Uncovering Streptomyces-derived compounds as cosmeceuticals for the development of improved skin photoprotection products: an in-silico approach to explore multi-targeted agents

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Table S1. Clustering of the 1981 selected compounds by *Flexophore* descriptor.

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1	Clorobiocin	CO[C@H]1[C@H](OC(=O)c2ccc([nH]2)C)[C@@H](O)[C@@H](OC1(C)C)Oc1ccc2c(c1Cl)oc(=O)c(c2O)NC(=O)c1ccc(c(c1)CC=C(C)C)O	1	Yes
2	2,2,4-Trimethyl-5,8-dihydroxy-6-isopentyl-2,7-dihydroanthra[9,1-de][1,3]oxazine-7-one	CC(CCC1=c2c3C(=C(C1=O)C)OC(Nc3c1=CC=CC(=O)c1c2O)(C)C)C	2	Yes
3	RK-682	CCCCCCCCCCCCCCCC(=O)C1=C(O)[C@H](OC1=O)CO	3	Yes
4	Spindomycin B	O=C1C(=C(C)[C@@]2(C3=C1CCC3)c1ccccc1N(C2=O)C)O	4	Yes
5	Spindomycin A	O=C1[C@H](O)[C@@H](C)[C@@]2(C3=C1CCC3)c1ccccc1N(C2=O)C	4	No
6	Aestivophoenin C	CC(=CCn1c2cccc(c2[nH]c2c1cccc2CC=C(C)C)C(=O)O[C@@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1O)O)O)C	5	No
7	Aminotrihydroxybacteriohopane	NC[C@@H]([C@@H]([C@@H](CCC([C@H]1CCC2C1CC[C@@]1(C2CCC2[C@@]1(C)CCC1[C@]2(C)CCCC1(C)C)C)C)O)O)O	5	No
8	Aminotrihydroxybacteriohopene	NC[C@@H]([C@@H]([C@@H](CCC([C@H]1CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC[C@H]2[C@@]1(C)CC[C@@H]1[C@]2(C)CCCC1(C)C)C)C)C)O)O)O	5	Yes
9	LMPR04000005	NC[C@@H]([C@@H]([C@@H](CCC(C1CC[C@]2(C1CC[C@@]1(C2CCC2[C@@]1(C)CCC1[C@]2(C)CCCC1(C)C)C)C)C)O)O)O	5	No
10	Mansouramycin D	CNC1=CC(=O)c2c(C1=O)cnc(c2)c1c[nH]c2c1cccc2	6	Yes
11	Pepticinnamin E	CC/C=C/Cc1ccccc1/C=C/C(=O)N[C@@H](C(=O)[C@@](N(C(=O)[C@H](Cc1ccc(c(c1Cl)O)OC)NC)C)(C(=O)OC[C@H]1NC(=O)CNC1=O)Cc1ccccc1)Cc1ccc(cc1)O	7	Yes
12	Norcodeine	COc1ccc2c3c1OC1C43CCNC(C2)C4C=CC1O	8	Yes
13	Coelimycin P1	C/C=C/C(=O)C1=C/C(=C/2\NCCC=C2)/SC[C@@H](C(=O)O1)NC(=O)C	9	Yes
14	C12392	Cc1cc(O)c2c(c1)C(N)C1=C2C(=O)c2c(C1=O)c(O)ccc2	10	Yes
15	Hatomarubigin E	C[C@@H]1C[C@H](O)C2=C(C1)C=CC1C2C(=O)c2c(C1=O)c(O)ccc2O	10	No
16	Kinobscurinone	Cc1cc(O)c2c(c1)c(=O)c1=c2c(=O)c2c(c1=O)c(O)ccc2	10	No
17	Prekinamycin	N#Cn1c2cc(C)cc(c2c2c1C(=O)c1c(O)cccc1C2=O)O	10	No
18	Frenolicin B	CCC[C@H]1O[C@@H]2CC(=O)O[C@@H]2C2=C1C(=O)c1c(C2=O)cccc1O	10	No
19	BU-4704	C#[N+]/C(=C\c1ccc(cc1)OS(=O)(=O)O)/C(=C/c1ccc(cc1)OC)/[N+]#C	11	Yes
20	Dechlororoseophilin	COc1cc(oc1C1=C2N=C3C=C2C(C1CCCCCCCC3)(C)C)c1ccc[nH]1	12	Yes
21	Camporidine B	CCCCCC[C@H]1CN(O)[C@@H]2[C@]3([C@@H]1O3)C(=C/C=C/C(=O)O)C=C2	13	Yes
22	Neopentalenolactone D	O=C1O[C@@H](C)[C@]23[C@@H](C1)C(=C[C@@H]3CC(C2)(C)C)C(=O)O	14	No
23	Pentalenolactone D	O=C1OC[C@@H]2[C@@]3([C@@H]1C)CC(C[C@H]3C=C2C(=O)O)(C)C	14	No
24	1-Deoxy-11-oxopentalenic acid	O=C1C[C@@H]2[C@@]3([C@@H]1C)CC(C[C@H]3C=C2C(=O)O)(C)C	14	No
25	Pentalenic acid	OC(=O)C1=C[C@H]2[C@@]3([C@H]1CC[C@H]3C)CC([C@@H]2O)(C)C	14	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
26	1-Deoxy-11beta-hydroxypentalenic acid	O[C@@H]1C[C@@H]2[C@@]3([C@@H]1C)CC(C[C@H]3C=C2C(=O)O)(C)C	14	Yes
27	Isofuranonaphthoquinone G	O=C1NC2(Nc3c1cccc3)c1coc(c1C(=O)c1c2cc(O)c(c1O)O)C	15	Yes
28	Lorneic acid H	OCc1cc(C)ccc1/C=C/CCCC(=O)O	16	Yes
29	2-Methyl-8-hydroxybenzeneheptanoic acid	OC(=O)CCCCC[C@@H](c1ccccc1C)O	16	No
30	Ketomemicin B5	CC(=O)N[C@H](C(=O)C[C@H](C(=O)O)Cc1ccccc1)Cc1ccc(cc1)O	17	Yes
31	Ketomemicin B6	CC(=O)N[C@H](C(=O)C[C@H](C(=O)O)Cc1ccccc1)Cc1ccccc1	18	Yes
32	Jomthonic acid F	C/C=C(/C=C/C(=O)NC(C(c1ccccc1)C)C(=O)O)\C	18	No
33	Streptenol E	C/C=C/CCC(=O)CC(CCNC(=O)C)O	19	Yes
34	N1-Acetyl-N7-O-hydroxyphenylacetyl cadaverine	O=C(Cc1ccccc1O)NCCCCCNC(=O)C	19	No
35	Phaeochromycin F	Cc1cc(=O)c2c(o1)cccc2Cc1cc(O)c(c(=O)o1)Cc1c(O)cc(oc1=O)Cc1cccc2c1c(=O)cc(o2)C	20	Yes
36	N-Butylbenzenesulfonamide	CCCCNS(=O)(=O)c1ccccc1	21	Yes
37	Sceliphrolactam	O=C1NCC(C)/C=C/C=C/C=C(\C)/C=C/C=C\C(=O)C(C(C(/C=C/C=C(/C=C/C(=C\1)/O)\C)O)O)O	22	Yes
38	2-Amino-9,13-dimethyl heptadecanoic acid	CCCCC(CCCC(CCCCCCC(C(=O)O)N)C)C	23	Yes
39	Cis-[2,(4,5-dihydroxy-4-methylhexyl)cyclopropyl]acetic acid	OC(=O)CC1CC1CCCC(C(O)C)(O)C	24	Yes
40	(+)-Austrosene	OC(=O)c1ccc(cc1)[C@](CCCC(O)(C)C)(O)C	25	Yes
41	Lobocompactol	C/C/1=C\CCC(=C)[C@@H](CC(CC1)C1=CCC(OC1)C(O)(C)C)O	26	Yes
42	Akashin A	O[C@@H]1[C@@H](O)[C@H](N)[C@H](O[C@@H]1n1c(C2=Nc3c(C2=O)cc(cc3)Cl)c(c2c1ccc(c2)Cl)O)C	27	Yes
43	N,N'-((1Z,3Z)-1,4-bis(4-Methoxyphenyl)buta-1,3-diene-2,3-diyl)diformamide	COc1ccc(cc1)/C=C(/C(=C/c1ccc(cc1)OC)/NCC=O)\NCC=O	28	Yes
44	A80915g	CC(=CCC12OC2(CC=C(C)C)C(=O)c2c(C1=O)cc(O)cc2O)CCC=C(C)C	29	Yes
45	Napyradiomycin A3	C/C(=C\C[C@]12OC(C)(C)[C@@H](C=C1C(=O)c1c(C2=O)cc(cc1O)O)O)/CCC(C(=C)C)O	29	No
46	Merochlorin B	CC(=CCC[C@]1(C)OC2=C(Cl)C(=O)c3c([C@@]42[C@H]1CC(=C(C)C)C4)cc(O)cc3O)C	30	Yes
47	7-Chloro-10-ethyl-1-[[2-[[2-hydroxyethyl]amino]ethyl]amino]-3-[4-	OCCNCCNc1cc(cc2c1c(=O)c1c(n2CC)ccc(c1)Cl)c1ccc(cc1)C(F)(F)F	31	Yes
48	Iromycin	CCCc1c(C/C=C(/C/C=C/C(C)C)\C)[nH]c(=O)c(c1O)C	32	Yes
49	3,6-disubstituted Indole B	O/N=C\Cc1c[nH]c2c1ccc(c2)CC=C(C)C	33	Yes
50	Vnezueline E	CCCC(=O)OCc1ccc2c(c1)nc1c(o2)cc(=O)c(c1)NC(=O)C	34	Yes
51	Vnezueline A	OCc1cc2nc3cc(NC(=O)C)c(=O)cc3oc2cc1Cc1ccc(c(c1)NC(=O)C)O	34	No
52	(5Z,8Z,11R*,12R*)-11,12-Dihydroxytetradeca-5,8-dienamide	CCC(C(C/C=C\C/C=C\CCCC(=O)N)O)O	35	Yes
53	TA 3037A	O=c1oc2cccc(c2[nH]/c/1=C\c1ccccc1)C(=O)O	36	Yes
54	Mycemycin G	Clc1ccc2c(c1)C(=O)Nc1c(O2)c(C)ccc1C(=O)C	36	No
55	Myxochelin A	OC[C@@H](NC(=O)c1cccc(c1O)O)CCCCNC(=O)c1cccc(c1O)O	37	Yes
56	Rosmarinic acid	O=C(O[C@@H](C(=O)O)Cc1ccc(c(c1)O)O)/C=C/c1ccc(c(c1)O)O	37	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
57	[6-hydroxy-2,2,6-trimethyl-3-(3-methylbut-2-en-1-yl)cyclohexyl]methyl acetate	CC(=O)OCC1C(C)(O)CCC(C1(C)C)CC=C(C)C	38	Yes
