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Supporting Information

Potential inhibitors for SARS-CoV-2 Mpro from Marine compounds

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Table S1. List of marine compounds and docking energy to SARS-CoV-2 Mpro.

N⁰	Name	SMILES	ΔG_{Dock}	Marine source
1	**M1**	Cc1cc2c(c(c1)O)C(=O)c1c(ccc(c3c(C)cc(c4c3C(=O)c3cccc(c3C4=O)O)O)c1O)C2=O	-10.6	*Laurenica spectabilis*
2	**M2**	C1(=C)C[C@@H]2[C@@H]3[C@]4([C@@H]1C[C@H]4C(O[C@@H]1[C@H]4[C@@H]3[C@@H](C[C@@H]2Cl)[NH2+][C@H]4[C@]2([C@H]1CC[C@@]1([C@]2(C)CC[C@H]2[C@@]31[C@@H]([C@H]([C@H](O2)C(=C)C)O)O3)O)C)(C)C)O	-10.2	*Mucor irregularis*
3	**M3**	c1ccc2c(c1)N=C([N+](C2=O)[C@H]1C[C@]2(OC1=O)c1c(N3[C@H]2NC2(C3=O)CC2)cccc1)C(=O)N	-9.9	*Aspergillus versicolor* LZD-14-1
4	**M4**	C1(=C)C[C@@H]2[C@@H]3[C@H]4[C@@H]1C[C@H]4C(O[C@@H]1[C@H]4[C@@H]3[C@@H](C[C@@H]2Cl)[NH2+][C@H]4[C@]2([C@H]1CC[C@@]1([C@]2(C)CC[C@H]2[C@@]31[C@@H]([C@H]([C@H](O2)C(=C)C)O)O3)O)C)(C)C	-9.9	*Mucor irregularis*
5	**M5**	c1ccc2c(c1)N=C1[N+](C2=O)[C@@H]2C(=O)N[C@@H]1N1[C@@H]3[C@](C2)(c2c(N3C(=O)C31CC3)cccc2)O	-9.8	*Aspergillus versicolor* LCJ-5-4
6	**M6**	[C@H]12N3C(=O)[C@@H](N(C(=O)[C@@H]3C[C@]1(c1ccccc1N2)[C@]12[C@H](N3C(=O)[C@@H](N(C(=O)[C@@H]3C1)C)Cc1ccccc1)Nc1c2cccc1)C)Cc1ccccc1	-9.8	Mangrove endophytic fungus Gx-3a
7	**M7**	c1ccc2c(c1)N=C1[N+](C2=O)[C@@H]2C(=O)N[C@H]1O[C@@]1([C@@H]3NC4(C(=O)N3c3c1cccc3)CC4)C2	-9.7	*Aspergillus versicolor* LZD-14-1
8	**M8**	c1(c(cc(c2c1cccc2O)O)c1ccccc1)C1=CC(=C(C(=O)[OH+]1)CC1=C(C=C([OH+]C1=O)[C@@H]1[C@](CC(=O)c2c1cccc2O)(c1ccccc1)O)O)O	-9.7	*Streptomyces* sp.
9	**M9**	c1(c(cc(c2c1cccc2O)O)c1ccccc1)C1=CC(=C(C(=O)[OH+]1)CC1=C(C=C([OH+]C1=O)[C@H]1[C@](CC(=O)c2c1cccc2O)(c1ccccc1)O)O)O	-9.7	*Streptomyces* sp.
10	**M10**	c1ccc2c(c1)N=C1[N+](C2=O)[C@@H]2C(=O)N3[C@H]1O[C@@]1([C@@H]4N(C3)[C@H](C(=O)N4c3c1cccc3)C)C2	-9.6	*Aspergillus versicolor* LZD-14-1
11	**M11**	c1ccc2c(c1)N=C1[N+](C2=O)[C@@H]2C(=O)N[C@@H]1N1[C@@H]3[C@](C2)(c2c(N3C(=O)[C@H]1C)cccc2)O	-9.6	*Aspergillus versicolor* LCJ-5-4
12	**M12**	C1CC[C@H]2[C@@H](C1)[NH2+]C[C@H]2[C@@]12[C@@H]3[C@H](CCCC3)N[C@@H]1N1[C@]3([C@H]2O)C(=O)N([C@@](C1=O)(C)SSS3)C	-9.6	*Acrostalagmus luteoalbus*
13	**M13**	[C@]12([C@H]3C(=C)C[C@@H]4[C@@H]1[C@H]1[C@@H](C[C@H]4Cl)[NH2+][C@@H]4[C@H]1[C@@H](OC([C@H]2C3)(C)C)O[C@]1([C@]4([C@@]2([C@@](CC1)([C@]13[C@H](CC2)O[C@@H]([C@@H]([C@H]1O3)O)C(=C)C)O)C)C)OC)O	-9.5	*Mucor irregularis* QEN-189
14	**M14**	c1ccc2c(c1)[nH+]c1c2cc([nH]c1C(=O)C)C(=O)NCC[C@H]1[C@H]2[C@H]([NH2+]C1)CCCC2	-9.4	*Marinactinospora thermotolerans* SCSIO 00652

15	**M15**	C1[C@@H]([C@@H]([C@H]([C@@H](O1)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)Oc1c(c2c(c(c1)OC)C(=O)c1c([OH+]2)cccc1)OC)O)O)O)O)O)O	-9.4	*Phomopsis* sp. ZH76
16	**M16**	[C@@]123OC(=O)CC/C=C(/C(=O)[C@H](C/C=C/[C@H]1[C@@H](C(=C)[C@H]([C@H]2[C@@H](NC3=O)Cc1ccccc1)C)O)C)\C	-9.4	*Arthrinium arundinis* ZSDS1-F3
17	**M17**	O1[C@@]2([C@@H]3N(c4c2cccc4)C(=O)[C@@H](N3)C)C[C@H]2[N+]3C(=Nc4c(C3=O)cccc4)[C@]1(NC2=O)C	-9.3	*Aspergillus* sp.
18	**M18**	c12c(cc(cc1[OH+]c1c(C2=O)c(cc(c1)OC)[C@H]1[C@@H](c2c(C1=O)cc(cc2O)OC)c1c(cc(cc1O)C)O)C)O	-9.3	*Ascomycota* sp. SK2YWS-L
19	**M19**	O=C1c2cc(OC)cc(O)c2[C@H](c2c(O)cc(C)cc2O)[C@H]1c1cc(OC)cc2c1C(=O)c1c([OH+]2)cc(C)cc1O	-9.3	*Ascomycota* sp. SK2YWS-L
20	**M20**	c1cc(ccc1)C[C@@H]1NC(=O)CN(C(=O)[C@H]2N(C(=O)[C@H](N(C(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](N(C1=O)C)Cc1ccc(cc1)O)C(C)C)CC(C)C)C)Cc1ccc(cc1)O)CCC2)C	-9.2	*Acremonium persicinum* SCSIO115
21	**M21**	C1=C[C@H]2[C@@H](OC1(C)C)C[C@@H]1[C@H](C2)[C@@H]([C@H]([NH2+]1)C(C)(C=C)C)/C=C\1/C(=O)N2[C@@H](C(=O)N1)CCC2	-9.2	*Aspergillus versicolor*
22	**M22**	C1C[C@H]2[C@@H](CC1)[C@H](C[NH2+]2)C[C@@H]1[C@H]2[C@@]3(C(=O)N1)[C@H]([C@@H]([C@@]([C@H]2C)(C)O)C)/C=C/C[C@H](C)/C=C(/C(=O)[C@@H](O)CCC3=O)\C	-9.2	*Chaetomium globosum*
23	**M23**	O=c1c2ccccc2ncn1[C@@H]1C[C@]2([C@H]3N(C1=O)[C@H](C(=O)N3c1c2cccc1)C)O	-9.2	*Penicillium* sp.
24	**M24**	C1C[C@@H]2[C@@H](CC1)[C@@H](C[NH2+]2)C[C@@H]1[C@H]2[C@@]3(C(=O)N1)[C@H]([C@@H](C(=C2C)C)O)/C=C/C[C@H](C)/C=C(/C(=O)[C@@H](O)CCC3=O)\C	-9.1	*Chaetomium globosum*
25	**M25**	O1[C@H]([C@H]([C@H](C[C@@H]1O[C@@H]1C[C@@](O[C@@H]([C@H]1CC)C)([C@H]([C@@H]([C@@H]([C@@H]1[C@H](/C=C/C=C/C(=C)O[C@@H]([C@H](/C=C/C=C/C(=O)O1)C)[C@H]([C@H]([C@@H](C1=C[C@H]([C@@H]([C@H](O1)C)CC)O[C@H]1C[C@@H]([C@@H]([C@@H](O1)C)O)O)C)O)C)C)C)O)C)O)O)O)C	-9.1	*Streptomyces* sp.
26	**M26**	c1cccc(c1O)C1=N[C@@H](CO1)[C@@H]1SC[C@@H](N1C)CN1[C@@H]2C(=O)N([C@H](C1=O)CSSC2)C[C@@H]1N([C@@H](SC1)[C@H]1N=C(OC1)c1c(O)cccc1)C	-9.1	*Streptomyces olivaceus*
27	**M27**	[C@]123[C@@H]4CC[C@@H]([C@]4(CC[C@@H]1[C@]1(CC[C@@H](C[C@]1(OO2)C=C3)O)C)C)[C@H](C)/C=C/[C@@H](C(C)C)C	-9.1	*Paecilomyces lilacinus* ZBY-1
28	**M28**	C1CC[C@H]2[C@@H](C1)[NH2+]C[C@H]2[C@@]12[C@@H]3[C@H](CCCC3)N[C@@H]1N1[C@]3([C@H]2O)C(=O)N([C@@](C1=O)(CO)SSS3)C	-9.1	*Acrostalagmus luteoalbus* SCSIO F457
29	**M29**	C/C=C/[C@@H]1[C@H]2C[C@H](CC[C@@H]2C(=C[C@H]1C(=O)C1=C(C(=C[NH+]C1=O)c1ccc(cc1)O)O)C)C	-9.1	*Campylocarpon* sp. HDN13-307

30	**M30**	[C@]12([C@H]3C(=C)C[C@H]4[C@@H]1[C@@H]1[C@@H](C[C@H]4Cl)[NH2+][C@@H]4[C@H]1[C@@H](OC([C@H]2C3)(C)C)O[C@]1([C@]4([C@@]2([C@@](CC1)([C@]13[C@H](CC2)O[C@@H]([C@@H]([C@H]1O3)O)C(=C)C)O)C)C)O)O	-9.1	*Mucor irregularis* QEN-189
31	**M31**	C1(=C)C[C@@H]2[C@@H]3[C@H]4[C@@H]1C[C@H]4C(O[C@@H]1[C@H]4[C@@H]3[C@@H](C[C@@H]2Cl)[NH2+][C@H]4[C@]2([C@H]1CC[C@@]1([C@]2(C)CC[C@H]2C1=C([C@H]([C@H](O2)C(=C)C)O)O)O)C)(C)C	-9.1	*Mucor irregularis* QEN-189
32	**M32**	[C@@H]1([C@H](C[C@@H]2[C@H](C1)[C@@H](C[NH2+]2)[C@@H]1[C@H](C[NH2+]C1)[C@@H]1[C@@H]2[C@@H]([NH2+]C1)C[C@@H]([C@@H](C2)Cl)Cl)Cl)Cl	-9.1	*Marine actinomycete* NPS12745
33	**M33**	c1cc(ccc1)C[C@@H]1NC(=O)CN(C(=O)[C@H]2N(C(=O)[C@H](N(C(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](N(C1=O)C)Cc1ccc(cc1)O)[C@H](C)CC)CC(C)C)C)Cc1ccc(cc1)O)CCC2)C	-9	*Acremonium persicinum* SCSIO115
34	**M34**	c1ccc2c(c1)NC(=O)[C@H]2[C@@H]1C(=O)Nc2c1cccc2	-9	*Shewanella piezotolerans*
35	**M35**	c1ccc2c(c1)N=C1[N+](C2=O)[C@@H]2C(=O)N[C@@H]1N1[C@@H]3[C@](C2)(c2c(N3C(=O)[C@@H]1C[C@H](CC)C)cccc2)O	-9	*Aspergillus versicolor* LCJ-5-4
36	**M36**	[C@]123[C@@H]4CC[C@@H]([C@]4(CC=C1[C@]1(CC[C@@H](C[C@]1(OO2)C=C3)O)C)C)[C@H](C)/C=C/[C@H](C(C)C)C	-9	*Paecilomyces lilacinus* ZBY-1
37	**M37**	C1CC[C@H]2[C@@H](C1)[NH2+]C[C@H]2[C@@]12[C@@H]3[C@H](CCCC3)N[C@@H]1N1[C@]3(C2)C(=O)N([C@@](C1=O)(CO)SSS3)C	-9	*Acrostalagmus luteoalbus* SCSIO F457
38	**M38**	C1(=O)[C@H]2N(C(=O)[C@H](NC(=O)[C@H]([C@H](OC(=O)[C@@H](N(C)C(=O)CN1C)C(C)C)C)NC(=O)c1ccc(c3c1Nc1c(O3)c(c3c(c1C(=O)N[C@H]1[C@@H](C)OC(=O)[C@H](C(C)C)N(C(=O)CN(C)C(=O)[C@@H]4CCCN4C(=O)[C@@H](C(C)C)NC1=O)C)nc(o3)C)C)C(C)C)CCC2	-8.9	*Streptomyces* sp. IMB094
39	**M39**	c1ccc2c(c1)N=C1[N+](C2=O)[C@@H]2C[C@H]([C@]3(O[C@H]1NC2=O)[C@H]1N(c2c3cccc2)C(=O)[C@@H](N1)[C@@H](C)CC)O	-8.9	*Aspergillus versicolor* LZD-14-1
40	**M40**	C1=C[C@H]2[C@H](OC1(C)C)C[C@@H]1[C@@H](C2)[C@H]2C[C@]34[C@H](C[C@]5(N(C3=O)CCC5)C(=O)N4)C([C@@H]2[NH2+]1)(C)C	-8.9	*Aspergillus versicolor*
41	**M41**	[C@@H]12CC[C@]3([C@H]([C@]1(CC[C@@H](C2)C(C)(C)O)C)C(=O)C1=C(O3)C(=O)C(=CC1=O)[C@@H](C(=O)/C(=C/C)/C)C)C	-8.9	*Nigrospora* sp. MA75
42	**M42**	C1[C@H]2[C@@](O[C@@]31c1ccccc1[C@@H]1[C@@H]3CC(C1=C)(C)C)(C(C)(C(=O)C1=Nc3ccccc3C(=O)[N+]21)C)O	-8.9	*Neosartorya Fischeri*
43	**M43**	N1=C2[N+](C(=O)c3ccccc13)[C@@H](C(=O)N[C@H]2C(C)C)C[C@H]1C[NH2+][C@@H]2[C@H]1CCCC2	-8.9	*Neosartorya Fischeri*
44	**M44**	C1CC[C@H]2[C@@H](C1)[NH2+]C[C@H]2[C@@]12[C@@H]3[C@H](CCCC3)N[C@@H]1N1[C@]3([C@H]2O)C(=O)N([C@@](C1=O)(C)SS3)C	-8.9	*Acrostalagmus luteoalbus* SCSIO F457
45	**M45**	c12c([NH+]C(=O)[N+](C1=O)[C@@H]1c3ccccc3NC1=O)cccc2	-8.8	*Shewanella piezotolerans*

46	**M46**	c1ccc2c(c1)N=C1[N+](C2=O)[C@H]2C[C@]3([C@@H]4N([C@@H]1NC2=O)[C@@H](C(=O)N4c1c3cccc1)C)O	-8.8	*Aspergillus versicolor* LZD-14-1
47	**M47**	C1(=O)OC(C2=C[C@@H]3[C@]4([C@H]([C@@]5(C2=C1)CO5)C[C@@]1([C@@H]2C4=C(C(O[C@@H]2OC1=O)(C)C)O3)C)C)(C)C	-8.8	*Talaromyces amestolkiae* YX1
48	**M48**	C1[C@H]2[C@@](O[C@]31c1ccccc1CC3=O)(C(C)(C(=O)C1=Nc3ccccc3C(=O)[N+]21)C)O	-8.8	*Neosartorya fischeri*
49	**M49**	C1CC[C@H]2[C@@H](C1)[NH2+]C[C@H]2[C@@]12[C@@H]3[C@@H](CCCC3)N[C@@H]1N1[C@]3(C2)C(=O)N([C@@](C1=O)(CO)SS3)C	-8.8	*Acrostalagmus luteoalbus* SCSIO F457
50	**M50**	O=C1N2[C@@H](CCC2)C(=O)N[C@H]1C[C@@H]1[C@H]([NH2+][C@@H]2[C@@H]1CCCC2)CC=C(C)C	-8.7	*Penicillium* sp.
51	**M51**	N1c2c(C(=C)N[C@H](C(=O)N3[C@H](C(=O)Nc4c(C(=O)N([C@H](C1=O)C)C)cccc4)CCC3)C)cccc2	-8.7	*Aspergillus versicolor* LZD-14-1
52	**M52**	c1ccc2c(c1)[nH+]c1c2cc([nH]c1C(=O)C)C(=O)NCCc1ccc(cc1)O	-8.7	*Marinactinospora thermotolerans* SCSIO 00652
53	**M53**	c1cc(c2c(c1)C(=O)c1c(C2=O)c(c2c(c1O)c1c(C[C@H]2O)cc2c(c1O)C(=O)O[C@@](C2)(O)C)OC)O	-8.7	*Streptosporangium* sp.
54	**M54**	c1cc(c2c(c1)C(=O)c1c(C2=O)c(c2c(c1O)c1c(C[C@H]2O)cc2c(c1O)C(=O)O[C@@](C2)(OC)C)OC)O	-8.7	*Streptosporangium* sp.
55	**M55**	C1[C@H](OC(=O)C[C@H](OC(=O)c2c(cc(cc2O)O)C[C@H](OC(=O)C[C@@H](C)OC(=O)c2c(cc(cc2O)O)CC1=O)C)C)C	-8.7	*Hansfordia sinuosae*
56	**M56**	Cc1cc(c2c(c1)[OH+]C1=C([C@@H]3[C@@H]4[C@H](C1)[C@](C(=O)OCC)(O)O[C@@]4(C1=C3[OH+]c3cc(C)cc(c3C1=O)O)C(=O)OC)C2=O)O	-8.7	*Penicillium purpurogenum* G59
57	**M57**	c1ccc2c(c1)[nH+]c1c2cc([nH]c1C(=O)C)C(=O)NCCc1ccc(cc1)OC	-8.6	*Streptomyces* sp. CMN-62
58	**M58**	c1ccc2c(c1)[nH+]c1c2cc([nH]c1C(=O)C)C(=O)NCCc1ccccc1	-8.6	*Marinactinospora thermotolerans* SCSIO 00652
59	**M59**	C1C[C@@H]([C@H]2[C@H]3[C@@H]1N[C@H](C(=O)N[C@@H](C[C@H]3C[NH2+]2)CC[C@H]1O[C@H]([C@@H]([C@H]([C@@H]1O)O)O)CO)C(CC)(C)C)C(C)(C)C=C	-8.6	*Marinactinospora thermotolerans* SCSIO 00652
60	**M60**	c1ccc2c(c1)N=C1[N+](C2=O)[C@H](C(=O)NC1)C[C@@]1(c2c(cccc2)N2[C@H]1N[C@H](C2=O)C)O	-8.6	*Aspergillus versicolor* LZD-14-1
61	**M61**	[C@@H]1(C[C@@H]([C@@H]2[C@@H](C1)[C@@H]([C@@H]([NH2+]2)C(C)(C)C=C)C[C@H]1C(=O)N[C@H](C(=O)N1)C)C/C=C(\C)/CO)CC=C(C)C	-8.6	*Eurotium cristatum*
62	**M62**	C1=C[C@H]2[C@H](OC1(C)C)C[C@@H]1[C@@H](C2)[C@@H]2C[C@]34[C@@H](C[C@]5(N(C3=O)CCC5)C(=O)N4)C([C@H]2[NH2+]1)(C)C	-8.6	*Aspergillus versicolor*
63	**M63**	c1cccc(c1O)C1=N[C@@H](CO1)[C@@H]1SC[C@@H](N1C)CN1[C@@H]2C(=O)N([C@H](C1=O)CSSC2)C[C@@H]1N([C@H](SC1)[C@H]1N=C(OC1)c1c(O)cccc1)C	-8.6	*Streptomyces olivaceus*

64	**M64**	C1[C@@H](C[C@]2([C@](C1)([C@@H]1[C@@H](CC2=O)[C@H]2[C@](CC1)([C@H](CC2)[C@@H](/C=C/[C@@H](C(C)C)C)C)C)C)O)O	-8.6	*Aspergillus terreus* GX7-3B
65	**M65**	CC(=CC[N@H+]1[C@H]2C[C@H](CC[C@H]2[C@H]2[C@@H]1[C@H](C=C(C)C)N1C(=O)[C@@H]3CCCN3C(=O)[C@@]1(C2=O)O)OC)C	-8.6	*Neosartorya laciniosa* KUFC 7896
66	**M66**	[C@@H]1([C@H](C[C@@H]2[C@H](C1)[C@@H](C[NH2+]2)[C@@H]1[C@H]([C@H]([NH2+]C1)C(=O)OC)[C@@H]1[C@@H]2[C@H]([NH2+]C1)CC[C@@H](C2)Cl)Cl)Cl	-8.6	*Marine actinomycete* NPS12745
67	**M67**	c1ccc2c(c1O)C(=O)c1c([OH+]2)cc(c2c1O[C@@H]1[C@H]2C=CO1)OC	-8.6	*Aspergillus* sp. MF-93
68	**M68**	c1ccc2c(c1)[C@@]1([C@@H]3N2C(=O)[C@H](N3C(=O)[C@H](C1)[N+]1C(=O)c2c(N=C1)cccc2)[C@H](CC)C)O	-8.5	*Aspergillus versicolor* LZD-14-1
69	**M69**	C1(=C2[C@]34[C@H](C(=O)[C@H](CC1)C)[C@H]([C@@H]1[C@@]3(OC2=O)C[C@@H]([C@]([C@H]1O)(C)O4)C)S[C@@H]1CC(=O)[C@H](CCC(=O)C2=C3[C@]4([C@@H]1[C@@H]([C@@]([C@H](C4)C)(C)O3)O)OC2=O)C)O	-8.5	*Streptomyces koyangensis* SCSIO 5802
70	**M70**	C1=Cc2c(OC1(C)C)cc1c(c2)[C@]2(C(=N1)C([C@H]1[C@]3(C2)C(=O)N2[C@](C1)(C(=O)N3)CCC2)(C)C)O	-8.5	*Aspergillus versicolor*
71	**M71**	c12cccc3c1c(c(=O)[n+]2C)c1c(c3)C([N+]2C1=NC(=CC2=O)C)(C)C	-8.5	*Penicillium commune* DFFSCS026
72	**M72**	[C@@H]1(CC[C@@H]2[C@H](C1)[C@H]([C@H]1[C@H]([C@@]2(C)O)OC2=C(C1=O)C(=O)[NH+]C=C2c1ccc(cc1)O)/C=C/C)C	-8.5	*Campylocarpon* sp. HDN13-307
73	**M73**	C/C/1=C/C[C@@H](/C(=C\[C@@H]2[C@H](C=C(C[C@]32C(=O)/C(=C(\[C@]2(C)[C@H]1C=C[C@H]1[C@H]2[C@@H](C)C[C@H](C)[C@@H]1O[C@H]1C[C@H]([C@H]([C@H](COC(=O)C)O1)OC(=O)C)O[C@H]1CC[C@H]([C@H](C)O1)O[C@@H]1C[C@H]([C@H]([C@H](C)O1)O[C@H]1CC[C@H]([C@H](C)O1)O)O)/O)/C(=O)O3)C=O)O)/C)O[C@H]1C[C@@](C)([C@H]([C@@H](C(=O)OC)O1)N)N(=O)=O	-8.5	*Micromonospora carbonacea* LS276
74	**M74**	Cc1cc(c2c(c1)[OH+]C1=C([C@@H]3[C@@H]4[C@H](C1)[C@](C(=O)OC)(O)O[C@@]4(C1=C3[OH+]c3cc(C)cc(c3C1=O)O)C(=O)OC)C2=O)O	-8.5	*Penicillium purpurogenum* G59
75	**M75**	C1C[C@H]2[C@H](CC1)[C@H](C[NH2+]2)[C@@]1([C@@H]2CCCC[C@@H]2NC1=O)C1=CN[C@H]2[C@@H]1C=CC=C2	-8.4	*Shewanella piezotolerans*
76	**M76**	c1ccc2c(c1)[C@@]1([C@@H]3N2C(=O)[C@H](N3C(=O)[C@H](C1)[N+]1C=Nc2c(C1=O)cccc2)[C@H](CC)C)O	-8.4	*Aspergillus versicolor* LZD-14-1
77	**M77**	c1(=C)c(=C)c(=C)[n+]2c([nH]1)[C@H](NC(=O)[C@H]2C[C@@]1([C@H]2N(c3c1cccc3)C(=O)[C@@H](N2)[C@@H](CC)C)O)C	-8.4	*Aspergillus versicolor* LZD-14-1
78	**M78**	C1=C[C@@]23C(=NC4=C(NC(=C)[C@@H](N4[C@@]42O[C@H](CO3)C(O4)(C)C)Cc2ccccc2)C(C)C)OC=C1	-8.4	*Paecilomyces variotii*
79	**M79**	C1=Cc2c(OC1(C)C)cc1c(c2)[C@@]2(C(=O)N1)C([C@@H]1[C@@]3(C2)C(=O)N2[C@@](C1)(C(=O)N3)CCC2)(C)C	-8.4	*Aspergillus versicolor*

