Supporting information for Review of SARS-CoV-2 main protease inhibitors

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1 Summary of SARS-CoV-2 or SARS-CoV Mpro inhibitors

In this section, we provide a collection of 701 SARS-CoV-2 and SARS-CoV inhibitors published in the literature or databases. Compound SMILES strings, potency values, PDB IDs, and references are given.

SMILES string	SARS-CoV-2 IC50 (μM)	SARS-CoV IC50 (μM)	SARS-CoV-2 K_i (μM)	SARS-CoV K_i (μM)	PDB ID	Compound name
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)CO	0.00027 [1]	0.004 [1]			6xhm [1]	
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)COC1=CC=CC(=C1)N(C)C)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1				0.003 [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]1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1		1.7 [2]		0.0041 [2]		
COC1=C2C=C(NC2=CC=C1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.0063 [3]		
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)(C)C)C(=O)NC(CC1CCNC1=O)C(=O)CO		0.007 [1]				
O=C(On1nnc2ccccc21)c1ccc2[nH]ccc2c1				0.0075 [4]		
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)COC1=CC=C(O)C=C1)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1		1.2 [2]		0.011 [2]		
CCN(CC)C1=CC=C(C=C1)C(=O)ON1N=NC2=CC=CC=C12				0.0111 [4]		
CNC1=CC=C(C=C1)C(=O)ON1N=NC2=CC=CC=C12				0.0121 [4]		
O=C(ON1N=NC2=CC=CC=C12)C1=CC2=CC=CC=C2N1				0.0123 [4]		
FC1=CC=C2NC(=CC2=C1)C(=O)ON1N=NC2=CC=CC=C12				0.0138 [4]		
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)c2nc3=CC=CC=c3s2)C=C1		0.92 [2]		0.014 [2]		
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C1=CC=CC=C1C#N		0.017 [1]				
CN(C)C1=CC=C(C=C1)C(=O)ON1N=NC2=CC=CC=C12				0.0174 [4]		

NC1=CC=CC=C1C(=O)ON1N=NC2=CC=CC=C12				0.0195 [4]		
CCCCC(NC(=O)C1=CC2=C(N1)C=CC=C2OC)C(=O)NC(CC1CCNC1=O)C(=O)CO		0.02 [1]				
CC(C)(C)CC(NC(=O)C1=CC2=C(N1)C=CC=C2)C(=O)NC(CC1CCNC1=O)C(=O)CO		0.02 [1]				
CC(C)C[C@H](NC(=O)C1=NC2=CC=CC=C2N1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.022 [3]		
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)c1nc2=CC=CC=c2s1		2.3 [2]		0.022 [2]		
O=C(ON1N=NC2=CC=CC=C12)C1=CC2=C(NC=N2)C=C1				0.0229 [4]		
CC(C)C[C@H](NC(=O)C1=CC2=C(O)C=CC=C2N1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.026 [3]		
CC(C)C[C@H](NC(=O)C1=CC2=CC(Cl)=CC=C2N1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.028 [3]		
CN(C)c1ccc(C(=O)N[C@@H](Cc2ccccc2)C(=O)Nc2ccc([N+](=O)[O-])cc2Cl)cc1		0.06 [5]		0.03 [5]		
CC(C)COC1=C2C=C(NC2=CC=C1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.03 [3]		
O=C(Oc1cncc(Cl)c1)c1cccc2[nH]ccc12		0.03 [6]				
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CCC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)CO		0.034 [1]				
COCC(=O)C(CC1CCNC1=O)NC(=O)C(CC(C)(C)C)NC(=O)C1=CC2=C(N1)C=CC=C2OC		0.035 [1]				
CC(C)CC(NC(=O)C1=CC2=C(N1)C=CC=C2)C(=O)NC(CC1CCNC1=O)C(=O)CO		0.038 [1]				
CC(C)C[C@H](NC(=O)[C@H](CNC(=O)C(C)(C)C)NC(=O)OCc1ccccc1)C(=O)N[C@H](CCC(C)=O)C[C@@H]1CCNC1=O				0.038 [7]	2zu4 [7]	

Fc1cccc(C[C@H](NC(=O)c2[nH]c3ccccc3c2)C(=O)N[C@@H](C[C@@H]4CCNC4=O)C=O)c1	0.04 [8]				6m0k [8]	
O=C(Nc1ccc(NC(=O)c2cc(B(O)O)cc([N+](=O)[O-])c2)cc1)c1cc(B(O)O)cc([N+](=O)[O-])c1				0.04 [9]		
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC1CCCCC1)C(=O)NC(CC1CCNC1=O)C(=O)CO		0.044 [1]				
NC(=O)C1=CC2=C(C=C1)N(CC1=CC3=CC=CC=C3C=C1)C(=O) C2=O	0.045 [10]					
NC(=O)C1=CC2=C(C=C1)N(CC1=CC3=CC=C(Br)C=C3C=C1)C(=O)C2=O	0.047 [10]					
CC(C)C[C@H](NC(=O)C1=CC2=CC(OC(C)C)=CC=C2N1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.048 [3]		
OC(=O)CC1N[Zn]2(NC(CC(O)=O)C(=O)O2)OC1=O				0.05 [11]	2z9l [11]	JMF1586
O=C(Oc1cncc(Br)c1)c1ccco1		0.05 [12]				
O=C(Cn1nnc2ccccc21)N(Cc1ccsc1)c1ccc(-c2ccccc2)cc1		0.051 [13]				
CC(OC(C)(C)C)[C@H](NC(=O)Oc1ccccc1)C(=O)N[C@@H](CnC1CCCCC1)C(=O)N[C@H](C=O)C[C@@H]1CCNC1=O				0.053 [14]	2gx4 [14]	
O=C[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC2CCCCC2)NC(=O)c3[nH]c4ccccc4c3	0.053 [8]				6lze [8]	
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C1=CC=C(C=C1)C#N		0.053 [1]				
COCC(=O)C(CC1CCNC1=O)NC(=O)C(CC(C)C)NC(=O)C1=CC2=C(N1)C=CC=C2OC		0.053 [1]				
NC(=O)C1=CC2=C(C=C1)N(CC1=CC3=CC=CC=C3S1)C(=O)C2=O	0.053 [10]					
CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)OC(C)(C)C				0.058 [14]		
O=C(Oc1cncc(Cl)c1)c1ccco1		0.06 [12]				
O=C(Oc1cncc(Cl)c1)c1ccc(-c2ccc([N+](=O)[O-])cc2)o1		0.06 [15]				

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)c1ncc(s1)C1=CC=CC=C1				0.06 [2]		
O=C(Oc1cncc(Cl)c1)c1ccc(-c2ccc(Cl)cc2)o1		0.063 [12, 15]				
CC(C)[C@H](NC(=O)[C@H](C)NC(=O)[C@H](CO)NC(C)=O)C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@@H](Cc2c[nH] c[nH+]2)C=O		0.065 [16]			3avz [16]	
O=C(Oc1cncc(Cl)c1)c1cc2ccccc2[nH]1		0.065 [12]				
CC(C)C[C@H](NC(=O)C1=CC2=CC=CC=C2N1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.065 [3]		
COC1=CC=C2NC(=CC2=C1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.067 [3]		
CC(C)C(NC(=O)C(C)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC1=CNC2=CC=CC=C12)[C@@H](O)[C@H](O)[C@H](CC1=CNC2=CC=CC=C12)NC(=O)C(NC(=O)C(C)NC(=O)OCC1=CC=CC=C1)C(C)C				0.073 [17]		
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C1=C(C)C=CC=C1C		0.074 [1]				
COC1=CC=C(C=C1)C(=O)OCC(=O)C(CC1CCNC1=O)NC(=O)C(CC(C)C)NC(=O)C1=CC2=C(N1)C=CC=C2OC		0.079 [1]				
O=C(Oc1cncc(Cl)c1)c1cccc2cc[nH]c12		0.08 [6]				
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C1=CC=C(F)C=C1		0.082 [1]				
COC1=CC=CC2=C1C=C(N2)C(=O)N(C)C(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)CO		0.083 [1]				
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C1=CC=CC=C1		0.086 [1]				
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C1=CC=C(C) C=C1		0.087 [1]				
ClC1=CN=CC(OC(=O)C2=CC=CS2)=C1	0.088 [18]	0.5 [19]				MAC-5576

ClC1=CC(OC(=O)C2=CC=C3N(C=C C3=C2)S(=O)(=O)C2=CC=CC(=C2) N(=O)=O)=CN=C1		0.089 [6]				
CC(C)(C)CC(NC(=O)C1CCCO1)C (=O)NC(CC1CCNC1=O)C(=O)CO		0.091 [1]				
O=C(Oc1cncc(Cl)c1)c1cc2ccccc2s1		0.095 [12]				
COC1=CC=CC2=C1C=C(N2)C(=O)N C(CC(C)C)C(=O)NC(CC1CCNC1=O) C(=O)COC(=O)C1=CC=C(Cl)C=C1		0.097 [1]				
CC(C)[C@H](NC(=O)[C@@H](NC (C)=O)[C@@H](C)O)C(=O)N[C@@H] (CC1CCCCC1)C(=O)N[C@@H](Cc 2c[nH]c[nH+]2)C=O		0.098 [16]			3atw [16]	
CC(C)C[C@H](NC(=O)[C@@H](NC (=O)OCc1ccccc1)[C@@H](C)OC(C) (C)C)C(=O)N[C@H](CCC(=O)C2C C2)C[C@@H]3CCNC3=O				0.099 [7]	2zu5 [7]	
COC1=CC=CC2=C1C=C(N2)C(=O)N C(CC1=CC=CC=C1)C(=O)NC (CC1CCNC1=O)C(=O)CO		0.103 [1]				
COCC(=O)C(CC1CCNC1=O)NC(=O) C(CC(C)(C)C)NC(=O)C1=C C2=C(N1)C=CC=C2		0.105 [1]				
O=C(Oc1cncc(Cl)c1)c1cc2ccccc2oc1=O		0.108 [15]				
CC(=O)O[Hg]C1=CC=CC=C1	0.4 [20]		0.11 [20]			
CCOCC(=O)C(CC1CCNC1=O)NC (=O)C(CC(C)(C)C)NC(=O)C1=CC2 =C(N1)C=CC=C2		0.112 [1]				
CC(C)C[C@H](NC(=O)C1CC2= CC=CC=C2N1)C(=O)N[C@@H] (C[C@@H]1CCNC1=O)C(=O)c1n c2ccccc2s1				0.12 [3]		
NC(=O)c1ccc2c(c1)C(=O)C (=O)N2Cc1ccc2ccccc2c1		0.37 [21]		0.12 [21]		
O=C(Oc1cncc(Cl)c1)c1ccc(-c2c cc(Cl)cc2[N+](=O)[O-])o1		0.122 [15]				
O=C(Oc1cncc(Cl)c1)c1cccc2ccccc12		0.124 [15]				
COCC(=O)[C@H](C[C@@H]1CCNC1 =O)NC(=O)C(CCC(C)C)N(C)C(=O)C1 =CC2=C(N1)C=CC=C2		0.131 [1]				
CC(=O)N1CC2=C(CC1C(=O)OC1=C N=CC(Cl)=C1)C=CC=C2		0.14 [6]				
CC(C)C[C@H](NC(=O)OCc1ccccc1)C (=O)N[C@@H](C[C@@H]2CCNC2 =O)[C@@H](O)[S](O)(=O)=O	0.62 [22] 0.19 [23] 0.03 [24]	2.2 [22] 0.05 [23]			6wtj [23]	GC376

CC(C)C[C@H](NC(=O)C1=CC2=CC(O)=CC=C2N1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.16 [3]		
O=C(Oc1cncc(Cl)c1)c1ccncc1		0.164 [15]				
O=C(Oc1cncc(Cl)c1)c1cc2ccccc2o1		0.17 [12]				
CCCCC1CCC(CC1)OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	0.17 [22]	0.9 [22]				
O=N1=CC=CC=C1S[Zn]SC1=CC=CC=N1=O				0.17 [25]		
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)COC1=CC=CC(=C1)N(C)C)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1ncc(s1)C1=CC=CC =C1				0.17 [2]		
O=C(N[C@@H](CC1CCCCC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NCc1ccccc1)\C=C\C1=CC=CC=C1	0.18 [26]	0.71 [26]				
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C1CC1		0.182 [1]				
CC(C)CC(NC(=O)C(NC(=O)c1ccncc1)C(C)C)C(=O)NC(C=O)CC1CCCNC1=O		0.186 [27]				
O=C[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](Cc1ccccc1)NC(=O)\C=C\c1ccc(Cl)cc1F		0.2 [28]				
CCCCC1CCC(CC1)OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)[C@@H](O)S(O)(=O)=O	0.2 [22]	1.0 [22]				
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C1=C(OC)C=CC=C1OC		0.205 [1]				
O=C(Oc1cncc(Cl)c1)c1ccc(-c2ccccc2[N+](=O)[O-])o1		0.208 [15]				
CC1=C(C=CC(=C1)C2=CC(=C(C=C2)N=NC3=C(C4=C(C=C3)C(=CC(=C4N)S(=O)(=O)[O-])S(=O)(=O)[O-])O)C)N=NC5=C(C6=C(C=C5)C(=CC(=C6N)S(=O)(=O)[O-])S(=O)(=O)[O-])O. [Na+].[Na+].[Na+].[Na+]	0.2 [20]		0.21 [20]			Evans blue
COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(C)=O		0.22 [1]				
O=C(Oc1cncc(Cl)c1)c1ccc2cc[nH]c2c1		0.23 [6]				