58	CHEMBL1268	O=C1NC(=O)C(S1)Cc1ccc(cc1)OCCc1ccc(cn1)C(=O)C	39	Yes
59	3-n-Heptyl-3-hydroxy-1,2,3,4-tetrahydroquinoline-2,4-dione	CCCCCCCCC1(O)C(=O)Nc2c(C1=O)cccc2	40	Yes
60	N6-Dodecanoyl-L-lysine	CCCCCCCCCCCC(=O)NCCCC[C@@H](C(=O)O)N	41	Yes
61	N-alpha-Lauroyl-L-lysine	CCCCCCCCCCCC(=O)N[C@H](C(=O)O)CCCCN	41	No
62	Fragin	CCCCCCCC(=O)NCC(/[N+](=N/O)/[O-])C(C)C	42	Yes
63	Resorthiomycin	CSC(=O)c1c(C)c(CCC(O)C)c(c(c1O)C)O	43	Yes
64	Corydalmine	COc1cc2c(cc1OC)CCN1[C@H]2Cc2ccc(c(c2C1)OC)O	44	Yes
65	BRN 1329464	COc1cc2c(=O)c(coc2c(c1OC)O)c1ccc(c(c1)O)OC	44	No
66	Dihydroxyl-3-farnesylindole	C/C(=C\CC1CNc2c1cccc2)/CCC=C(CCC(C(O)(C)C)O)C	45	No
67	Separacene A	C=C[C@H]([C@@H](/C=C/C=C/C=C/C=C/C=C/[C@H]([C@H](O)C)O)O)O	45	Yes
68	Separacene B	C=C[C@H]([C@@H](/C=C/C=C/C=C/C=C/C=C/[C@@H]([C@H](O)C)O)O)O	45	No
69	Succinilene D	CC[C@@H]([C@@H](C/C=C/C=C/C=C/C=C/C[C@@H](/C(=C/[C@H]([C@H](O)C)C)/C)O)O)O	45	No
70	2-Hydroxy-2-propyl-5-(2-hydroxy-4-oxo-4H-pyran-6-ylmethyl)-2,3-dihydro-4H-1-benzopyran-4-one	CCCC1(O)CC(=O)c2c(O1)cccc2Cc1cc(O)cc(=O)o1	46	No
71	Anhydrosek4b	Oc1cc(oc(=O)c1)Cc1cc(=O)c2c(o1)cc(cc2C)O	46	No
72	CHEMBL487191	CCCc1cc(=O)c2c(o1)cccc2Cc1cc(O)cc(=O)o1	46	Yes
73	Bionectriamine B	O=C(Nc1ccccc1C(=O)O)/C=C/C(=O)Nc1ccccc1C(=O)O	47	Yes
74	DC 102 Antibiotic	CC/C=C\1/CC2N(C1)C(=O)c1c(NC2OC)ccc(c1)OC1OC(C)C(C(C1O)(C)O)NC	48	Yes
75	1,3-Diphenethylurea	O=C(NCCc1ccccc1)NCCc1ccccc1	49	Yes
76	Lydicamycin	OC(C/C=C(/C(C(CCC1C(=CC2C(C1(C)/C(=C\1/C(=O)CNC1=O)/O)CCC(C2O)O)C)C)O)\C)/C=C/C(C(/C=C/CC(/C(=C/CC(CC1CCCN1C(=N)N)O)/C)O)O)C	50	Yes
77	Aurachin SS	COc1c(C/C=C(/CCC=C(C)C)\C)c(C)[n+](c2c1cccc2)[O-]	51	Yes
78	SIA-7248	O[C@@H]1C[C@H](O)C[C@H](O)C[C@H](C[C@@H]([C@@H](O)C)O)OC(=O)c2c(/C=C/C=C/C=C/C=C(\C)/C[C@H](O)C[C@@H](C[C@@H](C[C@@H](C[C@@H](OC(=O)c3c(/C=C/C=C/C=C/C=C(/C[C@@H](C1)O)\C)cccc3O)C[C@@H]([C@@H](O)C)O)O)O)O)cccc2O	52	Yes
79	Juanlimycin B	C/C/1=C\C[C@H](O)c2cc(O)cc3c2[C@](Nc2cc(O)ccc2C(=O)O)(C(=O)/C=C/C(=C/C[C@@H](c2c4[C@](C(=O)\C=C1)(Nc1ccccc1C(=O)O)C(=C)Nc4cc(c2)O)O)/C)C(=O)N3	53	Yes
80	Juanlimycin A	C/C/1=C\C[C@H](O)c2cc(O)cc3c2[C@](Nc2ccccc2C(=O)O)(C(=O)/C=C/C(=C/C[C@@H](c2c4[C@](C(=O)\C=C1)(Nc1ccccc1C(=O)O)C(=C)Nc4cc(c2)O)O)/C)C(=O)N3	53	No
81	Lavanduquinocin	C[C@H](CC1=C(C)C(=O)C(=O)c2c1[nH]c1c2cc(cc1)CC1=C(C)CC(CC1)(C)C)O	54	No
82	Carquinostatin B	CC(=CCc1ccc2c(c1)c1C(=O)C(=O)C(=C(c1[nH]2)[C@@H]([C@H](O)C)O)C)C	54	No
83	Neocarazostatin B	COc1c(C)c(CC(O)C)c2c(c1O)c1cc(CC=C(C)C)ccc1[nH]2	54	No
84	Neocarazostatin A	COc1c(C)c(C(C(O)C)O)c2c(c1O)c1cc(CC=C(C)C)ccc1[nH]2	54	Yes
85	Neocarazostatin C	COC(c1c(C)c(OC)c(c2c1[nH]c1c2cc(cc1)CC=C(C)C)O)C(O)C	54	No
86	Carquinostatin A	C[C@H](CC1C(C)C(=O)C(=O)c2c1[nH]c1c2cc(cc1)CC=C(C)C)O	54	No
87	Spiroindimicin F	COC(=O)c1[nH]cc2c1C1(CN(c3c1cccc3)C)c1c2c2cc(Cl)ccc2[nH]1	55	No
88	Spiroindimicin E	COC(=O)c1[nH]cc2c1C1(CN(c3c1cc(Cl)cc3)C)c1c2c2ccccc2[nH]1	55	No
89	Spiroindimicin C	COC(=O)c1[nH]cc2c1[C@]1(CNc3c1cc(Cl)cc3)c1c2c2cc(Cl)ccc2[nH]1	55	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
90	Spiroindimicin D	COC(=O)c1[nH]c(c2c1c1c3cc(Cl)ccc3[nH]c1[C@]12CN(c2c1cc(Cl)cc2)C)C(=O)OC	55	No
91	Spiroindimicin B	COC(=O)c1[nH]cc2c1[C@]1(CN(c3c1cc(Cl)cc3)C)c1c2c2cc(Cl)ccc2[nH]1	55	Yes
92	Wailupemycin F	OC1CC(=O)c2c(C1)c(c1cc(O)cc(=O)o1)c(cc2O)c1ccccc1	56	Yes
93	Phaeochromycin B	CCCc1cc(O)c2c(c1c1cc(O)cc(=O)o1)CC(CC2=O)O	56	No
94	Fijiolide B	O=C1OC[C@H](O)c2ccc3c(c2Cl)C2=CC=C[C@@]2([C@@H]3Oc2c(cc([C@H](C1)N)cc2Cl)O)OC1OC(C)(C)C(C(C1O)O)N(C)C	57	Yes
95	CHEMBL517944	CCCCCOc1ccc2c(c1)ccc(c2)S(=O)(=O)N[C@@H](C(=O)O)CCC(=O)O	58	Yes
96	Acetamide, N-[2-hydroxy-5-[[8-(hydroxymethyl)-3-oxo-3H-phenoxazin-2-yl]amino]phenyl]-	OCc1ccc2c(c1)nc1c(o2)cc(=O)c(c1)Nc1ccc(c(c1)NC(=O)C)O	59	Yes
97	U 68204	C=C/C(=C/[C@@]1(CC)SC(=C(C1=O)CC(=O)N)O)/C	60	Yes
98	Goadsporin	CC[C@@H]([C@@H](C(=N[C@H](c1scc(n1)C(=N[C@H](C(=NCC(=NCc1nc(c(o1)C)C(=N[C@H](C(=NC(=C)c1occ(n1)C(=N[C@H](C(=NCc1scc(n1)C(=N[C@H](C(=O)O)C(C)C)O)O)C)O)O)O)CO)O)CC(C)C)O)N=C(c1nc(oc1C)C(=C)N=C([C@H](C(C)C)N=C(c1nc(oc1C)[C@@H](N=C(O)C)C)O)O)O)C	61	Yes
99	Linearolide B	COC1CCC(C1/C=C/C(=C/C(C(O)C)C)/C)C(/C=C/C(C(/C=C(/C1OC(O)(CC)C(C(C1C)O)OC)\OC)C)OC1OC(C)C(C(C1)NC(=O)C)O)(O)C	62	Yes
100	Juniperolide A	CO/C(=C\[C@@H]([C@H](/C(=C/CC[C@@H]([C@H](/C(=C/C=C/C([C@H](O)C)C)/C)O)C)/C)O[C@H]1C[C@@H](NC(=O)C)[C@@H]([C@H](O1)C)O)C)/[C@H]1OC(O)(CC)C[C@@H]([C@@H]1C)O	62	No
101	Marineosin B	CO[C@H]1CC(=N[C@]21O[C@@H](C)C[C@H]1[C@H]2c2ccc([nH]2)CCCCCCC1)c1[nH]ccc1	63	Yes
102	CHEBI:66676	CO[C@@H]1C/C(=C/2\C=CC=N2)/N[C@@]21O[C@@H](C)C[C@H]1[C@H]2c2ccc([nH]2)CCCCCCC1	64	Yes
103	Bohemamine G	O=C(NC1=CC(=O)[C@]2(N1[C@@H](C)CC2)C)/C=C/C(C)C	65	Yes
104	Bohemamine I	C[C@H]1CC[C@@]2(N1C(=CC2=O)NC(=O)c1ccccc1)C	65	No
105	Streptenol I	C/C=C/CCC(=O)C[C@H](CCO[C@]1(OCC[C@@H](C1)O)CC/C=C/C)O	66	Yes
106	Niizalactam A	C/C/1=C\C=C\[C@H]2[C@H](O)[C@H](CN2C(=O)CC(=O)/C=C/C(=C/C=C/[C@H]([C@@H]([C@@H](C(=O)/C=C\C=C1)O)O)O)/C)C	67	Yes
107	Niizalactam B	C/C/1=C\C=C\[C@H]2[C@H](O)[C@H](CN2C(=O)CC(=O)/C=C/C(=C/C=C/C[C@@H]([C@@H](C(=O)/C=C/C=C1)O)O)/C)C	67	No
108	Donghaesulfin A	COc1cccc2c1[C@@H](OC)c1c([C@H]2O)c2C(=O)C[C@H]([C@@H](c2cc1Sc1cc2[C@@H](O)[C@H](C)CC(=O)c2c2c1[C@H](OC)c1c(OC)cccc1[C@@H]2O)O)C	68	Yes
109	Donghaesulfin B	COc1cccc2c1[C@@H](OC)c1c([C@H]2O)c2C(=O)C[C@H]([C@@H](c2cc1Sc1cc2[C@@H](O)[C@H](C)CC(=O)c2c2c1[C@@H](O)c1c(OC)cccc1C2=O)O)C	68	No
110	Galbonolide G	CC[C@@H](/C(=C/C(=C)C[C@@H](/C=C(/C[C@@]1(CO)OC(=O)C(=C1O)C)\C)C)/C)O	69	Yes
111	Lauroyl vanillylamide	CCCCCCCCCCCC(=O)NCc1ccc(c(c1)OC)O	70	No
112	Alkylresorcylic acid	CC(CCCCCCCCCCCCc1c(C)c(O)cc(c1C(=O)O)O)C	70	Yes