80	**M80**	C1=C[C@H]2[C@H](OC1(C)C)C[C@H]1[C@@H](C2)[C@H]([C@H]([NH2+]1)C(C)(C=C)C)C[C@H]1C(=O)N2[C@@H](C(=O)N1)CCC2	-8.4	*Aspergillus versicolor*
81	**M81**	[C@@H]1(CC[C@H]2[C@H](C1)[C@H]([C@@]1(C=C2C)C(=O)C2=C(O1)C(=C[NH+]C2=O)c1ccc(cc1)O)/C=C/C)C	-8.4	*Campylocarpon* sp. HDN13-307
82	**M82**	C1[C@H]2[C@H]3[C@@]4(C(=O)N2)[C@H](C=C([C@]3([C@@H]2[C@@H]1[C@@H]1[C@H]([NH2+]2)CCCC1)C)C)/C=C/C[C@H](C)/C=C(/C(=O)C(=O)CCC4=O)\C	-8.4	*Penicillium chrysogenum* V11
83	**M83**	O1C(=O)CC[C@]2([C@](C1(C)C)([C@@H](C[C@]1([C@@H]2Cc2c(O1)c(c1c(c2OC)C(=O)OC1)C)C)O)O)C	-8.4	*Aspergillus aureolatus* HDN14-107
84	**M84**	C1CC(=O)C=C2[C@]1([C@@H]1C(=C3[C@](CC1)([C@H](CC3)[C@H](/C=C/C(=C)C(C)C)C)C)C=C2)C	-8.4	*Aspergillus* sp.
85	**M85**	c1cc(c2c(c1)C(=O)c1c(C2=O)c(c2c(c1O)c1c(C[C@H]2OC(=O)C(C)C)cc2c(c1O)C(=O)O[C@H](C2)C)OC)O	-8.4	*Streptosporangium* sp.
86	**M86**	c1cc(c2c(c1)C(=O)c1c(C2=O)c(c2c(c1O)c1c(C[C@H]2OC(=O)CC)cc2c(c1O)C(=O)O[C@H](C2)C)OC)O	-8.4	*Streptosporangium* sp.
87	**M87**	c12c(c(ccc1O)[C@@H]1CCC(=O)c3c1cccc3O)C(=O)[C@](C2=O)(CC(=O)C)O	-8.4	*Cladosporium cladosporioides* HDN14-342
88	**M88**	N1C(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H]2N(C(=O)[C@@H](OC(=O)[C@@H](N(C(=O)[C@@H]1Cc1ccc(cc1)OCCC(=C)C)C)C)Cc1ccccc1)CCC2)C)C)[C@H](CC)C	-8.4	*Bionectria ochroleuca*
89	**M89**	C[C@H]1C/C=C/[C@H]2[C@H]3[C@@](C)([C@@H](C)[C@H]4[C@H](Cc5cccc5)N=C([C@@]24C(=O)/C=C/C(=O)[C@@H](/C(=C/1)/C)OC(=O)C)O)O3	-8.4	*Jishengella endophytica* 161111
90	**M90**	Cc1cc(cc(c1C(=O)c1c2c3cc(cc(c3c(=O)c3c(cc(C)c(c23)[oH+]c1=O)O)O)O)O)O	-8.4	*Aspergillus glaucus*
91	**M91**	N1C(=O)[C@@]2(c3cc(c4c(c13)C=CC(O4)(C)C)Cl)C([C@H]1[C@]3(C(=O)N4CCC[C@]4(C1)C(=O)N3)[C@H]2O)(C)C	-8.4	*Aspergillus westerdijkiae* DFFSCS013
92	**M92**	c1c(c(ccc1)O)/C=C/1\NC(=O)[C@@]2(NC1=O)Cc1c(O2)cccc1	-8.4	*Hansfordia sinuosae*
93	**M93**	c1ccc2c3c1O[C@]14c5c(C(=O)[C@@H]6[C@H]1O6)c(ccc5O[C@]3([C@@H](CC2=O)O)O)O4)O	-8.4	*Lasiodiplodia theobromae* ZJ-HQ1
94	**M94**	c1cc(c2c3c1c1c4c(c3C=CC2=O)[C@H]([C@H](Oc4c(cc1)O)C(=O)O)O)O	-8.4	*Alternaria* sp.
95	**M95**	c1cc(c2c3c1c1c4c(c3C=CC2=O)C[C@](Oc4c(cc1)O)(C(=O)O)O)O	-8.4	*Alternaria* sp.
96	**M96**	Cc1cc(cc(c1C(=O)c1c2c3cc(cc(c3c(=O)c3c(cc(C)c(c23)[oH+]c1=O)O)O)O)O)O	-8.4	*Aspergillus glaucus*
97	**M97**	C[C@H]1C(=O)N2[C@@H]3N1[C@H]1C4=Nc5ccccc5C(=O)[N+]4[C@@H](C[C@]3(c3ccccc23)O)C(=O)N1	-8.4	*Aspergillus versicolor* MST-MF495
98	**M98**	c1(ccc(cc1)C[C@@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)O)C(C)C)C[C@H]1[C@@H]2[C@H]([NH2+]C1)CCCC2)N)O	-8.3	*Aspergillus* sp. SCSIO 41501
99	**M99**	c1ccc2c(c1)c1c([nH+]2)c([nH]c(c1)C(=O)O)c1cc(oc1)CO	-8.3	*Jishengella endophytica* 161111
100	**M100**	c1ccc2c(c1)N=C1[N+](C2=O)[C@H]2C[C@]3([C@@H]4N([C@@H]1NC2=O)[C@H](C(=O)N4c1c3cccc1)CO)O	-8.3	*Aspergillus versicolor* LZD-14-1

101	**M101**	[C@@H]1(CC[C@H]2[C@H](C1)[C@H]([C@]1(C=C2C)C(=O)C2=C(O1)C(=C[NH+]C2=O)c1ccc(cc1)O)/C=C/C)C	-8.3	*Campylocarpon* sp. HDN13-307
102	**M102**	[C@@H]1(CC[C@@H]2[C@H](C1)[C@H]([C@H]1[C@H]([C@]2(C)O)OC2=C(C1=O)C(=O)[NH+]C=C2c1ccc(cc1)O)/C=C/C)C	-8.3	*Campylocarpon* sp. HDN13-307
103	**M103**	c12c(c(ccc1O)[C@@H]1CCC(=O)c3c1cccc3O)C(=O)[C@H]([C@@H]([C@@H]2OC)O)Cl	-8.3	*Cladosporium cladosporioides* HDN14-342
104	**M104**	c12c(cc(cc1[OH+]C1=C(C2=O)[C@]2([C@H]3[C@@H]1C1=C(C[C@H]3[C@@](O2)(C(=O)OC)O)[OH+]c2c(C1=O)c(cc(c2)C)O)C(=O)OC)C)O	-8.3	*Penicillium* sp. ZJ-SY2
105	**M105**	[C@@]123[C@H]([C@@]4(c5ccccc5N[C@@H]4N1C(=O)[C@](SS2)(N(C3=O)C)[C@H](C)O)[C@]12[C@@H]([C@]34N([C@H]2Nc2c1cccc2)C(=O)[C@](SS3)(N(C4=O)C)[C@H](C)O)O)O	-8.3	*Bionectria ochroleuca*
106	**M106**	[C@@H]12C[C@H]3[C@@H]4CC[C@@H](C[C@@H]4[NH2+][C@@H]3[C@@H](N1C(=O)[C@@H]1CCCN1C2=O)C=C(C)C)OC	-8.3	*Aspergillus* sp. BRF 030
107	**M107**	C1[C@@H](C[C@]2([C@](C1)([C@@]1([C@@H](CC2=O)[C@@H]2[C@](CC1)([C@H](CC2)[C@@H](/C=C/[C@@H](C(C)C)C)C)C)O)C)O)O	-8.3	*Aspergillus versicolor* ZBY-3
108	**M108**	c1ccc2c3c1O[C@]14c5c(C(=O)[C@H]([C@H]1O)Cl)c(ccc5O[C@]3([C@@H](CC2=O)OC)O4)O	-8.3	*Lasiodiplodia theobromae* ZJ-HQ1
109	**M109**	c1ccc2c3c1O[C@]14c5c(C(=O)[C@@H]6[C@H]1O6)c(ccc5O[C@]3(CCC2=O)O4)O	-8.3	*Lasiodiplodia theobromae* ZJ-HQ1
110	**M110**	c1ccc2c3c1O[C@]14c5c(C(=O)[C@@H]6[C@H]1O6)c(ccc5O[C@]3(C=CC2=O)O4)O	-8.3	*Lasiodiplodia theobromae* ZJ-HQ1
111	**M111**	[C@@H]1(CC[C@@H]2[C@H](C1)[C@@H](C[NH2+]2)[C@@H]1[C@H]([C@H]([NH2+]C1)C(=O)OC)[C@@H]1[C@@H]2[C@H]([NH2+]C1)CC[C@@H](C2)Cl)Cl	-8.3	*Marine actinomycete* NPS12745
112	**M112**	N1([C@H](C(=O)Nc2c(C(=O)N3[C@H](C(=O)Nc4c(C(=O)N[C@H](C1=O)C)cccc4)CCC3)cccc2)C)C	-8.2	*Aspergillus versicolor* LZD-14-1
113	**M113**	C1(=O)C[C@H]([C@@H]2[C@@]34C(=C(C(=O)CC[C@@H]1C)C(=O)O3)O[C@@]([C@H](C4)C)([C@H]2O)C)[C@@H]1C(=O)C(=C(O1)O)C	-8.2	*Streptomyces koyangensis* SCSIO 5802
114	**M114**	C1CC[C@@H]2[C@H](C1)[C@@H]([C@H]([NH2+]2)C(C)(C=C)C)/C=C\1/[NH+]C(=O)/C(=C/C)/[NH+]C1=O	-8.2	*Eurotium* sp. SCSIO F452
115	**M115**	C1=Cc2c(OC1(C)C)cc1c(c2)[C@](C(=O)N1)(C[C@H]1C(=O)N2[C@H](C(=O)N1)CCC2)C(C)(C)C=C	-8.2	*Aspergillus versicolor*
116	**M116**	c12cccc3c1[C@@](C(=O)N2)([C@H]1[C@@H](C3)CNC1=O)O	-8.2	*Penicillium commune* DFFSCS026
117	**M117**	C1([C@@H](CC[C@]2([C@@H]1CC[C@@]1([C@@H]2Cc2c(O1)c(c1c(c2O)C(=O)OC1)C)C)C)O)(C)C	-8.2	*Aspergillus aureolatus* HDN14-107
118	**M118**	[C@@H]1(C([C@H]2[C@](CC1)([C@@]1([C@@H](CC2)C)Oc2c(C1)c(cc1c2CN(C1=O)CCCC(=O)OC)O)C)(C)C)O	-8.2	*Stachybotrys chartarum* 952

119	**M119**	C1(=C([C@H](OC1=O)O)c1ccc(cc1)O)Cc1ccc2c(c1)CCC(O2)(C)C	-8.2	*Aspergillus terreus*
120	**M120**	N12C(=O)[C@H](OC(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H]1CCC2)CO)C)C(C)C)Cc1ccc(cc1)OCC=C(C)C)C)C)Cc1ccccc1	-8.2	*Bionectria ochroleuca*
121	**M121**	CC[C@@H](C)[C@@H]1C(=O)N(C)[C@H]([C@H](c2ccccc2)O)/C(=N/c2ccccc2/C(=N/[C@H](C)/C(=N/1)/O)/O)/O	-8.2	*Aspergillus terreus* SCSGAF0162
122	**M122**	C[C@]1(c2cccc(c2C(=C2[C@@H]1C[C@H]1[C@@H](C(=O)C(=C([C@]1(C2=O)O)O)C(=N)O)N(C)C)O)O)O	-8.2	*Streptomyces* BL 567201
123	**M123**	C1C2=C[C@@H]([C@@H]3[C@@H]([C@]2(CC[C@@H]1O)C)CC[C@]1([C@H]3CC[C@H]1[C@@H](/C=C/[C@H](C(C)C)C)C)C)O	-8.1	*Aspergillus* sp.
124	**M124**	[C@H]1(C(=O)NCC(=O)N([C@H](C(=O)N[C@H](C(=O)N1C)C)c1ccccc1)C)Cc1ccccc1	-8.1	*Aspergillus versicolor* LZD-14-1
125	**M125**	c1(ccccc1)C[C@@H](N(C(=O)[C@@H](N)[C@@H](CC)C)C)C(=O)N[C@H](C(=O)Nc1ccccc1C(=O)O)C(C)C	-8.1	*Simplicillium obclavatum* EIODSF 020
126	**M126**	N1[C@H](C2=Nc3c(C(=O)[N+]2[C@@H]2[C@@H](C1=O)C=CC=C2)cccc3)CCC(=O)N	-8.1	*Penicillium aurantiogriseum*
127	**M127**	c1ccc2c(c1)[C@@]1(C(=N2)C([C@@H]2[C@@]3(C1)CN1[C@@](C2)(O[NH2+]3)CCC1)(C)C)O	-8.1	*Penicillium purpurogenum* G59
128	**M128**	c1ccc2c(c1)[C@@]13C(=N2)C([C@H]2[C@](C1)([C@@H](N1[C@H](C2)CCC1)C#N)NC(=O)O3)(C)C	-8.1	*Aspergillus versicolor*
129	**M129**	C(C[C@@H](CCCCCC/C=C/C(=O)N[C@@H]1[C@H](O[C@@H]([C@@H]([C@@H]1O)O)C[C@@H](O)[C@@H]1[C@@H]([C@@H]([C@@H](O1)[N+]1C(=O)[NH+]C(=O)C=C1)O)O)O[C@@H]1O[C@H]([C@@H]([C@@H]([C@@H]1NC(=O)C)O)O)CO)C)C	-8.1	*Streptomyces xinghaiensis* SCSIO S15077
130	**M130**	C[C@@H]1C2=Nc3c(cccc3O)C(=O)[N+]2c2ccccc2C(=O)N1	-8.1	*Aspergillus westerdijkiae* SCSIO 05233
131	**M131**	CC(C)C[C@@H](c1ccc2c(c1OC)C(=O)OCc1cc(C)cc(c1O2)O)O	-8.1	*Penicillium* sp. ZLN29
132	**M132**	C1CC[C@H]2[C@H](C1)[C@H](C[N@H+]2C)C(=O)N1CCN(CC1)[C@@H]1[C@H](CCCC1)OC	-8.1	*Aspergillus sydowii* SCSIO 00305
133	**M133**	COc1ccc2C=C(C(=O)[OH+]c2c1OC)NC(=O)C1=NO[C@H]2[C@@H](C=C[C@H]([C@]2(C1)O)Cl)O	-8.1	*Trichoderma virens*
134	**M134**	C1(=C)C[C@@H]2[C@H]([C@H]3[C@@H]1C[C@@H]3C(O)(C)C)[C@H]1[C@@H](CC2)[NH2+][C@@H]2[C@H]1[C@H]([C@H]1[C@]2([C@@]2([C@@](CC1)([C@]13[C@H](CC2)O[C@@H]([C@@H]([C@H]1O3)O)C(=C)C)O)C)C)OC	-8.1	*Mucor irregularis* QEN-189
135	**M135**	CC[C@H](C)C(=O)O[C@H]1CCC=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@H](CC(=O)O3)O)[C@@H]12	-8.1	*Penicillium solitum*
136	**M136**	c1(ccccc1)C[C@H]1N(C(=O)[C@@H](OC(=O)[C@@H](NC(=O)[C@@H](OC(=O)[C@@H](N(C(=O)[C@H](NC1=O)C)C)C)C(C)(C)O)C)CC(C)C)C	-8.1	*Spicellum roseum*

137	**M137**	COc1ccc2c(c1)[nH]c1c2[C@@H]([C@@]2(N([C@H]1C=C(C)C)C(=O)[C@@H]1CCCN1C2=O)O)O	-8	*Aspergillus* sp.
138	**M138**	c1(ccc(cc1)O)C[C@@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)O)C(C)C)C(C)C)C)N	-8	*Aspergillus* sp.
139	**M139**	c1(ccccc1)C[C@H](N(C(=O)[C@@H](N)C(C)C)C)C(=O)N[C@H](C(=O)Nc1ccccc1C(=O)O)CC(C)C	-8	*Simplicillium obclavatum* EIODSF 020
140	**M140**	c1cc(ccc1)C[C@@H]1NC(=O)CN(C(=O)[C@H]2N(C(=O)[C@H](N(C(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](N(C1=O)C)Cc1ccc(cc1)O)C(C)C)CC(C)C)C)Cc1ccccc1)CCC2)C	-8	*Acremonium persicinum* SCSIO115
141	**M141**	c1ccc2c(c1)c1c([nH+]2)c([nH]cc1)c1cc(oc1)CO	-8	*Jishengella endophytica* 161111
142	**M142**	c1ccc(c(c1)C(=O)OC)[N+]1C(=Nc2c(C1=O)cccc2)[C@@H]1CCC(=[NH2])N1	-8	*Penicillium aurantiogriseum*
143	**M143**	C1[C@@H](C[C@H]2[C@@H](C1)[C@H]([C@H]([NH2+]2)C(C)(C)C=C)C[C@@H]1C(=O)N[C@@](C(=O)N1)(C)OC)CC=C(C)C	-8	*Eurotium cristatum*
144	**M144**	O1[C@@H](CC(=O)O[C@@H](CC(=O)Cc2c(C1=O)c(cc(c2)O)O)C)C	-8	*Hansfordia sinuosae*
145	**M145**	c12c(c(ccc1O)[C@@H]1CCC(=O)c3c1cccc3O)C(=O)CC[C@@H]2OC	-8	*Cladosporium cladosporioides* HDN14-342
146	**M146**	c1c(cc2c(c1O)C(=O)c1c(C2=O)cc(cc1O)O)C[C@H](O)C	-8	*Penicillium* sp. SCSGAF 0023
147	**M147**	c1ccc2c(c1O)C(=O)c1c(C2=O)cc(c(c1O)[C@@H](CCO)CO)O	-8	*Aspergillus* sp. F40
148	**M148**	c1cc(c2c(c1)[OH+]c1c(C2=O)c(cc2c1[C@]1([C@@](O2)(O[C@@H](C1)OC)C)C)OC)O	-8	*Aspergillus* sp. F40
149	**M149**	C1C[C@](c2c(C1)c1c(c(c2)O)[C@@H]2[C@](CC1)([C@@H](CO2)O)C)(C)CO	-8	*Aspergillus wentii* SD-310
150	**M150**	C1C[C@](c2c(C1)c1c(c(c2)O)[C@@H]2[C@](CC1)([C@H](CO2)O)C)(C)CO	-8	*Aspergillus wentii* SD-310
151	**M151**	C[C@H]1C[C@H]2[C@H](C)Oc3c(cnc(c3[C@@H]2[C@@H](C)[C@@H]1O)O)c1ccc(cc1)O	-8	*Chaunopycnis* sp. CMBMF028
152	**M152**	N1C(=O)[C@@]2(c3ccc4c(c13)C=CC(O4)(C)C)C([C@H]1[C@]3(C(=O)N4CCC[C@]4(C1)C(=O)N3)[C@@H]2O)(C)C	-8	*Aspergillus westerdijkiae* DFFSCS013
153	**M153**	c1ccc2c(c1)C1=C(C2)[C@]2([C@H](C1)CC[C@@H]1[C@@]2(CC[C@H]2C1=C[C@H]([C@H](C2)C(C)(C)O)O)C)C	-8	*Mucor irregularis* QEN-189
154	**M154**	C[C@@H]1CCC/C=C\[C@@H]2CCC[C@H]2[C@H](/C=C\C(=O)O1)O	-8	*Penicillium* sp. PSU-F44
155	**M155**	O=c1c2ccccc2ncn1[C@H]1C(=O)N([C@@H]2[C@@](C1)(O)c1ccccc1N2)[C@H](C)C(=O)OC	-8	*Penicillium* sp.
156	**M156**	c12c(cccc1)c(c[nH]2)C[C@H]1C(=O)N2[C@H](C(=O)N1)CCC2	-7.9	*Aspergillus* sp.
157	**M157**	C1C[C@@H]2[C@H](CC1)[C@@H](C[NH2+]2)[C@]1([C@@H]2CCCC[C@H]2NC1=O)OC	-7.9	*Shewanella piezotolerans*
158	**M158**	c1ccc2c(c1)N=C1[N+](C2=O)[C@H](C(=O)NC1)C[C@]12c3c(cccc3)N3[C@H]1N(C1(C3=O)CC1)CO2	-7.9	*Aspergillus versicolor* LZD-14-1

159	**M159**	[C@H]1([C@]23N([C@@H]4[C@]1(c1c(N4)cccc1)[C@@]14c5c(N[C@@H]1N1[C@]6([C@H]4O)C(=O)N([C@@](C1=O)(CO)[S@@]6=S=S)C)cccc5)C(=O)[C@@](N(C2=O)C)(C)[S@]3=S=S)O	-7.9	*Acrostalagmus luteoalbus* HDN13-530
160	**M160**	C1CC[C@H]2[C@@H](C1)[C@H](C[N@H+]2C/C=C(\C)/CO)C[C@H]1C(=O)N[C@H](C(=O)N1)C	-7.9	*Eurotium cristatum*
161	**M161**	c12cccc3c1[C@@]1(C(=O)N2C)[C@H]2[C@@H](C3)C(N3[C@]2([C@](O1)([C@](C3=O)([C@H](C)O)O)O)O)(C)C	-7.9	*Penicillium commune* DFFSCS026
162	**M162**	C1CC[C@H]2[C@H](C1)[C@H]1[C@H]([NH2+]2)C([C@@H]2[C@]3(C1)CN1[C@@](C2)(O[NH2+]3)CCC1)(C)C	-7.9	*Penicillium purpurogenum* G59
163	**M163**	[C@H]1([C@H]([C@H]([C@@H]([C@H]2[C@@]1(C=C([C@H]([C@@H]2/C=C(/C(=O)O)\C)/C(=C/C[C@@H](C[C@H]([C@@H]([C@H](C(C)C)O)C)O)O)/C)C)C)C)O)O)O	-7.9	*Streptomyces* sp. SCSGAA 0027
164	**M164**	[C@H]1(CC[C@@H]([C@H]2[C@@]1(C=C([C@H]([C@@H]2/C=C(/C(=O)O)\C)/C(=C/C[C@@H](C[C@H]([C@@H]([C@H](C(C)C)O)C)O)O)/C)C)C)C)O	-7.9	*Streptomyces* sp. SCSGAA 0027
165	**M165**	c1(c(cc2c(c1C)c(c1c(c2)[C@@H](OC1=O)[C@]1([C@@H](C(=CC(=O)[C@@H]1OC)OC)O)O)O)OC)C(=O)OC	-7.9	*Saccharothrix* sp. 10-10
166	**M166**	C1(=C([C@H](OC1=O)OC)c1ccc(cc1)O)Cc1ccc(c(c1)CC=C(C)C)O	-7.9	*Aspergillus terreus*
167	**M167**	c1cc(c2c(c1)C(=O)c1c(C2=O)c(c2c(c1O)c1c(C[C@H]2O)cc(c(c1O)C(=O)O)CC(=O)C)OC)O	-7.9	*Streptosporangium* sp.
168	**M168**	c1c(cc2c(c1O)[OH+]C(=CC2=O)c1c(c(cc(c1)O)O)O)O	-7.9	*Penicillium* sp. SCSGAF 0023
169	**M169**	C1(=O)[C@@]([C@@H]([C@@H]2C(=C1)C=C(OC2)/C=C/[C@@]([C@H]([C@H](CC)C)O)(O)C)O)(O)C	-7.9	*Penicillium sclerotiorum* M-22
170	**M170**	C(=O)(c1ccc(cc1)[N](=O)O)O[C@H]1[C@@H]2[C@@]([C@@]3(C(=C1)C(=O)OC3)O)(CCC[C@]2(C)CO)C	-7.9	*Aspergillus ochraceus* Jcma1F17
171	**M171**	N1C(=O)[C@@H](NC(=O)/C/1=C/[C@@H]1[C@H]([NH2+][C@H]2[C@@H]1CCCC2)C(C)(C=C)C)C	-7.9	*Microsporum* sp. MFS-YL
172	**M172**	c1ccc2c3c1O[C@]14c5c([C@H]([C@@H]6[C@H]1O6)O)c(ccc5O[C@]3(C=CC2=O)O4)O	-7.9	*Lasiodiplodia theobromae* ZJ-HQ1
173	**M173**	C1[C@@H](C(c2c(C1)c1c(c(c2)O)[C@@H]2[C@](CC1)([C@@H](CO2)O)C)(C)C)O	-7.9	*Aspergillus wentii* SD-310
174	**M174**	C1CC(c2c(C1)c1c(c(c2)O)[C@@H]2[C@](CC1)([C@@H](CO2)O)C)(C)C	-7.9	*Aspergillus wentii* SD-310
175	**M175**	COc1cc2cc3COC(=O)c3c(c3ccc4c(c3)OCO4)c2cc1OC	-7.9	*Nocardia* sp. ALAA 2000
176	**M176**	CC(=C[C@H]1[C@]2(C=C3C(=O)N4CCC[C@H]4C(=O)N13)c1ccc(cc1N=C2O)OC)C	-7.9	*Aspergillus sydowi* PFW1-13
177	**M177**	[C@@H]1(O)CC2=CC(=O)C3=C([C@]2(CC1)C)CC[C@]1([C@@H]3CC[C@@H]1[C@@H](/C=C/[C@@H](C(C)C)C)C)C	-7.8	*Aspergillus* sp.
178	**M178**	CC/C=C\[C@@H]([C@@H](C1=C(C(=O)[C@]2(O1)C(=O)N([C@]([C@@H]2O)(C(=O)c1ccccc1)OC)C(=O)Cc1ccccc1)O)O)O	-7.8	*Aspergillus* sp.