COC1=CC=CC2=C1C=C(N2)C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C(C)(C)C		0.23 [1]				
CCCC1CCC(CC1)OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)[C@@H](O)S(O)(=O)=O	0.23 [22]	1.7 [22]				
O=C(N[C@@H](CC1CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NCc1ccccc1)\C=C\c1ccccc1		0.24 [29]			5n5o [29]	
CN1C2=NC(=O)N(C(=O)C2=NC(=N1)C3=CC=C(C=C3)C(F)(F)F)C	0.26 [30]					walrycin B
CC(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@H](C=O)Cc1c[nH]cn1)C(C)C		0.27 [16]				
O=C(Oc1cncc(Cl)c1)c1cscn1		0.27 [12]				
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)c2ncc(s2)C2=CC=CC=C2)C=C1				0.27 [2]		
CCCC1CCC(CC1)OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	0.28 [22]	1.7 [22]				
O=N(=O)O[Hg]C1=CC=CC=C1				0.3 [25]		
Cc1cc(c(Cl)cc1Cl)S(=O)(=O)c1c(cc(cc1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O		0.3 [31]			2gz7 [31]	
ClCC(=O)[C@H](CC1=CC=CC=C1)NC(=O)OCC1=CC=CC=C1				0.31 [32]		
COc1ccccc1NCC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.33 [33]		
COC1=CC=C2C=C(NC2=C1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.33 [3]		
CC(C)C[C@H](NC(=O)\C=C1\cccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NCc1ccccc1		0.33 [29]				
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)COC1=CC=CC(=C1)N(C)C)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1ncc(C)s1				0.33 [2]		
O=C(Oc1cncc(Cl)c1)c1ccccc1[N+](=O)[O-]		0.333 [15]				
CC(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@H](C=O)Cc1c[nH]cn1)C(C)C		0.34 [16]				

COc1cccc(C(=O)Oc2cncc(Cl)c2)c1		0.34 [12]				
O[C@H]([C@H](CC1=CNC2=CC=CC=C12)NC(=O)OCC1=CC=CC=C1)[C@H](O)[C@H](CC1 =CNC2=CC=CC=C12)NC(=O)OCC1=CC=CC=C1				0.34 [17]		
Cc1ccc(S(=O)(=O)N2C=CC3C=C(C(=O)Oc4cncc(Cl)c4)C=CC32)cc1		0.37 [6]				
ClCC(=O)[C@H](CC1=CC2=CC=CC=C2C=C1)NC(=O)OCC1=CC=CC=C1				0.37 [32]		
FC1=CC=C(C[C@H](NC(=O)OCC2=CC=CC=C2)C(=O)CCl)C=C1				0.38 [32]		
CC(=O)N[C@@H](CO)C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@H](C=O)Cc1c[nH]cn1)C(C)C		0.39 [16]				
COc1cccc(NCC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)c2nc3ccccc3s2)c1				0.39 [33]		
CC(C)C[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CC1CCNC1=O)C=O	0.4 [23]	0.07 [23]			6wtk [23]	GC373
CC(=O)n1ccc2cc(C(=O)Oc3cncc(Cl)c3)ccc21		0.4 [6]				
CC(C)(C)OC(=O)C[C@H](NC(=O)OCC1=CC=CC=C1)C(=O)CBr				0.4 [32]	3d62 [32]	
CC(C)C[C@H](NC(=O)OC1CCC(F)(F)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)[C@@H](O)S(O)(=O)=O	0.41 [22]	2.2 [22]				
COc1ccc(CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)c2nc3ccccc3s2)cc1				0.42 [33]		
CC(C)C[C@H](NC(=O)OC1CCC(F)(F)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	0.43 [22]	2.3 [22]				
O=C(Oc1cncc(Cl)c1)c1ccc(Cl)cc1		0.434 [15]				
CC(C)C[C@H](NC(=O)OCC1CCC(F)(F)CC1)C(=O)N[C@@H](C[C@@H]2CCNC2=O)[C@@H](O)[S](O)(=O)=O	0.45 [22]	1.1 [22]			6xmk [22]	
CCCC(C(=O)C(=O)NCC1=CC=CC=N1)NC(=O)C(CC(C)C)NC(=O)OCC2=CC=CC=C2	0.45 [24]					Calpain inhibitor XII
CC(C)C[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.42 [33]		

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)c2ncc(s2)C2=CC=CC=C2OC)C=C1				0.47 [2]		
CC(C)C[C@H](NC(=O)OCC1CCC(F)(F)CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	0.48 [22]	1.2 [22]				
[H]C(=O)[C@H](C[C@@H]1CCNC1=O)N C(=O)[C@H](CC1=CC=CC=C1)NC(=O)\C=C\C1=CC=C(C=C1)N(C)C		0.5 [28]				
O=C(Oc1cncc(Br)c1)c1cccs1		0.5 [34]				
O=C(Oc1cncc(Cl)c1)c1ccc(-c2cccc([N+](=O)[O-])c2)o1		0.5 [15]				
CC(C)C[C@H](NC(=O)/C=C/c1ccccc1)C(=O)N[C@H](C=O)C[C@@H]1CCCNC1=O		0.508 [27]			6lny [27]	
CCP(CC)(CC)=[Au]S[C@@H]1O[C@H](COC(C)=O)[C@@H](OC(C)=O)[C@H](OC(C)=O)[C@H]1OC(C)=O	0.51 [35]					Auranofin
COC(=O)CC(NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)CF				0.51 [32]		
Clc1ccc(SSc2nnco2)cc1		0.516 [36]				
CCOC(=O)/C=C/C(Cc1ccccc1)NC(=O)C(Cc1ccccc1)NC(=O)\C=C\c1ccc(N(C)C)cc1		0.52 [37]				
CC(C)C[C@H](NC(=O)COc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2cc ccc2s1				0.56 [33]		
[Na+].[O-]C(=O)c1ccccc1S[Hg]CC	0.6 [20]		0.6 [20]			Thimerosal
CC(C)C(NC(=O)[C@@H](C)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@H](CC1=CC=CC=C1)C(O)C(O)[C@@H](CC1=CC=CC=C1)NC(=O)C(NC(=O)[C@@H](C)NC(=O)OCC1=CC=CC=C1)C(C)C				0.6 [38]		
CC(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(=O)N(C)C)C(=O)Cn1[nH]c(=O)c2c([N+](=O)[O-])cccc2c1=O)[C@H](C)OCc1ccccc1)C(C)C		0.6 [39]				
COc1ccc(CCC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)c2nc3ccccc3 s2)cc1				0.61 [33]		

CC(C)C[C@@H](NC(=O)[C@H](NC(=O)COC1=CC=C(C=C1)N(C)C)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1		0.65 [2]				
CCOC(=O)\C=C\[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C				0.66 [14]		
CC(C)C[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1ncc(-c2ccccc2)s1				0.66 [33]		
COC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C				0.66 [33]		
CC(C)C[C@H](NC(=O)OC1CCCCC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)[C@@H](O)S(O)(=O)=O	0.65 [22]		3.8 [22]			
CC(C)(C)OC(=O)NC1=CC=CN([C@@H](CC2CC2)C(=O)N[C@@H](C[C@@H]3CCNC3=O)[C@@H](O)C(=O)NCc4ccccc4)C1=O	0.67 [26]		0.9 [26]		6y2g [26]	
O=C1N([Se]C2=CC=CC=C12)C1=CC=CC=C1	0.67 [40]					Ebselen
CC(C)C[C@H](NC(=O)C1=CNC2=C1C=CC=C2)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2cccccc2s1				0.68 [3]		
O=C(Oc1cncc(Cl)c1)c1cccc([N+](=O)[O-])c1		0.684 [15]				
Clc1ccc(SSc2ncccn2)cc1		0.684 [36]				
CC(C)C[C@H](NC(=O)/C=C/c1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.69 [33]		
O=C(Oc1cncc(Cl)c1)c1cccnc1		0.697 [15]				
Brc1ccc(SSc2ncccn2)cc1		0.697 [36]				
CC(=O)O[Hg]C1=CC=CC=C1				0.7 [25]		Phenylmercuric acetate
[H]C(=O)[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)\C=C\C1=CC=CC(Br)=C1		0.7 [28]				
OC(=O)c1cc(C(O)=O)c(cc1C(O)=O)C(O)=O				0.7 [11]	2z9g [11]	PMA
COc1ccc(/C=C/C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)c2nc3ccccc3s2)cc1				0.7 [33]		

COc1ncccc1-c1ccc(N(Cc2ccsc2)C(=O)Cn2nnc3ccccc32)cc1		0.7 [13]				
COC1=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]2CCNC2=O)C(=O)c2nc3=CC=CC=c3s2)=CC=C1		0.75 [2]				
CC(C)C[C@H](NC(=O)C1=NC2=CC=CC=C2S1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.8 [3]		
CC1=CC[C@]2(C)CC[C@]3(C)C4=CC=C5C(=CC(=O)C(O)=C5C)[C@]4(C)CC[C@@]3(C)[C@@H]2C1				0.8 [41]		
CC(C)C[C@H](NC(=O)OC1CCCCC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	0.82 [22]		3.9 [22]			
CC(C)CC(NC(=O)/C=C/c1ccccc1)C(=O)NC(C=O)CC1CCNC1=O			0.83 [27]		6lo0 [27]	
CC(C)CC(NC(=O)COC1=CC=C(C=C1)N(C)C)C(=O)NC(CC1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1				0.84 [33]		
CC(C)C[C@H](NC(=O)COc1cccc(N(C)C)c1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				0.84 [33]		
O=[N+]([O-])c1ccccc1SSc1ncccn1		0.883 [36]				
O=C(Oc1ccc(S(=O)(=O)c2ccc(OC(=O)C(Cl)=C(Cl)Cl)cc2)cc1)C(Cl)=C(Cl)Cl		0.9 [31]				
Cc1cc(C)nc(SSc2ccccc2[N+](=O)[O-])n1		0.921 [36]				
O=C\1c3c(O)c(O)c(O)cc3O\C(=C\1)c2ccccc2	0.94 [42]				6m2n [42]	Baicalein
O=C1C(=O)N(Cc2cc3ccccc3s2)c2ccc(I)cc21		0.95 [43]				
CC(C)CC(C(=O)NC(CC(C)C)C(=O)NC(CCSC)C=O)NC(=O)C	0.97 [24]					
O=C(Cn1nnc2ccccc21)N(Cc1ccsc1)c1ccc(-c2cccnc2)cc1		0.97 [13]				
O=C1C(=O)N(Cc2cc3ccccc3s2)c2c(Br)cccc21		0.98 [43]				
CCNCCC1=CC=C(C=C1)C(=O)CN1N=NC2=CC=CC=C12				1.0 [4]		
CCN(C(=S)S[Zn]SC(=S)N(CC)C1=CC=CC=C1)C1=CC=CC=C1				1.0 [25]		
CC(C)CC(NC(C)=O)C(=O)NC(CC1CCNC1=O)C(=O)COC(=O)C1=C(Cl)C=CC=C1Cl		1.028 [1]				

CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3C)CC1		1.04 [44]				
CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccccc2)CC1		1.69 [44]				
COCC(=O)C(CC1CCNC1=O)NC(=O)C(CC(C)(C)C)NC(=O)C1CCCO1		1.076 [1]				
CC(=O)N1C=CC2=C(C=CC=C12)C(=O)OC1=CN=CC(Cl)=C1		1.08 [6]				
O=C1C(=O)N(Cc2ccc3ccccc3c2)c2ccc(I)cc21		1.1 [21]				
COC(=O)c1ccccc1SSc1nnco1		1.118 [36]				
Cc1cc(C)nc(SSc2ccc(Br)cc2)n1		1.121 [36]				
CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3)CC1		1.18 [44]				
O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1) OCc1ccccc1				1.2 [33]		
Cc1ccc(SSc2nccs2)cc1		1.25 [36]				
COC(=O)c1ccccc1SSc1nc(C)co1		1.264 [36]				
O=C(N[C@@H](CC1CCCC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NCc1ccccc 1)\C=C\c1ccccc1		1.27 [29]				
COC1=C(C=CC(=C1)C2=CC(=C(C=C2)N=NC3=C(C4=C(C=C3)C(=CC(=C4N)S(=O)(=O)[O-])S(=O)(=O)[O-])O)OC)N=NC5=C(C6=C(C=C5)C(=CC(=C6N)S(=O)(=O)[O-])S(=O)(=O)[O-])O.[Na+].[Na+].[Na+].[Na+]	7.7 [20]		1.3 [20]			Chicago Sky Blue
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)c2ncc(s2)C2=CC=C(Cl)C=C2)C=C1				1.3 [2]		
COc1ccc(/C=C/C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)c2nc3ccccc3s2)cc1OC				1.3 [33]		
CN(C)c1ccc(cc1)C(O)=O				1.38 [45]	2v6n [45]	
CC1=CC2=C(S[Zn]S2)C=C1				1.4 [25]		