113	n-Lauryl-5-hydroxyanthranilate	CCCCCCCCCCCCNc1ccc(cc1C(=O)[O-])O	70	No
114	Panosialin WA	CC(CCCCCCCCCCCCc1cc(O)cc(c1)OS(=O)(=O)O)C	71	No
115	Panosialin WB	CCCCCCCCCCCCCCCc1cc(O)cc(c1)OS(=O)(=O)[O-].[Na+]	71	No
116	Panosialin A	CC(CCCCCCCCCCCCc1cc(cc(c1)OS(=O)(=O)[O-])OS(=O)(=O)[O-])C.[Na+].[Na+]	71	No
117	Panosialin-IA	CCCCCCCCCCCCCCCCc1cc(cc(c1)OS(=O)(=O)O)OS(=O)(=O)O	71	Yes
118	Homodimericin A	C/C=C/C=C/[C@@]1(O)[C@@H]2C=C3[C@@]45[C@]([C@@H]1[C@@H]1C(=O)C(=C(C(=O)[C@]41CC3=O)O)C)([C@H]2C)C(=O)C(=C(C5=O)C)O	72	Yes
119	Tetroazolemycin A	CN1[C@H](CS[C@H]1[C@@H]1COC(=N1)c1ccccc1O)CN1[C@@H]2CSSC[C@H](C1=O)N(C2=O)C[C@H]1CS[C@H](N1C)[C@@H]1COC(=N1)c1ccccc1O	73	Yes
120	Tetroazolemycin B	CN1[C@H](CS[C@@H]1[C@@H]1COC(=N1)c1ccccc1O)CN1[C@@H]2CSSC[C@H](C1=O)N(C2=O)C[C@H]1CS[C@H](N1C)[C@@H]1COC(=N1)c1ccccc1O	73	No
121	HMS1844K12	COc1ccc(cc1)c1noc(n1)CSc1nnc(n1c1ccc(cc1)OC)C	74	Yes
122	FD-594	CCC[C@H]1OC(=O)c2c(C1)cc1c(c2O)c2c(O)c3C(=O)C4C(Oc3c(c2[C@@H]([C@H]1O)O)OC)C=CC(=C4O)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)OC1CC(OC)C(C(O1)C)O	75	Yes
123	7-Acetyl-3,6-dihydroxy-8-methyl-tetralone	OC1CC(=O)c2c(C1)cc(c(c2C)C(=O)C)O	76	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
124	(R)-7-Acetyl-3,6-dihydroxy-8-propyl-3,4-dihydronaphthalen-1(2H)-one	CCCc1c2C(=O)C[C@@H](Cc2cc(c1C(=O)C)O)O	76	No
125	Gastrophenzine	CCOC(=O)Nc1cccc2c1CN(C)CC2c1ccc(cc1)Cl	77	Yes
126	Telomestatin	Cc1oc2nc1c1occ(n1)c1occ(n1)c1occ(n1)c1occ(c3nc(C4=NC(c5nc2c(C)o5)CS4)co3)n1	78	Yes
127	Xantholipin B	COc1c(Cl)ccc2c1oc1c3OCO[C@H]4c3c(c(c1c2=O)O)c1c(C4)c(O)c2c(c1O)c(=O)[nH]c(c2)C	79	Yes
128	Lysolipin I	CO[C@H]1N(C)C(=O)c2c([C@H]1O)cc1c(c2O)c2c3C([C@H]1OC)OCOc3c1c(c2O)c(=O)c2c(o1)c(OC)c(cc2)Cl	80	Yes
129	Xantholipin	COc1c(Cl)ccc2c1oc1c3OCO[C@H]4c3c(c(c1c2=O)O)[C@@]1([C@H](C4)C(=O)c2c(C1=O)c(=O)[nH]c(c2)C)O	81	Yes
130	2-Benzylthio-8-methyl-7-phenylpyrano [2,3-f]benzoxazol- 6(h)-one	O=C1C(C)c2ocnc2C2=C1CC=C(O2)c1ccccc1SCc1ccccc1	82	Yes
131	2,18-seco-Lankacidinol B	OC/C=C(/C=C/[C@H](C/C=C(/C=C/[C@H](C[C@H]1OC(=O)C(=C([C@@H]1C)O)C)O)\C)O)\C	83	Yes
132	2-Methoxy-4,5-diphenyl-6-(2'-phenylethyl)pyrimidine	COc1cc(c2ccccc2)c(cc1c1cc(CCc2ccccc2)nc(n1)c1ccccc1)c1ccccc1	84	Yes
133	SF2738 F	COc1cc(nc2c1scc2)c1ccccn1	85	Yes
134	SF2738D	COc1cc(nc(c1SC)C#N)c1ccccn1	86	Yes
135	(4-Methoxy-3-methylsulfanyl-6-pyridin-2-ylpyridin-2-yl)methanol	COc1cc(nc(c1SC)CO)c1ccccn1	86	No
136	Acidomycin	OC(=O)CCCCCC1SCC(=O)N1	87	Yes
137	7-[1-(Thiophene-5-yl)-1-formamido]-3-propylenyl-3-cephem-4-carboxylic acid	C=CCC1=C(C(=O)O)N2C(SC1)[C@@H](C2=O)NC(=O)c1cccs1	88	Yes
138	(+)-Blastmycinone	CCCC[C@H]1C(=O)O[C@H]([C@@H]1OC(=O)C(C)C)C	89	Yes
139	AgB	O=C(NC12CC3CC(C2)CC(C1)C3)NCc1ccc(cc1)N=C(N)N	90	Yes
140	Phthoxazolin	C/C(=C/C=C\C=C\Cc1ocnc1)/[C@H](C(C(=O)N)(C)C)O	91	No
141	Inthomycin B	C/C(=C/C=C/C=C/Cc1ocnc1)/[C@@H](C(C(=O)N)(C)C)O	91	Yes
142	Phthoxazolin B	OC(c1ocnc1)C=CC=CC=C(C(C(C(=O)N)(C)C)O)C	91	No
143	Antibiotic X 14885A	C[C@@H]1CCC2(O[C@@H]1Cc1oc3c(n1)c(C(=O)O)c(cc3)O)CC[C@H](C(O2)C(C(=O)c1ccc[nH]1)C)C	92	Yes
144	Cezomycin	C[C@@H]1CCC2(O[C@@H]1Cc1nc3c(o1)cccc3C(=O)O)O[C@@H](C(CC2C)C)C(C(=O)c1[nH]ccc1)C	92	No
145	Luteoride D	COC(=O)C1=NOC2C(C1)(O)c1cccc(c1N2)/C=C/C(=C)C	93	Yes
146	Lorneic acid I	CCCC(c1cc(C)ccc1/C=C/CCCC(=O)O)SSCC(C(=O)O)NC(=O)C	94	Yes
147	beta-Sitosteryl glucoside-3'-O-heptadecoicate	CC[C@@H](C(C)C)CC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@@]2(C)CC=C2[C@]1(C)CCC(C2)OC(=O)/C=C/c1ccc(c(c1)OC)O)C	95	No
148	UK-2A	COc1ccnc(c1O)C(=O)N[C@H]1COC(=O)[C@@H]([C@H]([C@@H](OC1=O)C)OC(=O)C(C)C)Cc1ccccc1	95	No
149	Antimycin A3a	CCCCC1C(=O)OCC(C(=O)OC(C1OC(=O)C(CC)C)C)NC(=O)c1cccc(c1O)NC=O	95	No
150	Antimycin A8a	O=CNc1cccc(c1O)C(=O)NC1COC(=O)C(C(C(OC1=O)C)OC(=O)C(CC)C)CCC(C)C	95	No
151	Uk-2c,D	CCC(C(=O)OC1C(C)OC(=O)C(COC(=O)C1Cc1ccccc1)NC(=O)c1nccc(c1O)OC)C.COc1ccnc(c1O)C(=O)NC1COC(=O)C(C(C(OC1=O)C)OC(=O)CC(C)C)Cc1ccccc1	95	Yes
152	4,4'-(3-hydroxypropane-1,1-diyl)diphenol	OCCC(c1ccc(cc1)O)c1ccc(cc1)O	96	Yes
153	Diolmycin B1	OC(C(Cc1ccc(cc1)O)O)Cc1ccc(cc1)O	97	Yes
154	Diolmycin A1	Oc1ccc(cc1)CC(C(Cc1c[nH]c2c1cccc2)O)O	97	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
155	Epocarbazolin B	CCC(CCC1(C)OC1c1c(C)c(O)cc2c1[nH]c1c2c(CO)ccc1O)C	98	Yes
156	Epocarbazolin A	OCc1ccc(c2c1c1cc(O)c(c(c1[nH]2)C1OC1(C)CCC(C)C)C)O	98	No
157	Ketoconazole	Clc1ccc(c(c1)Cl)[C@]1(OC[C@@H](O1)COc1ccc(cc1)N1CCN(CC1)C(=O)C)Cn1cncc1	99	Yes
158	Asenjonamide A	CCCC/C=C(/C(=O)C(C(=O)NCCO)C)\C	100	Yes
159	N-(2-Hydroxyethyl)dodecanamide	CCCCCCCCCCCC(=O)NCCO	101	Yes
160	Avermectin B1a 4"-beta-D-glucoside	O=C(CC=C(C)C)NCCCCCNC(=O)C	102	Yes
161	N1-Acetyl-N7-4"-methyl-pentoyl cadaverine	CC(CCC(=O)NCCCCCNC(=O)C)C	102	No
162	N1-Acetyl-N7-phenylacetyl cadaverine	O=C(Cc1ccccc1)NCCCCCNC(=O)C	102	No
163	NSC33451	Clc1cccc2c1C(=O)/C(=C\1/Nc3c(C1=O)c(Cl)ccc3)/N2	103	Yes
164	Actinoplanic acid A	CCC(C(=O)CC/C/1=C/C(C)C/C(=C/C(C)C(O)C(C)CCC(OC(=O)CC(CC(=O)OC1)C(=O)O)CCCC/C=C/C(CCC(OC(=O)CC(C(=O)O)CC(=O)O)C)C)/C)CC(C(=O)O)C	104	Yes
165	Actinoplanic acid C	OCC(C(=O)CC/C/1=C/C(C)C/C(=C/C(C)C(O)C(C)CCC(OC(=O)CC(CC(=O)OC1)C(=O)O)CCCC/C=C/C(CCC(OC(=O)CC(C(=O)O)CC(=O)O)C)C)/C)CC(C(=O)O)C	104	No
166	Actinoplanic acid B	CCC(C(=O)CC/C(=C/C(C/C(=C/C(C(C(CCC(OC(=O)CC(C(=O)O)CC(=O)O)CCCC/C=C/C(CCC(CC(C(=O)O)CC(=O)O)C)C)C)O)C)/C)C)/C)CC(C(=O)O)C	104	No
167	Actinoplanic acid D	OC/C(=C\C(C/C(=C/C(C(C(CCC(OC(=O)CC(C(=O)O)CC(=O)O)CCCC/C=C/C(CCC(OC(=O)CC(C(=O)O)CC(=O)O)C)C)C)O)C)/C)C)/CCC(=O)C(CC(C(=O)O)C)CO	104	No
168	RK-270B	O[C@@H](C(O)(C)C)Cc1ccc2c(c1)NC(=O)C2=C(C)C	105	Yes
169	RK-270C	NC(=O)/C(=C/Cc1ccc2c(c1)NC(=O)C2=C(C)C)/C	105	No
