoleoyl-3-acetyl-rac-glycerol	-6.3268423
Ruzasvir	-6.3249669
Bosentan	-6.3217754
Muraglitazar	-6.3117418
NADP nicotinamide-adenine-dinucleotide phosphate	-6.3117328
Elobixibat	-6.3088441
(S)-4-Phenyl-1-[3-(3-pyridyl)propyl]butyl N-[difluoro(3,4,5-trimethoxy)acetyl]-L-pipecolate	-6.3084021
Cilofexor	-6.3075676
Motuporin	-6.3067598
CID 53340771	-6.2961597
Sitravatinib	-6.2925801
Hydrocortisone cypionate	-6.28916
Lifitegrast	-6.28518
N-n-Butyl-N-methyl-11-(3,17beta-dihydroxyestra-1,3,5(10)-trien-7alpha-yl)undecanamide	-6.2850342
Ethyl (E,4S)-4-[[[(2S)-2-[[[(2S)-2-[[[(2S)-2-(furan-3-carbonylamino)-3-methylbutanoyl]amino]-3-methylbutanoyl]amino]-4-methylpentanoyl]amino]-5-[(3S)-2-oxopyrrolidin-3-yl]pent-2-enoate	-6.284081
Fenebrutinib	-6.2834244
Region IV (C480-C488) of SARS-CoV-2 spike*	-6.27480

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\*positive control.