179	**M179**	C1(=O)[C@H](NC(=O)CC(=O)/C=C/C[C@H](OC(=O)[C@@H]2N1CCC2)CCC)Cc1ccccc1	-7.8	*Sarocladium kiliense* HDN11-112
180	**M180**	C1(=O)[C@H](N(C(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]2N(C(=O)[C@@H](N1)C(C)C)CCC2)Cc1ccc(cc1)OC)Cc1ccc(cc1)OC)C)Cc1ccc(cc1)O	-7.8	*Aspergillus* sp. SCSIO 41501
181	**M181**	c12cccc3c1c(c(=O)[nH+]2)c1c(c3)C(N(C1=O)C(=O)CC(=O)C)(C)C	-7.8	*Penicillium commune* DFFSCS026
182	**M182**	c12cccc3c1c(c(=O)[nH+]2)c1c(c3)C(NC1=O)(C)C	-7.8	*Penicillium commune* DFFSCS026
183	**M183**	c1cc(ccc1C(=O)OC[C@@]1([C@H]2[C@](CCC1)([C@@]1([C@@H](C[C@H]2O)C(=O)OC1)O)C)C)[N](=O)O	-7.8	*Aspergillus ochraceus* Jcma1F17
184	**M184**	c1(c(cc2c(c1C)c(c1c(c2)[C@H](OC1=O)[C@]1([C@@H](C(=CC(=O)[C@@H]1O)OC)O)O)O)OC)C(=O)OC	-7.8	*Saccharothrix* sp. 10-10
185	**M185**	[C@@H]1(CC[C@@H](O[C@@H]1C)O[C@H]1[C@](C[C@@H](O[C@@H]1C)O[C@H]1[C@@H]([C@H](O[C@H](C1)c1c(c2c(cc1)C(=O)C1=C(C2=O)[C@@H]([C@@H]([C@@]2([C@]1([C@H](C=C(C2)C)O[C@H]1O[C@H]([C@H]([C@@H](C1)OC)O)C)O)O)CC(=O)C)C)O)C)O)(O)C)OC(=O)N	-7.8	*Streptomyces pratensis* NA-ZhouS1
186	**M186**	C1(=O)OC(C2=CC(=O)[C@]3([C@H]([C@@]4(C2=C1)CO4)C[C@@]1([C@@H]2[C@H]3C(=O)[C@H](O[C@@H]2OC1=O)C)C)(C)C	-7.8	*Talaromyces amestolkiae* YX1
187	**M187**	c1c(cc(c(c1CCC(=O)/C=C/C)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1c(c(cc(c1)O)O)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1cc(cc(c1)O)O)C)C)C)C)O)O	-7.8	*Hansfordia sinuosae*
188	**M188**	c12c(c(ccc1O)[C@@H]1CCC(=O)c3c1cccc3O)C(=O)[C@@](C2=O)(CC(=O)C)O	-7.8	*Cladosporium cladosporioides* HDN14-342
189	**M189**	[C@@H]1([C@](C[C@H]2[C@]3(C([C@H](CC[C@]13C)Cl)(C)C)O2)(C)OCc1c(c2c([C@H](OC2=O)OC)c(c1O)C=O)OC)C(=O)O	-7.8	*Acremonium strictum*
190	**M190**	C12=CC(=O)OC(C1=C[C@@H]1[C@]3([C@H]([C@H]2C)C[C@@]2([C@@H]4[C@]3([C@@]([C@@H](O[C@@H]4OC2=O)C)(O1)O)C(=O)OC)C)C)(C)C	-7.8	*Penicillium* sp. 303
191	**M191**	[C@]12([C@H]([C@H]3[C@@H]4CC[C@@H](C[C@@H]4[NH2+][C@@H]3[C@@H](N1C(=O)[C@H]1CCCN1C2=O)C=C(C)C)OC)O)O	-7.8	*Aspergillus* sp. BRF 030
192	**M192**	CC(=CCc1ccc2c(c1OC)C(=O)OCc1cc(C)cc(c1O2)O)C	-7.8	*Penicillium* sp. ZLN29
193	**M193**	[C@@H]12[C@H]3CC[C@@H]([C@]3(CC[C@H]1[C@]1(CC[C@@H](C[C@]31O[C@H]3C2=O)O)C)C)[C@H](C)/C=C/[C@H](C(C)C)C	-7.8	*Paecilomyces lilacinus* ZBY-1
194	**M194**	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)OC)O	-7.8	*Microsporum* sp. MFS-YL
195	**M195**	[C@@H]12OC3=C(C(=O)[NH+]C=C3c3ccc(cc3)O)C(=O)[C@@H]1[C@@H]([C@H]1C[C@H](CC[C@@H]1[C@]2(C)O)C)/C=C/C	-7.8	*Campylocarpon* sp. HDN13-307
196	**M196**	c1(ccccc1O)C(=O)[C@@H]1[N@H+]([C@H]([C@H](C1)Cl)Cl)[C@@H]1[C@H]([C@H]([NH2+][C@@H]1C(=O)[C@H]1CCCC[C@@H]1O)Cl)Cl	-7.8	*Actinomycete* strain CNQ-418
197	**M197**	CC(=CC(=O)[C@@H]1[C@H](C[C@H]2C(=O)N3CCC[C@H]3C(=N2)O)[C@@H]2CC[C@@H](C[C@@H]2[NH2+]1)OC)C	-7.8	*Aspergillus sydowi* PFW1-13

198	**M198**	O=c1c2ccccc2ncn1[C@H]1C(=O)N([C@@H]2[C@@](C1)(O)c1ccccc1N2)[C@H](C)C(=O)O	-7.8	*Penicillium* sp.
199	**M199**	O[C@@H]1CC2=CC=C3[C@H]4[C@@]([C@H](CC4)[C@H](C)/C=C/[C@@H](C(C)C)C)(CC[C@@H]3[C@]2(CC1)C)C	-7.7	*Aspergillus* sp.
200	**M200**	C[C@@H]1CCC/C=C/C=C/[C@@H](C[C@H]([C@@H](/C=C\C=C\[C@@H](C/C=C/C=C\C(=O)O1)O)O)O)O	-7.7	*Bacillus amyloliquefaciens* SCSIO 00856
201	**M201**	C[C@@H]1[C@H](OC=C2C1=C(C(=C(C2=O)CC1=C(C(=C([OH+]C1=O)C)C)O)O)C)C	-7.7	*Aspergillus* sp. 16-02-1
202	**M202**	[C@@H]12[C@H](CC(=O)[C@H](CCC1=O)C)[C@@H]1[C@@]3(OC2=O)C[C@@H]([C@]([C@H]1O)(C)OC3=O)C	-7.7	*Streptomyces koyangensis* SCSIO 5802
203	**M203**	c12c(cccc1)N=C([N+](C2=O)c1c(cccc1)C(=O)O)[C@H]1NC(=[NH2])CC1	-7.7	*Penicillium aurantiogriseum*
204	**M204**	C[C@H]1/C=C/C(=O)O[C@H](C)[C@H](/C=C\C=C\C(=O)[C@](C)(C[C@H](C)[C@@H]1O[C@H]1[C@@H]([C@H](C[C@@H](C)O1)OC)O)O)CO[C@H]1[C@@H]([C@@H]([C@@H]([C@@H](C)O1)O)OC)OC	-7.7	*Streptomyces* sp. HK-2006-1
205	**M205**	c12cccc3c1[C@@]1(C(=O)N2C)[C@H]2[C@@H](C3)C(N3[C@]2([C@](O1)([C@](C3=O)(CC(=O)C)O)O)O)(C)C	-7.7	*Penicillium commune* DFFSCS026
206	**M206**	c1(c(cc2O[C@@]3([C@@H]([C@@H]4c2c1[C@@H]([C@H](O4)C)C)C)C(=O)/C(=C(\[C@@H](CCCCCC)C)/O)/C(=O)N3C)O)C	-7.7	*Penicillium citrinum*
207	**M207**	c1ccc2c(c1)N=C([NH+]C2=O)[C@]([C@](C(=O)Nc1c(cccc1)C(=O)N)(C)O)(O)C	-7.7	*Penicillium commune* 366606
208	**M208**	C1(=C[C@@H]2[C@]3(CC1)[C@@]1([C@]4([C@H](O2)C[C@H]1OC(=O)C/C=C/C=C(/OCC/C(=C/C(=O)OC3)/C)\C(=O)C)CO4)C)C	-7.7	*Stachybotrys chartarum*
209	**M209**	[C@]12([C@H]([C@H](C[C@H]1O)C(C)C)C[C@]1([C@H](C2)[C@H](CC[C@@H]2C3=C1C(=O)O[C@]3(C[C@@H]2C)C)C)O)C	-7.7	*Alternaria alternata* k21-1
210	**M210**	O1[C@]2(CC[C@]3([C@](C1(C)C)([C@@H](C[C@]1([C@@H]3Cc3c(O1)c(c1c(c3OC)C(=O)OC1)C)C)C(=O)OC)O2)C)O	-7.7	*Aspergillus aureolatus* HDN14-107
211	**M211**	O1[C@H]([C@H]([C@H](C[C@@H]1O[C@@H]1C[C@@](O[C@@H]([C@H]1CC)C)([C@H]([C@@H]([C@@H]([C@@H]1[C@H](/C=C/C=C/C(=C)O[C@@H]([C@H](/C=C/C=C/C(=O)O1)C)[C@H]([C@H]([C@@H]([C@]1(C[C@H]([C@@H]([C@H](O1)C)CC)O[C@H]1C[C@@H]([C@@H]([C@@H](O1)C)O)O)O)C)O)C)C)O)C)O)O)O)C	-7.7	*Streptomyces* sp. 7-145
212	**M212**	[C@@H]1(CC(=C2[C@]([C@H]1O)(Oc1c(C2=O)c(c(cc1)c1ccc2c(c1O)C(=O)C1=C(C[C@@H]([C@@H]([C@@]1(O2)C(=O)OC)O)C)O)O)C(=O)OC)O)C	-7.7	*Penicillium* sp. SCSGAF 0023
213	**M213**	C1[C@@H](C[C@@]23[C@](C1)([C@@]1(C(=C4[C@](CC1)([C@H](C[C@@H]4O)[C@@H](/C=C/[C@@H](C(C)C)C)C)C)C=C2)OO3)C)O	-7.7	*Aspergillus niger* MA-132
214	**M214**	C[C@@]1(Cc2c(C[C@H]1O)c(c1C(=O)C=C(C(=O)c1c2O)OC)O)O	-7.7	*Nigrospora* sp. 1403
215	**M215**	C(=O)([C@H](CC(C)C)NC(=O)[C@H](Cc1ccc(cc1)O)N(C)C(=O)[C@H]([C@@H](CC)C)NC(=O)C)OC	-7.7	*Simplicillium obclavatum* EIODSF 020e

216	**M216**	c1cc(ccc1[N](=O)O)C(=O)OC[C@@]1([C@H]2[C@](CCC1)([C@@]1([C@@H](C[C@H]2O)C(=O)OC1)O)C)C	-7.7	*Aspergillus ochraceus* Jcma1F17
217	**M217**	C[C@]1([C@@H](C[C@H]2[C@@H]([C@H]1O)C(=O)c1c(C2=O)c(cc(c1)OC)O)O)O	-7.7	*Stemphylium globuliferum*
218	**M218**	c1(ccccc1O)C(=O)[C@@H]1[N@H+]([C@H]([C@H]([C@@H]1Br)Cl)Cl)[C@@H]1[C@H]([C@H]([NH2+][C@@H]1C(=O)[C@H]1CCCC[C@@H]1O)Cl)Cl	-7.7	*Actinomycete* strain CNQ-418
219	**M219**	CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@H](CC(=O)O3)O)[C@@H]12	-7.7	*Aspergillus terreus*
220	**M220**	O1[C@@]2(Oc3cccc4c3c1ccc4O)[C@@H]1[C@@H]([C@@H](c3c2c(ccc3O)O)O)O1	-7.7	*Ascochyta* sp. NGB4
221	**M221**	C/C=C/C=C/C=C/C(=O)O[C@@H]1C=C2COC(=O)[C@@]2([C@@]2(C)CCCC(C)(C)[C@H]12)O	-7.7	*Aspergillus ustus*
222	**M222**	C1(=O)N[C@@H](C(=O)N2[C@H]1CCC2)Cc1ccccc1	-7.6	*Aspergillus* sp.
223	**M223**	[C@@H]1(O)C[C]23=C([C@H](O)C4=C([C@]2(CC1)C)CC[C@]1([C@@H]4CC[C@@H]1[C@@H](/C=C/[C@@H](C(C)C)C)C)C)O3	-7.6	*Aspergillus* sp.
224	**M224**	O=C1N2[C@H]([C@]3(C=C2C(=O)N2[C@H]1CCC2)c1c(NC3=O)cc(OC)cc1)C=C(C)C	-7.6	*Aspergillus* sp.
225	**M225**	c12c(cc(cc1[OH+]C1=C(C2=O)[C@]2([C@H]3[C@@H]1C1=C(C[C@@H]3[C@](O2)(C(=O)OC)O)[OH+]c2c(C1=O)c(cc(c2)C)O)C(=O)OC)C)O	-7.6	*Penicillium* sp. ZJ-SY2
226	**M226**	C(=O)(/C=C/[C@@H]1[C@@]23C(=C(C(=O)CC[C@H](C)O)C(=O)O2)O[C@@]([C@H](C3)C)([C@H]1O)C)O	-7.6	*Streptomyces koyangensis* SCSIO 5802
227	**M227**	c1(c(cc2c(c1)nc1c(n2)C(=O)[NH+]C(=O)[NH+]1)C)C	-7.6	*Jishengella endophytica* 161111
228	**M228**	C1C[C@H]2[C@@H](CC1)[C@@H](C[NH2+]2)[C@@]1([C@H]2CCCC[C@@H]2NC1=O)OC	-7.6	*Shewanella piezotolerans*
229	**M229**	c1ccc2c(c1O)N=C1[N+](C2=O)[C@H](C(=O)NC1)C[C@H]1[C@H]2[C@@H](CCCC2)[NH2+]C1	-7.6	*Aspergillus versicolor* LZD-14-1
230	**M230**	C[C@H]1CCC(=O)O[C@H](C)[C@@H](CO[C@H]2[C@@H]([C@@H]([C@@H]([C@@H](C)O2)O)OC)OC)[C@H]2[C@H](/C=C/C(=O)[C@](C)(C[C@H](C)[C@H]1O[C@H]1[C@@H]([C@H](C[C@@H](C)O1)OC)O)O)O2	-7.6	*Streptomyces* sp. HK-2006-1
231	**M231**	c1c(c(c2c(c1C(=O)OC)C(=O)c1c([OH+]2)cc(nc1)C)OC(=O)C)OC	-7.6	*Diaporthe phaseolorum* SKS019
232	**M232**	C1(=C[C@H]2[C@](CC1)([C@@]1([C@](O2)(CCC1)CO[C@H]1O[C@@H]([C@H]([C@@H]([C@@H]1O)O)O)CO)C)C)C	-7.6	*Stachybotrys chartarum*
233	**M233**	c1(c(cc2c(c1C)c(c1c(c2)[C@H](OC1=O)[C@]1([C@@H](C(=CC(=O)[C@@H]1OC)OC)O)O)O)OC)C(=O)OC	-7.6	*Saccharothrix* sp. 10-10
234	**M234**	C([C@@H](CC/C(=C/[C@@H]1O[C@H]2[C@@](C1)(OC1=C(C2)C(=O)[C@H](CC1)O)C)/C)O)(C)(C)O	-7.6	*Alternaria alternata* k21-1
235	**M235**	C1(=O)OC(C2=CC(=O)[C@]3([C@H](C(=C2C1)COC(=O)CC(C)C)C)C[C@@]1([C@@H]2[C@H]3C(=O)[C@H](O[C@@H]2OC1=O)C)C)(C)C	-7.6	*Talaromyces amestolkiae* YX1

236	**M236**	[C@@H]1(C([C@H]2[C@](CC1)([C@@]1([C@@H](CC2)C)Oc2c(C1)c(cc1c2CN(C1=O)CC(=O)OC)O)C)(C)C)O	-7.6	*Stachybotrys chartarum* 952
237	**M237**	c1c(cc(c(c1CCC(=O)C[C@@H](C)O)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1c(c(cc(c1)O)O)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1cc(cc(c1)O)O)C)C)C)C)O)O	-7.6	*Hansfordia sinuosae*
238	**M238**	C1[C@@]23[C@@H]([C@H]4/C(=C(\CC[C@H](C)OC(=O)C4)/O)/C(=O)O2)[C@H]([C@@](OC3=O)([C@@H]1C)C)O	-7.6	*Streptomyces koyangensis* SCSIO 5802
239	**M239**	C1[C@@H](C[C@]2([C@](C1)([C@@H]1[C@@H](CC2=O)[C@]2([C@](CC1)([C@H](CC2)[C@@H](/C=C/[C@@H](C(C)C)C)C)C)O)C)O)O	-7.6	*Aspergillus terreus* GX7-3B
240	**M240**	c1cc(c2c(c1O)C(=O)c1c(C2=O)cc(cc1)C)O	-7.6	Mangrove endophytic fungus No.5094
241	**M241**	CC1=CC(=O)C2=C([OH+]1)O[C@]1(CC[C@H]3[C@@](CC[C@H]4C(C)(C)[C@H]([C@H](C[C@]34C)OC(=O)C)OC(=O)C)([C@@H]1C2)C)C	-7.6	Neosartorya laciniosa KUFC 7896
242	**M242**	c1(c(cc(cc1)COc1cc(ccc1[C@@](CCCC(C)C)(C)O)CO)O)[C@@](CCCC(C)C)(C)O	-7.6	*Aspergillus* sp.
243	**M243**	COC(=O)[C@H]1[C@@H](C=CC2=C1C(=O)c1c(cc(cc1[OH+]2)CO)O)O	-7.6	*Neosartorya fischeri* 1008F1
244	**M244**	[C@H]12N(C(=O)[C@H](NC1=O)Cc1ccc(cc1)O)CCC2	-7.6	*Aspergillus versicolor* ZBY-3
245	**M245**	C1(=O)C2=C(C(=C([OH+]1)C)C)O[C@@]1(C2)C(=C[C@H]([C@@H]2[C@]3(C=CC(=O)C([C@@H]3CC[C@@]12C)(C)C)C)O)C	-7.6	*Penicillium* sp.
246	**M246**	C1(=O)C2=C(C(=C([OH+]1)C)C)O[C@@]1(C2)C(=CC[C@@H]2[C@]3(C=CC(=O)C([C@@H]3CC[C@@]12C)(C)C)C)C	-7.6	*Penicillium* sp.
247	**M247**	C12=C(C(=O)[N+]3C(=N1)[C@](NC(=O)[C@@H]3Cc1ccccc1)(C(C)C)OC)C=CC=CO2	-7.6	Paecilomyces variotii EN-291
248	**M248**	C[C@]1([C@@H]([C@H](C2=C([C@H]1O)C(=O)c1c(C2=O)c(cc(c1)OC)O)O)O)O	-7.6	*Stemphylium globuliferum*
249	**M249**	c1c(c(c2c(c1C(=O)OC)C(=O)C1=C([OH+]2)C=C(O[C@@H]1OC)C)O)OC	-7.6	*Chaetomium* sp. strain Gö 100/2
250	**M250**	C[C@@H]1CCC/C=C/C(=O)c2c(cc(cc2O)O)CC(=O)O1	-7.6	*Curvularia* sp. strain no. 768
251	**M251**	C[C@@H]([C@@H](/C=C/C=C/C(=O)O[C@@H]1C=C2COC(=O)[C@@]2([C@@]2(C)CCCC(C)(C)[C@H]12)O)O)O	-7.6	*Aspergillus ustus*
252	**M252**	CC(C)C[C@H]1C(=O)N2CCCC[C@H]2/C(=N/[C@@H](CCCCCC(=O)[C@@H]2CO2)/C(=N/[C@H](Cc2ccccc2)/C(=N\1)/O)/O)/O	-7.6	*Petriella* sp.
253	**M253**	CC(=CC[C@H]1CCC[C@H]2[C@@H](C[C@H]3C(=N[C@@H](C)C(=O)N3O)O)C[NH2+][C@@H]12)C	-7.6	*Aspergillus sydowi* PFW1-13
254	**M254**	c12c(c[nH]c2cccc1)c1c2c([nH]c1)cccc2	-7.5	*Aspergillus* sp.
255	**M255**	C1(=O)/C=C/[C@@H]2[C@@]34C(=C(C(=O)CC[C@H](C)O1)C(=O)O3)O[C@@]([C@H](C4)C)([C@H]2O)C	-7.5	*Streptomyces koyangensis* SCSIO 5802
256	**M256**	C1(=O)[C@H]2N(C(=O)[C@H](NC(=O)[C@H]([C@H](OC(=O)[C@@H](N(C)C(=O)CN1C)C(C)C)C)NC(=O)c1ccc(c3c1Nc1c(O3)c(c3c(c1C(=O)N[C@H]1[C@@H](C)OC(=O)[C@H](C(C)C)N(C(=O)CN(C)C(=O)[C@@H]4CCCN4C(=O)[C@@H](CC)NC1=O)C)nc(o3)CCC(=O)O)C)C(C)C)CCC2	-7.5	*Streptomyces* sp. IMB094