170	Cerebroside A	CCCCCCCCCCCC/C=C/C(C(=O)NC(C(/C=C/CC/C=C(/CCCCCCCCC)\C)O)CO[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)O	106	Yes
171	Phosphatidylinositol	CCCCCCCCCCCCCCCCCC(=O)OC[C@@H](OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)COP(=O)(OC1[C@H](O)[C@H](O)C([C@@H]([C@H]1O)O)O)O	106	No
172	2-Heptyl-3-hydroxy-4-quinolone	CCCCCCCc1[nH]c2ccccc2c(=O)c1O	107	Yes
173	Benzastatin K	CC(=CCCC1=CCc2c(NC1)ccc(c2)C(=O)O)C	108	No
174	Methylbenzastatin K	CC(=C(CCC1=CCc2c(NC1)ccc(c2)C(=O)O)C)C	108	Yes
175	4-[(2-Hydroxybenzoyl)amino]benzoic acid	O=C(c1ccccc1O)Nc1ccc(cc1)C(=O)O	108	No
176	Violaceol II	Cc1cc(O)c(c(c1)O)Oc1cc(C)cc(c1O)O	109	Yes
177	Violaceol I	Cc1cc(Oc2cc(C)cc(c2O)O)c(c(c1)O)O	109	No
178	Pentacyclo[19.3.1.1(3,7).1(9,13).1(15,19)]octacosa-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-25,26,27,28-tetrol,5,11,17,23-tetrakis(1,1-dimethylethyl)	CC(c1cc2Cc3cc(cc(c3O)Cc3cc(cc(Cc4c(c(Cc(c1)c2O)cc(c4)C(C)(C)C)O)c3O)C(C)(C)C)C(C)(C)C)(C)C	110	Yes
179	Diorcinol	Cc1cc(Oc2cc(C)cc(c2)O)cc(c1)O	111	Yes
180	Austramide	Cc1cc(Oc2cc(C)c(c(c2)O)C(=O)N)cc(c1)O	111	No
181	M-Bis(M-phenoxyphenoxy)benzene	c1ccc(cc1)Oc1cccc(c1)Oc1cccc(c1)Oc1cccc(c1)Oc1ccccc1	112	Yes
182	9,11-Diamino-3-{[(4-bromophenyl)methyl]sulfanyl}-10-chloro-6-(methoxymethyl)-2-	COCc1cc2C(=[N+](c3c2c(n1)c(N)c(c3N)Cl)C)SCc1ccc(cc1)Br	113	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	methyl-2,7-diazatricyclo[6.3.1.0^{4,12}]dodeca-1(11),2,4,6,8(12),9-hexaen-2-ium			
183	9,11-Diamino-10-chloro-3-(ethylsulfanyl)-6-(methoxymethyl)-2-methyl-2,7-diazatricyclo[6.3.1.0^{4,12}]dodeca-1(11),2,4,6,8(12),9-hexaen-2-ium	COCc1cc2C(=[N+](c3c2c(n1)c(N)c(c3N)Cl)C)SCC	113	Yes
184	9,11-Diamino-10-chloro-3-[(2-acetamidoethyl)sulfanyl]-6-(methoxymethyl)-2-methyl-2,7-diazatricyclo[6.3.1.0^{4,12}]dodeca-1(11),2,4,6,8(12),9-hexaen-2-ium	COCc1cc2C(=[N+](c3c2c(n1)c(N)c(c3N)Cl)C)SCCNC(=O)C	113	No
185	Sulfotanone	CC(CCCCCCCCCCCCCCCCCC(=O)[C@@H](CS(=O)(=O)O)O)C	114	Yes
186	FR900452	CSC[C@@H]1N/C(=C\2/CC=CC2=O)/[C@@H](NC1=O)[C@H]([C@@H]1C(=O)N(c2c1cccc2)C)C	115	Yes
187	FR 900452	CSC[C@@H]1N/C(=C/2\CC=CC2=O)/C(NC1=O)[C@H](C1C(=O)N(c2c1cccc2)C)C	115	No
188	Deoxypyoluteorin	Oc1ccccc1C(=O)c1[nH]c(c(c1)Cl)Cl	116	Yes
189	Panobinostat	ONC(=O)/C=C/c1ccc(cc1)CNCCc1c(C)[nH]c2c1cccc2	117	Yes
190	Belinostat	ONC(=O)/C=C/c1cccc(c1)S(=O)(=O)Nc1ccccc1	118	Yes
191	Antibiotic S 632-C	CC(C(=O)CC1CC(CC(=O)N)CC(=O)O1)/C=C(/C=C/C)\C	119	Yes
192	Azalomycin	CC[C@]1(C)C[C@@H](OC(=O)CSc2n[nH]c(n2)N)[C@]2(C)CC[C@H]([C@@]3([C@H]([C@@H]1O)C)[C@H]2C(=O)CC3)C	120	Yes
193	Bagrelactone A	O=C1Oc2ccc(cc2)[C@@H](CNc2cc1ccc2O)O	121	Yes
194	Boshramycinone A	Cc1ccc2=C(O)C3C(C=c2c1)C(=O)c1c(C3=O)c(O)ccc1	122	Yes
195	Boshramycinone B	Cc1ccc2=C(O)C3C(C=c2c1)C(=O)c1c(C3=O)cccc1O	122	No
196	WS 9761 A	Oc1cc(C)c2c(c1)C(C)(O)c1c(C2=O)c(O)c(cc1)C	122	No
197	WS 9761 B	OCc1ccc2c(c1O)C(=O)c1c(C2(C)O)cc(cc1C)O	122	No
198	rel-6R,7R,10R-7,10-Epoxy-3,7,11-trimethyldodec-2- ene-1,6,11-triol	OC/C=C(/CC[C@H]([C@@]1(C)CC[C@@H](O1)C(O)(C)C)O)\C	123	No
199	Heronapyrrole D	C/C(=C\Cc1c[nH]c(c1)N(=O)=O)/CC[C@@H]([C@@]1(C)CC[C@@H](O1)C(O)(C)C)O	123	Yes
200	Glyciapyrrole A	C/C(=C/C(=O)c1ccc[nH]1)/C=C/[C@@H]([C@@]1(C)CC[C@@H](O1)C(O)(C)C)O	123	No
201	SCHEMBL13815014	C/C(=C/C(=O)c1ccc[nH]1)/C=C/C1OC1(C)CCC=C(C)C	124	Yes
202	rel-6R,7R,10R-6,10-Epoxy-3,7,11-trimethyldodec-2-ene-1,7,11-triol	OC/C=C(/CC[C@H]1O[C@H](CC[C@@]1(C)O)C(O)(C)C)\C	125	Yes
203	(5S,6E,9E,13S,14R)-5-Hydroxy-5,9,13,14-tetramethyl-1-oxacyclotetradeca-6,9-diene-2,8-dione	O=C1CCC(C)(O)C=CC(=O)C(=CCCC(C(O1)C)C)C	126	No
204	7-O-Demethoxy-7-oxoalbocycline	C[C@H]1CC/C=C(\C)/C(=O)/C=C/[C@@](/C=C/C(=O)OC1)(C)O	126	No
205	Albocycline, 2,3-dihydro-	CO[C@H]1/C=C\[C@@](C)(O)CCC(=O)O[C@@H]([C@H](CC/C=C\1/C)C)C	126	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
206	Albocyclin	CO[C@H]1/C=C/[C@@](C)(O)/C=C/C(=O)O[C@@H]([C@H](CC/C=C/1\C)C)C	126	Yes
207	Diosgenone	C[C@@H]1CC[C@@]2(OC1)OC1C([C@@H]2C)[C@@]2(C(C1)C1CCC3=CC(=O)C=C[C@@]3(C1CC2)C)C	127	Yes
208	CHEBI:65482	C/C(=C\Cn1c2cc(ccc2[nH]c2c1cc(cc2C(=O)O)C(=O)c1ccccc1)C(=O)c1ccccc1)/CCC=C(C)C	128	Yes
209	PI 201	CC[C@H](C[C@H]1C(=CC2C([C@@H]1C(=O)OC)CCCC2)C)O	129	Yes
210	Homonactic acid methyl ester	CCC(CC1CCC(O1)C(C(=O)OC)C)O	129	No
211	Hydroxyvalerenic acid	C[C@@H]1CC[C@H](C2=C(C[C@H]([C@H]12)O)C)/C=C(/C(=O)O)\C	130	Yes
212	Limazepine G	C/C=C/C1=CN2[C@@H](C1)C(=O)Nc1c(C2=O)ccc(c1O)C	131	Yes
213	2-Acetylamino-3-hydroxyl-4-methyl-benzoic acid methyl ester	COC(=O)c1ccc(c(c1NC(=O)C)O)C	132	Yes
214	Geranylpyrrol A	COC(=O)c1[nH]cc(c1NC(=O)C)C/C=C(/CCC=C(C)C)\C	133	Yes
215	2-Hydroxylcyslabdan A	C=C/C(=C/C[C@H]1[C@](O)(CSC[C@H](C(=O)O)NC(=O)C)[C@@H](O)C[C@@H]2[C@]1(C)C[C@@H](O)CC2(C)C)/C	134	No
216	Cyslabdan	C=C/C(=C/C[C@H]1[C@@](O)(CSC[C@@H](C(=O)O)NC(=O)C)[C@@H](O)C[C@@H]2[C@]1(C)CCCC2(C)C)/C	134	Yes
217	17-Hydroxylcyslabdan A	C=C/C(=C/C[C@H]1[C@](O)(C(SC[C@H](C(=O)O)NC(=O)C)O)[C@@H](O)C[C@@H]2[C@]1(C)CCCC2(C)C)/C	134	No
218	Cyslabdan B	C=C/C(=C/C[C@H]1[C@@](O)(CSC[C@@H](C(=O)O)NC(=O)C)[C@@H](O)C[C@@H]2[C@]1(C)CCCC2(C)CO)/C	134	No
219	JBIR-77	COC1c2coc(c2C(=O)c2c1cc(O)c(c2O)OC)C	135	No
220	IIQ A	COc1c(O)cc2c(c1O)C(=O)c1c(C2=O)c[nH]c1C	135	No
221	Isofuranonaphthoquinone C	COc1cc2C(=O)c3coc(c3C(=O)c2c(c1O)O)C	135	No
222	Isofuranonaphthoquinone D	COc1c(OC)cc2c(c1O)C(=O)c1c(C2=O)coc1C	135	No
223	Isofuranonaphthoquinone E	COc1c(O)c(O)c2c(c1O)C(=O)c1c(C2=O)c(oc1)C	135	No
224	Isofuranonaphthoquinone A	O=C1c2coc(c2C(=O)c2c1cc(O)c(c2O)O)C	135	No
225	Isofuranonaphthoquinone B	COc1c(O)cc2c(c1O)C(=O)c1c(C2=O)coc1C	135	Yes
226	Isofuranonaphthoquinone F	COc1c(O)c2c(c(c1O)O)C(=O)c1c(C2=O)c(C)oc1	135	No