Oc1cc(cc(O)c1O)C(=O)Oc1cc(cc(O)c1O)C(=O)OC[C@H]1O[C@H](OC(=O)c2cc(O)c(O)c(OC(=O)c3cc(O)c(O)c(O)c3)c2)[C@H](OC(=O)c2cc(O)c(O)c(OC(=O)c3cc(O)c(O)c(O)c3)c2)[C@@H](OC(=O)c2cc(O)c(O)c(OC(=O)c3cc(O)c(O)c(O)c3)c2)[C@@H]1OC(=O)c1cc(O)c(O)c(OC (=O)	2.1 [20]		1.4 [20]			Tannic acid
Cc1ccc(S)c(S)c1				1.4 [11]	2z94 [11]	
Cc1cc(C)nc(SSc2ccc(Cl)cc2)n1		1.437 [36]				
O=C(N[C@@H](CC1CCC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NCc1ccccc1)\C=C\c1ccccc1		1.44 [29]				
CCCCCCCCCC(=O)NC1C(C(C(OC1OC2=C3C=C4C=C2OC5=C(C=C(C=C5)C(C6C(=O)NC(C7=C(C(=CC(=C7)O)OC8C(C(C(C(O8)CO)O)O)O)C9=C(C=CC(=C9)C(C(=O)N6)NC(=O)C4NC(=O)C1C2=CC(=CC(=C2)OC2=C(C=CC(=C2)C(C(=O)NC(CC2=CC(=C(O3)C=C2)Cl)C(=O)N1)N)O)O)O)C(=O)O)	1.46 [46]					Teicoplanin
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)c2ncc(s2)C2=CC=C(C)C=C2)C=C1				1.46 [2]		
Cc1ccc(SSc2nc(C)cc(C)n2)cc1		1.495 [36]				
O=C(Cn1nnc2ccccc21)N(Cc1ccsc1)c1ccc(NCc2ccccc2)cc1		1.5 [13]				
CC(C)(C)NC(=O)[C@H](N(C(=O)c1ccco1)c1ccc(cc1)C(C)(C)C) c1cccnc1		1.5 [34]				
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)c1nc2=CC=CC=c2s1		1.5 [2]		0.22 [2]		
CC(=O)Nc1cnc(SSc2ccccc2)s1		1.506 [36]				
Cc1ccc(SSc2ncccn2)cc1		1.522 [36]				
O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=CC=CC2=CC=C1	1.55 [47]					Tideglusib
CCOC(=O)c1ccccc1SSc1nnc(C)o1		1.557 [36]				
COc1ccc(OCC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)c2nc3ccccc3s2)cc1				1.56 [33]		
CCCC[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				1.6 [33]		
CC(=O)Nc1cnc(SSc2ccc(Br)cc2)s1		1.651 [36]				

COC(=O)c1ccccc1SSc1nnc(C)o1		1.679 [36]				
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)COC1=CC=C(C=C1)C(O)=O)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1		1.7 [2]				
CC(C)C[C@H](NC(=O)C1=CC=CN1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				1.7 [3]		
CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				1.71 [33]		
Cc1nnc(SSc2ccccc2[N+](=O)[O-])o1		1.713 [36]				
CC(=O)n1nc(SSc2ccccc2[N+](=O)[O-])nc1-c1cccnc1		1.762 [36]				
CCCCCCNC(=O)N1C=C(F)C(=O)NC1=O	1.82 [47]					
Clc1ccc(SSc2nccs2)cc1		1.871 [36]				
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)c1cc(C)on1)C(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)\C=C/C(=O)OCc3ccccc3				1.9 [48]	2hob [48]	
COC1=CC=CC=C1OCC(=O)N[C@H](C(C)C)C(=O)N[C@H](CC(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1		1.7 [2]		0.0041 [2]		
CC(=O)Nc1cnc(SSc2ccccc2[N+](=O)[O-])s1		1.947 [36]				
O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC1CCNC1=O)C(=O)C(=O)NCc1ccccc1)\C=C\c1ccccc1		1.95 [29]			5n19 [29]	
Cc1cc(C)nc(SSc2ccccc2)n1		1.991 [36]				
O=C1C(=O)N(Cc2cc3ccccc3s2)c2c1cccc2[N+](=O)[O-]		2.0 [43]				
O=C(Cn1nnc2ccccc21)N(Cc1ccsc1)c1ccc(-c2ccncc2)cc1		2.0 [13]				
Nc1ccc(cc1N)C(=O)N[C@@H](Cc1ccccc1)C(=O)Nc1ccc(cc1Cl)[N+]([O-])=O		2.0 [5]				
[H]N(C(C(C)O)C(=O)N[C@@H](Cc1ccccc1)C(=O)Nc1ccc(cc1Cl)[N+]([O-])=O)C(=O)CCC(=O)NC(C(C)O)C(=O)NC(CC1=CC=CC=C1)C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O		2.0 [5]				
[H]N(C(C(C)O)C(=O)N[C@@H](Cc1ccccc1)C(=O)Nc1ccc(cc1Cl)[N+]([O-])=O)C(=O)C(O)CC(=O)NC(C(C)O)C(=O)NC(CC1=CC=CC=C1)C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O		2.0 [5]				

[H]N(C(C(C)O)C(=O)N[C@@H](Cc1cccc1)C(=O)Nc1ccc(cc1Cl)[N+]([O-])=O)C(=O)C(O)C(O)C(=O)NC(C(C)O)C(=O)NC(CC1=CC=CC=C1)C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O		2.0 [5]				
COC1=C(SC2=NN=NN2C2=CC=C(OCC3=CC=CC=C3)C=C2)C(=O)NC2=C1C=CC=C2		2.0 [49]				
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)c1nc(C)c(C)s1		2.0 [2]				
O=[N+]([O-])c1ccccc1SSc1nccs1		2.029 [36]				
COC(=O)c1nc(SSc2ccccc2[N+](=O)[O-])[nH]c1C		2.075 [36]				
CNc1ccc(N(Cc2ccsc2)C(=O)Cn2nnc3ccccc32)cc1		2.1 [13]				
O=C1SN(C)C(N1CC2=CC=CC=C2)=O	2.15 [50]					TDZD-8
C[C@@H](NC(=O)[C@H](Cc1ccccc1)NC(=O)OCc1ccccc1)C(=O)CCO				2.2 [51]	2op9 [51]	
CCC(C)c1ccc(N(C(=O)c2ccco2)C(C(=O)NC2CCCC2)c2cccnc2)cc1		2.2 [34]				
Fc1ccc(SSc2nccs2)cc1		2.211 [36]				
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nccs1				2.2 [52]		
OC[C@H](Cc1ccccc1)NC(=O)[C@H](Cc1ccccc1)NC(=O)\C=C1\ccccc1				2.24 [53]	3sn8 [53]	
CC1CCCCN1S(=O)(=O)c1ccc2c(c1)C(=O)C(=O)N2		2.25 [44]				
CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C				2.26 [14]		
CC(C)(C)OC(=O)Nc1cccn(C(CC2CCCCC2)C(=O)NC(CC2CCNC2=O)C(=O)C(=O)NC2CC2)c1=O	2.39 [26]					
CC[Hg]SC1=CC=CC=C1C(=O)O[Na]				2.4 [25]		Thimerosal
CCOC(=O)c1ccccc1SSc1nc(C)cs1		2.452 [36]				
CCOC(=O)\C=C\C(Cc1ccccc1)NC(=O)C(Cc1ccccc1)NC(=O)\C=C\c1ccc(cc1)N(=O)=O				2.48 [37]		
CC1=C(C(=O)OCCc2ccccc2)C(c2cccc2[N+](=O)[O-])C2=C(CCCC2=O)N1		2.5 [54]				

COc1ccccc1-c1cnc(C(=O)[C@H](C[C@@H]2CCNC2=O)NC(=O)[C@H](CC(C)C)NC(=O)OCc2ccccc2)s1				2.5 [33]		
[O-][N+](=O)C(Br)(CO)CO	4.4 [20]			2.5 [20]		Bronopol
ClC1=CC=C(C=C1)C1C(N2C=CN=C2)C(=NN1C1=CC(Cl)=C(Cl)C=C1)C1=CC=C(Br)C=C1		2.5 [55]				
Cc1csc(SSc2ccccc2[N+](=O)[O-])n1		2.555 [36]				
CC(=O)Nc1cnc(SSc2ccc(F)cc2)s1		2.565 [36]				
NC1=NC2=NC3=C(SC(N)=N3)C=C2S1		2.6 [19]				MAC22272
CC(=O)Nc1cnc(SSc2ccc(Cl)cc2)s1		2.626 [36]				
ClC1=C(NCCN2CCOCC2)C(=O)c2nccc2C1=O	2.63 [30]					DA-3003-1
CC(C)C[C@H](NC(=O)C1CCC(=O)N1)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)c4nc3ccccc3s4				2.7 [3]		
CC(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)Cn1[nH]c(=O)c2ccccc2c1=O)C(C)OCc1ccccc1)C(C)C		2.7 [39]				
CC(=O)Nc1cnc(SSc2ccc(C)cc2)s1		2.803 [36]				
CC1CC(C)CN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3C)C1		2.820 [44]				
CC1C(C(C(C(O1)OC2C(C(OC(C2OC(=O)C=CC3=CC(=C(C=C3)O)O)COC4C(C(CO4)(CO)O)O)OCCC5=CC(=C(C=C5)O)O)O)O)O)O	2.88 [42]					Forsythoside B
CC(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)Cn1[nH]c(=O)c2ccccc2c1=O)C(C)O)C(C)C		2.9 [39]				
CCC(=O)Nc1ccc(N(Cc2ccsc2)C(=O)Cn2nnc3ccccc32)cc1		2.9 [13]				
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)COC1=CN=CC=C1)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1		2.9 [2]		0.22 [2]		
FC(F)(F)c1nnc(SC(=O)c2ccc(o2)C#Cc2ccccc2)[nH]1		3.0 [31]			2gz8 [31]	
O=C(CSc1nccc(-c2csc(-c3ccccc3)n2)n1)Nc1cc(Cl)cc(Cl)c1		3.0 [56]				

C1=C(C=C(C(=C1O)O)O)C(=O)OC2=CC(=CC(=C2O)O)C(=O)OCC3C(C(C(C(O3)OC(=O)C4=CC(=C(C(=C4)OC(=O)C5=CC(=C(C(=C5)O)O)O)O)O)OC(=O)C6=CC(=C(C(=C6)OC(=O)C7=CC(=C(C(=C7)O)O)O)O)O)OC(=O)C8=CC(=C(C(=C8)OC(=O)C9=CC(=C(C(=C9)O)O)O)O)O)OC(=O)C1=CC(=C(C(=C1)OC(=O)C1=CC(=C(C(=C1)O)O)O)O)O		3.0 [57]				Tannic acid
C13=C(OC(=CC1=O)C2=CC=C(O)C=C2)C=C(O)C(=C3O)O	3.02 [42]					Scutellarein
CCOC(=O)\C=C\C(Cc1ccccc1)NC(=O)C(Cc1ccccc1)NC(=O)\C=C1̨ccc2OCOc2c1				3.046 [37]		
COC(=O)[C@]1(C)CC[C@]2(C)CC[C@]3(C)C4=CC=C5C(=CC(=O)C(O)=C5C)[C@]4(C)CC[C@@]3(C)[C@@H]2C1		5.5 [41]		3.1 [41]		
CC(=O)n1nc(SSc2ccccc2[N+](=O)[O-])nc1C		3.13 [36]				
CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OCCC3=CC(=C(C=C3)O)O)O)O)OC(=O)C=CC4=CC(=C(C=C4)O)O)O)O)O	3.18 [42]					Forsythoside A
CC(C)C[C@H](NC(=O)Cc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				3.2 [33]		
COc1ccc(NCC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]2CCNC2=O)C(=O)c2nc3ccccc3s2)cc1				3.2 [33]		
Cc1cc2ncn(c2cc1C)C9OC(CO)C(OP3(=O)OC(C)CNC(=O)CCC5C4=C(C)C8=NC(=CC7=NC(=C(C)C6=NC(C)(C(N4[Co](O)O3)C5(C)CC(N)=O)C(C)(CC(N)=O)C6CCC(N)=O)C(C)(CC(N)=O)C7CCC(N)=O)C(CCC(N)=O)C8(C)C)C9O	3.29 [30]					Hydroxocobalamin
COC1=CC=CC=C1\N=C\C1=C(OC(C)=O)OC(=N1)C1=CC=CC=C1		3.3 [55]				
Brc1ccc(SSc2nccs2)cc1		3.321 [36]				
CC(=O)NC(C(=O)NC(C(=O)NC(CC(C)C)C(=O)NC(CC1CCNC1=O)C(=O)CN1NC(=O)C2C([N+](=O)[O-])=CC=CC2C1=O) C(C)O)C(C)C		3.4 [39]				
COCCC(=O)Nc1ccc(N(C(=O)Cn2nnc3ccccc32)C(C)c2ccsc2)cc1		3.4 [13]				

CC(C)C[C@@H](NC(=O)[C@H](NC(=O)COC1=CC=C(C=C1)N(=O)=O)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1		3.4 [2]				
CC(C)C(=O)Nc1ccc(N(Cc2ccsc2)C(=O)Cn2nnc3ccccc32)cc1		3.6 [13]				
CCOC(=O)c1c[nH]c(SSc2ccc(Cl)cc2)n1		3.675 [36]				
CC(C)(C)NC(=O)C(c1ccsc1)N(C(=O)Cn1nnc2ccccc21)c1ccc(NC(=O)C2CCC2)cc1		3.8 [13]				
CC(C)C[C@@H](C=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC(C)C)NC(=O)OCc1ccccc1	3.9 [24]					MG-132
COC(=O)c1ccccc1SSc1nc(C(=O)OC)c(C)[nH]1		3.957 [36]				
[H]C(C(SO)C(=O)N[C@@H](Cc1ccccc1)C(=O)Nc1ccc(cc1Cl)[N+]([O-])=O)C(=O)NC(CC1=CC=CC=C1)C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O		4 [5]				
CC1=C(O)C(=O)C=C2C1=CC=C1[C@@]3(C)CC[C@@]4(C)CC(=O)[C@H](C)C[C@H]4[C@]3(C)CC[C@@]21C		9.9 [41]		4 [41]		
ClC=1C(=O)C(\Cl)=C(\Cl)C(=O)C=1Cl	4.1 [20]					
CC(C)C(=O)Nc1ccc(N(C(=O)Cn2nnc3ccccc32)C(C(=O)NC(C)(C)C)c2ccsc2)cc1		4.1 [13]				
O=C(Nc1ccc(N(Cc2ccsc2)C(=O)Cn2nnc3ccccc32)cc1)C1CC1		4.1 [13]				
COc1ccc(SSc2nc(-c3ccccc3)n(C(C)=O)n2)cc1		4.1 [36]				
COC(=O)c1nc(SSc2ccc(Cl)cc2)[nH]c1C		4.126 [36]				
[H][C@]12CN([C@H](C(=O)NC(CC3CCC3)C(=O)C(N)=O)[C@@]1([H])C2(C)C)C(=O)[C@@H](NC(=O)NC(C)(C)C)C(C)(C)C	4.13 [24]				7brq [58]	
CC(=O)n1nc(SSc2ccc(C)cc2)nc1-c1ccccc1		4.183 [36]				
CC1=C(O)C(=O)C=C2C1=CC=C1[C@@]3(C)CC[C@@]4(C)CC[C@@](C)(C(=O)O)C[C@H]4[C@]3(C)CC[C@@]21C		10.3 [41]		4.2 [41]		
Cc1ccc2nc(-c3ccc(N)cc3)sc2c1S(=O)(=O)O		4.3 [44]				
CC1CC(C)CN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3)C1		4.3 [44]				