257	**M257**	C1(=O)/C=C/[C@@H]2[C@@]34C(=C(C(=O)CC[C@@H]1C)C(=O)O3)O[C@@]([C@H](C4)C)([C@H]2O)C	-7.5	*Streptomyces koyangensis* SCSIO 5802
258	**M258**	C1C[C@H]([C@@H]2[C@H](C1)[C@@H]([C@@H]([NH2+]2)/C=C(/[C@@H](CO)O)\O)N[C@@H]1[C@@H](C(=O)O)CCCC1)C(=O)O	-7.5	*Streptomyces* sp. CMN-62
259	**M259**	C1(=C2[C@]34[C@H](C(=O)[C@H](CC1)C)[C@H]([C@@H]1[C@@]3(OC2=O)C[C@@H]([C@]([C@H]1O)(C)O4)C)S[C@@H]1[C@@H]2[C@@]34[C@]5([C@@H]1[C@@H]([C@@]([C@H](C5)C)(C)O3)O)OC(=O)C4=C(CC[C@@H](C2=O)C)O)O	-7.5	*Streptomyces koyangensis* SCSIO 5802
260	**M260**	c12cccc3c1c(c(=O)[n+]2C)c1c(c3)C(N(C1=O)[C@@H](CC(=O)C)C)(C)C	-7.5	*Penicillium commune* DFFSCS026
261	**M261**	C(C[C@@H](CCCCCC)C)C/C=C(/C=C/C(=O)[C@@H](CC[C@@H]1[C@H](C(=O)NC(=C)C(=O)NC[C@@H](C(=O)N[C@@H](C(=O)O1)CCC(=O)N)C)C)C)\C	-7.5	*Diaporthe phaseolorum* SKS019
262	**M262**	[C@H]1(CC[C@@H]([C@H]2[C@@]1(C=C([C@H]([C@@H]2/C=C(/C(=O)O)\C)/C(=C/C[C@@H](C[C@H](C[C@H]([C@@H]([C@H](C(C)C)O)C)O)O)O)/C)C)C)C)O	-7.5	*Streptomyces* sp. SCSGAA 0027
263	**M263**	[C@@]12([C@H]3[C@](CC[C@@H]1C(OC(=O)C=C2)(C)C)([C@@]12[C@@](C(=O)[C@@](C3)(C)C2=C)(O)[C@@H](C)OC1=O)C)C	-7.5	*Penicillium brasilianum*
264	**M264**	C1(=O)OC(C2=CC(=O)[C@]3([C@H](C(=C2C1)COC(=O)C)C[C@@]1([C@@H]2[C@H]3C(=O)[C@H](O[C@@H]2OC1=O)C)C)C)(C)C	-7.5	*Talaromyces amestolkiae* YX1
265	**M265**	c1(cc(c2c(c1)CC(=O)O[C@H](CCC/C=C/C2=O)C)O)O	-7.5	*Penicillium Sumatrense*
266	**M266**	c1c(cc(c(c1CCC(=O)C)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1c(c(cc(c1)O)O)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1cc(cc(c1)O)O)C)C)C)C)O)O	-7.5	*Hansfordia sinuosae*
267	**M267**	c1c(cc(c(c1CCC(=O)C[C@@H](C)OC)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1c(c(cc(c1)O)O)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1cc(cc(c1)O)O)C)C)C)C)O)O	-7.5	*Hansfordia sinuosae*
268	**M268**	c1c(cc2c(c1O)C(=O)c1c(C2=O)cc(cc1O)O)C	-7.5	*Penicillium* sp. SCSGAF 0023
269	**M269**	C1C[C@](c2c(C1)c1c(c(c2)O)[C@@H]2[C@](CC1)([C@@H](CO2)O)C)(C)COC(=O)C	-7.5	*Aspergillus wentii* SD-310
270	**M270**	c12c([OH+]C(=O)C=C1)c(c1c(c2C)cco1)CC=C(C)C	-7.5	*Penicillium* sp. ZH16
271	**M271**	N(C(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H]1N(C(=O)[C@H](O)Cc2ccccc2)CCC1)CO)C)[C@H](CC)C)[C@H](C(=O)O)Cc1ccc(cc1)OCC=C(C)C	-7.5	*Bionectria ochroleuca*
272	**M272**	c1c(cc2c(c1C(=O)OC)C(=O)c1c([OH+]2)cc(c(c1)O)C)O	-7.5	*Phomopsis* sp. SK7RN3G1
273	**M273**	CC(=CCC/C(=C\COc1cc2[C@H](C)N(c3ccc(cc3OCC=C(C)C)OC)C(=O)c2c(c1C)OC)/C)C	-7.5	*Stachylidium* sp.
274	**M274**	CC(=CCc1c(C)cc(cc1Oc1cc(C)cc(c1)O)O)C	-7.5	*Aspergillus versicolor*
275	**M275**	c1ccc2c(c1)C(=O)[N+]1c3ccccc3C(=N[C@@H](CCC(=N)O)C1=N2)O	-7.5	*Penicillium aurantiogriseum*
276	**M276**	C[C@@]1(CC2=C(C[C@H]1O)C(=O)c1c(C2=O)cc(cc1O)OC)O	-7.5	*Stemphylium globuliferum*

277	**M277**	C1CC[C@H]2[C@H](C1)[C@H](C[NH2+]2)[C@@H]1[C@H]([C@H]([NH2+][C@@H]1C(=O)OC)C(=O)OC)[C@H]1[C@@H]2[C@H]([NH2+]C1)CC[C@@H](C2)Cl	-7.5	*Marinispora sp.* NPS12745
278	**M278**	c12c(cc(cc1O)C)C(=O)c1c(C2=O)c(ccc1)OC	-7.5	*Nocardia* sp. ALAA 2000
279	**M279**	c1c(c(c2c(c1C(=O)OC)C(=O)C1=C([OH+]2)C=C(OC1)C)O)OC	-7.5	*Chaetomium* sp. strain Gö 100/2
280	**M280**	c1(c(cc2c(c1C(=O)O)C(=O)C1=C([OH+]2)C=C(O[C@@H]1OC)C)O)O	-7.5	*Chaetomium* sp. strain Gö 100/2
281	**M281**	CC1(C)CCC[C@@]2(C)[C@H]1[C@@H](C=C1COC(=O)[C@]21O)OC(=O)/C=C/C=C/C(=O)O	-7.5	*Aspergillus ustus*
282	**M282**	[C@H]1(NC(=O)[C@H]2N(C1=O)C[C@H](C2)O)Cc1ccccc1	-7.4	*Aspergillus* sp.
283	**M283**	c12c3c([nH]c2CCCC1)cncc3	-7.4	*Aspergillus* sp.
284	**M284**	C1C[C@H]([C@@H]2[C@@H]3[C@@H]1N[C@H](C(=O)N[C@@H](C[C@@H]3C[NH2+]2)CO)[C@H](CC)C)C(C)(C)C=C	-7.4	*Marinactinospora thermotolerans* SCSIO 00652
285	**M285**	c12cccc3c1c(c(=O)[nH+]2)c1c(c3)C(N(C1=O)[C@@H](CC(=O)C)C)(C)C	-7.4	*Penicillium commune* DFFSCS026
286	**M286**	c12cccc3c1[C@@](C(=O)N2C)([C@H]1[C@@H](C3)CNC1=O)O	-7.4	*Penicillium commune* DFFSCS026
287	**M287**	c1c(cc2c(c1C(=O)OC)C(=O)c1c([OH+]2)cc(nc1)CO)O	-7.4	*Diaporthe phaseolorum* SKS019
288	**M288**	c1c(cc2c(c1O)C(=O)c1c(C2=O)cc(nc1)C)OC	-7.4	*Diaporthe phaseolorum* SKS019
289	**M289**	C1=C[C@]2([C@H]3[C@]([C@@H]1O)([C@@]1(C(=C[C@H]3OC2=O)COC(=O)C1)O)C)C	-7.4	*Aspergillus wentii* SD-310
290	**M290**	C([C@@H](CC/C(=C/[C@@H]1O[C@H]2[C@@](C1)(OC1=C(C2)C(=O)CC[C@@H]1O)C)/C)O)(C)(C)O	-7.4	*Alternaria alternata* k21-1
291	**M291**	c1(cc(c2c(c1C=O)O[C@](C=C2)(CC/C=C(/C)\CC[C@@H](O)C(C)(O)C)C)O)COC(=O)C	-7.4	*Stachybotrys chartarum* 952
292	**M292**	c1c(cc(c(c1O)C(=O)O)c1cc(c2c(c1C)scn2)O)OC	-7.4	*Alternaria* sp.
293	**M293**	c1c(cc(c(c1C)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1c(c(cc(c1)O)O)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1cc(cc(c1)O)O)C)C)C)C)O)O	-7.4	*Hansfordia sinuosae*
294	**M294**	c1c(cc(c(c1CCC(=O)/C=C/C)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1c(c(cc(c1)O)O)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1c(c(cc(c1)O)O)C(=O)O)C)C)C)C)O)O	-7.4	*Hansfordia sinuosae*
295	**M295**	c1c(cc2c(c1O)C(=O)c1c(C2=O)cc(cc1O)O)CO	-7.4	*Penicillium* sp. SCSGAF 0023
296	**M296**	C/C(=C/CC1=C(C=C(C)[OH+]C1=O)O)/CC/C=C(/C)\CC[C@@H]1C(=C)CC[C@@H](C1(C)C)OC(=O)C	-7.4	*Neosartorya laciniosa* KUFC 7896
297	**M297**	c1(c(cc(cc1)Cc1c(cc(c(c1)C(CCCC(C)C)(C)C)O)CO)O)[C@@](CCCC(C)C)(C)O	-7.4	*Aspergillus* sp.
298	**M298**	[C@H]12N(C(=O)[C@H](NC1=O)Cc1ccccc1)CCC2	-7.4	*Aspergillus versicolor* ZBY-3
299	**M299**	O[C@H]1C=CC[C@@H]2C[C@]34SS[C@@]5(C[C@@H]6[C@@H](O)C=C[C@H](O)[C@H]6N5C3=O)C(=O)N4[C@H]12	-7.4	*Penicillium brocae* MA-231
300	**M300**	c1ccc2c3c1O[C@]14c5c(C(=O)[C@H]([C@H]1OC)Cl)c(ccc5O[C@]3([C@@H](CC2=O)OC)O4)O	-7.4	*Lasiodiplodia theobromae* ZJ-HQ1

301	**M301**	CC(=O)O[C@@H]1[C@H](C2=C([C@H]([C@]1(C)O)O)C(=O)c1c(C2=O)c(cc(c1)OC)O)O	-7.4	*Stemphylium globuliferum*
302	**M302**	C1C([C@@](C(=CC1=O)C)(O)/C=C/C(=C\C(=O)O[C@@H]1[C@H]([C@@H](C=C(C1=O)CO)O)O)/C)(C)C	-7.4	*Nigrospora* sp.
303	**M303**	C[C@H]1[C@H](C)OCc2c1c(C)c(c(c1c(c(C)c3[C@H](C)[C@@H](C)OCc3c1O)O)c2O)O	-7.4	*Aspergillus* sp. MF-93
304	**M304**	c1(ccccc1)C[C@H]1N(C(=O)[C@@H](OC(=O)[C@@H](NC(=O)[C@@H](OC(=O)[C@@H](N(C(=O)[C@H](NC1=O)C)C)C(C)C)C)CC(C)C)C	-7.4	*Spicellum roseum*
305	**M305**	c1ccc(cc1)CC1=CC(=O)C(=C[OH+]1)C(=O)N	-7.4	*Aspergillus carbonarius*
306	**M306**	[C@H]1(NC(=O)[C@@H]2N(C1=O)CCC2)Cc1ccc(cc1)O	-7.3	*Aspergillus* sp.
307	**M307**	O=C1N2[C@H](CCC2)C(=O)N[C@@H]1Cc1ccccc1	-7.3	*Aspergillus* sp.
308	**M308**	C1CCC[C@H]2[C@@H]1[C@H](C[N@H+]2CC=C(C)C)C[C@@H](C(=O)OC)NC(=O)[C@H](CC1CCCCC1)O	-7.3	*Aspergillus* sp. SCSIO XWS03F03
309	**M309**	c1c(cc2c(c1C(=O)OC)C(=O)c1c([OH+]2)cc(nc1)C)OC	-7.3	*Diaporthe phaseolorum* SKS019
310	**M310**	c1c(c(c2c(c1C(=O)OC)C(=O)c1c([OH+]2)cc(nc1)C)OC)OC	-7.3	*Diaporthe phaseolorum* SKS019
311	**M311**	C1CC[C@H]2[C@@H](C1)[NH2+][C@@H]([C@H](C2=O)C(=O)O)[C@@H]1CCC[NH2+]1	-7.3	*Penicillium* sp.
312	**M312**	[C@H]1(C[C@H]([C@@H]([C@H]2[C@@]1(C=C([C@H]([C@@H]2/C=C(/C(=O)O)\C)/C(=C/C[C@@H](C[C@H](C[C@H]([C@@H]([C@H](C(C)C)O)C)O)O)O)O)/C)C)C)C)O)O	-7.3	*Streptomyces* sp. SCSGAA 0027
313	**M313**	c1(ccc(cc1)[N](=O)O)C(=O)O[C@@H]1C[C@@H]2[C@@]([C@@]3([C@@H]1[C@@](CCC3)(C)CO)C)(COC2=O)O	-7.3	*Aspergillus ochraceus* Jcma1F17
314	**M314**	C1[C@@H](C([C@H]2[C@](C1)(C1=CC(=C)[C@@]([C@H](C1=CC2)O)(C=C)C)O)(C)C)O	-7.3	*Aspergillus wentii* SD-310
315	**M315**	C(=CCC/C(=C/[C@@H]1O[C@H]2[C@@](C1)(OC1=C(C2)C(=O)CC[C@@H]1O)C)/C)(C)C	-7.3	*Alternaria alternata* k21-1
316	**M316**	[C@@]1([C@H]2[C@](CC[C@@H]1C(O)(C)C)([C@@]13[C@@](C(=O)[C@@](C2)(C)C3=C)(O)[C@@H](C)OC1=O)C)(C)CCC(=O)OC	-7.3	*Penicillium brasilianum*
317	**M317**	c1(cc(c2c(c1)CC(=O)O[C@H](CCCCC2=O)[C@@H](C)O)O)O	-7.3	*Penicillium Sumatrense*
318	**M318**	c1c(cc(c(c1O)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1cc(cc(c1)O)O)C)C)CC(=O)C[C@H](O)C)O	-7.3	*Hansfordia sinuosae*
319	**M319**	c1(cc(c2c(c1)[C@](OC2=O)(c1c(c(ccc1O)CC=C(C)C)O)C)O)C	-7.3	*Ascomycota* sp. SK2YWS-L
320	**M320**	N12C(=O)[C@H](OC(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H]1CCC2)CO)C)[C@@H](C)CC)Cc1ccc(cc1)OCC=C(C)C)C)C)Cc1ccccc1	-7.3	*Bionectria ochroleuca*
321	**M321**	C1(=O)[C@@](C(=O)[C@@H]2C(=C1Cl)C[C@@H]([N@@H+](C2)CCCC[N@H+]1C[C@H]2C(=O)[C@@](C(=O)C(=C2C[C@@H]1/C=C/C(=C/[C@@H](CC)C)/C)Cl)(C)OC(=O)C)/C=C/C(=C/[C@H](CC)C)/C)(C)OC(=O)C	-7.3	*Penicillium* sp. 303

322	**M322**	O1C(=C(C(=O)[C@]21C(=O)N[C@@]([C@@H]2O)(OC)C(=O)c1ccccc1)C)[C@H]([C@H](/C=C\CC)O)O	-7.3	*Aspergillus* sp. BRF 030
323	**M323**	c1c(ccc(c1)/C=C(/C(=C/c1ccc(cc1)O)/[N]#C)\[N]#C)O	-7.3	*Penicillium commune* SD-118
324	**M324**	c1(c(cc2c(c1O)C(=O)c1c(C2=O)cc(c(c1O)[C@H](CCCCC)O)O)OC)Cl	-7.3	*Aspergillus* sp. SCSIO F063
325	**M325**	c1ccc2c(c1)C(=C(C(=O)[NH+]2)OC)c1cc(ccc1)O	-7.3	*Aspergillus versicolor* Y31-2
326	**M326**	CC(C)C(=O)Cc1c(C)cc(cc1Oc1cc(C)cc(c1)O)O	-7.3	*Aspergillus versicolor*
327	**M327**	Cc1cc(c2c(c1)[OH+]C1=C(C[C@@H]([C@](C[C@H](C(=O)OC)O)(C(=O)OC)O)S1)C2=O)O	-7.3	*Penicillium oxalicum* SCSGAF 0023
328	**M328**	C1C2=C(C(=O)c3c([OH+]2)cc(cc3O)C)C(=O)C1	-7.3	*Penicillium oxalicum* SCSGAF 0023
329	**M329**	[C@@H]1(CC[C@H]2[C@H](C1)[C@H](C[NH2+]2)[C@@H]1[C@H]([C@H]([NH2+][C@@H]1C(=O)OC)C(=O)OC)[C@H]1[C@@H]2[C@H]([NH2+]C1)CC[C@@H](C2)Cl)Cl	-7.3	*Marinispora*. sp. NPS12745
330	**M330**	c1cc(ccc1)C[C@@H](O[C@@H](CC(C)C)C(=O)O[C@@H]1[C@H]([C@@H](C=C(C1=O)CO)O)O)C(=O)OC	-7.3	*Nigrospora* sp.
331	**M331**	CC1(C)CCC[C@@]2(C)[C@H]1[C@@H](C=C1COC(=O)[C@]21O)OC(=O)/C=C/C=C/C=O	-7.3	*Aspergillus ustus*
332	**M332**	[C@H]1(NC(=O)[C@H]2N(C1=O)CCC2)Cc1ccccc1	-7.2	*Aspergillus* sp.
333	**M333**	C1(=O)N[C@H](C(=O)N2[C@H]1CCC2)Cc1ccccc1	-7.2	*Aspergillus* sp.
334	**M334**	c1(ccccc1)C[C@@H](N(C(=O)[C@@H](NC(=O)C)C(C)C)C)C(=O)N[C@H](C(=O)O)CC(C)C	-7.2	*Simplicillium obclavatum*
335	**M335**	C1(C[C@@H]2/C(=C\[C@@H]([C@@H](C(=C)CC[C@@]12O)NC(=O)/C=C(/CCO)\C)O)/CO)(C)C	-7.2	*Hansfordia sinuosae*
336	**M336**	C1[C@@H](C([C@H]2[C@](C1)(C1=CC(=C)[C@@]([C@@H](C1=CC2)O)(C=C)C)O)(C)C)O	-7.2	*Aspergillus wentii* SD-310
337	**M337**	C(/C=C/C/C(=C/[C@@H]1O[C@H]2[C@@](C1)(OC1=C(C2)C(=O)CC[C@@H]1O)C)/C)(OO)(C)C	-7.2	*Alternaria alternata* k21-1
338	**M338**	[C@H]1([C@@H]([C@@H]2[C@@H](CC1)[C@@]([C@@H](C(=C2)C)/C(=C/C)/C)(/C=C/C=C/C=C/C=C/C(=O)O)C)O)C	-7.2	*Janthinobacterium* spp. ZZ145
339	**M339**	O1[C@H]([C@H]([C@H](C[C@@H]1O[C@@H]1C[C@@](O[C@@H]([C@H]1CC)C)([C@H]([C@@H]([C@@H]([C@@H]1[C@H](/C=C/C=C/C(=C)O[C@@H]([C@H](/C=C/C=C/C(=O)O1)C)[C@H]([C@H]([C@@H]([C@]1(C[C@H]([C@@H]([C@H](O1)C)CC)O[C@H]1C[C@@H]([C@@H]([C@@H](O1)C)O)O)O)C)O)C)C)O)C)OC)O)O)C	-7.2	*Streptomyces* sp. 7-145
340	**M340**	c1c(cc(c(c1CCC(=O)C[C@@H](C)OC)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1c(c(cc(c1)O)O)C(=O)O)C)C)C)O)O	-7.2	*Hansfordia sinuosae*

341	**M341**	C([C@@H](C)O)C(=O)Cc1cc(cc(c1C(=O)O[C@@H](CC(=O)O[C@@H](Cc1c(c(cc(c1)O)O)C(=O)O[C@@H](CC(=O)O)C)C)C)O)O	-7.2	*Hansfordia sinuosae*
342	**M342**	C1[C@@](Oc2c(C1=O)c(ccc2c1ccc(c2c1O[C@](CC2=O)(C(=O)OC)[C@@H]1[C@H](CC(=O)O1)C)O)O)([C@]1([C@H](CC(=O)O1)C)C)C(=C)OC	-7.2	*Penicillium* sp. SCSGAF 0023
343	**M343**	c1c(cc2c(c1C(=O)OC)C(=O)c1c(cc(cc1O)CO)[OH+]2)O	-7.2	*Penicillium* sp. ZJ-SY2
344	**M344**	c1ccc2c(c1C(=O)OC)C(=O)c1c(cc(cc1O)C)[OH+]2	-7.2	*Penicillium* sp. ZJ-SY2
345	**M345**	c1ccc2c(c1C(=O)OC)C(=O)c1c(cc(cc1O)CO)[OH+]2	-7.2	*Penicillium* sp. ZJ-SY2
346	**M346**	[C@@]12(C3=CC(=O)OC[C@H]3[C@@H]([C@H]3OC(=O)[C@@](CCC1)([C@@H]23)C)O)C	-7.2	*Aspergillus terreus* GX7-3B
347	**M347**	C(=O)(C(C)C)OC[C@]1([C@H]2[C@@]3(C4=C([C@H]([C@@](CC4)(C)C=C)O)C(=O)[C@@H]2O)[C@@H](C[C@H]1OC(=O)C)C3)C	-7.2	*Eutypella* sp. FS46
348	**M348**	[C@@]123[N+](c4ccccc4[C@@]1(C=C(C(=O)N2/C(=C/c1c[nH]c[nH+]1)/C(=O)N3)O)C(C)(C=C)C)OC	-7.2	*Penicillium commune* SD-118
349	**M349**	c1c(cc2c(c1)C(=O)C1=C(C2=O)[C@H]([C@H]([C@H](O1)C)O)O)O	-7.2	*Acaromyces ingoldii* FS121
350	**M350**	C[C@@]1([C@@H](C2=C(C(=O)c3c(cc(c(c4c(cc(c5c4C(=O)C4=C(C5=O)[C@@H]([C@H]([C@](C)([C@@H]4O)O)O)O)O)O)OC)c3C2=O)OC)O)[C@@H]([C@H]1O)O)O)O	-7.2	*Stemphylium globuliferum*
351	**M351**	c1c(cccc1C(=O)O[C@@H]1[C@H]([C@@H](C=C(C1=O)CO)O)O)O	-7.2	*Nigrospora* sp.
352	**M352**	CC(C)CCCCCC(=O)N[C@H](Cc1ccc(cc1)O)C(=O)N[C@@H](CO)C(=O)N[C@H](CC(C)C)C(=O)N[C@@H](C[C@@H]1C[NH2+][C@H]2CCCC[C@H]12)C(=O)N[C@@H](CCCN=C(N)N)C(=O)OC	-7.2	*Brevibacillus laterosporus* PNG276
353	**M353**	c1(ccc(cc1)O)C[C@@H]1NC(=O)[C@H](N(C(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]2N(C1=O)CCC2)C(C)C)C(C)C)C)Cc1ccc(cc1)O	-7.2	*Aspergillus versicolor* MST-MF495
354	**M354**	c1c(ccc(c1)C[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](N)C)C(C)C)C(C)C)C(=O)O)O	-7.1	*Aspergillus* sp. SCSIO 41501
355	**M355**	C1CC[C@@H]2[C@H](C1)[C@@H](C[NH2+]2)C[C@@H]1CNC[C@H](N1)C	-7.1	*Serinicoccus profundi* sp.
356	**M356**	C1(=C[C@@]2([C@]3(N(C1=O)[C@H](C(=O)N3)C)[N+](c1c2cccc1)O)C(C)(C)C=C)O	-7.1	*Aspergillus versicolor* LZD-14-1
357	**M357**	C[C@@H]1CCC/C=C/C=C/[C@@H](C[C@H]([C@@H](/C=C\C=C\[C@H](C/C=C/C=C/C(=O)O1)O)O)O)O	-7.1	*Bacillus amyloliquefaciens* SCSIO 00856
358	**M358**	C1=C2[C@@](C(=C)C1=O)([C@H]1[C@@](C2)(CC(C1)(C)C)O)C	-7.1	*Chondrostereum* sp.
359	**M359**	C1(=O)[C@@](C[C@]2(C(=C1)C=C[C@H]([C@@H]2C)OC(=O)/C=C/C(=C/C(C)C)/C)C)(C(=C)C=O)O	-7.1	*Cochliobolus lunatus* SCSIO41401
360	**M360**	c1(cc(c2c(c1)OCc1c2nc(cc1)C)C(=O)O)O	-7.1	*Phomopsis* sp. 33
361	**M361**	c1c(cc(c(c1O)C(=O)O[C@@H](CC(=O)O[C@@H](Cc1cc(cc(c1)O)O)C)C)C[C@H](OC(=O)C[C@H](O)C)C)O	-7.1	*Hansfordia sinuosae*
362	**M362**	[C@@H]1(CC(=C2[C@]([C@@H]1O)(Oc1c(C2=O)c(c(cc1)c1ccc2c(c1O)C(=O)C1=C(C[C@@H]([C@H]([C@@]1(O2)C(=O)OC)O)C)O)O)C(=O)OC)O)C	-7.1	*Penicillium* sp. SCSGAF 0023