227	Bostrycoidin-9-methyl ether	COc1cc(OC)c2c(c1O)C(=O)c1c(C2=O)cnc(c1)C	136	Yes
228	Naphthgeranine A	COc1cc(OC)c2c(c1)C(=O)C1=C(C2=O)OC(C2C1C=C(C)CC2)(C)C	136	No
229	Hybrubin B	C/C=C/1\NC(=O)C(C1=O)/C=C\c1[nH]c(cc1OC)c1[nH]ccc1	137	Yes
230	BRN 0400664	CCC(=O)NCCc1c[nH]c2c1cccc2	138	Yes
231	WS 30581B	CCCCc1ncc(o1)c1c[nH]c2c1cccc2	138	No
232	Vnezueline F	CC(=O)Nc1cc(COCc2ccc(c(c2)NC(=O)C)O)ccc1O	139	Yes
233	Neoansamycin B	CCCCC[C@@H]1C(=O)N[C@]23[C@H]1[C@]1(C)C(=O)[C@@H](OC)CCC/C(=C/4\[C@@]1(C2)c1c(C3=O)ccc(c1O4)O)/CC	140	Yes
234	Neoansamycin C	CCCC[C@@H]1C(=O)N[C@]23[C@H]1[C@]1(C)C(=O)[C@@H](OC)CCC/C(=C/4\[C@@]1(C2)c1c(C3=O)ccc(c1O4)O)/CC	140	No
235	Neoansamycin A	CCCCC[C@H]1/C=C(\C)/C(=O)[C@@H](OC)CCC[C@H](C(=O)c2c3C(=O)C=C(NC1=O)C(=O)c3ccc2O)CC	140	No
236	Lugdunomycin	COc1cccc2c1[C@H](O)[C@]13[C@]([C@H]2Oc2cc(C)cc4c2cc(O)cc4)(C[C@H](C1)O)C(=O)NC3=O	141	Yes
237	T22-azaphilone	C/C=C/C=C/C1=CC2=CC(=O)[C@@](C(=O)C2=CO1)(C)OC(=O)C[C@@H](O)C	142	Yes
238	Galbonolide F	CC[C@@H]1OC(=O)[C@H](C)C(=O)c2coc(c2)C[C@H](CC(=C)/C=C\1/C)C	143	Yes
239	Lorneic acid K	CCCC(c1cc(C)ccc1/C=C/CCCC(=O)O)O	144	Yes
240	Lorneic acid E	CC/C=C/c1cc(C)ccc1/C=C/CC(CC(=O)O)O	144	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
241	Ammosamide G	Clc1ccc(cc1)N=c1n(C)c2c3c1cc(nc3c(c(c2N)Cl)N)C(=O)N	145	Yes
242	Cryptolepinone	O=c1c2ccccc2n(c2c1[nH]c1c2cccc1)C	146	Yes
243	3-((2E,4E,6E,8E)-13-Hydroxytetradeca-2,4,6,8-tetraenamido)propanoic acid	CC(CCC/C=C/C=C/C=C/C=C/C(=O)NCCC(=O)O)O	147	Yes
244	1,19-bis(3-Hydroxyazetidin-1-yl)nonadeca-5,14-diene-1,8,12,19-tetraone	OC1CN(C1)C(=O)CCCC=CCC(=O)CCCC(=O)CC=CCCCC(=O)N1CC(C1)O	148	Yes
245	Epicatechin	Oc1cc2O[C@H](c3ccc(c(c3)O)O)[C@@H](Cc2c(c1)O)O	149	No
246	Catechin	Oc1cc2O[C@H](c3ccc(c(c3)O)O)[C@H](Cc2c(c1)O)O	149	No
247	Luteolin	Oc1cc(O)c2c(c1)oc(cc2=O)c1ccc(c(c1)O)O	149	No
248	BE 14348B	Oc1ccc(cc1)[C@H]1Oc2cc(O)cc(c2C(=O)[C@H]1C)O	149	No
249	Naringenin	Oc1ccc(cc1)[C@@H]1CC(=O)c2c(O1)cc(cc2O)O	149	No
250	Chalconaringenin	Oc1ccc(cc1)/C=C/C(=O)c1c(O)cc(cc1O)O	149	No
251	3',4',7-Trihydroxyisoflavone	Oc1ccc2c(c1)occ(c2=O)c1ccc(c(c1)O)O	149	No
252	Gliricidin	COc1c(O)cc(cc1O)c1coc2c(c1=O)ccc(c2)O	149	No
253	5,7,4'-trihydroxy-3'-methoxyisoflavone	COc1cc(ccc1O)c1coc2c(c1=O)c(O)cc(c2)O	149	No
254	5,7,3'-trihydroxy-4'-methoxyisoflavone	COc1ccc(cc1O)c1coc2c(c1=O)c(O)cc(c2)O	149	No
255	Orobol	Oc1cc(O)c2c(c1)occ(c2=O)c1ccc(c(c1)O)O	149	Yes
256	L 694746	OC(=O)COc1ccc(cc1)C[C@@H](C(=O)N[C@@H]1C(O)Cc2c1cccc2)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)O	150	Yes
257	1,3-Diphenyl-4H-1,2,4-triazoline-5-thione	S=c1nc([nH]n1c1ccccc1)c1ccccc1	151	Yes
258	Dinotefuran	CC(Oc1ccccn1)COc1ccc(cc1)Oc1ccccc1.CN=C(N[N+](=O)[O-])NCC1COCC1	152	Yes
259	CHEBI:70277	C/C(=C\CC[C@@]1(C)O[C@@H]1Cc1c[nH]c(c1)N(=O)=O)/CCC=C(C)C	153	Yes
260	CHEBI:70279	C/C(=C\C/C=C(/[C@@H](Cc1c[nH]c(c1)N(=O)=O)O)\C)/CCC=C(C)C	153	No
261	1R)-9-Hydroxy-1-methyl-1H,3H,4H,5H,10H-naphtho[2,3-c]pyran-5,10-dione	C[C@H]1OCCC2=C1C(=O)c1c(C2=O)cccc1O	154	No
262	Utahmycin A	Cc1nc(C)c2c(c1)C(=O)c1c(C2=O)c(O)ccc1.COC(c1coc(c1)C(=O)OC)O	154	Yes
263	Bhimamycin A	Cc1oc(c2c1C(=O)c1c(C2=O)cccc1O)C(O)C	154	No
264	Bhimamycin I	Oc1cccc2c1C(=O)c1c(C2=O)c2n(c1C)CCOC2C	154	No
265	Antibiotic A 121	COC(C(C(=O)CC1(C)C=COC1(C)C(C(=C)(C)C)O)C(O)C	155	Yes
266	Venezueline D	OCOCNc1cc2Nc3cc(CO)ccc3Oc2cc1OCOCO	156	Yes
267	Jomthonic acid D	C/C=C(/C=C/C(=O)NC(C(c1ccccc1)C)C(=O)OC(C(C(=O)NC(C(=O)O)CCC(=O)N)C)C)\C	157	Yes
268	Jomthonic acid E	OC/C=C(/C=C/C(=O)NC(C(c1ccccc1)C)C(=O)OC(C(C(=O)O)C)C)\C	158	No
269	Jomthonic acid A	C/C=C(/C=C/C(=O)N[C@@H]([C@@H](c1ccccc1)C)C(=O)O[C@@H]([C@H](C(=O)O)C)C)\C	158	Yes
270	Jomthonic acid B	C/C=C/C=C/C(=O)N[C@@H]([C@@H](c1ccccc1)C)C(=O)O[C@@H]([C@H](C(=O)O)C)C	158	No
271	Jomthonic acid C	C/C=C(/C=C/C(=O)N[C@@H]([C@@H](c1ccccc1)C)C(=O)O[C@@H](CC(=O)O)C)\C	158	No
272	2,5-bis(5-tert-Butyl-2-benzoxazolyl)thiophene	CC(c1ccc2c(c1)nc(o2)c1ccc(s1)c1nc2c(o1)ccc(c2)C(C)(C)C)(C)C	159	Yes
273	Anandin A	OCCN1C(=O)C=C2C1=CC[C@]1([C@H]2CC[C@@H]1[C@@H](/C=C/[C@@H](C(C)C)C)C)C	160	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
274	Anandin B	OCCN1C(=O)C=C2[C@]1(O)CC[C@]1([C@H]2CC[C@@H]1[C@@H](/C=C/[C@@H](C(C)C)C)C)C	160	No
275	Griseorhodin F	COC(=O)CCc1cc2cc(C)oc(=O)c2c(c1O)O	161	Yes
276	4-Benzoxazolecarboxylic acid, 5-hydroxy-2-(2-hydroxyphenyl)-	Oc1ccccc1c1oc2c(n1)c(C(=O)O)c(cc2)O	161	No
277	7beta-Hydroxydigoxin	O=C1OCC(=C1)C1CCC2(C1(C)C(O)CC1C2C(O)CC2C1(C)CCC(C2)OC1CC(O)C(C(O1)C)OC1CC(C)C(C(C1)O)OC1CC(C)C(C(C1)O)O)O	162	Yes
278	Cogoxin	O=C1OCC(=C1)C1CCC2(C1(C)C(O)CC1C2CCC2C1(C)CCC(C2)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)O)O	162	No
279	7-Hydroxydigitoxin	O=C1OCC(=C1)[C@H]1CCC2([C@]1(C)CCC1C2[C@@H](O)CC2[C@]1(C)CC[C@@H](C2)O[C@H]1O[C@H](C)[C@H]([C@H](C1)O[C@@H]1C[C@H](O)[C@@H]([C@H](O1)C)O)O[C@@H]1C[C@H](O)[C@@H]([C@H](O1)C)O)O	163	Yes
280	ULDF4	OC1CCC(OC1C)OC1CC(O)C2=C(C1O)Cc1c(C2=O)c(O)c2c3c1OCOC3Cc1c2c(O)c2c(c1)CC1(N(C2=O)CCO1)C	164	Yes
281	Cuevaene A	CO/C(=C\C(=C\C1CCCC2C1c1cc(O)ccc1O2)\C)/C=C/C(=O)O	165	No
282	Cuevaene C	CO/C(=C/C(=C/C1CCCc2c1c1cc(O)ccc1o2)/C)/C=C/C(=O)O	165	Yes
283	Cuevaene D	C/C(=C\C1CCCc2c1c1cc(O)ccc1o2)/C=C(/C=C/C(=O)N)\OC	165	No
284	Jietacin D	CC[C@@H](CCCCCC(=O)CCCCCCCN[N+](=O)C=C)C	166	Yes
285	Jietacin C	CCCCCCCCC(=O)CCCCCCCN[N+](=O)C=C	166	No
286	JBIR-133	OC(=O)CCc1nc(cc2c1[nH]c1c2cccc1)C(=O)O	167	Yes
287	Oxopropaline G	OCCC(=O)c1ncc(c2c1[nH]c1c2cccc1)C	167	No
288	3-Hydroxypropane-1,2-diyl dipalmitate	CCCCCCCCCCCCCCCC(=O)OCC(OC(=O)CCCCCCCCCCCCCCC)CO	168	Yes
289	N-(1-(2,2-Dimethyl- 5-undecyl-1,3-dioxolan-4-yl)-2-hydroxyethyl)stearamide	CCCCCCCCCCCCCCCCCC(=O)NC(C1OC(OC1CCCCCCCCCCC)(C)C)CO	168	No