O=C1Nc2ccc(S(=O)(=O)N3CCCCC3)cc2C1=O		4.45 [44]				
CCOC(=O)c1ccccc1SSc1nc(-c2ccncc2)n(C(C)=O)n1		4.511 [36]				
CNC1=CC=C(C=C1)C(=O)CN1N=NC2=CC=CC=C12				4.5 [4]		
OB(O)C1=CC(=CC(=C1)C(=O)OC1=CC=C(OC(=O)C2=CC(=CC(=C2)B(O)O)N(=O)=O)C=C1)N(=O)=O				4.5 [9]		
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@H](C#N)CCC(N)=O		4.6 [59]			3vb5 [59]	
COC1=C(C=CC(=C1)C(=S)N2CCOCC2)O	4.6 [20]					Vanitiolide
CC1CC(C)CN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccccc2)C1		4.7 [44]				
CC(C)(C)NC(=O)[C@H](N(C(=O)c1ccco1)c1ccc(cc1)C(C)(C)C)c1cccnc1		4.8 [34]			3v3m [34]	
O=C1C(=O)N(Cc2cc3ccccc3s2)c2ccc(F)cc21		4.82 [43]				
CN(C)CCCSc1ccccc1NC(=O)/C=C/c1ccccc1		5.0 [13]				
Cc1noc(NC(=O)c2ccc(-c3cc(C(F)(F)F)nn3C)s2)c1[N+](=O)[O-]		5.0 [31]				
CC(C)(C)NC(=O)C(c1cccnc1)N(C(=O)c1ccc(Cl)o1)c1ccc(C(C)(C)C)cc1		5.2 [34]				
CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OCCC3=CC(=C(C=C3)O)O)O)OC(=O)C=CC4=CC(=C(C=C4)O)O)O)O)O)O	5.47 [42]					Forsythoside I
N#Cc1ccc(N2N=C(c3ccccc3)/C(=C/c3ccc(C(=O)O)cc3)C2=O)cc1		5.5 [60]				
CC(C)(C)NC(=O)C(c1cnccn1)N(C(=O)c1ccco1)c1ccc(C(C)(C)C)cc1		5.5 [34]				
CN1C(=O)C(=O)c2cc(S(=O)(=O)N3CCN(c4ccccn4)CC3)ccc21		5.52 [44]				
CCOc1cccc(c1)C(=O)c2ccc(O)c(O)c2O		10.6 [20]		5.6 [20]		
CCOC(=O)c1ccccc1SSc1nc(-c2cccnc2)n(C(C)=O)n1		5.654 [36]				
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)[C@H](CO)NC(C)=O)C(C)C)C(=O)N[C@@H](Cc1c[nH]c[nH+]1)C=O		5.7 [16]			3aw0 [16]	
CC(=O)N[C@@H](CO)C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C=O)Cc1c[nH]cn1)C(C)C		5.7 [16]				

CCCCC(NC(=O)C1[C@@H]2[C@H](CN1C(=O)C(NC(=O)NC1(CS(=O)(=O)C(C)(C)C)CCCCC1)C(C)(C)C)C2(C)C)C(=O)C(=O)NC1CC1		5.73 [24]				Narlaprevir
COc1ccc(SSc2nc(-c3cccnc3)n(C(C)=O)n2)cc1		5.794 [36]				
O[C@H]([C@@H]([C@@H](O)[C@H](C)O1)O)[C@H]1OC[C@@H]2[C@H]([C@@H]([C@@H](O)[C@H](OCCC3=CC(O)=C(O)C=C3)O2)OC(/C=C/C4=CC(O)=C(O)C=C4)=O)O	5.85 [42]					Isoforsythiaside
CC(C)CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				5.9 [33]		
CC1=C(C2=CC3=NC(=CC4=NC(=CC5=C(C(=C(N5)C=C1N2)C(C)O)C)C(=C4CCC(=O)O)C)C(=C3C)CCC(=O)O)C(C)O	3.9 [20]		5.9 [20]			Hematoporphyrin
CCOC(=O)c1ccccc1SSc1nc(C(=O)OC)c(C)[nH]1		5.954 [36]				
Nc1ncc(S(=O)(=O)c2ccc(Cl)cc2)c(N)n1		6.0 [31]				
CC(C)(C)NC(=O)C(c1cccnc1)N(C(=O)C1=NC=NC1)c1ccc(C(C)(C)C)cc1		6.0 [34]				
OB(O)C1=CC(=CC(=C1)N(=O)=O)C(=O)OCC1=CC=CC=C1COC(=O)C1=CC(=CC(=C1)N(=O)=O)B(O)O				6.0 [9]		
N#Cc1c(-c2ccc(Cl)cc2)nc(SCc2ccc([N+](=O)[O-])cc2)[nH]c1=O		6.1 [60]				
CCC(C)(C)NC(=O)[C@H](N(C(=O)Cn1nnc2ccccc12)c1ccc(NC(C)=O)cc1)c1cccn1C		6.2 [13]			4mds [13]	
O=C(N[C@@H](C1CC1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NCc1ccccc1)\C=C\c1ccccc1		6.27 [29]				
O=C3\C=C(/Oc2cc(O[C@@H]1O[C@H](C(=O)O)[C@@H](O)[C@H](O)[C@H]1O)c(O)c(O)c23)c4ccccc4	6.41 [42]					Baicalin
CCOC(=O)\C=C\C(Cc1ccccc1)NC(=O)C(Cc1ccccc1)NC(=O)\C=C\c1ccc(cc1)C1=CC=CC=C1				6.44 [37]		

CC1=C(C=C(C=C1)C(=O)NC2=C3C(=CC(=CC3=C(C=C2)S(=O)(=O)[O-])S(=O)(=O)[O-])S(=O)(=O)[O-])NC(=O)C4=CC(=CC=C4)NC(=O)NC5=CC=CC(=C5)C(=O)NC6=C(C=CC(=C6)C(=O)NC7=C8C(=CC(=CC8=C(C=C7)S(=O)(=O)[O-])S(=O)(=O)[O-])S(=O)(=O)[O-])C.[Na+].[Na+].[Na+].[Na+].[Na+].[Na+]	6.5 [30]					Suramin sodium
CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OCCC3=CC(=C(C=C3)O)O)O)O)O)O)O)O	6.68 [42]					Forsythoside E
COC1=CC=C2NC(C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]3CCNC3=O)C(=O)c3nc4ccccc4s3)=C(C)C2=C1				6.7 [3]		
CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)c2cocc2)C(C)C)C(C)C				6.7 [61]	2amd [61]	
CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CCC(C)C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)c1ccco1)C(C)C)C(C)C				6.7 [36]		
CN(C)C1=CC=C(C=C1)C(=O)CN1N=NC2=CC=CC=C12				6.7 [4]		
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)c1nccs1		6.8 [2]				
CC(C)C(C(=O)NC(CC(=O)OC)C(=O)CF)NC(=O)C(CCC(=O)OC)NC(=O)C(CC(=O)OC)NC(=O)OCC1=CC=CC=C1	6.81 [30]					Z-DEVD-FMK
O=C(O)c1ccc(/C=C2\C(=O)N(c3ccc(F)cc3)N=C2c2ccccc2)cc1		6.8 [60]				
COC1=CC=C(C=C1)N1C(=O)NC(=O)\C(=C/C2=CC(Cl)=C(OCC3=CC(=CC=C3)C(O)=O)C(Cl)=C2)C1=O		6.86 [62]				
CCC(=O)Nc1ccc(N(C(=O)Cn2nnc3ccccc32)C(C(=O)NC(C)(C)C)c2ccsc2)cc1		6.9 [13]				
COC(=O)c1cc2c(O)cc(C(F)(F)F)nc2o1		7.0 [19]				
O[C@@H]1CC2=C(O)C=C(O)C=C2OC1C1=CC2=C(C=C(O)C(O)=C2C(=O)C(O)=C1)C1OC2=C(C[C@@H]1OC(=O)C1=CC(O)=C(O)C(O)=C1)C(O)=CC(O)=C2		7.0 [57]				TF2B

O=C1C=CC(=O)C2=CN(CC3=CC=CC=C3)C=C12		7.0 [55]				
CC1=C(SC2=C1C=C(Cl)C=C2)C(=O)CC1OC(=O)C(Cl)=C1Cl		7.0 [19]				MAC-30731
COC1=CC(=O)OC(CS(=O)C2=NC3=C(S2)N=CC=C3)=C1		7.2 [55]				
Cc1noc(C)c1CN1C(=O)C(=O)c2cc(C#N)ccc21		7.2 [43]				
CC(C)C[C@H](NC(=O)CCc1cccnc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				7.4 [33]		
CCC1=C(NC2=CC=C(OC)C=C12)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				7.5 [3]		
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)CNCC1=CC=CC=C1)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1		7.5 [2]				
CC(=O)OC1=C(SC2=C(Cl)C(Cl)=CC(Cl)=C2OC(C)=O)C(Cl)=C(Cl)C=C1Cl		7.6 [63]				
CC(=O)Nc1ccc(N(C(=O)Cn2nnc3ccccc32)C(C(=O)NC(C)(C)C)c2ccsc2)cc1		7.72 [13]				
O=C(OC1=CN=CC=C1)C1CCCO1		7.9 [34]				
CC1=CC(=O)C2=CC=CC=C2C1=O	7.96 [35]					Vitamin K3
O=C(N[C@H](C(N[C@@H](CC(C)C)C(N[C@H](C([H])=O)CCC)=O)=O)CC(C)C)OCC1=CC=CC=C1	3.14 [24] 12.7 [30]					MG-115
CCCN1C(NCC2=CC=C(C=C2)N2N=C(CC2C2=CC=CC=C2)C2=CC=CC=C2)=NC2=CC=CC=C12		8.0 [55]				
CCCCN1C(NCC2=CC=C(C=C2)N2N=C(CC2C2=CC=CC=C2)C2=CC=CC=C2)=NC2=CC=CC=C12		8.1 [55]				
O=C(Nc1ccc(N(Cc2ccsc2)C(=O)Cn2nnc3ccccc32)cc1)C1CCC1		8.1 [13]				
CC(=C)C1CCC2(CCC3(C)C(CCC4C5(C)CCC(O)C(C)(C)C5CCC34C)C12)C(O)=O		10.0 [64]		8.2 [64]		
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](CO)NC(=O)[C@H](CCC(O)=O)NC(C)=O)[C@@H](C)O)C(=O)N[C@H](CO)CCC(N)=O				8.27 [53]	3sne [53]	

O=c1cc(-c2ccc(O)c(-c3c(O)cc(O)c4c(=O)cc(-c5ccc(O)cc5)oc34)c2)oc2cc(O)cc(O)c12		8.3 [65]		13.8 [65]		
O=C(O)c1ccc(/C=C2\C(=O)N(c3cccc([N+](=O)[O-])c3)N=C2c2ccccc2)cc1		8.4 [60]				
CC(C)C[C@H](NC(=O)COc1ccc(O)cc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				8.4 [33]		
CCN1C(NCC2=CC=C(C=C2)N2N=C(CC2C2=CC=CC=C2)C2=CC=CC=C2)=NC2=CC=CC=C12		8.4 [55]				
CCCC[C@H](NC(=O)\C=C1\ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NCc1ccccc1		8.5 [29]				
CCCC[C@H](NC([C@@H](NC([C@@H](NC(C)=O)CC(C)C)=O)CC(C)C)=O)C=O	8.6 [24]					Calpain inhibitor I
S=C=NCCC1=CC=CC=C1	10.13 [35]					Phenethyl isothiocyanate
Cc1cc(C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](/C=C/C(=O)OCc2ccccc2)C[C@@H]2CCNC2=O)C(C)C)no1				9.0 [36]		
CCOC1=CC=C(C=C1)C(=O)C2=C(C(=C(C=C2)O)O)O	9.0 [20]					
CCOC(=O)\C=C\C(Cc1ccccc1)NC(=O)C(Cc1ccccc1)NC(=O)\C=C1\ccc(OC)cc1OC				9.049 [37]		
O=C1OC[C@H](CC2=CC=C3OCOC3=C2)\C1=C/C1=CC=C2OCOC2=C1		25 [64]		9.1 [64]		
CC(C)(C)NC(=O)C(c1ccsc1)N(C(=O)Cn1nnc2ccccc21)c1ccc(NC(=O)C2CC2)cc1		9.1 [13]				
OC(=O)C1=C(C=CC(Br)=C1)C1=CC=C(O1)\C=C1\C(=O)NN(C1=O)C1=CC(Cl)=C(Cl)C=C1		9.19 [62]				
O=C1C2=C([C@H](NCC3=CC=CC=C3)[C@H](O)C(C)(C)O2)C(C4=C1C=CC=C4)=O	9.2 [30]					CAY-10581
OC1=C(C=C(Cl)C=C1SC1=C(O)C(=CC(Cl)=C1)N(=O)=O)N(=O)=O		9.2 [63]				
CCN(CC)C(=S)SSC(=S)N(CC)CC	9.35 [47]					Disulfiram
CSCCC(NC(=O)OCC1=CC=CC=C1)C(=O)NC(CC1CCNC1=O)C(=O)c1nc2=CC=CC=c2s1				9.4 [33]		
O=C1C(=O)N(Cc2ccc(F)cc2Cl)c2ccc(I)cc21		9.4 [43]				