363	**M363**	[C@H]1(CC(=C2[C@@]([C@H]1O)(Oc1c(C2=O)c(ccc1c1c(O)c2C(=O)C3=C(O)C[C@@H]([C@H]([C@@]3(Oc2cc1)C(=O)OC)O)C)O)C(=O)OC)O)C	-7.1	*Penicillium* sp. SCSGAF 0023
364	**M364**	c1c(cc(c(c1C(=O)OC)C(=O)c1c(ccc(c1O)CC=C(C)C)O)O)C	-7.1	*Ascomycota* sp. SK2YWS-L
365	**M365**	c1(ccc2c(c1C(=O)OC)C(=O)c1c(cc(cc1O)C)[OH+]2)O	-7.1	*Penicillium* sp. ZJ-SY2
366	**M366**	c1(ccc2c(c1C(=O)OC)C(=O)c1c(cc(cc1O)CO)[OH+]2)O	-7.1	*Penicillium* sp. ZJ-SY2
367	**M367**	CC(=CCC/C(=C\COc1cc2[C@@H](C)N(c3ccc(cc3OCC=C(C)C)OC)C(=O)c2c(c1C)OC)/C)C	-7.1	*Stachylidium* sp.
368	**M368**	C1(=O)[C@@]([C@@H]([C@@H]2C(=C1Cl)C=C(OC2)/C=C/[C@H]([C@@]([C@H]([C@@H](CC)C)O)(O)C)O)O)(O)C	-7.1	*Penicillium sclerotiorum* M-22
369	**M369**	CCCCCC[C@@H](C)C(=O)C1=C([C@@]2([C@H](C)[C@@H]3c4c(cc(c(C)c4[C@H](C)[C@@H](C)O3)O)O2)N(C)C1=O)O	-7.1	*Penicillium citrinum*
370	**M370**	CC1=CC(=O)c2c(cc(c([C@@H]3C[C@H](C(=O)O3)OC)c2[OH+]1)OC)O	-7.1	*Rhytidhysteron rufulum*
371	**M371**	O=C1N[C@H](C(=O)N[C@@H]1Cc1ccccc1)C(C)C	-7.1	*Cladosporium* sp. F14
372	**M372**	c1(ccc(cc1)O)C[C@@H]1NC(=O)[C@H](N(C(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]2N(C1=O)CCC2)C(C)C)[C@@H](C)CC)C)Cc1ccc(cc1)O	-7.1	*Aspergillus versicolor* MST-MF495
373	**M373**	C1(=O)O[C@H](c2c(C1)cc(cc2O)O)CCCCCC[C@@H](C)O	-7.1	*Pestalotiopsis* sp.
374	**M374**	c1(cc(c2c(c1)[OH+]C(=CC2=O)CCCCCCC)CC(=O)O)O	-7.1	*Pestalotiopsis* sp.
375	**M375**	C/C=C\[C@@H]([C@@H](C1=C(C)C(=O)[C@]2([C@H]([C@](C(=O)c3ccccc3)(N=C2O)OC)O)O1)O)O	-7.1	*Aspergillus sydowi* PFW1-13
376	**M376**	C1=C[C@]2([C@H]([C@@H](C1=O)C)[C@@H](C(=O)[C@]1([C@@H]2CC[C@@H]2[C@@]1(C[C@@H](/C/2=C(\CCCC(C)(C)O)/C(=O)O)OC(=O)C)C)C)OC(=O)C)C	-7.1	*Aspergillus sydowi* PFW1-13
377	**M377**	c1(cc2c(cc1C)nc(c(c2O)O)C(=O)O)C	-7	*Aspergillus* sp.
378	**M378**	C1(=O)N[C@H](C(=O)N2[C@H]1CCC2)Cc1ccc(cc1)O	-7	*Aspergillus* sp.
379	**M379**	S1SSC[C@H]2NC(=O)[C@H](NC(=O)C[C@@H](/C=C/CC1)OC(=O)[C@@H](NC(=O)/C(=C/C)/NC2=O)C(C)C)C(C)C	-7	*Chromobacterium* sp. HS-13-94
380	**M380**	c1(ccccc1)C[C@@H](N(C(=O)[C@@H](NC(=O)C)[C@@H](CC)C)C)C(=O)N[C@H](C(=O)O)CC(C)C	-7	*Simplicillium obclavatum* EIODSF 020
381	**M381**	c1ccc2c(c1)[C@]1([C@](N2)(N2[C@@H](C1)C(=O)N[C@H](C2=O)C)C(C)(C=C)C)O	-7	*Eurotium* sp. SCSIO F452
382	**M382**	c1(cc(c(cc1)[C@](CCCC(C)C)(C)O)O)C(=O)O	-7	*Aspergillus* sp.
383	**M383**	[C@@H]1([C@@]([C@@H]2[C@@](C1)(CC(=O)C(=CC2)C)C)(C(C)C)O)O	-7	*Trichoderma virens*
384	**M384**	C1(=O)[C@@](C[C@]2(C(=C1)C=C[C@H]([C@@H]2C)OC(=O)/C=C/C(=C/C(C)C)/C)C)(C(=C)/C(=N\O)/C)OC	-7	*Cochliobolus lunatus* SCSIO41401
385	**M385**	C1=C[C@]2([C@H]3[C@](C1=O)([C@@]1(C(=C[C@H]3OC2=O)COC(=O)C1)O)C)C	-7	*Aspergillus wentii* SD-310
386	**M386**	c1(c(cc2c(c1C)c(c1c(c2)C(=O)[C@]2([C@@](C1=O)(C(=CC(=O)[C@@H]2OC)OC)O)O)O)OC)C(=O)OC	-7	*Saccharothrix* sp. 10-10

387	**M387**	c1(cc(c2c(c1)OCc1c2nc(cc1)C)C(=O)O)OC	-7	*Phomopsis* sp. 33
388	**M388**	c1(cc(c2c(c1O)OCc1c2nc(cc1)C)C(=O)O)OC	-7	*Phomopsis* sp. 33
389	**M389**	O1[C@H]([C@H]([C@H](C[C@@H]1O[C@@H]1C[C@@](O[C@@H]([C@H]1CC)C)([C@H]([C@@H]([C@@H]([C@@H]1[C@H](/C=C/C=C/C(=C)O[C@@H]([C@H](/C=C/C=C/C(=O)O1)C)[C@H]([C@H]([C@@H]([C@]1(C[C@H]([C@@H]([C@H](O1)C)C)O[C@H]1C[C@@H]([C@@H]([C@@H](O1)C)O)O)OC)C)O)C)C)O)C)OC)O)O)C	-7	*Streptomyces* sp. 7-145
390	**M390**	[C@H]1([C@@H]([C@@H]2[C@@H](CC1)[C@@]([C@@H](C(=C2)CO)/C(=C/C)/C)(/C=C/C=C/C=C/C=C/C(=O)O)C)O)C	-7	*Janthinobacterium* spp. ZZ145
391	**M391**	c1(cc(c2c(c1)CC(=O)O[C@H](CCCCC2=O)[C@@H](C)O)O)O	-7	*Penicillium Sumatrense*
392	**M392**	c1(cc(c2c(c1)CC(=O)O[C@H](CCCCCC2=O)C)O)O	-7	*Penicillium Sumatrense*
393	**M393**	O1[C@H]([C@H]([C@H](C[C@@H]1O[C@@H]1C[C@@](O[C@@H]([C@H]1CC)C)([C@H]([C@@H]([C@@H]([C@@H]1[C@H](/C=C/C=C/C(=C)O[C@@H]([C@H](/C=C/C=C/C(=O)O1)C)[C@H]([C@H]([C@@H]([C@]1(C[C@H]([C@@H]([C@H](O1)C)CC)O[C@H]1C[C@@H]([C@@H]([C@@H](O1)C)O)O)OC)C)O)C)C)O)C)OC)O)O)C	-7	*Streptomyces* sp. 7-145
394	**M394**	C=C1CC[C@H]2[C@@](C)(CC[C@H]3C(C)(C)[C@H](CC[C@]23C)OC(=O)C)[C@@H]1CC1=C(C=C(C)[OH+]C1=O)O	-7	*Neosartorya laciniosa* KUFC 7896
395	**M395**	c1(cc(c2c3c1[C@H](OC(=O)c3c(cc2C)O)C(=O)OC)O)O	-7	*Penicillium purpurogenum* G59
396	**M396**	C1CC(=[NH2])N[C@@H]1C1=Nc2c(C(=O)[N+]1c1c(C(=O)O)cccc1)cccc2	-7	*Penicillium aurantiogriseum*
397	**M397**	COC(=O)c1ccccc1[N+]1C(=Nc2ccccc2C1=O)[C@@H]1CCC(=N)N1	-7	*Penicillium aurantiogriseum*
398	**M398**	c1c(cc2c(c1O)C(=O)C1=C([OH+]2)C=C[C@@H]([C@H]1C(=O)OC)O)CO	-7	*Engyodontium album* DFFSCS021
399	**M399**	c1ccc2c(c1O)C(=O)C1=C(C2=O)[C@H]([C@H]([C@H](O1)C)O)O	-7	*Acaromyces ingoldii* FS121
400	**M400**	c1ccccc1C[C@@H]1N2C(=O)[C@]3(C=CC=COC3=NC2=C(C(C)C)NC1=O)OCC(=O)C(C)C	-7	Paec*ilomyces variotii* EN-291
401	**M401**	C[C@@]12CCCCC1=CC=C1C2=CC=CC1=O	-7	*Pseudomonas stutzeri* CMG 1030
402	**M402**	CC(C)CCCCC/C(=N/[C@H](C[C@H]1CC[C@@H](CC1)O)/C(=N/[C@@H](CO)/C(=N/[C@H](CC(C)C)/C(=N/[C@@H](C[C@H]1C[NH2+][C@H]2CCCC[C@@H]12)/C(=N/[C@@H](CCCNC(=N)N)C(=O)O)/O)/O)/O)/O)/O	-7	*Brevibacillus laterosporus* PNG276
403	**M403**	c1cc(ccc1C/C(=N/O)/C(=O)OC[C@@H]([C@@H](COC(=O)/C(=N\O)/Cc1ccc(cc1)O)O)O)O	-7	*Aspergillus aculeatus* CRI323-04A
404	**M404**	c1(cc(c2c(c1)[OH+]C(=CC2=O)CCCCCCC)CC(=O)OC)O	-7	*Pestalotiopsis* sp.
405	**M405**	c1(cc(c2c(c1)[OH+]C(=CC2=O)CCCCC[C@@H](C)O)CC(=O)OC)O	-7	*Pestalotiopsis* sp.
406	**M406**	c1(cc(c2c(c1)[OH+]C(=CC2=O)CCCCC[C@@H](C)O)CC(=O)OCC)O	-7	*Pestalotiopsis* sp.
407	**M407**	CC(=C1C(=O)/C(=C\2/C=CC[C@H](C)O2)/C(=N1)O)C	-6.9	*Cladosporium* sp. OUCMDZ-1635
408	**M408**	c1(ccc(cc1)O)C[C@@H](N(C(=O)[C@@H](NC(=O)C)[C@@H](CC)C)C)C(=O)N[C@H](C(=O)O)CC(C)C	-6.9	*Simplicillium obclavatum* EIODSF 020

409	**M409**	c1(ccc(cc1)O)C[C@@H](N(C(=O)[C@@H](NC(=O)C)[C@@H](CC)C)C)C(=O)N[C@H](C(=O)OC)CC(C)C	-6.9	*Simplicillium obclavatum* EIODSF 020
410	**M410**	c1c(ccc(c1)C[C@@H]1[C@@H](C)N=C(N=C1)Cc1ccc(cc1)OC)OC	-6.9	*Eurotium* sp. SCSIO F452
411	**M411**	C[C@H]1/C=C/C(=O)O[C@H](C)[C@@H](CO[C@H]2[C@@H]([C@@H]([C@@H]([C@@H](C)O2)O)OC)OC)[C@H]2[C@H](/C=C/C(=O)[C@](C)(C[C@H](C)[C@H]1O[C@H]1[C@@H]([C@H](C[C@@H](C)O1)OC)O)O)O2	-6.9	*Streptomyces* sp. HK-2006-1
412	**M412**	C1(=O)[C@@]([C@@H]2[C@@](C1)(CC(=O)C(=CC2)C)C)(C(C)C)O	-6.9	*Trichoderma virens*
413	**M413**	[C@]12(CC[C@]3([C@H]([C@@H]1[C@@H]1[C@]([C@H]4C(=C(CC4)C(=O)O)C2)(C1)C)[C@H](CC3)C(C)C)C)CO	-6.9	*Aspergillus* sp. 16-5c
414	**M414**	c1(cc(c2c(c1)OCc1c2nc(cc1)C)C(=O)OC)O	-6.9	*Phomopsis* sp. 33
415	**M415**	c1(cc(c2c(c1)CC(=O)O[C@H](CCCC2=O)C[C@H](C)O)O)O	-6.9	*Penicillium Sumatrense*
416	**M416**	c1(cc(c2c(c1)CC(=O)O[C@@H](CCCC2=O)C[C@H](C)O)O)O	-6.9	*Penicillium Sumatrense*
417	**M417**	C12=C(C[C@@H]3[C@]4(C(=C1C)C[C@@]1([C@@H]5[C@]4([C@@]([C@@H](O[C@@H]5OC1=O)C)(O3)O)C(=O)OC)C)C)C(OC(=O)C2)(C)C	-6.9	*Penicillium* sp. 303
418	**M418**	c1cccc(c1C(=O)O)N/C=N/c1occc1	-6.9	*Penicillium paneum* SD-44
419	**M419**	C=C[C@H]1CC[C@@]2([C@@H]3CC[C@H](C(C)(C)C)C3=C(C(=O)C2=C1)O)O)O	-6.9	*Eutypella scoparia* FS26
420	**M420**	CC(C)C[C@H]1[C@@H]2[C@H](C)C(=C[C@@H]3/C=C(/C)\CCCC(=O)C[C@H](C(=O)[C@@]23C(=N1)O)SC)C	-6.9	*Aspergillus* sp.
421	**M421**	c1(ccccc1)CCOC(=O)[C@H]1NC(=O)CC1	-6.9	*Aspergillus versicolor* ZBY-3
422	**M422**	c1c(cc2c(c1O)C(=O)C1=C([OH+]2)C=C[C@H]([C@H]1C(=O)OC)O)CO	-6.9	*Engyodontium album* DFFSCS021
423	**M423**	[C@@H]12[C@@H]([C@]3([C@H]4[C@]([C@@H]1O2)(C1=CC(=C)OCC1=C[C@H]4OC3=O)C)C)O	-6.9	*Aspergillus dimorphicus* SD317
424	**M424**	C1=C[C@]2([C@H]3[C@]([C@@H]1O)(C1=CC(=O)OCC1=C[C@H]3OC2=O)C)C	-6.9	*Aspergillus wentii* EN-48
425	**M425**	CC1(C)[C@@H](C(=O)O)N2C(=O)[C@H]([C@H]2S1)/N=C(/Cc1ccccc1)\O	-6.9	*Penicillium mold*
426	**M426**	C[C@H]1CC(=O)C/C=C/[C@@H]2CCC[C@H]2[C@@H](/C=C/C(=O)O1)O	-6.9	*Penicillium* sp. PSU-F44
427	**M427**	O=C1N2[C@H](C(=O)N[C@H]1Cc1ccccc1)CCC2	-6.9	*Cladosporium* sp. F14
428	**M428**	C[C@@H]1CCC/C=C\[C@]2(CC(=O)c3c(cc(cc3O2)O)CC(=O)O1)O	-6.9	*Curvularia* sp. 768
429	**M429**	c1(cc(c2c(c1)[OH+]C(=CC2=O)CCCCCCC)CC(=O)OCC)O	-6.9	*Pestalotiopsis* sp.
430	**M430**	c1(cc(c2c(c1)[OH+]C(=CC2=O)CCCCC)CC(=O)OC)O	-6.9	*Pestalotiopsis* sp.
431	**M431**	[C@H](CCCCCCCCCCCCC)([C@@H]1OC(=O)[C@H](NC(=O)CN(C(=O)/C=C/C(=C)NC(=O)[C@H]1C)C)[C@@H](C(=O)N)O)C	-6.8	*Micromonospora chalcea* FIM 02-523
432	**M432**	C1C(=O)[C@@H]([C@@]2([C@H]1[C@H](C1=C2CC(C1=O)(C)C)O)C)C	-6.8	*Chondrostereum* sp.
433	**M433**	[C@]12([C@@]3(C[C@H](CC1)C([C@@]3(O)C)(C)C)[C@@H](C[C@@H]2C)O)O	-6.8	*Streptomyces* sp. SCSIO 10355
434	**M434**	C1CC([C@]2([C@](C1)(C1=C([C@@H](C2=O)O)[C@H]([C@](CC1)(C=C)C)O)C)O)(C)C	-6.8	*Eutypella scoparia* FS26
435	**M435**	C1CC([C@H]2[C@]3(C1)[C@@]1([C@@](CC2=O)([C@H]([C@](CC1)(C=C)C)O)OC3=O)O)(C)C	-6.8	*Aspergillus wentii* SD-310

436	**M436**	C1CC(C2=CC(=O)C3=C([C@@]2(C1)O)CC[C@@]([C@@H]3O)(C=C)C)(C)C	-6.8	*Aspergillus wentii* SD-310
437	**M437**	C1CC(C2=CC(=O)C3=C([C@]2(C1)O)CC[C@@]([C@@H]3O)(C=C)C)(C)C	-6.8	Aspergillus wentii SD-310
438	**M438**	[C@@]12([C@H]3[C@](CC[C@@H]1[C@@]1(OC(=O)[C@H]([C@H]2O)C1)C)([C@@]12[C@@](C(=O)[C@@](C3)(C)C2=C)(O)[C@@H](C)OC1=O)C)C	-6.8	*Penicillium brasilianum*
439	**M439**	[C@@H]1(CC[C@@H](O[C@@H]1C)O[C@H]1[C@](C[C@@H](O[C@@H]1C)O[C@H]1[C@@H]([C@H](O[C@H](C1)c1c(c2c(cc1)C(=O)C1=C(C2=O)[C@@H]([C@@H]([C@@]2([C@]1([C@H](C=C([C@H]2O)C)O[C@H]1O[C@H]([C@H]([C@@H](C1)OC)O)C)O)O)CC(=O)C)C)O)C)O)(O)C)OC(=O)N	-6.8	*Streptomyces pratensis* NA-ZhouS1
440	**M440**	c1(cc(c2c(c1C=O)O[C@](C=C2)(CC/C=C(/C)\CC[C@@H](O)C(C)(C)OC)C)O)COC(=O)C	-6.8	*Stachybotrys chartarum* 952
441	**M441**	c1cccc(c1C(=O)O)N/C(=N/CC(C)(C)O)/C	-6.8	*Penicillium paneum* SD-44
442	**M442**	Cc1cc(c(C)c(c1)O[C@@H]1C(=O)C(=C(C(=O)[C@@]1(C)OC)O)C)O	-6.8	*Aspergillus aculeatus*
443	**M443**	CC[C@@H](CC(=O)C(Cl)Cl)[C@H](C)c1ccc(cc1)[N](=O)O	-6.8	*Nocardia* sp. ALAA 2000
444	**M444**	C[C@H]1C[C@H](C/C=C/[C@@H]2CCC[C@H]2[C@@H](/C=C/C(=O)O1)O)O	-6.8	*Penicillium* sp. PSU-F44
445	**M445**	C1[C@H](C=C2[C@H]([C@H]1OC(=O)C(CC)(C)C)[C@H]([C@H](C=C2)C)CC[C@@H]1C[C@H](CC(=O)O1)O)C	-6.8	*Aspergillus terreus*
446	**M446**	C1(=C(C=C([OH+]C1=O)/C(=C/[C@@H](CC(=O)O)C)/C)OC)CO	-6.8	*Petriella* sp.
447	**M447**	c1(c(c2c(cc1C)C(=O)C[C@H](O2)/C=C/C)C)O	-6.7	*Aspergillus* sp.
448	**M448**	c1c(c2c(c(c1O)C)[C@H]([C@@H](OC2=O)C)C)O	-6.7	*Aspergillus* sp.
449	**M449**	[C@H](CCCCCCCCCCCCCCC)([C@@H]1OC(=O)[C@H](NC(=O)CN(C(=O)/C=C/C(=C)NC(=O)[C@H]1C)C)[C@@H](C(=O)N)O)C	-6.7	*Micromonospora chalcea* FIM 02-523
450	**M450**	[C@H](CCCCCCCCCCCCCCC)([C@@H]1OC(=O)[C@H](NC(=O)CN(C(=O)/C=C/C(=C)NC(=O)[C@H]1C)C)[C@@H](C(=O)N)O)C	-6.7	*Micromonospora chalcea* FIM 02-523
451	**M451**	C(=O)([C@H](CSc1ccc[n+]2c1[C@]([C@H]([C@@H]2/C=C(\C)/C=C/C1CC1)O)(C)O)CC(=O)C)O	-6.7	*Streptomyces* sp. HZP-2216E
452	**M452**	C1(=C[C@@]2([C@]3(N(C1=O)CC(=O)N3)[N@H+]([C@@H]1[C@@H]2C=CC=C1)O)C(C=C)(C)C)OC	-6.7	*Aspergillus versicolor* LZD-14-1
453	**M453**	C1=C2[C@@]([C@H](C1=O)C)([C@]1(C(=C2)C(=O)C(C1)(C)C)O)C	-6.7	*Chondrostereum* sp.
454	**M454**	C1(=O)C=C([C@@H]2[C@]1([C@H]([C@@H]1[C@H]2CC(C1)(C)C)O)C)C	-6.7	*Chondrostereum* sp.
455	**M455**	[C@@H]1([C@@]([C@@H]2[C@@](C1)(CC=C(CC2)C(=O)O)C)(C)C)O)O	-6.7	*Trichoderma virens*
456	**M456**	[C@@]12(CC[C@]3([C@H]([C@@H]1CC(=C1[C@@H]([C@H]2O)[C@H](CC1)C)C)CC(CC3)(C)C)C)C	-6.7	*Aspergillus* sp. 085242
457	**M457**	[C@@]12(CC[C@]3([C@H]([C@@H]1CC(=C1[C@@H]([C@H]2O)[C@H]([C@@H](C1)O)C)C)CC(CC3)(C)C)C)C	-6.7	*Aspergillus* sp. 085242
458	**M458**	c1(cc(c2c(c1C=O)O[C@](C=C2)(CC/C=C(/C)\CC[C@@H](O)C(C)(O)C)C)O)C	-6.7	*Stachybotrys chartarum* 952
459	**M459**	c1c(cc(c(c1O)C(=O)O)c1cc(c(cc1C)O)O)OC	-6.7	*Streptomyces olivaceus*
460	**M460**	c1c(cc(cc1O)c1cc(c(cc1C)O)O)OC	-6.7	*Streptomyces olivaceus*