290	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl) ethyl ester	CCCCCCCCCCCCCCCC(=O)OC(CO)CO	169	No
291	Glycerol Linoleate	CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@H](CO)O	169	No
292	1-Monolinolein	CCCCC/C=C\C/C=C\CCCCCCCC(=O)OCC(CO)O	169	No
293	Hexadecanoic acid, 2,3-dihydroxypropyl ester	CCCCCCCCCCCCCCCC(=O)OCC(CO)O	169	Yes
294	Aggreceride C	OCC(COC(=O)CCCCCCCCCCCCCC(C)C)O	169	No
295	Aggreceride A	CC[C@@H](CCCCCCCCCC(=O)OC[C@@H](CO)O)C	169	No
296	Pyridinopyrone A	COc1cc(/C=C/C=C/C(=C/C=C/c2cccnc2)/C)oc(=O)c1	170	Yes
297	Zoumbericin B	COc1cc(Cc2cccc(c2)O)oc(=O)c1	170	No
298	Gombapyrone A	C=CC(c1cc(C)ccc1C=CC=CC(=CCc1oc(=O)c(c(c1C)OC)C)C)O	171	No
299	Gombapyrone B	C=CCc1cc(C)ccc1C=CC=CC(=CCc1oc(=O)c(c(c1C)O)C)C	171	No
300	Gombapyrone C	C=CCc1cc(C)ccc1C=CC=CC=CCc1oc(=O)c(c(c1C)OC)C	171	No
301	Gombapyrone D	C=CCc1cc(C)ccc1C=CC=CC(=CCc1oc(=O)c(c(c1C)OC)C)C	171	Yes
302	Pladienolide analog 10	CC[C@@H]([C@H]([C@H]1O[C@@H]1C[C@@H](/C=C/C=C(/[C@H]1OC(=O)C[C@H](O)CC[C@@]([C@H](/C=C/[C@@H]1C)OC(=O)NCCCC[C@@H](C(=O)N(CCN(C(=O)CCCC[C@H]1SC[C@@H]2[C@H]1NC(=O)N2)C)C)NC(=O)c1ccc(cc1)C1(N=N1)C(F)(F)F)(C)O)\C)C)C)O	172	Yes
303	Lavendiol	CC(C(=O)/C=C/C=C/C=C/C)[C@H](CCO)O	173	Yes
304	LMA-P3	CCCCCCCCC(CC(C(C(=O)OC)O)O)O	173	No
305	3-((1H-Indol-3-yl)methyl)-6-(4-	Oc1ccc(cc1)CC1(O)C(=O)NC(C(=O)N1C)Cc1c[nH]c2c1cccc2	174	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	hydroxybenzyl)-6-hydroxy-1-methylpiperazine-2,5-dione			
306	p-Thaxtomin A	Oc1cccc(c1)CC1(O)C(=O)N(C)C(C(=O)N1C)Cc1c[nH]c2c1cccc2	174	No
307	6-((1H-Indol-3-yl)methyl)-3-(4-hydroxybenzyl)-3-hydroxy-1-methylpiperazine-2,5-dione	Oc1ccc(cc1)CC1(O)NC(=O)C(N(C1=O)C)Cc1c[nH]c2c1cccc2	174	No
308	3,6-bis(1H-Indol-3-ylmethyl)piperazine-2,5-dione	O=C1NC(Cc2c[nH]c3c2cccc3)C(=O)NC1Cc1c[nH]c2c1cccc2	174	No
309	Cyclo-l-Trp-l-Tyr	Oc1ccc(cc1)C[C@@H]1NC(=O)[C@@H](NC1=O)Cc1c[nH]c2c1cccc2	174	Yes
310	Streptovaricin C	COC(=O)[C@@H]1[C@H](O)[C@H](C)C(O)[C@H](C)/C=C\C=C(/C)\C(=O)NC2=C(C(=c3c4=C(/C(=C/[C@@]([C@@H]([C@@H]([C@H]1O)C)O)(C)O)/C)OCOc4c(C)c(c3C2=O)O)OC(=O)C)C	175	Yes
311	2-Bromo-1-hydroxyphenazine	Brc1ccc2c(c1=O)nc1c([nH]2)cccc1	176	No
312	Phenazine 2	CC(=CCn1c2ccccc2nc2c1ccc(c2=O)Br)C	176	Yes
313	Phenazine 1	CC1=C(CCC(C1)(C)C)Cn1c2ccccc2nc2c1ccc(c2=O)Br	176	No
314	WS 9659 B	CC1=C(CCC(C1)(C)C)Cn1c2ccccc2nc2c1ccc(c2=O)Cl	176	No
315	JBIR-47	CC(=CCc1ccc(c2c1nc1c(=O)ccc(c1[nH]2)CC=C(C)C)O)C	177	Yes
316	(+)-Sydowic acid	Oc1cc(ccc1[C@@]1(C)CCCC(O1)(C)C)C(=O)O	178	Yes
317	Olivetolic acid	CCCCCc1cc(O)cc(c1C(=O)O)O	179	No
318	Sorbicillin	C/C=C/C=C/C(=O)c1cc(C)c(c(c1O)C)O	179	No
319	Chrysin	Oc1cc(O)c2c(c1)oc(cc2=O)c1ccccc1	179	Yes
320	(2S)-Pinocembrin	Oc1cc2O[C@@H](CC(=O)c2c(c1)O)c1ccccc1	179	No
321	Salaceyin A	CC(CCCCCCCCc1cccc(c1C(=O)O)O)C	180	Yes
322	Pyrrolostatin	C/C(=C\Cc1c[nH]c(c1)C(=O)O)/CCC=C(C)C	180	No
323	alpha-Lipomycin	OC(=O)CCC1N(C)C(=O)/C(=C(\C=C\C=C\C=C\C=C\C(=C\C(C(C(C)C)O[C@H]2C[C@H](O)[C@@H]([C@H](O2)C)O)C)\C)/O)/C1=O	181	Yes
324	Oleficin	OC(=O)CCC1C(=O)/C(=C(\C=C\C=C\C=C\C=C\C=C\C(=C\C(C(C(C)C)O[C@@H]2C[C@H](O)[C@@H]([C@H](O2)C)O)C)\C)/O)/C(=O)N1C	181	No
325	Tiancilactone G	OCC[C@H]1[C@H](C)[C@@H](OC)CC2[C@]1(C)CCC1[C@]2(C)CC[C@@H]([C@@]1(C)OC(=O)c1cc(Cl)ccc1NC)O	182	Yes
326	Tiancilactone F	O/C=C(/[C@H]1[C@H](C)[C@@H](OC)CC2[C@]1(C)CCC1[C@]2(C)CC[C@@H]([C@@]1(C)OC(=O)c1cc(Cl)ccc1NC)O)\C=O	182	No
327	Tiancilactone J	CNc1ccc(cc1C(=O)OC[C@]1(C)[C@@H](O)CC[C@]2(C1CC[C@]1(C2CC(=O)[C@H]([C@@H]1C1=C(O)C(=O)OC1O)C)C)C)Cl	183	Yes
328	Tiancilactone C	CO[C@H]1CC2[C@@]3(C)CCC([C@@](C3CC[C@@]2([C@H]([C@@H]1C)C1=C(O)C(=O)OC1O)C)CO)OC(=O)c1cc(Cl)ccc1NC	183	No
329	Tiancilactone A	CO[C@H]1CC2[C@@]3(C)CC[C@@H]([C@@](C3CC[C@@]2([C@H]([C@@H]1C)C1=C(O)C(=O)OC1O)C)(C)COC(=O)c1cc(Cl)ccc1NC)O	183	No
330	Tiancilactone K	COC1CC2[C@@]3(C)CC[C@@H]([C@@](C3CC[C@@]2([C@H]([C@@H]1C)C1=C(O)C(=O)OC1O)C)(C)COC(=O)c1cc(Cl)ccc1NC)O	183	No
331	Tiancilactone I	CNc1ccc(cc1C(=O)OC[C@]1(C)[C@@H](O)CC[C@]2(C1CC[C@]1(C2C[C@@H]([C@H]([C@@H]1C1=C(O)C(=O)OC1O)C)O)C)C)Cl	183	No
332	Sannastatin	CN[C@H]1[C@@H](O)C[C@@H](O[C@@H]1C)O[C@H]1C/C=C(\C)/C[C@](C)(O)[C@H](C)/C=C/CC[C@@H](CNC(=O)/C=C/C=C/[C@@H]1C)C	184	Yes
333	Vicenistatin	CN[C@H]1[C@@H](O)C[C@@H](O[C@@H]1C)O[C@H]1C/C=C(\C)/C/C(=C/C=C/CC[C@@H](CNC(=O)/C=C/C=C/[C@@H]1C)C)/C	184	No
334	Cytochalasin J	CC1CC=CC2C(O)C(=C)C(C3C2(C(C=CC(C1)(C)O)O)C(=O)NC3Cc1ccccc1)C	185	Yes
335	Cytochalasin H	CC(=O)O[C@@H]1/C=C/[C@@](C)(O)C[C@H](C/C=C/[C@@H]2C31C(=O)N[C@H]([C@@H]3[C@H](C)C(=C)[C@H]2O)Cc1ccccc1)C	185	No
336	Maremycin G	CSCc1nc2C3=C(CCC3=O)C3([C@@H](c2[nH]c1=O)C)C(=O)N(c1c3cccc1)C	186	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
337	SRB-1	CC(CC(=O)CCCC[C@H](C1=C(C)C(OC1=O)O)O)C	187	Yes
338	SRB-2	CCC(CC(=O)CCCC[C@H](C1=C(C)C(OC1=O)O)O)C	187	No
339	Bagremycin F	COC(=O)[C@H](NC(=O)C)CSc1c(ccc(c1N)O)C(=O)Oc1ccc(cc1)C=C	188	Yes
340	Bagremycin C	C=Cc1ccc(cc1)OC(=O)c1ccc(c(c1SC[C@H](C(=O)O)NC(=O)C)N)O	188	No
341	Divergolide A	CC[C@H]1/C=C\[C@H](OC(=O)/C(=C/CC(=O)Nc2c3O[C@@]4(CC1)CC(=O)[C@H]([C@H](O4)c3cc(c2)O)C)/C)[C@H](C=C(C)C)O	189	Yes
342	Mohangic acid C	OC(=O)C[C@H](/C=C/C=C/C=C/[C@H]([C@H]([C@@H](C[C@H]([C@@H](CC(=O)c1ccc(cc1)NC(=O)C)O)C)C)O)C)O	190	No
343	Mohangic acid D	OC(=O)C[C@H](/C=C/C=C/C=C/[C@H]([C@H]([C@@H](C[C@H]([C@@H](C[C@H](c1ccc(cc1)NC(=O)C)O)O)C)C)O)C)O	190	No
344	(2E)-17-(4'-Aminophenyl)-3,11,15-trihydroxy-10,12,14-trimethyl-17-oxo-heptadeca-4,6,8-trienoic acid	OC(=O)CC(/C=C/C=C/C=C/C(C(C(CC(C(CC(=O)c1ccc(cc1)N)O)C)C)O)C)O	190	Yes
345	Mohangic acid A	OC(=O)C[C@H](/C=C/C=C/C=C/[C@H]([C@H]([C@@H](C[C@H]([C@@H](CC(=O)c1ccc(cc1)N)O)C)C)O)C)O	190	No