OC1=CC2=C(C[C@H](OC(=O)C3=CC(O)=C(O)C(O)=C3)C(O2)C2=C3C=C(C=C(O)C(=O)C3=C(O)C(O)=C2)C2OC3=CC(O)=CC(O)=C3C[C@@H]2OC(=O)C2=CC(O)=C(O)C(O)=C2)C(O)=C1		9.5 [57]				TF3
COC1=CC=C(C=C1)C(C1=C(O)C2=C(OC1=O)C=CC(C)=C2)C1=C(O)C2=C(OC1=O)C=CC(C)=C2		9.56 [62]				
OC(=O)CCC=5C1=C\C6=N\C(=C/c3n2[Fe](Cl)N1C(=C\C4=N\C(=C/c2c(C=C)c3C)C(/C)=C4/C=C)/C=5C)C(\C)=C6\CCC(O)=O	9.68 [66]					Hemin
COC(=O)[C@@]1(C)CCCc2c1ccc1c2C(=O)C(=O)c2c(C)coc2-1				9.7 [67]		
COC1=CC2=C(C=C1)C1=NN(C(C1CC2)C1=CC(I)=CC=C1)C(C)=O		9.8 [55]				
NS(=O)(=O)C1=CC=CC2=C1C(=O)C1=CC=CC(O)=C1C2=O	9.84 [30]					LLL-12
CN1C(=O)C(=O)c2cc(S(=O)(=O)N3CCOCC3)ccc21		9.91 [44]				
C1=CC=C2C(=C1)C3=C(N2)C4=[N+](C=C3)C5=CC=CC=C5C4=O	9.96 [30]					Fascaplysin
Cc1ccc(C(=O)N/C(=C/c2ccc(-c3ccc([N+](=O)[O-])cc3)o2)C(=O)NCCCN(C)C)cc1		10.0 [63]				
CC(=O)N[C@@H](CC(N)=O)C(=O)N[C@H](C(=O)N[C@@H](CC1CCCCC1)C(=O)N[C@H](C=O)Cc1c[nH]cn1)C(C)C		10.0 [16]				
Cc1oc(C(C)(C)C)cc1-c1cc(NS(=O)(=O)c2cccs2)[nH]n1		10.0 [31]				
CC(C)(C)NC(=O)C(c1ccnnc1)N(C(=O)c1ccco1)c1ccc(C(C)(C)C)cc1		10.0 [34]				
Cn1nc(-c2ccc(-c3ccnc(SCC(=O)Nc4ccc(Cl)cc4)n3)s2)cc1C(F)(F)F		10.0 [56]				
CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@H](CO)NC(=O)OC(C)(C)C)C(C)C		10.0 [68]				
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCc1ccccc1)C(C)C)C(=O)NC(Cc1ccccc1)C(=O)C(F)(F)F		10.0 [33]				
OC1=C(SC2=NN=NN2C2=CC=C(OCC3=CC=CC=C3)C=C2)C(=O)NC2=C1C=CC=C2		10.0 [49]				
OC1=CC=C(C=C1)N1N=NN=C1SC1=C(O)C2=C(NC1=O)C=C(Cl)C=C2Cl		10.0 [49]				

O=C1Nc2ccc(S(=O)(=O)N3CCN(C(=O)c4ccco4)CC3)cc2C1=O		10.07 [44]				
CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OCCC3=CC(=C(C=C3)O)O)OC(=O)C=CC4=CC(=C(C=C4)O)O)O)O)O)O)O	10.17 [42]					Forsythoside H
CCCN1C(=O)C(=O)C2=C1C=CC(=C2)C(N)=O	10.2 [10]					
CC(C)COC(=O)Nc1ccc(N(Cc2ccsc2)C(=O)Cn2nnc3ccccc32)cc1		10.3 [13]				
CC[C@H](C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](CCC(=O)OC(C)(C)C)C(=O)N[C@@H](C)C(=O)N[C@H](C=O)CC(C)C	10.38 [24]					PSI
CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)c2cc(C)on2)C(C)C				10.7 [61]	1wof [61]	
CCCCC(C=O)NC(=O)C(CC(C)C)NC(=O)OCC1=CC=CC=C1	10.69 [24]					Calpeptin
N#Cc1c(-c2cccc([N+](=O)[O-])c2)nc(SCc2ccc([N+](=O)[O-])cc2)[nH]c1=O		10.6 [60]				
O=C(N[C@@H](CC#C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)C(=O)NCc1ccccc1)\C=C\c1ccccc1		10.68 [29]				
OC(=O)C1=CC=C(\C=C2/C(=O)N(N=C2C2=CC=CC=C2)C2=CC=CC(Cl)=C2)C=C1		10.8 [60]				
O=N(=O)C1=C(C=CC=C1)C1N(CCN1C1=CC=CC=C1)C1=CC=CC=C1				11.0 [69]		MP521
CC(=O)Nc1ccc(cc1)N([C@H](C(=O)NC(C)(C)C)C1=CSC=C1)C(=O)N1C=C(N=N1)C1=CC=CC=C1		11.0 [13]				
CSC1=C(C(C)=C(S1)C1=NC(C)=CS1)C1=NC(SCC(=O)NC2=CC=C(Cl)C=C2)=NC=C1		11.0 [56]				
CC(=O)Nc1ccc(N(C(=O)Cn2cc(-c3ccccc3)nn2)C(C(=O)NC(C)(C)C)c2ccsc2)cc1		11.0 [13]				
C=CCC=CCC=CCCCCCCCC1=C(C(=CC=C1)O)C(=O)O	11.04 [30]					Anacardic acid
O=C1C(=O)N(Cc2cc3ccccc3s2)c2cccc(Cl)c21		11.2 [43]				
FCC(=O)C(NC(=O)C(NC(=O)OCc1ccccc1)Cc2ccccc2)C	11.39 [30]					Z-FA-FMK
CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3C)CC1		11.83 [44]				

O=[N+]([O-])c1cc(C(F)(F)F)c cc1S(=O)(=O)c1ccc(Cl)cc1		12.0 [31]				
COC1=CC=C(C=C1)N1N=C(\C(=C\ C2=CC=C(C=C2)C(O)=O)C1=O)C1 =CC=CC=C1		12.0 [60]				
CSC1=C(C(C)=C(S1)C1=NC(C)=C S1)C1=NC(SCC(=O)NC2=C(Cl) C=CC=C2)=NC=C1		12.0 [56]				
COc1ncc(-c2ccc(N(Cc3ccsc3)C (=O)Cn3nnc4ccccc43)cc2)cn1		12.5 [13]				
NC(=O)c1ccc2c(c1)C(=O)C(=O) N2Cc1ccccc1		12.5 [21]				
O=C(Nc1ccc(Cl)cc1)c1ccc(CN2 C(=O)C(=O)c3cc(I)ccc32)s1		12.57 [43]				
O=C1Nc2ccc(S(=O)(=O)N3CCOCC3) cc2C1=O		12.66 [44]				
CCOC(=O)\C=C\C(CC1=CC=CC=C1) NC(=O)C(CC(=O)C(NC(=O)C1=NOC (C)=C1)C(C)C)CC1=CC=CC=C1		13.0 [37]				
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)CCC1=CC=CC=C1)C(C)C)C(=O) N[C@H](C[C@H]1CCNC1=O)C(=O)c1 nccs1		13.0 [2]				
ClC1=CC=C(C=C1)C1=CC=C(O1)C(=O)CC1=CN=CC(Br)=C1		13.0 [70]				
Cc1ccc(S(=O)(=O)c2nc(C)c([N+] (=O)[O-])c(C)c2C#N)cc1		13.0 [31]				
Cc1nc(S(=O)(=O)c2ccccc2)c(C#N) c(C)c1[N+](=O)[O-]		13.0 [31]				
C=C(Cc1cccc(C)c1)C1=CC=C(c2ccc(C) cc2)C1		13.0 [34]				
O=C1C(=O)N(Cc2cc3ccccc3s2)c2cccc c21		13.11 [43]				
CC(C)(C)C(=O)Nc1ccc(N(Cc2ccsc2)C (=O)Cn2nnc3ccccc32)cc1		13.3 [13]				
O[C@@H]1[C@@H](O)[C@H](O)[C@ @H](CO)O[C@@H]1S[Au]	13.32 [66]					Aurothioglucose
CC1(CCC2=C(O1)C3=CC=CC=C3C (=O)C2=O)C	13.33 [30]					Beta lapachone
O=C1C(=O)N(CC2COc3ccccc3O2)c2c cc(I)cc21		13.5 [43]				
CC1=[N+](C2=C(N1CCOC)C(=O)C3 =CC=CC=C3C2=O)CC4=NC=CN =C4.[Br-]	13.6 [30]					Sepantronium bromide
OC1=C(CC2=C(Cl)C(Cl)=CC(Cl)= C2O)C(Cl)=C(Cl)C=C1Cl		13.7 [25]				Hexachlorophene

[H][C@]12C[C@]1(NC(=O)[C@]1([H])C[C@H](C[C@@]1([H])C(=O)N(C)CCCC\C=C/2)OC1=CC(=NC2=C1C=CC(OC)=C2C)C1=NC(=CS1)C(C)C)C(=O)NS(=O)(=O)C1CC1	13.74 [24]					Simeprevir
NC1=NC=NC2=C1N=C(N2)C(F)(F)F		13.9 [71]				
OC(=O)C1=CC=C(\C=C2/C(=O)N(N=C2C2=CC=CC=C2)C2=CC=C(Cl)C=C2)C=C1		13.9 [60]				
O=C1C(=O)N(Cc2ccccc2)c2ccc(S(=O)(=O)N3CCOCC3)cc21		13.86 [44]				
CN1C(=O)C(=O)c2cc(S(=O)(=O)N3CCN(CCc4ccccc4)CC3)ccc21		13.86 [44]				
O=C1C(=O)N(Cc2ccccc2)c2ccc(S(=O)(=O)N3CCCCC3)cc21		14.0 [44]				
CC(C)C[C@H](NC(=O)C1=CC2=CC=CC=C2O1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2cc ccc2s1				14.0 [3]		
CC1=CSC(=N1)C1=NC(=CS1)C1=NC(SCC(=O)NC2=CC=C(Cl)C=C2)=NC=C1		14.0 [56]				
Cc1cccc2c3c(ccc12)C1=C(C(=O)C3=O)[C@@H](C)CO1		14.4 [67]		11.2 [67]		
CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)[C@H](CO)NC(=O)OC(C)(C)C)C(C)C		15.0 [68]				
CSc1[nH]nc(NC(=O)c2cccs2)c1S(=O)(=O)c1ccccc1		15.0 [31]				
O=[N+]([O-])c1ccc(S(=O)(=O)c2ccc(Cl)cc2)[n+]([O-])c1		15.0 [31]				
CSC1=NNC(NC(=O)C2=CC=CS2)=C1S(=O)(=O)C1=CC=C(Cl)C=C1		15.0 [31]				
CC(C)CC(NC(=O)OCc1ccccc1)C(=O)NC(CC1=CC=CC=C1)C(=O)C(F)(F)F		15.0 [72]				
ClC1=CC=C(NC(=O)CSC2=NC=CC(=N2)C2=CC(=NO2)C2=CC=CC=C2)C=C1		15.0 [56]				
FC(F)(F)C1=CC=C(NC(=O)CSC2=NC=CC(=N2)C2=CC(=NO2)C2=CC=C(Cl)C=C2Cl)C=C1		15.0 [56]				
ClC1=CC=C(NC(=O)CSC2=NC=CC(=N2)C2=CC(=NO2)C2=CC=CC=C2Cl)C=C1		15.0 [56]				