461	**M461**	O1[C@H]([C@H]([C@H](C[C@@H]1O[C@@H]1C[C@@](O[C@@H]([C@H]1CC)C)([C@H]([C@@H]([C@@H]([C@@H]1[C@H](/C=C/C=C/C(=C)O[C@@H]([C@H](/C=C/C=C/C(=O)O1)C)[C@H]([C@H]([C@@H]([C@]1(C[C@H]([C@@H]([C@H](O1)C)C)O[C@H]1C[C@@H]([C@@H]([C@@H](O1)C)O)O)O)C)O)C)C)O)C)O)O)O)C	-6.7	*Streptomyces* sp. 7-145
462	**M462**	C1CC(C2=C(C(=O)C3=C[C@@](CC(=O)[C@@]3([C@]2(C1)C)O)(C)C=C)O)(C)C	-6.7	Fungal strain HS-1
463	**M463**	Cc1cc(c2c(c1)[OH+]C1=C(C[C@@H]([C@](CC(=O)OC)(C(=O)OC)O)S1)C2=O)O	-6.7	*Penicillium oxalicum* SCSGAF 0023
464	**M464**	[C@@H]12[C@@H]([C@]3([C@H]4[C@]([C@@H]1O)(C1=CC(=O)OCC1=C[C@H]4OC3=O)C)C)O2	-6.7	*Aspergillus wentii* EN-48
465	**M465**	C1=C[C@]2([C@@H]3[C@]([C@H]1O)(C(=O)O[C@@H]3C=C1C2=CC(=O)OC1)C)C	-6.7	*Aspergillus wentii* EN-48
466	**M466**	[C@]12(C(=O)O[C@@H]3[C@@H]1[C@]([C@@H](CC2)O)([C@H]1[C@H](C3)COC(=O)C1)C)C	-6.7	*Aspergillus wentii* SD-310
467	**M467**	O[C@H]1/C=C\C=C\[C@@H](CCC[C@H](C)OC(=O)/C=C/1)O	-6.7	*Streptomyces lividan*
468	**M468**	O[C@@H]1/C=C\C=C\[C@@H](CCC[C@H](C)OC(=O)/C=C/1)O	-6.7	*Streptomyces lividan*
469	**M469**	CCCCCCCCCCCCCCCCc1cc(cc(c1C(=O)Oc1cc(C)c(c(c1)O)C(=O)O)O)O[C@H]1[C@@H]([C@H]([C@H]([C@@H](CO)O1)O)O)O	-6.7	*Cosmospora* sp. SF-5060
470	**M470**	C/C=C(/C)\[C@H]1[C@@H](/C=C/C=C(/C)\[C@H]([C@@H](C)CO)O)[C@@H]2C[C@H]([C@@](C)(C[C@H]2[C@H]2[C@]1(C)O2)O)Cl	-6.7	*Aspergillus* sp.
471	**M471**	C/C=C/[C@@H]1CO[C@]2(C)[C@H]1CC1=C(C=C(C)[OH+]C1=O)O2	-6.7	*Penicillium* sp. PSU-F44
472	**M472**	c1ccc(cc1)CC1=CC(=C(C(=O)[NH+]1)C=O)O	-6.7	*Aspergillus carbonarius*
473	**M473**	C1(=C(C=C([OH+]C1=O)/C(=C/[C@@H](CC(=O)O)C)/C)OC)C	-6.7	*Petriella* sp.
474	**M474**	C1(=O)O[C@H](c2c(C1)cc(cc2O)O)CCCCCC[C@@H](C)OC(=O)C	-6.7	*Pestalotiopsis* sp.
475	**M475**	CCOC(=O)[C@H](CCCNC(=N)N)/N=C(/[C@H](C[C@H]1C[NH2+][C@H]2CCCC[C@@H]12)/N=C(/[C@@H](CC(C)C)/N=C(/[C@H](CO)/N=C(/[C@@H](C[C@H]1CC[C@H](CC1)O)/N=C(/CCCCCC(C)C)\O)\O)\O)\O)\O	-6.7	*Brevibacillus laterosporus* PNG276
476	**M476**	C1(=O)O[C@H](c2c(C1)cc(cc2O)O)CCCCCCCCOC(=O)C	-6.7	*Pestalotiopsis* sp.
477	**M477**	[C@H]1([C@@]23N([C@@H]4[C@]1(c1c(N4)cccc1)[C@@]14c5c(N[C@@H]1N1[C@]6([C@H]4O)C(=O)N([C@@](C1=O)(CO)[S@]6=S=S)C)cccc5)C(=O)[C@](N(C2=O)C)(CO)[S@@]3=S=S=S)O	-6.6	*Acrostalagmus luteoalbus* HDN13-530
478	**M478**	c1ccc2c(c1)[C@]1([C@@](N2)(N2[C@@H](C1)C(=O)NCC2=O)C(C)(C=C)C)O	-6.6	*Eurotium* sp. SCSIO F452
479	**M479**	C1(C[C@@H]2/C(=C\[C@@H]([C@@H](C(=C)C[C@@H]([C@@]12O)OC(=O)C)NC(=O)/C=C(/CCO)\C)O)/CO)(C)C	-6.6	*Hansfordia sinuosae*
480	**M480**	c1(ccc(cc1)[C@@](CCCC(C)C)(O)C)CO	-6.6	*Aspergillus* sp.
481	**M481**	C1C(=O)[C@@H]([C@@]2([C@H]1C(=O)C1=C2CC(C1=O)(C)C)C)C	-6.6	*Chondrostereum* sp.
482	**M482**	[C@@H]1([C@@]([C@@H]2[C@@](C1)(CC(=O)C(=CC2)C)C)(C(C)(C)O)O)O	-6.6	*Trichoderma virens*

483	**M483**	C1C[C@@H]([C@@H]2[C@@H](C1=C)[C@@H](CC(=C2)C(=O)O)O)C(C)C	-6.6	*Cochliobolus lunatus* SCSIO41401
484	**M484**	C1CC(C2=C(C(=O)C3=C[C@](CC[C@@]3([C@]2(C1)C)O)(C=C)C)O)(C)C	-6.6	*Eutypella scoparia* FS26
485	**M485**	C1CC([C@]2([C@]3(C1)C1=C([C@H]([C@@]2(OC3)O)O)[C@H]([C@](CC1)(C=C)C)O)O)(C)C	-6.6	*Eutypella scoparia* FS26
486	**M486**	C1[C@@H](C([C@H]2[C@](C1)(C1=C(C(=O)C2)C[C@](C[C@@H]1O)(C=C)C)C)(C)C)O	-6.6	*Aspergillus wentii* SD-310
487	**M487**	C1/C=C/[C@H](C/C=C/[C@H](CC(=O)O[C@@H]1C)O)O	-6.6	*Dendrodochium* sp.
488	**M488**	C1C(=C[C@]2(C1)[C@@H]1[C@H](CC[C@@H]2C)[C@@H](C(=O)O1)C)CO	-6.6	*Penicilliumsp*.FJ-1
489	**M489**	O1C(=O)c2c([C@@H]1CCCCCCC)c(c(c(c2)O)O)O	-6.6	*Acremonium strictum*
490	**M490**	C=C[C@]1(C)C=C2C(=O)[C@@]3([C@]4(C(C)(C)CCC[C@]4(CO3)[C@]2([C@@H](C1)O)O)O)O	-6.6	*Eutypella scoparia* FS26
491	**M491**	c1c(cc2c(c1O)C(=O)C1=C([OH+]2)CC[C@H]1OC)C	-6.6	The the diethyl sulfate (DES) mutagenesis of *Penicillium purpurogenum* G59
492	**M492**	Cc1cc(c(C)c2c1C(=O)[C@]1(C(=O)C(=C(C(=O)[C@@]1(C)OC)O)C)O2)O	-6.6	*Aspergillus aculeatus*
493	**M493**	c1(cc(c2c3c1COC(=O)c3c(cc2C)O)O)O	-6.6	The the diethyl sulfate (DES) mutagenesis of *Penicillium purpurogenum* G59
494	**M494**	CC1(C)C[C@@H]2[C@H](C1)[C@@H]([C@@]1(C)CCC(=C21)C(=O)O)O	-6.6	*Chondrostereum* sp.
495	**M495**	[C@H]1(C[C@]2([C@H]3[C@](C1)(C1=CC(=O)OCC1=C[C@H]3OC2=O)C)C)O	-6.6	*Aspergillus dimorphicus* SD317
496	**M496**	c1c(cc(c2c1C=C(C(=O)[OH+]2)[C@@H]([C@@H](C)O)O)OC)OC	-6.6	*Pestalotiopsis* sp.
497	**M497**	c1c(cc(c2c1C=C(C(=O)[OH+]2)C[C@@H](CO)O)OC)OC	-6.6	*Pestalotiopsis* sp.
498	**M498**	c1c(cc(c2c1C=C(C(=O)[OH+]2)C[C@@H](CO)O)O)OC	-6.6	*Pestalotiopsis* sp.
499	**M499**	c1cc(c(cc1)NC[C@]1([C@H]([C@@H]([C@H](O1)CO)O)O)OC)C(=O)O	-6.5	*Streptomyces* sp. CMN-62
500	**M500**	c1(cc(c(cc1)[C@](CCCC(C)C)(C)O)O)CO	-6.5	*Aspergillus* sp.
501	**M501**	C1[C@@H](C(C2=C(C(=O)C3=C[C@](C[C@H]([C@@]3([C@]2(C1)C)O)O)(C=C)C)O)(C)C)O	-6.5	*Eutypella scoparia* FS26
502	**M502**	C1CC([C@H]2[C@]3(C1)C1=C([C@H]([C@@H]2O)O[C@H]3OC)[C@H]([C@](CC1)(C=C)C)O)(C)C	-6.5	*Aspergillus wentii* SD-310
503	**M503**	[C@@H]1(C([C@H]2[C@](C[C@@H]1O)([C@@]1([C@@H](CC2)C)Oc2c(C1)c(cc(c2C=O)CO)O)C)(C)C)OC(=O)C	-6.5	*Stachybotrys chartarum* 952
504	**M504**	CC(C)CC1=NC=C([C@H](C(C)C)O)[N+](C1=O)O	-6.5	Fungus strain CF07002
505	**M505**	C(=O)([C@@H](/C=C/CCCCCCCCCCCC)O)N[C@@H](CO[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)O)CO)[C@@H](/C=C/CC/C=C(/CCCCCCCCC)\C)O	-6.5	*Paecilomyces lilacinus* ZBY-1
506	**M506**	CC[C@@H](C)C[C@H](/C=C(/C)\[C@@H]([C@H](C)/C=C(/C)\[C@@H]([C@H](C)/C=C/[C@@H]([C@H](C)/C=C(/C)\C=O)O)O)O)CO	-6.5	*Pestalotiopsis clavispora*
507	**M507**	CCCCCC/C(=C/C(=O)/C=C\1/O[C@@H](C(=O)N1)CCCC)/C	-6.5	*Marinispora* strain NPS008920

508	**M508**	C1(=C(C(=O)[OH+]C(=C1)/C(=C/[C@@H](CCCC(=O)O)C)/C)CO)OC	-6.5	*Petriella* sp.
509	**M509**	C1CC[C@@H]2[C@@H](C1)[C@@H]([C@@H]([NH2+]2)C(C)(C=C)C)C(=O)N	-6.4	*Eurotium* sp. SCSIO F452
510	**M510**	c1c(cc2c(c1O)CN(C2=O)CCCCC(=O)OC)O	-6.4	*Diaporthe phaseolorum* SKS019
511	**M511**	C1(C[C@@H]2/C(=C/C=C\[C@@](C[C@@H]([C@@]12O)OC(=O)C)(C)O)/CO)(C)C	-6.4	*Hansfordia sinuosae*
512	**M512**	c1(cc(c(cc1)[C@@]1(C)OC(CCC1)(C)C)O)CO	-6.4	*Aspergillus* sp.
513	**M513**	[C@@H]1([C@@]([C@@H]2[C@@](C1)(CC(=O)[C@]1([C@@H](C2)O1)C)C)(C(C)C)O)O	-6.4	*Trichoderma virens*
514	**M514**	C1[C@@H](C(C2=C(C(=O)C3=C[C@](CC[C@@]3([C@]2(C1)C)O)(C=C)C)O)(C)C)O	-6.4	*Eutypella scoparia* FS26
515	**M515**	C1=C[C@]2([C@@H](C(C1=O)(C)C)[C@H]([C@@H](C1=C[C@](CC[C@]21O)(C=C)C)O)O)C	-6.4	*Eutypella* sp. FS46
516	**M516**	C1[C@@H](C([C@H]2[C@](C1)(C1=C(C(=O)C2)[C@H]([C@](CC1)(C=C)C)OC(=O)C)C)(C)C)O	-6.4	*Aspergillus wentii* SD-310
517	**M517**	c1c(cc(c(c1O)C(=O)O)c1c2c(c(cc1C)O)ncs2)OC	-6.4	*Alternaria* sp.
518	**M518**	c1c(cc(c(c1C(=O)O)C(=O)c1c(cccc1O)O)O)C	-6.4	*Penicillium* sp. ZJ-SY2
519	**M519**	c1c(cc(c(c1C(=O)OC)C(=O)c1c(cccc1O)O)O)C	-6.4	*Penicillium* sp. ZJ-SY2
520	**M520**	C(=O)(CC[C@@]1([C@H](CCc2c(c(c(cc12)O)C)C=C)C(=C)C)C)OC	-6.4	Endophytic fungus J3
521	**M521**	C=C[C@@]1(C)CC[C@]2(C(=C1)C(=O)C(=C1C(C)(C)CC[C@H]([C@]21C)O)O)O	-6.4	*Eutypella scoparia* FS26
522	**M522**	C(=O)(C)O[C@H]1[C@H]2O[C@H]2C2=CC(=O)[C@]3(C[C@@]2([C@H]1C)C)O[C@]3(C)CO	-6.4	*Penicilliumsp*. PR19 N-1
523	**M523**	C1CC([C@]2([C@]3(C1)[C@@H]1C(=C[C@@](CC1=O)(C)C=C)C(=O)[C@]2(O)OC3)O)(C)C	-6.4	Fungal strain HS-1
524	**M524**	C1CC([C@]2([C@]3(C1)[C@@]1(C(=C[C@@](C[C@H]1O)(C)C=C)C(=O)[C@]2(O)OC3)O)O)(C)C	-6.4	Fungal strain HS-1
525	**M525**	c1(cc(c2c(c1)[OH+]C1=C(C2=O)C[C@H]([C@@]1(O)C(=O)OC)SC[C@@H](C(=O)OC)O)O)C	-6.4	*Penicillium purpurogenum* G59
526	**M526**	C(=O)([C@@H](/C=C/CCCCCCCCCCCCCC)O)N[C@@H](CO[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)O)CO)[C@@H](/C=C/CC/C=C(/CCCCCCCCC)\C)O	-6.4	*Paecilomyces lilacinus* ZBY-1
527	**M527**	C(CCCCC/C(=C/C(=O)/C=C\1/O[C@@H](C(=O)N1)CCCCC)/C)C	-6.4	*Marinispora* strain NPS008920
528	**M528**	OC[C@@H]1O[C@H](C[C@H]1O)[N+]1C(=O)NC(=O)C(=C1)C	-6.3	*Aspergillus* sp.
529	**M529**	[C@@H]1(C[C@@H]([C@H]2[C@]([C@@H]1O)(CC[C@](C2)(C(=C)C)O)C)C)O	-6.3	*Penicillium* sp. J-54
530	**M530**	[C@@H]1(C[C@@H]([C@]2([C@]([C@@H]1O)(CC[C@H](C2)C(=C)C)C)O)C)O	-6.3	*Penicillium* sp. J-54
531	**M531**	[C@@H]1([C@@]([C@@H]2[C@@](C1)(C[C@H](C(=C)CC2)O)C)(C(C)C)O)O	-6.3	*Trichoderma virens*
532	**M532**	C(/C=C/C(C)(C)OC)[C@]([C@@H]1CC[C@@]([C@H]1C)(C)O)(O)C	-6.3	*Trichoderma harzianum* X-5
533	**M533**	[C@@H]1([C@@H]([C@](CC1)(C)O)C)[C@](CCC[C@@H](C)C(=O)OC)(C)O	-6.3	*Trichoderma harzianum* X-5
534	**M534**	C1CC(C2=CC(=O)C3=C([C@]2(C1)O)CC[C@@]([C@H]3O)(C=C)C)(C)C	-6.3	*Aspergillus wentii* SD-310

535	**M535**	[C@@]12([C@H]3[C@](CC[C@@H]1[C@@]1(OC(=O)[C@H]([C@H]2O)C1)C)([C@@]1(C(=O)[C@@](C(=O)[C@@](C3)(C)C1=C)(C)O)C(=O)OC)C)C	-6.3	*Penicillium brasilianum*
536	**M536**	C1[C@H]2[C@H]([C@H](C/C=C/[C@H](CC(=O)O[C@@H]1C)O)O)O2	-6.3	*Dendrodochium* sp.
537	**M537**	C1[C@H](C[C@H](C/C=C/[C@H](CC(=O)O[C@@H]1C)O)O)O	-6.3	*Dendrodochium* sp.
538	**M538**	c1(cc(cc(c1)C[C@H](OC(=O)C[C@@H](C)O)C)O)O	-6.3	*Hansfordia sinuosae*
539	**M539**	c1(ccc(cc1)CCO)OC[C@@H](O)C(C)(C)O	-6.3	*Penicilliumsp*.FJ-1
540	**M540**	c1(c(c(cc(c1)O)O)C(=O)CCCCCCC)CC(=O)OC	-6.3	*Dothiorella* sp.
541	**M541**	c1ccc2c(c1)c(=C)[nH+]c([nH]2)[C@@H](C)O	-6.3	*Penicillium commune* SD-118
542	**M542**	CC(C)CC1=CN=C(CC(C)C)C(=O)[N+]1O	-6.3	marine-derived fungus strain CF07002
543	**M543**	c1cc2[C@H](CCC(=O)c2c(c1)O)O	-6.3	*Aspergillus fumigatus*
544	**M544**	O=C1/C=C\[C@@H](OC)/C=C\CCC[C@H](C)OC(=O)/C=C/1	-6.3	*Pestalotiopsis microspore*
545	**M545**	c1c(cc(c2c1C=C(C(=O)[OH+]2)C[C@@H](C)O)OC)OC	-6.3	*Pestalotiopsis* sp.
546	**M546**	C([C@H]1NC(=O)[C@H](NC1=O)Cc1ccc(cc1)O)C(C)C	-6.2	*Aspergillus* sp.
547	**M547**	c1(c(c2c(c(c1O)C)[C@@H]([C@H](OC2)C)C)O)C(=O)O	-6.2	*Aspergillus* sp.
548	**M548**	C1(=O)C[C@H]([C@@H]2[C@@]34C(=C(C(=O)CC[C@@H]1C)C(=O)O3)O[C@@]([C@H](C4)C)([C@H]2O)C)O	-6.2	*Streptomyces koyangensis* SCSIO 5802
549	**M549**	c1(ccc(cc1)O)C[C@@H](N(C(=O)[C@@H](NC(=O)C)[C@@H](CC)C)C)C(=O)O	-6.2	*Simplicillium obclavatum* EIODSF 020
550	**M550**	C1(=C[C@@]2([C@]3(N(C1=O)CC(=O)N3)[N@H+]([C@@H]1[C@@H]2C=CC=C1)OC)C(C=C)(C)C)OC	-6.2	*Aspergillus versicolor* LZD-14-1
551	**M551**	c1c(cc2c(c1O)CN(C2=O)CCO)O	-6.2	*Diaporthe phaseolorum* SKS019
552	**M552**	[C@@]12([C@@H]([C@@]3([C@]([C@@H]1OC(=O)C)([C@H](C=C3)O)C)CO)CC2(C)C)O	-6.2	*Hansfordia sinuosae*
553	**M553**	[C@@H]1(C[C@@H]([C@H]2[C@]([C@@H]1O)(CC[C@H](C2)C(=C)C)C)C)O	-6.2	*Penicillium* sp. J-54
554	**M554**	[C@@H]12C[C@@]([C@@H]3[C@](C1)([C@H](C[C@H]3O)C)CC=C2C)(C)O	-6.2	*Penicillium bilaiae* MA-267
555	**M555**	C1[C@H]([C@H]2C(C(=C1C)CC/C(=C/[C@@H](C/C(=C/C2)/C)OC)/C)(C)C)O	-6.2	*Trichoderma harzianum* X-5
556	**M556**	C1[C@@H](CC(=O)C/C=C/[C@H](CC(=O)O[C@@H]1C)O)O	-6.2	*Dendrodochium* sp.
557	**M557**	C1/C=C/[C@@H](C/C=C/[C@H](CC(=O)O[C@@H]1C)O)O	-6.2	*Dendrodochium* sp.
558	**M558**	C1=C([OH+]c2c(C1=O)c(cc(c2[C@@H](OC)C[C@H](C(=O)O)OC)OC)O)C	-6.2	*Rhytidhysteron rufulum*
559	**M559**	[C@H]12C(=C[C@H]([C@H](O1)/C=C/C)O)C(=O)O[C@H]2/C=C/C	-6.2	*Acremonium Strictum*
560	**M560**	c1cccc(c1C(=O)O)/N=C(/C(=O)C)\C	-6.2	*Penicillium paneum* SD-44
561	**M561**	C[C@H]1C[C@@H]([C@@H]2[C@@](C)(C(=O)CCO)[C@@](C)(C=C[C@]2(C1)O)O)O	-6.2	*Aspergillus sulphureus* KMM 4640
562	**M562**	Br/C=C/C#CCCCCCC/C=C/C#CCCCCCCCC(=O)N[C@@H](CCl)N	-6.2	*Xestospongia* sp.
563	**M563**	C1[C@H]([C@@H](C[C@@]2([C@H](C[C@H](C=C12)O)C)C)C(=C)C)O	-6.2	*Penicilliumsp*. PR19 N-1
564	**M564**	C1=C([OH+]c2c(C1=O)c(cc(c2[C@@H](OC)C[C@H](C(=O)OC)OC)OC)O)C	-6.2	*Rhytidhysteron rufulum*
565	**M565**	CN1/C(=C/c2ccccc2)/C(=O)N(C)[C@@](CO)(C1=O)SC	-6.2	Pleosporales strain CRIF2
566	**M566**	c1(c(c(cc(c1)O)O)C(=O)CCCCCC[C@@H](C)O)CC(=O)OC	-6.2	*Pestalotiopsis* sp.