346	Fexofenadine	OC(=O)C(c1ccc(cc1)C(CCCN1CCC(CC1)C(c1ccccc1)(c1ccccc1)O)O)(C)C	191	Yes
347	Ansaetherone	CC=C1/C=C(\C)/[C@H]2Oc3c(NC(=O)C(C1=O)C)cc(cc3[C@H]([C@@H]2C)O[C@H]1CC[C@H](C(O1)C)O)O	192	Yes
348	(S)-2-(5(2,3-Dihydroxy-3-methylbutyl)-1H-indol-3-yl)acetonitrile	O[C@H](C(O)(C)C)Cc1ccc2c(c1)c(CC#N)c[nH]2	193	Yes
349	(R)-6-(2,3-Dihydroxy-3-methylbutyl)indole	O[C@@H](C(O)(C)C)Cc1ccc2c(c1)[nH]cc2	193	No
350	Alnumycin S	CCC[C@H]1OC(=Cc2c1c(O)c1c(c2)C(=O)C=C(C1=O)C1O[C@H]([C@H](O1)CO)CO)C	194	No
351	Alnumycin A	CCC[C@H]1OC(=Cc2c1c(O)c1c(c2)C(=O)C=C(C1=O)C1OC[C@@H]([C@H](O1)CO)O)C	194	No
352	Alnumycin B2	CCC[C@H]1OC(=Cc2c1c(O)c1c(c2)C(=O)C=C(C1=O)[C@H]1O[C@@H]2[C@H](O1)CO[C@H]2O)C	194	No
353	Alnumycin B1	CCC[C@H]1OC(=Cc2c1c(O)c1c(c2)C(=O)C=C(C1=O)[C@@H]1O[C@@H]2[C@H](O1)CO[C@H]2O)C	194	Yes
354	Prealnumycin	CCC[C@H]1OC(=Cc2c1c(O)c1c(c2)C(=O)C=CC1=O)C	194	No
355	Esterastin	CCCCC/C=C/C/C=C/CC(CC1OC(=O)C1CCCCCC)OC(=O)C(NC(=O)C)CC(=O)N	195	No
356	Orlistat	CCCCCCCCCCC[C@@H](C[C@@H]1OC(=O)[C@H]1CCCCCC)OC(=O)[C@H](CC(C)C)NC=O	195	No
357	Lipstatin	CCCCC/C=C\C/C=C\C[C@@H](C[C@@H]1OC(=O)[C@H]1CCCCCC)OC(=O)[C@H](CC(C)C)NC=O	195	Yes
358	Naphthomycin K	O[C@@H]1/C=C/[C@H](C)[C@H](O)[C@@H](C)/C=C(/C)\C(=O)c2c(O)c(C)cc3c2C(=O)C(=C2C43[C@H](/C=C/C([C@H](CC(=O)/C(=C/C1)/C)O)C)C=CC(O4)C(=O)N2)Cl	196	Yes
359	3-((3E,6E,8E,10R,11R,12E)-11-Hydroxy-4,8,10,12-tetramethyltetradeca-3,6,8,12-tetraenamido)butanoic acid	C/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/CC(=O)NC(CC(=O)O)C)/C)\C)C)O)\C	197	Yes
360	3E,6E,8E,10R,11R,12E)-11-Hydroxy-4,8,10,12-tetramethyltetradeca-3,6,8,12-tetraenoic acid	C/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/CC(=O)O)/C)\C)C)O)\C	198	Yes
361	4-Hydroxy-6-(2',4',6'-trioxotridecyl)-2-pyrone	CCCCCCCC(=O)CC(=O)CC(=O)Cc1cc(O)cc(=O)o1	199	Yes
362	Pladienolide D	CCC(C(C1OC1CC(C=CC=C(C1OC(=O)CC(O)CCC(C(C=CC1C)OC(=O)C)(C)O)C)(O)C)C)O	200	No
363	Pladienolide B	CCC(C(C1OC1CC(C=CC=C(C1OC(=O)CC(O)CCC(C(C=CC1C)OC(=O)C)(C)O)C)C)C)O	200	Yes
364	Pladienolide	CCC(C(C1OC1CC(C=CC=C(C1OC(=O)CC(O)CCC(C(CCC1C)O)(C)O)C)C)C)O	200	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
365	Spirofungin A	C/C(=C\C[C@H]1O[C@]2(CC[C@@H]1C)CC[C@@H]([C@@H](O2)/C=C/C(=C/C(=O)O)/C)C)/C=C/[C@@H]([C@H](/C=C/C(=O)O)C)O	201	Yes
366	Reveromycin E	CCCCCC[C@]1(CC[C@@]2(O[C@H]1/C=C/C(=C/C(=O)O)/C)CC[C@@H]([C@H](O2)C/C=C(/C=C/[C@@H]([C@H](/C=C/C(=O)O)C)O)\C)C)OC(=O)CCC(=O)O	202	No
367	(2E,4S,5S,6E,8E)-10-[(2S,3R,6S,8R,9S)-2-[(1E,3E)-4-Carboxy-3-methylbuta-1,3-dienyl]-3-(3-carboxypropanoyloxy)-9-methyl-3-(3-methylbutyl)-1,7-dioxaspiro[5.5]undecan-8-yl]-5-hydroxy-4,8-dimethyldeca-2,6,8-trienoic acid	CC(CC[C@]1(CC[C@@]2(O[C@H]1/C=C/C(=C/C(=O)O)/C)CC[C@@H]([C@H](O2)C/C=C(/C=C/[C@@H]([C@H](/C=C/C(=O)O)C)O)\C)C)OC(=O)CCC(=O)O)C	202	No
368	Reveromycin A	CCCC[C@]1(CC[C@@]2(O[C@H]1/C=C/C(=C/C(=O)O)/C)CC[C@@H]([C@H](O2)C/C=C(/C=C/[C@@H]([C@H](/C=C/C(=O)O)C)O)\C)C)OC(=O)CCC(=O)O	202	No
369	Reveromycin D	CCCCC[C@]1(CC[C@@]2(O[C@H]1/C=C/C(=C/C(=O)O)/C)CC[C@@H]([C@H](O2)C/C=C(/C=C/[C@@H]([C@H](/C=C/C(=O)O)C)O)\C)C)OC(=O)CCC(=O)O	202	Yes
370	(2E,6E,8E)-10-[2-Butyl-2-[(2E,4E)-5-carboxy-1-(3-carboxypropanoyloxy)-4-methylpenta-2,4-dienyl]-8-methyl-1,10-dioxaspiro[4.5]decan-9-yl]-5-hydroxy-4,8-dimethyldeca-2,6,8-trienoic acid	CCCC[C@@]1(CC[C@@]2(O1)CC[C@@H]([C@H](O2)C/C=C(/C=C/[C@@H]([C@H](/C=C/C(=O)O)\C)O)\C)C)[C@@H](OC(=O)CCC(=O)O)/C=C/C(=C/C(=O)O)/C	202	No
371	Reveromycin	CCCCC1(CCC2(OC1/C=C\C(=C\C(=O)O)\C)CCC(C(O2)C/C=C(/C=C/C(C(/C=C\C(=O)O)C)O)\C)C)OC(=O)CCC(=O)O	202	No
372	Pyrrolnitrin	Clc1c[nH]cc1c1cccc(c1N(=O)=O)Cl	203	Yes
373	Methicillin	COc1cccc(c1C(=O)N[C@@H]1C(=O)N2[C@@H]1SC([C@@H]2C(=O)O)(C)C)OC	204	Yes
374	Xiamenmycin B	CC(=CCC[C@]1(C)Oc2ccc(cc2C[C@@H]1O)C(=O)O)C	205	Yes
375	Xiamenmycin C	CC(=CCC[C@]1(C)Oc2ccc(cc2C[C@@H]1O)C(=O)N)C	205	No
376	(S)-Methyl 2-(4-bromobenzamido)butanoate	CC[C@@H](C(=O)OC)NC(=O)c1ccc(cc1)Br	206	Yes
377	Stubomycin	COC1CC2C(=C1O)C(=O)CC(O)CC/C=C/CC(NC(=O)/C=C/C=C/C(=C\2)/C)c1ccccc1	207	Yes
378	2,4,6,8-Nonatetraenamide, N-(2-hydroxy-5-oxo-1-cyclopenten-1-yl)-9-(2-methylphenyl)-, (2E,4E,6E,8E)-	O=C(NC1=C(O)CCC1=O)/C=C/C=C/C=C/C=C/c1ccccc1C	208	No
379	4-E-Annimycin	CC/C=C/C=C(/C=C/C=C/C(CC(=O)NC1=C(O)CCC1=O)O)\C	208	No
380	4-Z-Annimycin	CC/C=C/C=C(/C=C/C=C\C(CC(=O)NC1=C(O)CCC1=O)O)\C	208	Yes
381	Protoasukamycin	C/C=C/C=C/C=C/C(=O)Nc1cc(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)ccc1O	208	No
382	4-Pentenamide, N-(2-hydroxy-5-oxo-1-cyclopenten-1-yl)-5-(2-methylphenyl)-, (4E)-	O=C(NC1=C(O)CCC1=O)CC/C=C/c1ccccc1C	209	Yes
383	Aminoansamycin F	O=C1C=C2NC(=O)[C@@H](C)[C@H](O)/C=C/C=C/C[C@H](C(=C1)C2=O)Nc1ccccc1C(=O)O	210	Yes
384	Huperzine A	C/C=C/1\C2C=C(CC1(N)c1c(C2)[nH]c(=O)cc1)C	211	Yes
385	Virantmycin B	COC[C@@]1(CCC(=C(C)C)C)Nc2ccc(cc2C[C@H]1O)C(=O)NC1=C(O)CCC1=O	212	Yes
386	Virantmycin C	COC[C@@]([C@@H]1Nc2c(C1)cc(cc2)C(=O)NC1=C(O)CCC1=O)(CCC(=C(C)C)C)O	212	No
387	Val-geninthiocin	C/C=C\1/N=C(O)C(N=C(O)c2csc(n2)c2ccc(nc2c2coc(n2)C(=C)N=C(O)C(=C)N=C(c2nc(C(=C)N=C(C(N=C(C(=C)N=C(c3nc1oc3)O)O)C(C)C)O)oc2C)O)C(=O)NC(=C)C(=NC(=C)C(=N)O)O)C(O)C	213	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
388	Mycophendic acid	COc1c(CCC(CCC(=O)O)C)c(O)c2c(c1C)COC2=O	214	Yes
389	6,8-Dimethoxy-7-hydroxy-methyl-isocoumarin	COc1cc2cc(C)oc(=O)c2c(c1O)OC	215	No
390	6,7,8-Trimethoxy-3-methylisocoumarin	COc1cc2cc(C)oc(=O)c2c(c1OC)OC	215	No
391	5,6,8-Trimethoxy-3-methylisocoumarin	COc1cc(OC)c2c(c1OC)cc(oc2=O)C	215	Yes
392	1H-2-Benzopyran-1-one, 6,8-dimethoxy-3-methyl-	COc1cc2cc(C)oc(=O)c2c(c1)OC	215	No