CC(C)[C@H](N1CCCNC1=O)C(=O)N[C@H](C[C@H](O)[C@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C)CC1=CC=CC=C1				15.0 [73]		Lopinavir
CCC[C@@H](C(=O)C(=O)NC1CC1)NC(=O)[C@@H]2[C@H]3CCC[C@H]3CN2C(=O)[C@H](C(C)(C)C)NC(=O)[C@H](C4CCCCC4)NC(=O)c5cnccn5	15.25 [66]					Telaprevir
O=C(ON1C(=O)CCC1=O)C1=CC2=C(C=C1)N(CC1=CC=CC=C1)C(=O)C2=O	15.5 [10]					
CC(=CCC(C1=CC(=O)C2=C(C=CC(=C2C1=O)O)O)O)C	15.75 [47]					Shikonin
CC1(C)CC(=O)c2c(NCc3ccco3)sc(C#N)c2C1		16.0 [31]				
O=C(O)c1ccc(S(=O)(=O)c2cc(Br)c(O)c(Br)c2)cc1		16.0 [31]				
CCOC(=O)/C(C#N)=C/Nc1ccc(S(=O)(=O)c2ccc(/N=C/C(C#N)=C(O)OCC)cc2)cc1		16.0 [31]				
CC(=O)c1ccccc1S(=O)(=O)c1ccccc1C(=O)O		16.0 [31]				
OB(O)C1=CC=CC(COC(=O)C2=CC(=CC(=C2)B(O)O)N(=O)=O)=C1				16.0 [9]		
ClC1=CC=C(C=C1)C1=C(C#N)C(=O)NC(SCCC2=CC=CC=C2)=N1		16.9 [60]				
O=C1C(C)=CC(C2=C1C=CC=C2O)=O	17.1 [20]					Plumbagin
Cc1cc2cc(CN(CCc3ccccc3C)C(=O)NCc3ccccc3)c(=O)[nH]c2cc1C		17.2 [74]				
CCOC(=O)C1=CC=C(C=C1)N2C(=O)/C(=C\C3=CC=C(O3)[N+](=O)[O-])/C(=O)N2	17.38 [66]					PYR-41
O=C1C(=O)N(Cc2ccc(C(=O)N3CCCCC3)s2)c2ccc(I)cc21		17.5 [43]				
CCCCN1C(=O)C(=O)C2=C1C=CC(=C2)C(N)=O	17.8 [10]					
CC1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccc3ccccc3c2)CC1		17.82 [31]				
OCCSC1=C(SCCO)C(=O)C2=CC=CC=C2C1=O	17.93 [30]					NSC 95397
CSc1nn(-c2c([N+](=O)[O-])c(C)nn2C)c(-c2cccs2)c1C#N		18.0 [31]				
O=[S](=O)(Cc1[s+]cc(n1[H])c2ccc([Cl])[s]2)c3ccc[s]3		18.0 [31]				

CCOC(=O)C1OC1C(=O)N(CCC(N)=O)NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)C(CC(C)C)NC(=O)OCC1=CC=CC=C1		18.0 [75]				
CSC1=NN(C2=C(C(C)=NN2C)N(=O)=O)C(C2=CC=CS2)=C1C#N		18.0 [31]				
ClC1=CC=C(S1)C1=CSC(CS(=O)(=O)C2=CC=CS2)=N1		18.0 [31]				
OC(=O)C1=CC=C(\C=C2/C(=O)N(N=C2C2=CC=CC=C2)C2=CC=CC=C2)C=C1		18.0 [60]				
CC1=CC2=C(C=C1C)N(C=N2)C3C(C(C(O3)CO)OP(=O)(O)OC(C)CNC(=O)CCC4(C(C5C6(C(C(C(=N6)C(=C7C(C(C(=N7)C=C8C(C(C(=N8)C(=C4[N-]5)C)CCC(=O)N)(C)C)CCC(=O)N)(C)CC(=O)N)C)CCC(=O)N)(C)CC(=O)N)C)CC(=O)N)C)O.[C-]#N.[Co+2]	18.02 [30]					Vitamin B12
CN1C=NC2=C1C=CC(NC(=O)C1=CC=C(Cl)C=C1)=C2		18.2 [71]				
O=C(CSc1nc(C2CCCCC2)nc2cccccc12)NCc1ccco1		18.2 [74]				
O=C1/C(C=C(C2=CC=CC=C2)N1C3=CC=C(C(O)=O)C=C3)=C\C4=CC=C(C5=CC=C([N+]([O-])=O)C=C5)O4	18.28 [30]					4E1RCat
CCCCN1C(=O)C(=O)c2cc(C(N)=O)ccc21		19.0 [21]				
CC1=CC(=CC(=C1C2=CC=C(C=C2)C(C)(C)C)C)OC(CCC(F)(F)F)C3=CC=C(C=C3)C(=O)NCCC(=O)O	19.18 [30]					Adomeglivant
O=c1cc(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12		20.0				
Cc1nn(C)c(NCc2ccc(-c3cccs3)s2)c1[N+](=O)[O-]		20.0 [31]				
CN1N=C(C)C(=C1NCC1=CC=C(S1)C1=CC=CS1)N(=O)=O		20.0 [31]				
FC(F)(F)C(=O)C(CC1=CC=CC=C1)NC(=O)C(CC1=CC=CC=C1)NC(=O)OCc1ccccc1		20.0 [72]				
COC1=CC=C(C=C1)C1=C(C#N)C(=O)NC(SCCC2=CC=CC=C2)=N1		20.3 [76]				
COC1=CC=C(C=C1)C1=C(C#N)C(=O)NC(SCCC2=CC=CC=C2)=N1	20.49 [30]					TBB
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@@H](CCC(=O)N1CCOCC1)C(=O)C(F)(F)F				21.0 [52]		

O=C2N[C@]7(C(=O)O)C[C@H]7/C=C\CCCCC[C@H](NC(=O)OC1CCCC1)C(=O)N6[C@H]2C[C@@H](Oc3cc(nc4c3ccc(OC)c4)c5nc(sc5)NC(C)C)C6	20.77 [66]					Ciluprevir
CC(C)C1=Cc2ccc3c(c2C(=O)C1=O)CCCC3(C)C		21.1 [67]				
CCC(C)SSC1=NC=CN1	21.39 [47]					PX-12
COC1=CC(\C=C2/S\C(=N\C3=CC=CC=C3)N(C2=O)C2=CC=CC=C2)=CC=C1OCC1=CC=CC(=C1)C(O)=O		21.49 [62]				
CC1=C(C=C(C=C1)N2C(=O)C(=C(N2)C)N=NC3=CC=CC(=C3O)C4=CC(=CC=C4)C(=O)O)C.C(CO)N.C(CO)N	21.52 [30]					Eltrombopag olamine
C1=CC=C(C=C1)C(CN(CCCOC2=CC=CC(=C2)CC(=O)O)CC3=C(C(=CC=C3)C(F)(F)F)Cl)C4=CC=CC=C4	21.52 [30]					GSK-3965
OC(C(Br)=C1)=C(Br)C=C1/C=C(C2=CC(I)=CC=C2N3)\C3=O	21.52 [30]					GW5074
C1=C(C(=C(C(=C1Cl)Cl)CC2=C(C(=CC(=C2Cl)Cl)Cl)O)O)Cl	21.52 [30]					Hexachlorophene
ClC(C=C3)=CC=C3CN(C(CC(C)(C(O)=O)C)=C2SC(C)(C)C)C1=C2C=C(C(C)C)C=C1	21.52 [30]					MK-886
Cc1c(O)c(O)cc2c1CC=C1[C@@]3(C)CC[C@@]4(C)CC[C@@](C)(C(=O)O)C[C@H]4[C@]3(C)CC[C@]12C		21.7 [41]				
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)c2ncc(s2)C2=CC3=CC=CC=C3C=C2)C=C1				22.0 [2]		
O=C(Nc1ccc(N(Cc2ccsc2)C(=O)Cn2nnc3ccccc32)cc1)C1CCCCC1		22.1 [13]				
FC(F)(F)c3c(F)cc(c1nc(c(s1)CSc2cc(c(OCC(=O)O)cc2)C)C)cc3	22.27 [30]					GW-0742
Cc1coc2c1C(=O)C(=O)c1c-2ccc2c1CCCC2(C)CO		24.8 [67]				
CC(C)(C)NC(=O)C(c1ccsc1)N(C(=O)Cn1nnc2ccccc21)c1ccc(NC(=O)C(C)(C)C)cc1		22.5 [13]				
CC\1=C(/C/2=C/C3=N/C(=C\C4=C(C(=C(N4)/C=C\5/C(=C(C(=N5)/C=C1\N2)C=C)C)C=C)C)/C(=C3CCC(=O)O)C)CCC(=O)O	23.0 [20]					Protoporphyrin IX
CC(C)C[C@H](NC(=O)CN1C(=O)CSC1=S)C(=O)N[C@@H](CC1=CC=CC=C1)[C@@H](O)C[C@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		23.0 [38]				

CC(C)C[C@H](NC(=O)OC(C)(C)C)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				23.0 [33]		
O=C1C(=O)N(C/C=C/c2cc3ccccc3s2)c2ccc(I)cc21		23.5 [43]				
O=C(\C=C1ccc(O)c(OC)c1)CC(=O)\C=C2cc(OC)c(O)cc2		23.5 [41] 40.0 [64]				Curcumin
CCCCCCCCCCCCCCCCCC(C(=O)O)C(CC(=O)O)(C(=O)O)O	23.54 [30]					Agaric acid
O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12		23.8 [65]				Quercetin
CC(C)C[C@H](NC(=O)C1=CC2=CC=CC=C2N1)C(=O)N[C@@H](CC1=CC=CC=C1)C(O)C[C@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		24.0 [38]				
COC1=CC=C(\C=C\C(=O)NC(CC(C)C)C(=O)N[C@H](CC2=CC=CC=C2)C(O)C[C@@H](CC2=CC=CC=C2)NC(=O)COC2=C(C)C=CC=C2C)C=C1		24.0 [38]				
CC(C)C[C@@H](NC(=O)[C@H](NC(C)=O)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nccs1		24.0 [2]				
CC1OC(OC2=C(OC3=C(C(O)=CC(O)=C3)C2=O)C2=CC=C(O)C(O)=C2)C(O)C(O)C1O		24.14 [77]				
C[C@H]1[C@@H]([C@@](C[C@@H](O1)O[C@H]2[C@H]3C(=O)N[C@H](C4=C(C(=CC(=C4)O)O)C5=C(C=CC(=C5)[C@H](C(=O)N3)NC(=O)[C@H]6C7=CC(=C(C(=C7)OC8=C(C=C(C=C8)[C@H]([C@H](C(=O)N[C@H](C(=O)N6)CC(=O)N)NC(=O)[C@@H](CC(C)C)NC)O)Cl)O[C@H]9[C@@H]	24.15 [30]					Oritavancin
OC(C[C@H](C#CC)C(C=C1)=CC=C1OCC2=CC(C3=CC=C(C(F)(F)F)C=C3)=CC=C2)=O	24.15 [30]					AMG-837
OC(=O)C1=CC=C(\C=C2/C(=O)N(N=C2C2=CC=CC=C2)C2=CC=C(Cl)C(Cl)=C2)C=C1		24.3 [60]				
COC1=CC2=CC=C(C=C2C=C1)C1=CC(=NN1[C@@H](C)C1=CC=C(C=C1)C(=O)NCCC(O)=O)C1=CC(Cl)=CC(Cl)=C1	24.33 [30]					MK-0893
NC(=O)C1=CC2=C(C=C1)N(CC1=CC3=CC=C(C=C3C=C1)C1=CC=CC=C1)C(=O)C2=O	24.9 [10]					

O=C1NC2=CC(C3=CC=CC=C3)=CC=C2/C1=C\C4=C(C)C(CCC(O)=O)=C(C)N4	24.97 [30]					SU 16f
CC(C)C[C@H](NC(=O)C1=CC=C(O1)N(=O)=O)C(=O)N[C@@H](CC1=CC=CC=C1)C(O)C[C@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		25.0 [38]				
CC(C)C[C@H](NC(=O)C1=CC(C)=CC=C1)C(=O)N[C@@H](CC1=CC=CC=C1)C(O)C[C@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		25.0 [38]				
CC(C)CC(NC(=O)C1=CC=C(C=C1)C(F)(F)F)C(=O)N[C@H](CC1=CC=CC=C1)C(O)C[C@@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		25.0 [38]				
CC(C)CC(NC(=O)C1=CCOC2=CC=C(CCl)C=C12)C(=O)N[C@H](CC1=CC=CC=C1)C(O)C[C@@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		25.0 [38]				
CCCN1C(=O)C(=O)c2cc(C(N)=O)ccc21		25.0 [21]				
O=[N+]([O-])c1ccc(S(=O)(=O)c2ccc([N+](=O)[O-])cc2)cc1		25.0 [31]				
CC(C)(C)NC(=O)C(c1ccsc1)N(C(=O)Cn1nnc2ccccc21)c1ccc(NS(C)(=O)=O)cc1		25.3 [13]				
CC(NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)CF				25.7 [32]		
CC(C)(C)NC(=O)C(c1ccsc1)N(C(=O)Cn1nnc2ccccc21)c1ccc(NC(=O)c2ccno2)cc1		26.0 [13]				
COc1ccc(-c2nc(SCc3ccc([N+](=O)[O-])cc3)[nH]c(=O)c2C#N)cc1		26.3 [76]				
OC1=C(C(O)=O)C(CCC2=CC=C(CCCCCCC)C=C2)=CC=C1	27.1 [30]					MG-149
O=C(C1=CC(O)=C(O)C(O)=C1)O[C@@H]([C@@H]([C@@H](COC(C2=CC(O)=C(O)C(O)=C2)=O)O3)OC(C4=CC(O)=C(O)C(O)=C4)=O)[C@H]([C@@H]3OC(C5=CC(O)=C(O)C(O)=C5)=O)OC(C6=CC(O)=C(O)C(O)=C6)=O	27.77 [30]					
CC(C)CC(NC(=O)C(NC(=O)C(NC(C)=O)C(C)C)C(C)O)C(=O)NC(CCC(=O)N(C)C)C(=O)CN1NC(=O)C2=C(C=CC=C2)C1=O		28.0 [39]				
FC(C(=O)C1=CC=C(O1)C1=CC=C(Cl)C=C1)C1=CN=CC(Br)=C1		28.0 [70]				
CC(C)c1ccc(cc1)N([C@@H](C(=O)NC(C)(C)C)c1cccnc1)C(=O)c1ccco1		28.1 [34]				