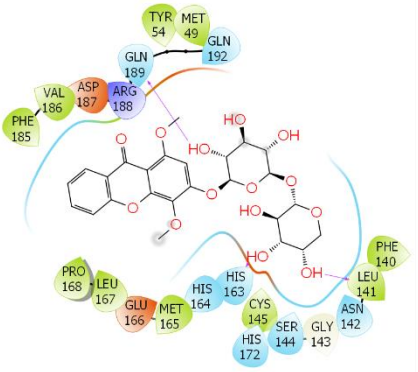
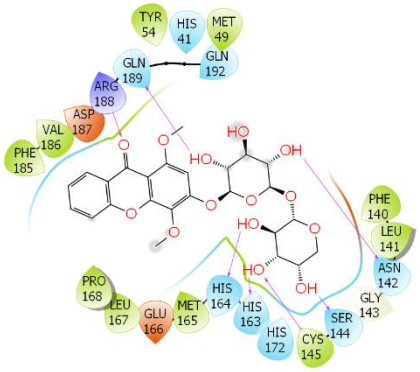
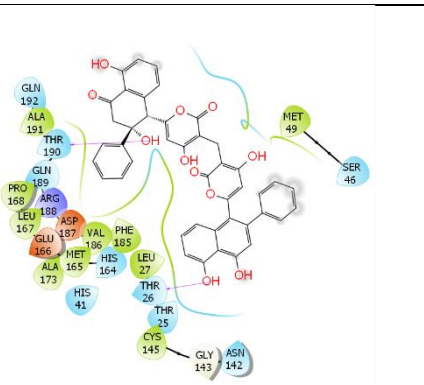
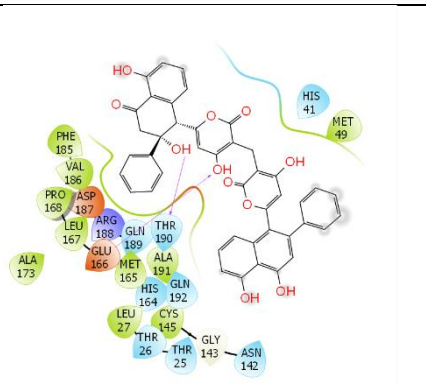
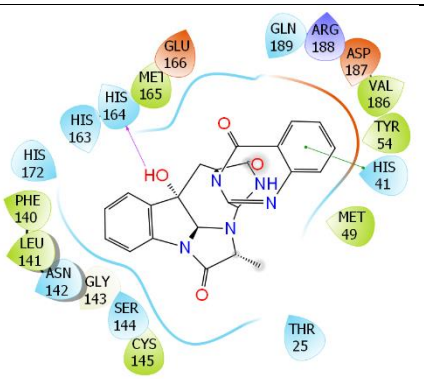
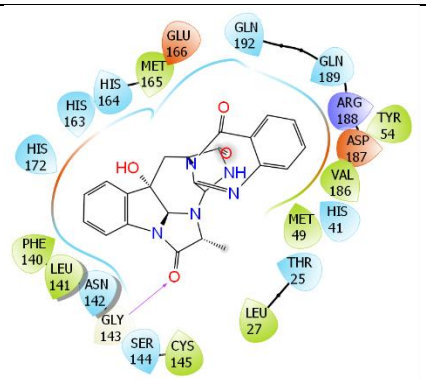
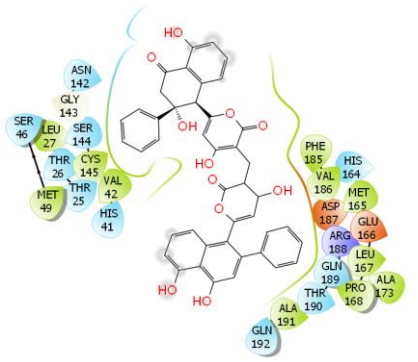
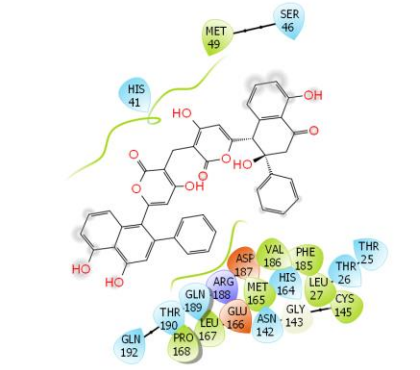
567	**M567**	c1(c(c(cc(c1)O)O)C(=O)CCCCCCCC)CC(=O)OC	-6.2	*Pestalotiopsis* sp.
568	**M568**	C1(=O)N[C@@H](C(=O)N2[C@H]1CCC2)[C@@H](CC)C	-6.1	*Aspergillus* sp.
569	**M569**	c1(C)c(c(C(=O)O)c(O)cc1[C@H]([C@H](O)C)C)O	-6.1	*Aspergillus* sp.
570	**M570**	C1(=O)[C@@H]([C@H](C)CC)NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@H](NC(=O)C[C@H](OC(=O)[C@H](N1)[C@H](CC)C)CCCCCCCCCCCCCC)CCC(=O)OC)CC(C)C)CC(C)C)CC(C)C)CC(=O)OC	-6.1	*Bacillus* sp. 176
571	**M571**	[C@@H]1([C@@]([C@@H]2[C@@](C1)(CC=C(CC2)C)C)(C(C)(C)O)O)O	-6.1	*Trichoderma virens*
572	**M572**	[C@@H]12C[C@@]([C@@H]3[C@](C1)([C@H](C[C@H]3O)C)CC=C2C)(C)OC(=O)C	-6.1	*Penicillium bilaiae* MA-267
573	**M573**	[C@]123[C@H]([C@]4([C@@H]([C@@H](CC1)C)C(=O)C4)C)C[C@H]([C@@H](C[C@H]2C)O)C3(C)C	-6.1	*Trichoderma harzianum* X-5
574	**M574**	[C@H]1([C@@H](CO[C@@H]([C@H]1O)CO)NC(=O)C)O	-6.1	*Virgibacillus dokdonensis* MCCC 1A00493
575	**M575**	C1[C@H](CC(=O)C/C=C/[C@H](CC(=O)O[C@@H]1C)O)O	-6.1	*Dendrodochium* sp.
576	**M576**	C1CC[C@@H](C/C=C/[C@H](CC(=O)O[C@@H]1C)O)O	-6.1	*Dendrodochium* sp.
577	**M577**	C1C[C@]([C@H]2[C@](C1)([C@H](C(=C)[C@H](C2)O)CC(=O)O)C)(C)C(=O)O	-6.1	*Aspergillus terreus* GX7-3B
578	**M578**	O1C(=O)/C=C\[C@](/C=C\[C@@H](/C(=C\CC[C@@H]([C@H]1C)C)/C)OC)(C)O	-6.1	*Eutypella* sp. FS46
579	**M579**	C(=O)(C)O[C@@H]1[C@]23[C@@H]([C@@H]([C@H]([C@@H](/C=C(/C1)\C)O)O)[C@@H](O3)O)CC2(C)C	-6.1	*Ascotricha* sp. ZJ-M-5
580	**M580**	C1(=O)C(=C(C=C([OH+]1)C[C@H](C)O)O)C	-6.1	*Aspergillus* sp. 16-02-1
581	**M581**	C(=O)([C@H](N(C)C(=O)[C@@H](NC(=O)C)[C@@H](CC)C)Cc1ccccc1)O	-6.1	*Simplicillium obclavatum* EIODSF 020e
582	**M582**	O[C@H]1/C=C\[C@@H](OC)/C=C\CCC[C@H](C)OC(=O)/C=C/1	-6.1	*Pestalotiopsis microspore*
583	**M583**	c1cc(c2c(c1)C(=O)C(=C([OH+]2)CO)C)OC	-6.1	*Penicillium* sp.
584	**M584**	C(CCCCC/C(=C/C(=O)CC(=N)O[C@H](C(=O)O)CCCC)/C)C	-6.1	*Marinispora* strain NPS008920
585	**M585**	C[C@H](CC[C@H]1c2cccc(c2C(=O)O1)OC)O	-6.1	*Pleosporales* strain CRIF2
586	**M586**	[C@@H]1(CC([C@H]2[C@](C1)([C@](C)([C@@H](CC2=O)C)(CO)O)C)(C)C)O	-6.1	*Aspergillus ustus*
587	**M587**	c1c(cc(c2c1C=C(C(=O)[OH+]2)CO)OC)O	-6.1	*Pestalotiopsis* sp.
588	**M588**	[C@H]1(NC(=O)[C@H]2N(C1=O)CCC2)CC(C)C	-6	*Aspergillus* sp.
589	**M589**	C1(=O)N[C@H](C(=O)N2[C@H]1CCC2)CC(C)C	-6	*Aspergillus* sp.
590	**M590**	C1(=O)[C@@H]([C@H](C)CC)NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@H](NC(=O)C[C@H](OC(=O)[C@H](N1)[C@H](CC)C)CCCCCCCCCCCCCCC)CCC(=O)OC)CC(C)C)CC(C)C)CC(C)C)CC(=O)OC	-6	*Bacillus* sp. 176
591	**M591**	c1(occc1)c1cncc(n1)C[C@@H]([C@H](CO)O)O	-6	*Jishengella endophytica* 161111
592	**M592**	[C@@H]1([C@@]([C@@H]2[C@@](C1)([C@@H](C=C(CC2)C)O)C)(C)C)O)O	-6	*Trichoderma virens*
593	**M593**	C1=CC2=CC(=O)[C@@](C[C@@]2([C@H](C1)C)C)(C(=C)CO)O	-6	*Cochliobolus lunatus* SCSIO41401
594	**M594**	C(CC=C(C)C)[C@]([C@@H]1[C@H](C[C@@]([C@H]1C)(C)O)O)(O)C	-6	*Trichoderma harzianum* X-5

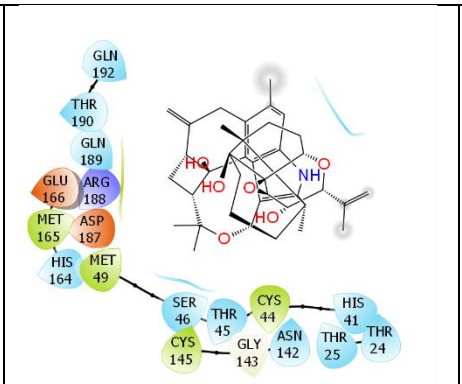
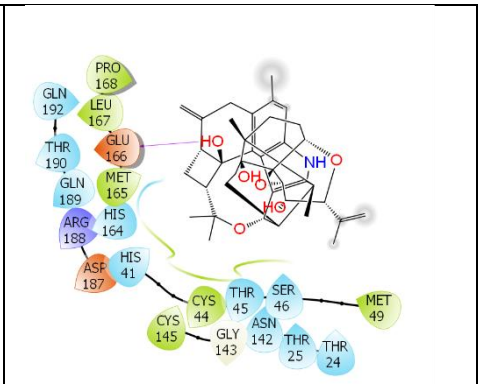
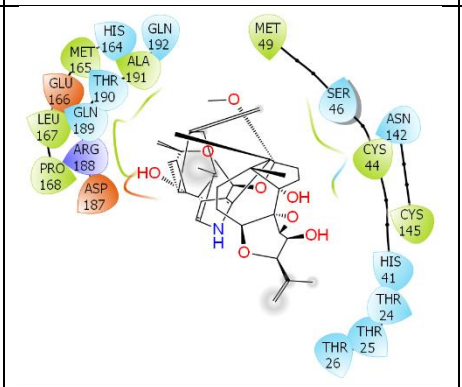
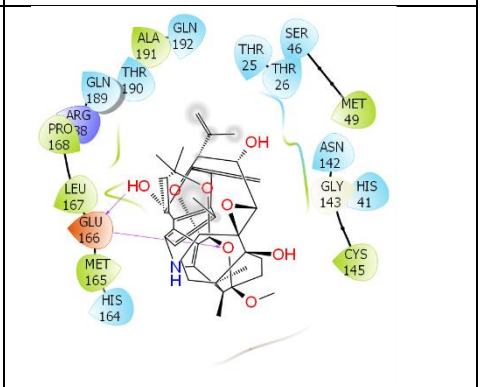
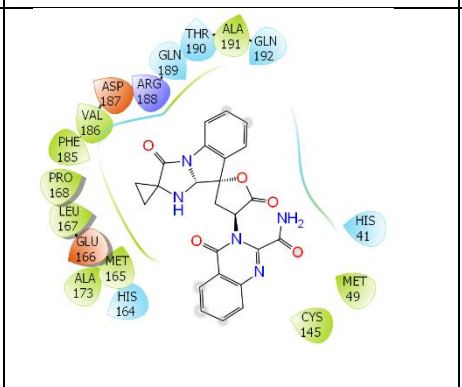
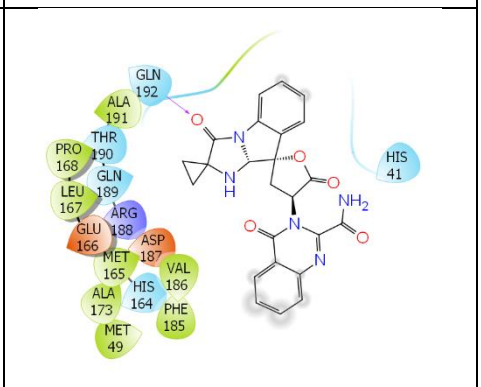
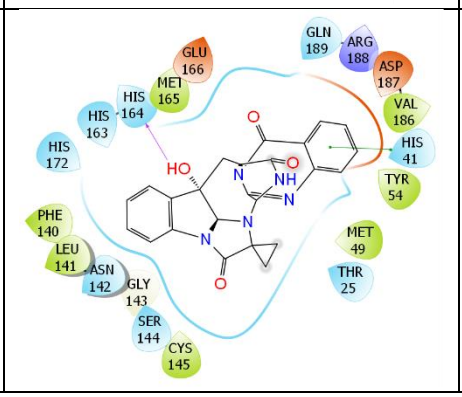
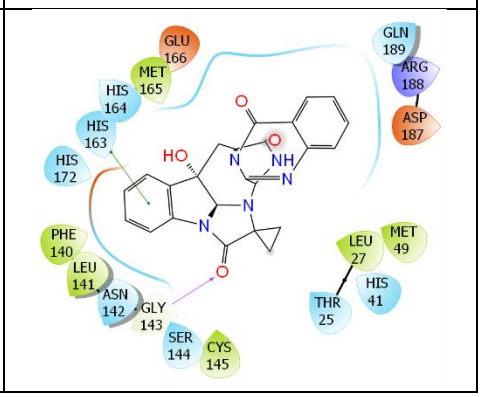
595	**M595**	C1CCC(=O)C/C=C/[C@H](CC(=O)O[C@@H]1C)O	-6	*Dendrodochium* sp.
596	**M596**	C1CC[C@H](C/C=C/[C@H](CC(=O)O[C@@H]1C)O)O	-6	*Dendrodochium* sp.
597	**M597**	C1CC[C@H](CCC[C@H](CC(=O)O[C@@H]1C)O)O	-6	*Dendrodochium* sp.
598	**M598**	O1C(=O)[C@@H](N(C(=O)[C@H](OC(=O)[C@@H](N(C(=O)[C@H](OC(=O)[C@@H](N(C(=O)[C@H]1C(C)C)C)Cc1ccccc1)C(C)C)C)Cc1ccccc1)C(C)C)C)Cc1ccccc1	-6	*Fusarium* sp. DZ27
599	**M599**	c1(c(c(cc(c1)O)O)C(=O)CCCCCCCC)CC(=O)OCC	-6	*Dothiorella* sp.
600	**M600**	[C@@H]12N(C(=O)[C@@H](NC1=O)CC(C)C)CCC2	-6	*Aspergillus versicolor* ZBY-3
601	**M601**	C1=C(C2=CC(=O)C(=C[C@@]2([C@H]([C@H]1OC(=O)C)C)C)O)Cl	-6	*Penicillium* sp. PR19N-1
602	**M602**	C(=O)(c1c(cc(cc1CCCCCCCCC)O)O)O	-6	*Lasiodiplodia* sp. 318
603	**M603**	CCCC[C@@H](CC)COC(=O)c1ccccc1C(=O)OC[C@H](CC)CCCC	-6	*Cladosporium* sp. F14
604	**M604**	[C@H]1(NC(=O)[C@H]2N(C1=O)C[C@@H](C2)O)CC(C)C	-5.9	*Aspergillus* sp.
605	**M605**	c1c(c(ccc1)C(=O)OCC(C)C)C(=O)OCCCC	-5.9	*Aspergillus* sp.
606	**M606**	C1(=O)[C@]([C@H](C(=C1C)[C@@H](CC/C=C/C)O)O)(O)C	-5.9	*Trichoderma* sp. HPQJ-34
607	**M607**	C1(=O)C2=C[C@@H]3[C@@]45[C@@]2(C(=C(CC[C@@H]1C)O)C(=O)O4)O[C@@]([C@H](C5)C)([C@H]3O)C	-5.9	*Streptomyces koyangensis* SCSIO 5802
608	**M608**	C1(C[C@@H]2/C(=C\[C@@H](/C=C(/C[C@@H]([C@@]12O)OC(=O)C)\C)O)/CO)(C)C	-5.9	*Hansfordia sinuosae*
609	**M609**	[C@@H]1(C[C@@H]([C@]2([C@]([C@@H]1O)(CC[C@](C2)(C(=C)C)O)C)O)C)O	-5.9	*Penicillium* sp. J-54
610	**M610**	C1(=C[C@H]2[C@](CC1)([C@@]1([C@](O2)([C@H](C[C@H]1O)OC)CO)C)C)C	-5.9	*Stachybotrys chartarum*
611	**M611**	[C@]123[C@H]([C@H](C(=O)C4=C1CC[C@@]([C@@H]4O)(C=C)C)O)[C@@]([C@@H](C[C@H]2C3)OC(=O)C)(CC(=O)C(C)C)C	-5.9	*Eutypella* sp. FS46
612	**M612**	C1/C=C/C(=O)C[C@H](C[C@H](CC(=O)O[C@@H]1C)O)OC	-5.9	*Dendrodochium* sp.
613	**M613**	C(=O)([C@@H](N(c1c(cccc1)C(=O)O)C(=O)[C@H](N(C)C(=O)[C@@H](N)C(C)C)Cc1ccccc1)CC(C)C)N	-5.9	*Simplicillium obclavatum* EIODSF 020e
614	**M614**	C(=O)(c1c(cc(cc1CCCCCCC[C@@H](C)O)O)O)O)OCC	-5.9	*Lasiodiplodia* sp. 318
615	**M615**	[C@@H]12[C@@H](C(=O)[C@@H](NC1=O)CC(=C)C)CCC2	-5.9	*Penicillium purpurogenum* G59
616	**M616**	C(=O)(C)O[C@@H]1[C@]23[C@@H]([C@@H]([C@H]([C@@H](/C=C(\C1)/C)O)OC)[C@@H](O3)O)CC2(C)C	-5.9	*Ascotricha* sp. ZJ-M-5
617	**M617**	[C@@H]12N(C(=O)[C@@H](NC1=O)[C@@H](CC)C)CCC2	-5.9	*Aspergillus versicolor* ZBY-3
618	**M618**	C(=O)([C@@H](CCCCCCCCCCCCCC)O)N[C@@H](CO[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO)[C@@H](/C=C/CC/C=C(/CCCCCCCCC)\C)O	-5.9	*Paecilomyces lilacinus* ZBY-1
619	**M619**	C(=O)([C@@H](CCCCCCCCCCCCCCCC)O)N[C@@H](CO[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO)[C@@H](/C=C/CC/C=C(/CCCCCCCCC)\C)O	-5.9	*Paecilomyces lilacinus* ZBY-1
620	**M620**	C1=C([OH+]c2c(C1=O)c(cc(c2[C@H](OC)C[C@H](C(=O)OC)OC)OC)O)C	-5.9	*Rhytidhysteron rufulum*
621	**M621**	CCCC[C@H]1c2cccc(c2C(=O)O1)OC	-5.9	Fungus strain CRIF2
622	**M622**	C1(=O)N[C@H](C(=O)N2[C@H]1CCC2)C(C)C	-5.8	*Aspergillus* sp.

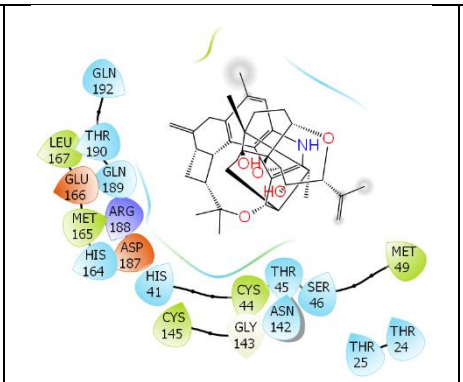
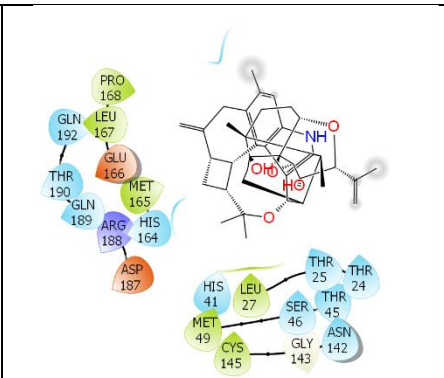
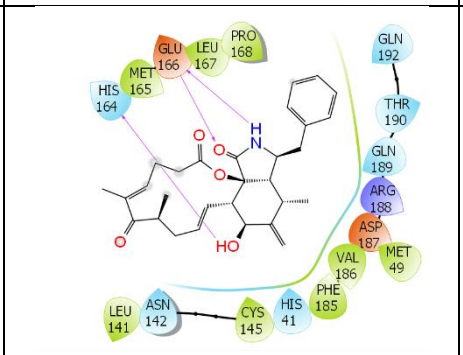
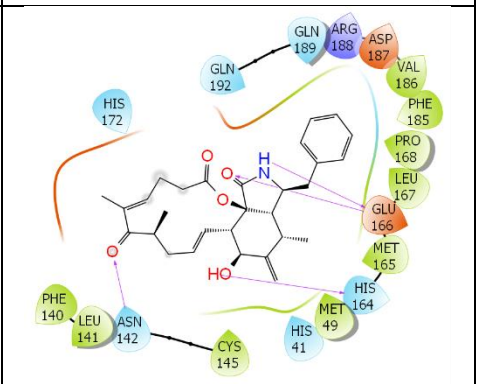
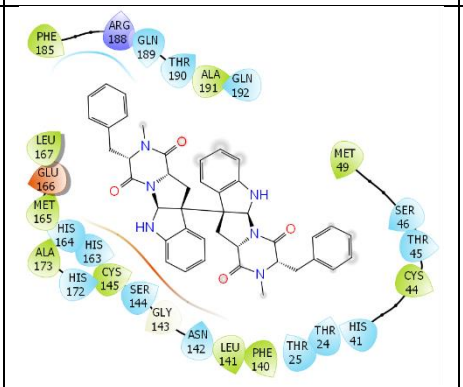
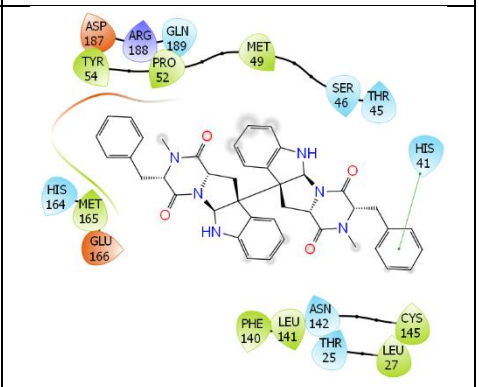
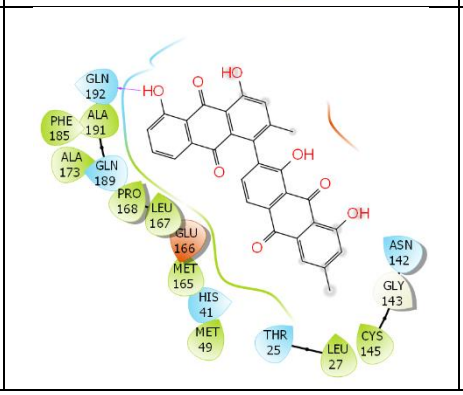
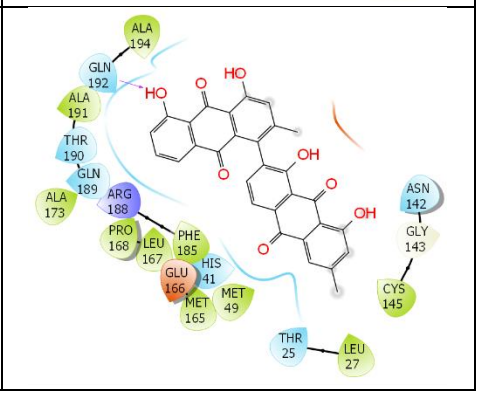
623	**M623**	C(C)[C@@H](C)[C@@H]1NC(=O)[C@H](NC1=O)CC(C)C	-5.8	*Aspergillus* sp.
624	**M624**	C1(=O)[C@@H](NC(=O)[C@H]2N1CCC2)CC(C)C	-5.8	*Aspergillus* sp.
625	**M625**	c1(cc(c2c(c1OC)C(=O)OC2)COC)C	-5.8	*Penicillium* sp. ZH58
626	**M626**	[C@H]1([C@H](OC(=O)C(=C1)[C@H]([C@H](C)O)Cl)C)O	-5.8	*Exophiala* sp.
627	**M627**	Cc1ccc(cc1C(=O)[C@H](C)O)O	-5.8	*Massarina* sp. CNT-016
628	**M628**	C1[C@@H](C([C@H]2[C@](C1)([C@H]([C@@H](CC2=O)C)CO)C)(C)C)O	-5.8	*Aspergillus ustus*
629	**M629**	C1(=C[C@]2([C@](CC1)([C@@]1(C[C@H](O2)C[C@H]1O)C)C)OCO)C	-5.7	*Stachybotrys chartarum*
630	**M630**	C1C=C(CC[C@]21[C@@H](C[C@H]([C@@H]2C)O)C(C)(C)O)C	-5.7	*Trichoderma harzianum* X-5
631	**M631**	[C@H](C(=C)C(=O)O)(C(=O)O)CCCCC(=O)C	-5.7	*Aspergillus niger*
632	**M632**	[C@H]1([C@H](C=C(C(=O)O1)[C@@H]([C@@H](C)O)OC)O)C	-5.7	*Aspergillus* sp. 16-02-1
633	**M633**	CC[C@@H](C)[C@H](NC(=O)C)C(=O)N(C)[C@@H](Cc1ccc(O)cc1)C(=O)O	-5.7	*Simplicillium obclavatum* EIODSF 020e
634	**M634**	C[C@@H]1[C@H]2CC(=O)[C@@H]([C@@]31[C@H](C(=C)OC3=O)O2)O	-5.7	*Massarina* sp. CNT-016
635	**M635**	C1[C@@H](C([C@H]2[C@](C1)([C@]([C@@H](CC2=O)C)(CO)O)C)(C)C)O	-5.7	*Aspergillus ustus*
636	**M636**	CC(=C1[C@H](C(=O)N(CCC(=O)OC)C1=O)O)C	-5.7	*Pestalotiopsis* sp.
637	**M637**	C(CCCCC/C(=C/C(=O)/C=C\1/O[C@@H](C(=O)N1)CCCC)/C)C	-5.7	*Marinispora* strain NPS008920
638	**M638**	c1c2c(ccc1)c(c[nH]2)CC(=O)O	-5.6	*Aspergillus* sp.
639	**M639**	[C@H]1(OC(=O)C(=C1)[C@H]([C@H](C)O)O)[C@H](C)O	-5.6	*Aspergillus* sp. 16-02-1
640	**M640**	[C@H]1([C@H](OC(=O)C(=C1)[C@@H]([C@@H](C)O)OC)C)O	-5.6	*Aspergillus* sp. 16-02-1
641	**M641**	[C@H](/C=C(/C=C/C(=C)C)\CO)(C)O	-5.6	*Aspergillus* sp. 16-02-1
642	**M642**	C1CCC[C@H]2[C@H]1[NH2+]C[C@@H]2C=O	-5.6	*Jishengella endophytica* 161111
643	**M643**	O1[C@H](C=C(C1=O)[C@H]([C@H](C)O)O)[C@H](C)O	-5.6	*Aspergillus* sp. 16-02-1
644	**M644**	C1(=O)N[C@H](C(=O)N2[C@H]1CCC2)C	-5.5	*Aspergillus* sp.
645	**M645**	[C@@H]1(O[C@H]([C@@H]([C@H]([C@H]1O)O)O)OC(C)C)CO	-5.5	*Aspergillus* sp.
646	**M646**	S([C@]12N([C@H]3C(=CC=C[C@@H]3O)C1)C(=O)[C@@](SC)(N(C2=O)C)CO)C	-5.5	*Aspergillus* sp.
647	**M647**	[C@H]1(OC(=O)C(=C1)[C@@H]([C@@H](C)O)O)[C@H](C)O	-5.5	*Aspergillus* sp. 16-02-1
648	**M648**	[C@H]1(OC(=O)C(=C1)[C@@H]([C@@H](C)O)OC)[C@H](C)O	-5.5	*Aspergillus* sp. 16-02-1
649	**M649**	[C@@H]1(OC(=O)/C(=C/[C@H](C)O)/[C@H]1O)[C@@H](C)O	-5.5	*Aspergillus ochraceus* MA-15
650	**M650**	[C@H]1([C@H](OC(=O)C(=C1)CC(=O)C)C)C	-5.5	*Aspergillus ochraceus* MA-15
651	**M651**	[C@@]12([C@@H]([C@@]3([C@](C[C@@H]1OC(=O)C)(C=C[C@H]3O)C)CO)CC2(C)C)O	-5.5	*Hansfordia sinuosae*
652	**M652**	O1[C@H](C=C(C1=O)[C@@H]([C@@H](C)O)O)[C@H](C)O	-5.5	*Aspergillus* sp. 16-02-1
653	**M653**	O1[C@H](C=C(C1=O)[C@@H]([C@@H](C)O)OC)[C@H](C)O	-5.5	*Aspergillus* sp. 16-02-1
654	**M654**	[C@H]1([C@H](C=C(C(=O)O1)C[C@H](C)O)O)C	-5.5	*Aspergillus* sp. 16-02-1
655	**M655**	[C@H]1([C@H](OC(=O)C(=C1)[C@@H]([C@H](C)Cl)O)C)O	-5.5	*Aspergillus versicolor* ZBY-3
656	**M656**	c1ccc(cc1)/C=C/C(=O)O	-5.5	*Penicillium* sp. PR19N-1
657	**M657**	c1c2[nH]cc(c2ccc1)CCO	-5.4	*Aspergillus* sp.
658	**M658**	[C@H]1(OC(=O)C(=C1)C[C@@H](C)O)[C@H](C)O	-5.4	*Aspergillus* sp. 16-02-1

659	**M659**	[C@H]1(OC(=O)C(=C1)C[C@H](C)O)[C@H](C)O	-5.4	*Aspergillus* sp. 16-02-1
660	**M660**	[C@H]1(OC(=O)C(=C1)CC(=O)[C@H](C)O)C	-5.4	*Aspergillus ochraceus* MA-15
661	**M661**	[C@H](C(=C)C(=O)O)(C(=O)OC)CCCCCCO	-5.4	*Aspergillus niger*
662	**M662**	[C@H](C(=C)C(=O)O)(C(=O)O)CCCCCCOC(=O)C	-5.4	*Aspergillus niger*
663	**M663**	O1[C@H](C=C(C1=O)C[C@@H](O)C)[C@H](C)O	-5.4	*Aspergillus* sp. 16-02-1
664	**M664**	c1c2c(ccc1)c(c[nH]2)C=O	-5.3	*Aspergillus* sp.
665	**M665**	C[C@@H]([C@H]1C=C(C(=O)O1)CC(=O)C)O	-5.3	*Aspergillus* sp. 16-02-1
666	**M666**	O1[C@H](C=C(C1=O)CC(=O)C)[C@H](C)O	-5.3	*Aspergillus* sp. 16-02-1
667	**M667**	O1[C@H](C=C(C1=O)C[C@H](O)C)[C@H](C)O	-5.3	*Aspergillus* sp. 16-02-1
668	**M668**	CC(=O)/C=C/C(=C/[C@@H](C)O)/CO	-5.3	*Aspergillus* sp. 16-02-1
669	**M669**	O[C@@H]1[C@@H](O)[C@@H]([C@H](O[C@H]1CO)OCCC)O	-5.2	*Aspergillus* sp.
670	**M670**	C1(OC(=O)C(=C1)CC[C@H](C)O)(C)C	-5.2	*Aspergillus* sp. 16-02-1
671	**M671**	C1[C@@H](CC(=O)C/C=C/[C@H](CC(=O)O[C@@H]1C)O)OC	-5.2	*Dendrodochium* sp.
672	**M672**	O1[C@H](C=C(C1=O)CC[C@H](C)O)C	-5.2	*Aspergillus* sp. 16-02-1
673	**M673**	C[C@@H](/C=C(/C=C/[C@@H](C)O)\CO)O	-5.2	*Aspergillus* sp. 16-02-1
674	**M674**	C[C@@H](C1=CC(=CC(=O)[OH+]1)OC)O	-5.2	*Nigrospora* sp.
675	**M675**	N12[C@H](C(=O)NCC1=O)CCC2	-5.1	*Aspergillus* sp.
676	**M676**	c1cc(ccc1)CCC(=O)O	-5.1	*Aspergillus* sp.
677	**M677**	C[C@@H](/C=C(/C=C/[C@H](C)O)\CO)O	-5.1	*Aspergillus* sp. 16-02-1
678	**M678**	c1cc(c(cc1)O)CC=O	-4.8	*Aspergillus* sp.
679	**M679**	C1=C(CO)C(=O)[C@H]2[C@@H]([C@@H]1O)O2	-4.8	*Nigrospora* sp.
680	**M680**	c1cc(ccc1)[C@H](CO)O	-4.7	*Aspergillus* sp.
681	**M681**	c1(c(cccc1)O)CN	-4.7	*Aspergillus* sp.
682	**M682**	c1ccc(cc1)C(=O)O	-4.6	*Aspergillus* sp.
683	**M683**	N1[C@@H](CCC1=O)[C@H](OC)O	-4.6	*Aspergillus* sp.
684	**M684**	C(CO)C(=O)[C@@H]1CC(=O)OC1	-4.5	*Penicillium* sp. PSU-F44
685	**M685**	n1cnc(c2c1nc[nH]2)N	-4.4	*Aspergillus* sp.
686	**M686**	[nH]1c(=O)[nH]c(=O)c(c1)C	-4.4	*Aspergillus* sp.
687	**M687**	c1(ccc(o1)CO)C=O	-4.4	*Penicillium chrysogenum* HGQ6
688	**M688**	O1[C@H](C=C(C1=O)CCO)C	-4.4	*Aspergillus* sp. 16-02-1
689	**M689**	c1c(=O)[nH]c(=O)[nH]c1	-3.9	*Aspergillus* sp.
690	**M690**	[C@H]([C@@H](O)C)(O)C	-3.1	*Aspergillus* sp.

Table S2. Docked and MD-refined structures of SARS-CoV-2 Mpro + top-lead ligands.

N^0	Name	Docked structure	MD-refined structure
1	**M15**		
2	**M8**		
3	**M11**		
4	**M9**		

5	**M2**		
6	**M13**		
7	**M3**		
8	**M5**		

9	**M4**		
10	**M16**		
11	**M6**		
12	**M1**		

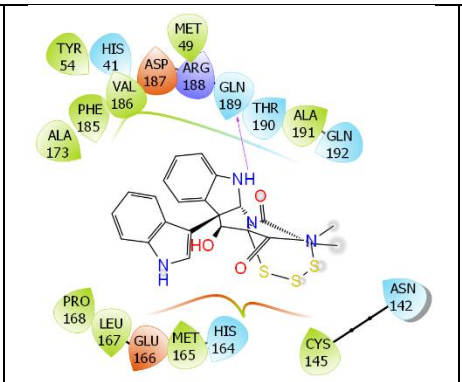
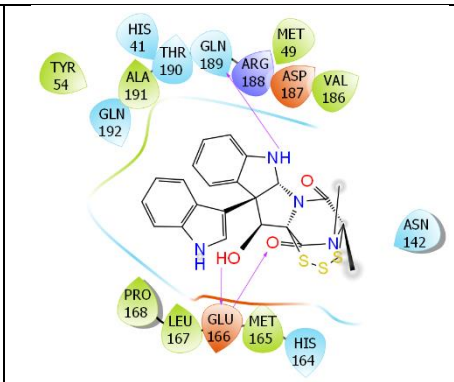
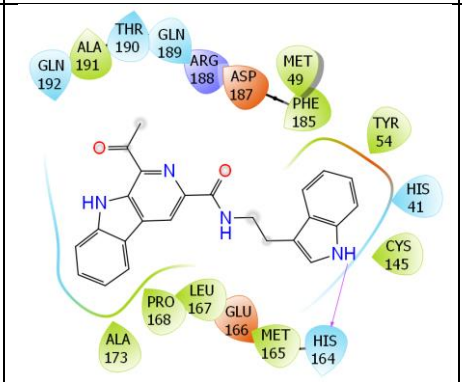
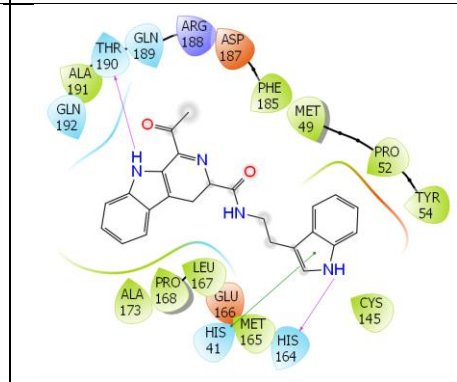
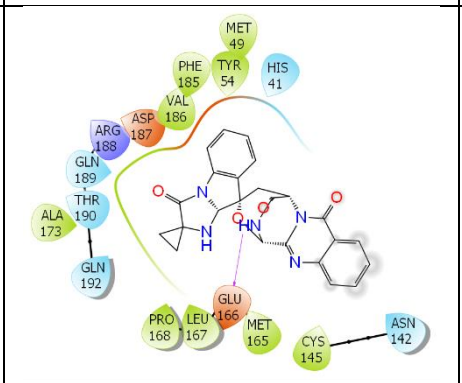
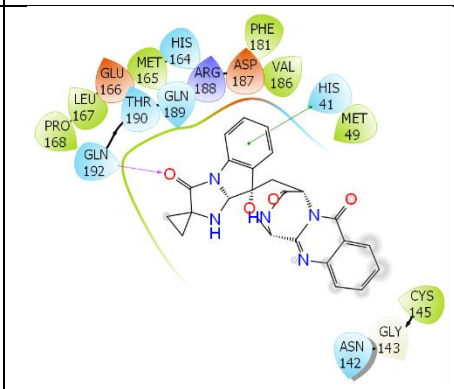
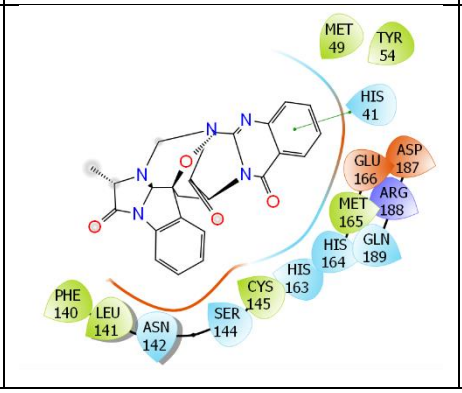
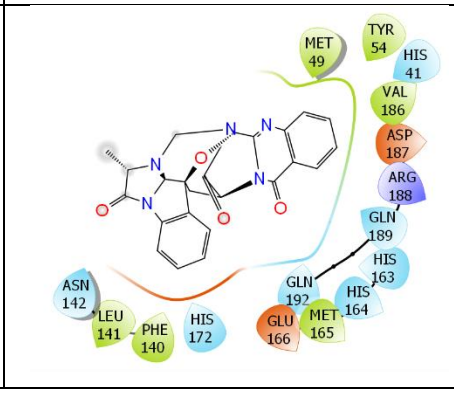
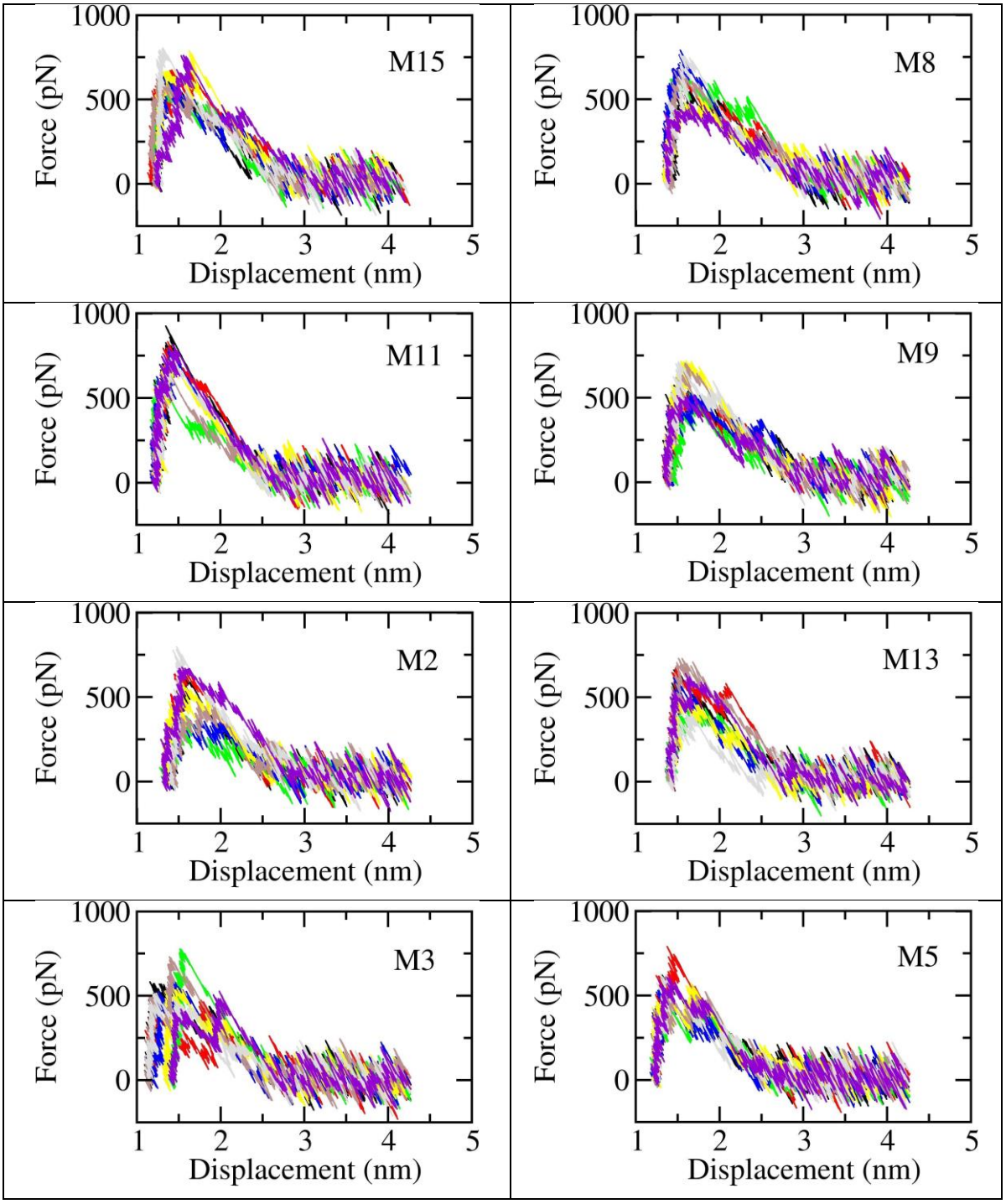
13	**M12**		
14	**M14**		
15	**M7**		
16	**M10**		

Table S3. The pulling force in displacement dependence over FPL simulations



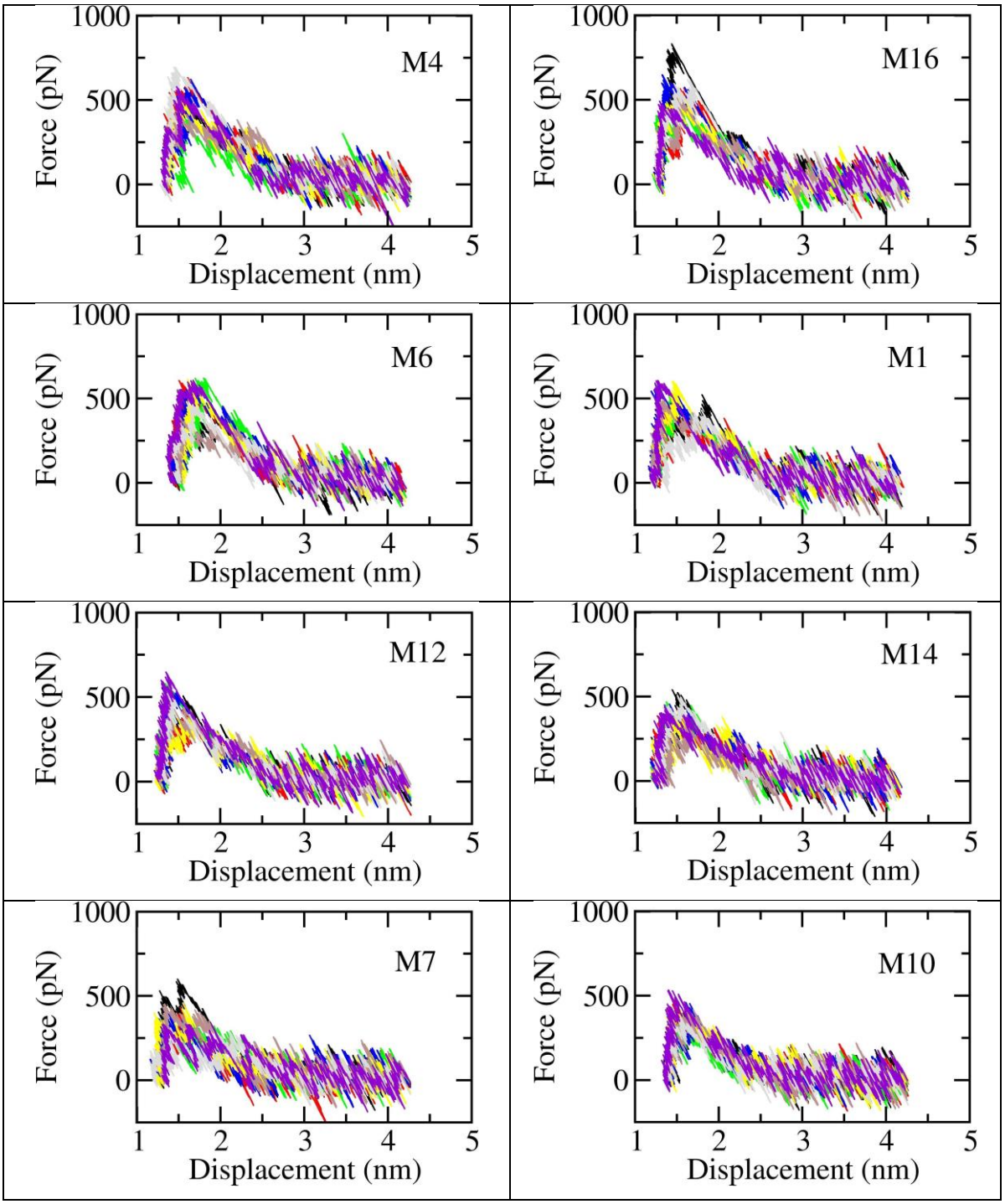

M4
M16
M6
M1
M12
M14
M7
M10
Force (pN)
Displacement (nm)
1000
500
0
1
2
3
4
5

Table S4. The computational values using FPL simulations of available inhibitors.

N⁰	Compound	F_{Max}	W	ΔG_{EXP}[a]
1	Atazanavir	762.8 ± 44.8	83.7 ± 3.5	-8.64
2	Candesartan Cilexetil	682.6 ± 15.7	68.2 ± 2.3	-9.23
3	Chloroquine	417.3 ± 40.9	34.5 ± 2.8	-8.56
4	Cimetidine	513.0 ± 29.7	46.5 ± 3.9	-7.51
5	Maribavir	377.0 ± 19.4	33.9 ± 1.5	-7.51
6	Omeprazole	361.4 ± 31.1	28.2 ± 2.4	-8.03
7	Oxytetracycline	448.1 ± 30.7	37.9 ± 2.7	-8.22
8	Roxatidine Acetate Hydrochloride	652.2 ± 31.7	62.2 ± 3.3	-8.05
9	Sulfacetamide	282.6 ± 19.0	16.0 ± 1.4	-7.51
10	Valacyclovir Hydrochloride	492.8 ± 20.9	49.8 ± 3.3	-8.16

[a]The experimental binding free energy was obtained through inhibition constant k_i.[1] The unit of energy and force are in kcal mol^{-1} and pN, respectively.

Table S5. ADME profile of potential compounds

Compound	Molecular Weight	HIA	BBR	Carcinogenicity	LD_{50} (mg/kg)	Toxicity prediction[a]
M8	722.18	0.6252	0.5804	0.9571	300	3
M9	722.18	0.6252	0.5804	0.9502	300	3
M11	429.14	0.6725	0.6995	0.7880	75	3
M15	552.15	0.9105	0.9401	0.9717	5000	5

[a]Toxicity prediction class: 1 → 6 (High toxicity to non-toxic). The ADME was calculated via admetSAR[2] and ProTOX-II[3] webserver.

Reference

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2. F. Cheng, W. Li, Y. Zhou, J. Shen, Z. Wu, G. Liu, P. W. Lee and Y. Tang, *J. Chem. Inf. Model.*, 2012, **52**, 3099-3105.
3. P. Banerjee, A. O. Eckert, A. K. Schrey and R. Preissner, *Nucleic Acids Res* 2018, **46**, W257-W263.