O=C(NC2=CC(C(F)(F)F)=CC(C(F)(F)F)=C2)C1=C(C(F)(F)F)N=C(Cl)N=C1	28.85 [30]					SP 100030
CC[C@@H](C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C(=O)c1nc2ccccc2s1				29.0 [33]		
CCCC1=NC(SCC(=O)NC2=CC=C(Cl)C=C2)=NC(O)=C1		30.0 [56]				
OC1COC(OC2=C(OC3=C(C(O)=CC(O)=C3)C2=O)C2=CC=C(O)C(O)=C2)C(O)C1O		31.62 [77]				
O=C1Nc2ccc(S(=O)(=O)N3CCN(Cc4ccccc4)CC3)cc2C1=O		31.71 [44]				
CCOC(=O)C(=CNc1ccc(S(=O)(=O)c2ccc(/N=C/C(C(=O)OCC)=C(\O)OCC)cc2)cc1)C(=O)OCC		32.0 [31]				
COc1cc(CN2CCN(S(=O)(=O)c3ccc4c(c3)C(=O)C(=O)N4)CC2)cc(OC)c1OC		32.08 [44]				
COc1cc(O)c2c(=O)cc(-c3ccc(OC)c(-c4c(O)cc(O)c5c(=O)cc(-c6ccc(O)cc6)oc45)c3)oc2c1		32.0 [65]		30.2 [65]		
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@@H](CCC(=O)N(C)Cc1ccccc1)C(=O)C(F)(F)F				34.1 [52]		
O=C1Nc2ccc(S(=O)(=O)N3CCN(CCc4ccccc4)CC3)cc2C1=O		34.91 [44]				
CC(C)C[C@H](NC(=O)CSC1=CC=CC=N1)C(=O)N[C@@H](CC1=CC=CC=C1)C(O)C[C@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		35.0 [38]				
O=C1NC(SCC2=CC=C(C=C2)N(=O)=O)=NC(C2=CC=CC=C2)=C1C#N		35.2 [76]				
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)OCc1ccc(cc1)N(=O)=O)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nccs1		36 [2]				
CCC(=C)C(=O)C1=C(Cl)C(Cl)=C(OCC(=O)NC(C)(C)C(N)=O)C=C1				35.3 [78]		
COc1ccc(-c2cc(=O)c3c(O)cc(O)c(-c4cc(-c5cc(=O)c6c(O)cc(OC)cc6o5)ccc4OC)c3o2)cc1		38.4 [65]		35.6 [65]		
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)[C@H](CO)NC(C)=O)C(C)C)C(=O)N[C@@H](CCC(=O)N(C)C)C=O		37.0 [16]				

Cc1ccc(-c2cnc(C(=O)[C@H](C[C@@H]3CCNC3=O)NC(=O)[C@H](CC(C)C)NC(=O)OCc3ccccc3)s2) cc1				37.0 [33]		
CN(C)CCCNC(=O)\C(=C\c1oc(cc1)c2cccc(c2)[N+](=O)[O-])\NC(=O)c3ccc(C)cc3		38.57 [79]		9.11 [79]		
CCOC(=O)\C=C\C(CC1=CC=CC=C1)NC(=O)C(CC1=CC=C(F)C=C1)NC(=O)C(NC(=O)C1=NOC(C)=C1)C(C)C		39.0 [37]				
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)C(CO)NC(=O)C(NC(=O)OCc1ccccc1)C(C)O)C(C)C)C(=O)N[C@@H](CCC(N)=O)C=N		39.0 [59]			3vb6 [59]	
CC(C)(C)NC(=O)C(c1cccnc1)N(C(=O)c1cnco1)c1ccc(C(C)(C)C)cc1		39.0 [34]				
Cc1coc2c1C(=O)C(=O)c1c-2ccc2c(C)cccc12		38.7 [67]		13.7 [67]		
NC(=O)CC1=CC2=C(C=C1)N(CC1=CC3=CC=CC=C3C=C1)C(=O)C2=O	39.2 [10]					
O=C(O)[C@]2(O)C[C@@H](O)[C@@H](O)[C@H](OC(=O)\C=C\c1ccc(O)c(O)c1)C2	39.48 [42]					Chlorogenic acid
O=C1C(=O)N(Cc2ccc3ccccc3c2)c2ccc(S(=O)(=O)N3CCOCC3)cc21		39.87 [44]				
O=C(Cc1nccs1)c1nccs1		40.0 [31]				
CC(C)CC(NC(=O)OC(C)(C)C)C(=O)NC(C)C(=O)C(F)(F)F		40.0 [72]				
CC(C)C[C@H](NC(=O)CC1=CC2=CC=CC=C2C=C1)C(=O)N[C@@H](CC1=CC=CC=C1)C(O)C[C@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		40.0 [38]				
CC(C)CC(NC(=O)CCNC(=O)OC(C)(C)C)C(=O)N[C@H](CC1=CC=CC=C1)C(O)C[C@@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		40.0 [38]				
CC(C)CC(NC(=O)COC1=CC2=CC=CC=C2C=C1)C(=O)N[C@H](CC1=CC=CC=C1)C(O)C[C@@H](CC1=CC=CC=C1)NC(=O)COC1=C(C)C=CC=C1C		40.0 [38]				
COC1=CC(=CC=C1)C1=C(C#N)C(=O)NC(SCC(=O)NC2=CC=C(C=C2)S(N)(=O)=O)=N1		40.0 [56]				
CC(C)C1=CC=C(NC(=O)CSC2=NC(=CC=N2)C2=CC=CS2)C=C1		40.0 [56]				
OC1=CC=C(Cl)C=C1C(=O)NC1=C(Cl)C=C(C=C1)N(=O)=O		40.0 [64]				

C[C@@H](O)[C@H](NC(=O)[C@H](CO)NC(=O)[C@H](CC(N)=O)NC(C)=O)C(=O)N[C@@H](CO)C(=O)N[C@H](CO)CCC(N)=O				40.98 [53]	3snc [53]	
CC(=O)N[C@@H](CC(O)=O)C(=O)N[C@@H](CO)C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(O)=O)C(=O)N[C@H](CO)CCC(N)=O				41.24 [53]	3snb [53]	
CN(C)CCCNC(=O)\C(=C\c1oc(cc1)c2ccccc2[N+](=O)[O-])\NC(=O)c3ccc(C)cc3		41.39 [79]		9.93 [79]		
CCCCN1C(=O)C(=O)C2=C1C=CC(I)=C2	41.8 [10]					
OC(=O)C1=CC=C(\C=C2/C(=O)N(N=C2C2=CC=CC=C2)C2=CC=C(OC(F)(F)F)C=C2)C=C1		42.0 [60]				
OC(=O)C(NC(=O)C(\NC(=O)C1=CC=C(Br)C=C1)=C/C=C/C1=CC=CC=C1)NC1=CC=CC=C1		42.19 [62]				
OCC1OC(OC2=C(OC3=C(C(O)=CC(O)=C3)C2=O)C2=CC=C(O)C(O)=C2)C(O)C(O)C1O		42.79 [77]				
CC(C)(C)NC(=O)C(c1ccncc1)N(C(=O)c1ccco1)c1ccc(C(C)(C)C)cc1		45.0 [34]				
COC1=CC=C(NC(=O)CSC2=NC(=CC(O)=N2)C2=CC=CC=C2)C=C1OC		45.0 [56]				
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@@H](CCC(=O)c1nccs1)C(=O)c1nccs1				45.2 [52]		
CCC(=C)C(=O)C1=C(Cl)C(Cl)=C(OCC(=O)NC(C)(C)C)C=C1				45.8 [78]		
CCOC(=O)C1=CC(=O)OC2=C1C=C(O)C(O)=C2		46.0 [80]				MC8
CC(C)(C)NC(=O)C(c1cccnc1)N(C(=O)c1ncco1)c1ccc(C(C)(C)C) cc1		47.0 [34]				
CC(=O)N[C@@H](CO)C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C=O)Cc1cccs1)C(C)C		48.0 [16]				
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OC(C)(C)C)C(C)C)C(=O)N[C@@H](CCC(N)=O)C=N		49.0 [59]			3vb4 [59]	
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)c1cc(C)on1)C(C)C)C(=O)N[C@@H](CCC(N)=O)C=N		49.0 [59]			3vb7 [59]	

CC(C)c1cc2c(cc1O)[C@@]1(C)CC CC(C)(C)[C@@H]1CC2		49.6 [65]				
CCN(CC)C(=O)CC[C@H](NC(=O)[C @H](CC(C)C)NC(=O)[C@@H](NC(= O)OCc1ccccc1)C(C)C)C(=O)c1n c2ccccc2s1				49.3 [52]		
CC(=O)CCC(=O)N1N=C(CC1C1=CC =C(Br)C=C1)C1=C(O)N=C2C=CC(C) =CC2=C1C1=CC=CC=C1		49.96 [62]				
O=C1C(=O)N(Cc2ccccc2)c2ccc(I) cc21		50.0 [21]				
CC(C)(C)NC(=O)C(c1cccnc1)N(C (=O)c1cccs1)c1ccc(C(C)(C)C) cc1		50.0 [34]				
O=C1Nc2ccc(S(=O)(=O)N3CCN(c4ccc cn4)CC3)cc2C1=O		51.33 [44]				
COc1ccc(-c2cnc(C(=O)[C@H](C[C@@ H]3CCNC3=O)NC(=O)[C@H](CC (C)C)NC(=O)OCc3ccccc3)s2)cc1				52.0 [33]		
CC(C)CC(NC(=O)C(NC(=O)C(NC(C) =O)C(C)C)C(C)O)C(=O)NC(CCC(=O) N(C)C)C(=O)CN1NC(=O)C2=C(C=C C=C2N(=O)=O)C1=O		53.0 [39]				
O[C@H]1CC2=C(OC1C1=C3C=C(C= C(O)C(=O)C3=C(O)C(O)=C1)C1OC3= CC(O)=CC(O)=C3C[C@H]1O)C=C(O) C=C2O		56.0 [57]				TF1
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)c2ncc (s2)C2=CC=C(OC)C=C2)C=C1				56.0 [2]		
CC1=CC(Br)=C(C=C1)N1C(=O)CC (SC2=CC=CC=C2C(O)=O)C1=O		56.24 [62]				
O=C[C@H](Cc1c[nH]cn1)NC[C@@H] 1C[C@H]2CCCC[C@@H]2CN1C (=O)c1ccc(F)cc1		57.0 [81]				
FC(F)(C(=O)C1=CC=C(O1)C1=CC=C (Cl)C=C1)C1=CN=CC(Br)=C1		57 [70]				
Nc1nc(CSc2nnc(c3cccc4ccccc34)n2 c5ccccc5)cs1		58.35 [79]				
COC1=CC(=CC=C1)C1=C(C#N)C(=O)NC(SCC(=O)NC2=CC=C(C=C2) C(C)=O)=N1		60.0 [56]				
CCC(SC1=NC(C2=CC=CC(OC)=C2)= C(C#N)C(=O)N1)C(=O)NC1=CC= CC(=C1)C(C)=O		60.0 [56]				
OCC1OC(OC2=CC3=C(C(O)=C2)C (=O)C(OC2OC(CO)C(O)C(O)C2O) =C(O3)C2=CC=C(O)C(O)=C2) C(O)C(O)C1O		61.46 [77]				

CC(=O)N[C@@H](CO)C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C=O)CC1CCCCC1)C(C)C		62.0 [16]				
Brc1ccc(cc1)C(=O)N1C[C@H]2CCCC[C@@H]2C[C@H]1CN[C@@H](Cc1cnc[nH]1)C=O		63.0 [81]			4tww [81]	
COc1cc(ccc1O)C2N(CCN(C)C)C(=O)C(=C2C(=O)c3ccc(OCC(C)C) cc3C)O		62.79 [79]				
CC(C)CC(NC(=O)C(NC(=O)C(NC(C)=O)C(C)C)C(C)OC1=CC=CC=C1)C(=O)NC(CCC(=O)N(C)C)C(=O)CN1NC(=O)C2=C(C=CC=C2)C1=O		64.0 [39]				
C[C@H](NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)CF				64.0 [32]		
CCCCN1C(=O)C(=O)c2cc(I)ccc21		66.0 [21]				
CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccccc2)CC1		67.2 [44]				
O=C[C@H](Cc1c[nH]cn1)NC[C@@H]1C[C@H]2CCCC[C@@H]2CN1C(=O)c1ccccc1		68.0 [81]				
CC(C)CC(NC(=O)C(NC(=O)C(NC(C)=O)C(C)C)C(C)OC1=CC=CC=C1)C(=O)NC(CCC(=O)N(C)C)C(=O)CN1NC(=O)C2=C(C=CC=C2N(=O)=O)C1=O		70.0 [39]				
CCOC(=O)/C=C/[C@H](C[C@@H]1CCNC1=O)NC(=O)[C@H](CC=C(C)C)CC(=O)[C@@H](NC(=O)c2cc(C)on2)C(C)C		70.0 [82]			2alv [82]	
CN1C(=O)C(=O)c2cc(C(N)=O)c cc21		71.0 [39]				
COc1ccc(-c2cc(=O)c3c(O)cc(O)cc3o2)cc1-c1c(O)cc(O)c2c(=O)cc(-c3ccc(O)cc3)oc12		72.3 [65]				
CC(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CO)C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CO)C(=O)N[C@H](CO)CCC(N)=O				72.73 [53]	3sna [53]	
Clc2cc(Cl)ccc2Oc1ccc(Cl)cc1O		75.0 [63]				Triclosan
ClC1=CC=C(C=C1)C1=NC=C(O1)C(=O)CC1=CN=CC(Br)=C1		75.0 [70]				
Cn1cnc(C(=O)N(c2ccc(C(C)(C)C)cc2)C(C(=O)NC(C)(C)C)c2cccnc2)c1		75.0 [34]				
CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3)CC1		76.74 [44]				

COc1cc(\C=N\NC(=O)\C(=C/c2ccccc2)\NC(=O)c3ccccc3)cc(OC)c1O		77.09 [79]				
CCOC(=O)CC[C@H](C[C@H]1CCNC1=O)NC(=O)[C@H](CC=C(C)C)CC(=O)[C@@H](NC(=O)[C@H](CO)NC(=O)OC(C)(C)C)C(C)C		80.0 [68]			2qiq [68]	
CCOC(=O)\C=C\C(CC1CCNC1=O)NC(=O)C(CC=C(C)C)CC(=O)C(NC(=O)C(CO)NC(=O)OC(C)(C)C)C(C)C		80.0 [68]				GRL-0155S
COC(=O)C1=C(C)N(CC2=CC=CN=C2)C(=O)\C1=C/C1=CC=C(OCC(=O)NCC2=CCCO2)C=C1		80.46 [62]				
CN1CCN(S(=O)(=O)c2ccc3c(c2)C(=O)C(=O)N3Cc2ccc3ccccc3c2) CC1		82.91 [44]				
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)OC1=CC=CC=C1)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nccs1		85 [2]				
Cc1coc2c1C(=O)C(=O)c1c-2ccc2c1CCCC2(C)C		89.1 [67]				
O=C(CSc1ncnc2c1sc3nc(N4CCOCC4)c5CCCCc5c23)NCc6occc6		90.72 [79]				
CCCCN(C)C[C@H]1O[C@H](CN[C@@H](CC2=CNC=N2)C=O)CC2CCCCC12		95.0 [83]				
OC1CC2=C(OC1C1=CC(O)=C(O)C(O)=C1)C=C(O)C=C2O		100.0 [57]				Catechin
CN1C=NC2=C1C(=O)N(C(=O)N2C)C		100.0 [57]				Caffeine
OC1CC2=C(OC1C1=CC(O)=C(O)C=C1)C=C(O)C=C2O		100.0 [57]				Epicatechin
OC1=CC2=C(CC(OC(=O)C3=CC(O)=C(O)C(O)=C3)C(O2)C2=CC(O)=C(O)C=C2)C(O)=C1		100.0 [57]				Epicatechin gallate
OC1=CC2=C(CC(OC(=O)C3=CC(O)=C(O)C(O)=C3)C(O2)C2=CC(O)=C(O)C(O)=C2)C(O)=C1		100.0 [57]				(-)-Epigallo-catechin gallte
Cn1c2c(c(=O)n(c1=O)C)[nH]cn2		100.0 [57]				Theophylline
C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C(=C3)O)O)O)O		100.0 [57]				Epigallocatechin
CC1=CC(=O)NC(SCC(=O)NC2=CC(Cl)=CC=C2OC2=CC=CC=C2)=N1		100.0 [56]				
Cc1nc(C)c(s1)C(=O)C2=C(O)C(=O)N(CCCN3CCOCC3)C2c4cccc(c4)[N+](=O)[O-]		101.38 [79]				
CC(C)COC(=O)N[C@@H](C(C)C)C(=O)CCl				105.0 [32]		
[H][C@]56C[C@@H](C(=O)N[C@]1			107.36 [84]			Dihydroer-

(C)O[C@]4(O)N(C1=O)[C@@H](Cc2ccccc2)C(=O)N3CCC[C@]34[H])CN(C)[C@]5([H])Cc7c[nH]c8cccc6c78						gotamine
O=C[C@H](Cc1cnc[nH]1)NC[C@@H]1C[C@H]2CCCC[C@@H]2CN1C(=O)c1ccc(cc1)-c1ccccc1		108.0 [81]			4twy [81]	
CCN(CC)C(=O)CC[C@H](NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)c1nccs1				112.0 [52]		
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@@H](CCC(=O)O)C(=O)C(F)(F)F				116.0 [52]		
CC(C)(C)OC(=O)N[C@@H](CC1=CC=CC=C1)[C@H](O)CCl				128.0 [32]		
CC(=O)Oc1cc2c(cc1C(C)C)CC[C@@H]1[C@]2(C)CCC[C@@]1(C)CO		128.9 [65]				
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[C@@H](CCC(C)=O)C(C)=O				134.5 [32]		
O=C[C@H](Cc1c[nH]cn1)NC[C@@H]1C[C@H]2CCCC[C@@H]2CN1C(=O)c1cccc(-c2ccccc2)c1		135.0 [81]				
O=C[C@H](Cc1c[nH]cn1)NC[C@@H]1C[C@H]2CCCC[C@@H]2CN1C(=O)c1ccccc1-c1ccccc1		135.0 [81]				
CC(C)C[C@H](NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)C(F)(F)F				135.0 [52]		
C=C1CC[C@H]2[C@](C)(CO)CCC[C@]2(C)[C@H]1CC/C(C)=C\CO		137.7 [65]				
CCN(CC)C(=O)CC[C@H](NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)c1nc2ccccc2s1				159.0 [52]		
CC(C)c1cc2c(cc1O)[C@@]1(C)CCC[C@@](C)(C=O)[C@@H]1CC2		163.2 [65]				
[H][C@]12CCCC[C@]1([H])CN([C@@H](CN[C@@H](Cc1cnc[nH]1)C=O)C2)C(=O)c1ccc(Br)cc1		175.0 [81]				
CC(C)C1=CC2=CC[C@H]3[C@](C)(C(=O)O)CCC[C@]3(C)[C@H]2CC1		189.1 [65]				
CCOC(=O)\C=C\C(CC1CCNC1=O)NC(=O)C(CC(C)C)NC(=O)C(NC(=O)C1=NOC(C)=C1)C(C)C		200.0 [68]				
CC1=CC(O)=NC(SCC(=O)NC2=CC=C(OC3=CC=C(Cl)C=C3)C=C2)=N1		200.0 [56]				

CC(C)C1=CC=C(NC(=O)CSC2=NC=CC(=N2)C2=CSC(COC3=CC=CC=C3Cl)=N2)C=C1		200.0 [56]				
COC(OC)C1=NC(SCC(=O)NC2=CC=C(C=C2)C(F)(F)F)=NC(O)=C1		200.0 [56]				
CCCCC1=CC(C)=C(NC(=O)CSC2=NC(C3CCCCC3)=C(C#N)C(=O)N2)C=C1		200.0 [56]				
FC(F)(F)C1=CC=CC(NC(=O)CSC2=NC(C3=CC=CC=C3)=C(C#N)C(=O)N2)=C1		200.0 [56]				
COC(=O)[C@]1(C)CCC[C@]2(C)c3ccc(C(C)C)cc3CC[C@H]21		207.0 []				
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)COC1=CC=CC=C1)C(C)C)C(=O)N[C@H](CC1=CNC=N1)C(=O)c1nccs1		210.0 [2]				
CC(C)c1cc2c(cc1O)[C@@]1(C)CCC[C@@](C)(CO)[C@@H]1CC2		220.8 [65]				
C[C@H]1COC2=C1C(=O)C(=O)c1c2ccc2c1CCCC2(C)C		226.7 [67]		9.0 [67]		
CC(C)c1cc2c(cc1O)[C@@]1(C)CC[C@H](O)C(C)(C)[C@@H]1CC2		233.4 [65]				
O=C[C@H](Cc1cnc[nH]1)NC[C@H]1C[C@@H]2CCCC[C@H]2CN1C(=O)c1ccc(cc1)-c1ccccc1		240.0 [81]			4wy3 [81]	
CCOC(=O)C1=C(N)N=C(SCC(=O)NC2=CC=C(C=C2)N(=O)=O)N=C1		250.0 [56]				
CC(C)COC(=O)N[C@H](C(C)C)C(=O)N[C@H](CC(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nccs1		250.0 [2]				
COc1c2c(cc(c1N3C[C@@H]4CCCN[C@@H]4C3)F)c(=O)c(cn2C5CC5)C(=O)O			249.0 [84]			Moxifloxacin
CCCCN(C)C[C@H]1O[C@@H](CN[C@@H](CC2=CNC=N2)C=O)CC2CCCCC12		260.0 [83]				
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N[C@H](CC1=CNC=N1)C(=O)c1nccs1		260.0 [2]				
CC(C)C[C@@H](NC(=O)[C@H](NC(=O)OCC(C)(C)C)C(C)C)C(=O)N[C@H](C[C@H]1CCNC1=O)C(=O)c1nccs1		280.0 [2]				
O=c1cc(-c2ccc(O)cc2)oc2cc(O)cc(O)c12		280.8 [65]				

C=C[C@@]1(C)CC[C@H]2C(=CC[C@H]3[C@](C)(C(=O)O)CCC[C@]23C)C1		283.5 [65]				
CC(C)CC(NC(=O)C(NC(=O)C(CCC(=O)OCC1=CC=CC=C1)NC(=O)OC(C)(C)C)C(C)C)C(N)=O				286.0 [32]		
CCCN(CCC)C(=O)CC[C@H](NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCc1ccccc1)C(C)C)C(=O)C(F)(F)F				297.0 [52]		
CCOC(=O)\C=C\C(CC1CCNC1=O)NC(=O)C(CC1=CC=CC=C1)NC(=O)C(NC(=O)C1=NOC(C)=C1)C(C)C		300.0 [68]				
CCOC1=CC=C(C=C1)N1C(=O)CC(SC2=NC(C)=CC(C)=N2)C1=O		300.0 [56]				
COC1=CC=CC(=C1)C1=C(C#N)C(=O)NC(SCC(=O)NC2=CC=C(C=C2)N(=O)=O)=N1		300.0 [56]				
CC(SC1=NC(C2=CC=CC=C2)=C(C#N)C(=O)N1)C(=O)NC1=CC=C(Cl)C=C1		300.0 [56]				
c1c(cc(c(c1F)CNC(=O)c2cn3c(c(c2=O)O)C(=O)N4[C@H]5CC[C@H](C5)O[C@@H]4C3)F)F			302 [84]			Bictegravir
CC(C)(C)C1=CC=C(NC(=O)CSC2=NC(C3CCCCC3)=C(C#N)C(=O)N2)C=C1		350.0 [56]				
CCCN(CCC)C(=O)CC[C@H](NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)C(F)(F)F				363.0 [52]		
CC1=CC=C(C=C1)C(NC(=O)OCC1=CC=CC=C1)NC(=O)OCC1=CC=CC=C1				366.0 [32]		
CC(C)[C@H](NC(=O)[C@H](CC1=CC=C(O)C=C1)NC(C)=O)C(=O)N[C@@H](C)C(=O)N[C@@H](CC(O)=O)C(=O)CCl				389.0 [32]		
COC1=CC=C(C=C1)C1=CC=NC(SCC(=O)NC2=CC=C(C=C2)C(C)C)=N1		400.0 [56]				
CCCCN(C)C[C@@H]1O[C@@H](CN[C@@H](CC2=CNC=N2)C=O)CC2CCCCC12		440.0 [83]				
CCN(CC)C(=O)CC[C@H](NC(=O)[C@H](CC(C)C)NC(=O)OCc1ccccc1)C(=O)c1nccs1				462.0 [52]		

CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)N[C@@H](CCC(=O)N1CCOCC1)C(=O)c1nccs1				478.0 [52]		
CC1=NC(SCC(=O)NC2=CC=C(Cl)C=C2F)=NC(=C1)C(F)(F)F		500.0 [56]				
O=S(=O)(c1ccc(N)cc1)N(CC(C)C)C[C@@H](O)[C@@H](NC(=O)O[C@H]2CO[C@H]3OCC[C@@H]23)Cc4ccccc4				518.0 [84]		Darunavir
CCCN(CCC)C(=O)CC[C@H](NC(=O)[C@H](CC(C)C)NC(=O)OCc1ccccc1)C(=O)C(F)(F)F				584.0 [52]		
CCN(CC)C(=O)CC[C@H](NC(=O)[C@@H](NC(=O)OCc1ccccc1)C(C)C)C(=O)c1nccs1				614.00 [52]		
CCCCN(C)C[C@@H]1O[C@@H](CN[C@@H](CC2=CNC=N2)C=O)CC2CCCCC12		780.0 [83]				
CCOC(=O)\C=C\[C@@H](C[C@@H]1CCNC1=O)NC(=O)C(CC=C(C)C)CC(=O)[C@H](NC(=O)C1=NOC(C)=C1)C(C)C		800.0 [68]				
C[C@H](NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)OCC1=CC=CC=C1)C(=O)N[C@@H](CCC(N)=O)C(=O)C(F)(F)F				844.0 [32]		
C[C@H](NC(=O)[C@H](CC1=CC=CC=C1)NC(=O)OCc1ccccc1)C(=O)N[C@@H](CCC(N)=O)C(=O)C(F)(F)F				844.4 [85]		
CCOC(=O)\C=C\C(CC1CCNC1=O)NC(=O)C(CC(=O)C(NC(=O)C1=NOC(C)=C1)C(C)C)CC1=CC=CC=C1		870.0 [68]				
CC(=O)N[C@@H](CO)C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C=O)Cc1ccccc1)C(C)C		2000 [16]				
CC1C(C(C(O1)OC2C(C(C(C(C2O)O)N=C(N)N)O)N=C(N)N)OC3C(C(C(C(O3)CO)O)O)NC)(C=O)O			2134 [84]			Streptomycin
Clc1cc2nccc(c2cc1)NC(C)CCCN(CC)CCO	3584 [46]					

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