393	5,6,7,8-Tetramethoxy-3-methyl-isocoumarin	COc1c2C[C@@H](C)OC(=O)c2c(c(c1OC)OC)OC	215	No
394	6,8-Dimethoxyl-3-methyl-isocoumarin	COc1cc2C[C@@H](C)OC(=O)c2c(c1)OC	215	No
395	Bireticulol	COc1c(O)c(c2c(O)c(OC)c(c3c2cc(C)oc3=O)O)c2c(c1O)c(=O)oc(c2)C	216	Yes
396	1-O-alpha-L-Rhamnosyl-12-hydroxy-8-O-methyltetrangulol	COc1cccc2c1C(=O)c1ccc3c(c1C2O)C(C[C@H](C3)C)O[C@@H]1O[C@@H](O)[C@@H]([C@H]([C@H]1O)C)O	217	Yes
397	Piceamycin	O=C1C=CC=CC=CC2(C)CC(=O)C(=C2C(=O)C=CC=CC=CC=CC=CC(CN1)C)O	218	No
398	Cyclamenol B	O=C1/C=C/[C@H]2C=C[C@@H]3[C@@H]4[C@@H]2[C@H](/C=C/C=C\[C@@H](CN1)C)O[C@@H]4[C@@H](C3)O	218	Yes
399	Cyclamenol C	O=C1/C=C/[C@@H]2C=C[C@H]3[C@H]4[C@H]2[C@@H](/C=C/C=C\[C@@H](CN1)C)O[C@H]4[C@@H](C3)O	218	No
400	Bombyxamycin B	O=C1/C=C\C=C/C=C/[C@@]2(C)O/C(=C\C(=O)/C=C/C=C\C=C/C=C/C=C\[C@H](CN1)C)/[C@H]([C@@H]2O)O	219	Yes
401	Cyclamenol D	C[C@H]1/C=C/C=C/[C@@H]2C=C[C@H]3[C@@H]([C@H]2/C=C/C(=O)CC(=O)NC1)C=CC[C@@H]3O	220	Yes
402	Indimicin E	Cn1cc(c(c1)[C@@]1(C)CN(c2c1cc(Cl)cc2)C)c1c[nH]c2c1cc(Cl)cc2	221	No
403	Indimicin B	Clc1ccc2c(c1)[C@@]1(C)c3cn(c(c3c3c([C@H]1N2C)[nH]c1c3cc(cc1)Cl)C)C	221	Yes
404	Indimicin A	Cn1cc2c(c1)[C@]1(C)c3cc(Cl)ccc3N([C@@H]1c1c2c2cc(Cl)ccc2[nH]1)C	221	No
405	Indimicin C	Clc1ccc2c(c1)[C@@]1(C)c3c[nH]c(c3c3c([C@H]1N2C)[nH]c1c3cc(cc1)Cl)C	221	No
406	Indimicin D	Clc1ccc2c(c1)[C@@]1(C)c3c[nH]cc3c3c([C@H]1N2C)[nH]c1c3cc(cc1)Cl	221	No
407	Chloroxaloterpin B	C=C[C@@]1(C)CC=C2[C@H](C1)CC[C@H]1[C@@]2(C)CC[C@H](C1(C)C)OC(=O)C(=O)Nc1ccccc1Cl	222	No
408	Chloroxaloterpin A	C=C[C@@]1(C)CC=C2[C@H](C1)CC[C@H]1[C@@]2(C)CC[C@H](C1(C)C)OC(=O)NC(=O)Nc1ccccc1Cl	222	Yes
409	Oxaloterpin B	OCCNC(=O)NC(=O)COC1CCC2(C(C1(C)C)CCC1C2=CCC(C1)(C)C=C)C	222	No
410	5-Hydroxy-4-methylnaphtho[1,2-beta]furan-3-one	O=C1COc2c1c(C)c(c1c2cccc1)O	223	Yes
411	16alpha-Hydroxydehydroepiandrosterone	O[C@H]1CC[C@]2(C(=CC[C@@H]3[C@@H]2CC[C@]2([C@H]3C[C@H](C2=O)O)C)C1)C	224	Yes
412	Streptoseolactone	CC(=CCCC1=C2[C@@H](OC1=O)C[C@]1([C@H]2CC[C@@H]2[C@]1(C)C(=O)[C@H]([C@@H]1[C@]2(C)CC[C@@H]([C@H]1C)O)O)C)C	225	Yes
413	2,8,10,19-Tetrahydroxy-18-methyldocosanoic acid	CCCC(C(CCCCCCCC(CC(CCCCCC(C(=O)O)O)O)O)C)O	226	No
414	Succinilene B	CC[C@@H]([C@@H](C/C=C/C=C/C=C/C[C@@H](/C(=C/[C@H]([C@H](OC(=O)CCC(=O)O)C)C)/C)O)O)O	226	Yes
415	Succinilene A	CC[C@H]([C@@H](C/C=C/C=C/C=C/C[C@@H](C(=C[C@H]([C@H](OC(=O)CCC(=O)O)C)C)C)O)O)O	226	No
416	Succinilene C	CCC(=O)[C@@H](C/C=C/C=C/C=C/C[C@@H](/C(=C/[C@H]([C@H](OC(=O)CCC(=O)O)C)C)/C)O)O	226	No
417	3,6,8,11-Tetrahydroxy-16,17-dimethyloctadecanoic acid	OC(CC(CCC(CC(=O)O)O)O)CCC(CCCCC(C(C)C)C)O	227	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
418	Frenolicin G	CCC[C@@H]1O[C@@H](CC(=O)O)CC2([C@]1(O)C(=O)c1c(O)cccc1C2=O)SC12C[C@@H](CC(=O)O)O[C@@H]([C@]2(O)C(=O)c2c(C1=O)cccc2O)CCC	228	Yes
419	(-)-BE-52440A	COC(=O)C[C@@H]1O[C@@H](C)[C@@]2([C@](C1)(S[C@]13C[C@H](CC(=O)OC)O[C@H]([C@@]3(O)C(=O)c3c(C1=O)cccc3O)C)C(=O)c1c(C2=O)c(O)ccc1)O	228	No
420	Chromomycin SA	CO[C@@H]([C@@H]1Cc2cc3cc(O[C@H]4C[C@@H](O[C@@H]5C[C@@H](O)[C@@H]([C@H](O5)C)OC)[C@@H]([C@H](O4)C)OC(=O)C)c(c(c3c(c2C(=O)[C@H]1O[C@H]1C[C@H](O[C@H]2C[C@H](O[C@@H]3O[C@@H](C)[C@@H]([C@](C3)(C)O)OC(=O)C)[C@@H]([C@H](O2)C)O)[C@@H]([C@H](O1)C)O)O)O)C)C(=O)O	229	Yes
421	Aburamycin B	CO[C@@H](C1Cc2cc3cc(O[C@H]4C[C@@H](O[C@@H]5C[C@@H](O)[C@H]([C@H](O5)C)OC)[C@H]([C@H](O4)C)OC(=O)C)c(c(c3c(c2C(=O)[C@H]1O[C@H]1C[C@@H](O[C@H]2C[C@@H](O[C@@H]3O[C@@H](C)[C@@H]([C@@](C3)(C)O)OC(=O)C)[C@@H]([C@H](O2)C)O)[C@@H]([C@H](O1)C)O)O)O)C)C(=O)[C@H]([C@H](O)C)O	230	Yes
422	Chromomycin	CO[C@@H]([C@@H]1Cc2cc3cc(OC4CC(OC5CC(O)C(C(O5)C)OC)C(C(O4)C)OC(=O)C)c(c(c3c(c2C(=O)[C@H]1OC1CC(OC2CC(OC3OC(C)C(C(C3)(C)O)OC(=O)C)C(C(O2)C)O)C(C(O1)C)O)O)O)C)C(=O)[C@H]([C@H](O)C)O	231	Yes
423	Chromomycin A3-1	COC(C1Cc2cc3cc(OC4CC(OC5CC(O)C(C(O5)C)OC)C(C(O4)C)OC(=O)C)c(c(c3c(c2C(=O)C1OC1OCC(C(C1)OC1CC(OC2OC(C)C(C(C2)(C)O)OC(=O)C)C(C(O1)C)O)O)O)O)C)C(=O)C(C(O)C)O	232	Yes
424	Chromomycin A3	CO[C@@H]([C@@H]1Cc2cc3cc(O[C@H]4C[C@@H](O[C@@H]5C[C@@H](O)[C@H]([C@H](O5)C)OC)[C@H]([C@H](O4)C)OC(=O)C)c(c(c3c(c2C(=O)[C@H]1O[C@H]1C[C@@H](O[C@H]2C[C@@H](O[C@@H]3O[C@@H](C)[C@@H]([C@@](C3)(C)O)OC(=O)C)[C@@H]([C@H](O2)C)O)[C@@H]([C@H](O1)C)O)O)O)C)C(=O)[C@H]([C@H](O)C)O	233	Yes
425	Chromomycin A2	CO[C@@H]([C@@H]1Cc2cc3cc(O[C@H]4C[C@@H](O[C@@H]5C[C@@H](O)[C@H]([C@H](O5)C)OC)[C@H]([C@H](O4)C)OC(=O)C)c(c(c3c(c2C(=O)[C@H]1O[C@H]1C[C@@H](O[C@H]2C[C@@H](O[C@@H]3O[C@@H](C)[C@@H]([C@@](C3)(C)O)OC(=O)C(C)C)[C@@H]([C@H](O2)C)O)[C@@H]([C@H](O1)C)O)O)O)C)C(=O)[C@H]([C@H](O)C)O	234	Yes
426	Chromomycin A2-1	COC(C1Cc2cc3cc(OC4CC(OC5CC(O)C(C(O5)C)OC)C(C(O4)C)OC(=O)C)c(c(c3c(c2C(=O)C1OC1OCC(C(C1)OC1CC(OC2OC(C)C(C(C2)(C)O)OC(=O)C(C)C)C(C(O1)C)O)O)O)O)C)C(=O)C(C(O)C)O	235	Yes
427	Demethylchromomycin A2	COC(C1Cc2cc3cc(OC4CC(OC5CC(O)C(C(O5)C)O)C(C(O4)C)OC(=O)C)c(c(c3c(c2C(=O)C1OC1CC(OC2CC(OC3OC(C)C(C(C3)(C)O)OC(=O)C(C)C)C(C(O2)C)O)C(C(O1)C)O)O)O)C)C(=O)C(C(O)C)O	236	Yes
428	Orinocin	COc1oc([C@@H]2OC/C(=C\c3ccc(cc3)N(=O)=O)/C2)c(c(=O)c1C)C	237	Yes
429	CHEMBL514407	COc1oc([C@@H]2OC[C@@]3(C2)[C@H]2C(=CC(=C[C@]2([C@H]3c2ccc(cc2)N(=O)=O)C)C)C)c(c(=O)c1C)C	238	Yes
430	CHEMBL459070	COc1oc(C2OC[C@@]3(C2)C2C(=CC(=C[C@]2([C@H]3c2ccc(cc2)N(=O)=O)C)C)C)c(c(=O)c1C)C	238	No
431	Luminacin D	CCCC(C(=O)c1cc(CC(C)C)c(c(c1O)C=O)O)C1CC(O)C2(C(O1)O)OC2CC	239	No
432	Luminacin	CC[C@@H]1OC21[C@H](O)CC(O[C@H]2O)C(C(=O)c1cc(C(C(C)C)OC)c(c(c1O)C=O)O)CC(C)C	239	No
433	Migracin A	CCC[C@H](C(=O)c1cc([C@H](C(C)C)OCC)c(c(c1O)C=O)O)[C@H]1C[C@@H](O)[C@]2([C@@H](O1)O)O[C@H]2CC	239	No
434	Luminacin I	CCCC(C(=O)c1cc(C(C(C)C)O)c(c(c1O)C=O)O)C1CC(O)C2(C(O1)O)OC2CC	239	Yes
435	Indinavir	O[C@H](CN1CCN(C[C@H]1C(=O)NC(C)(C)C)Cc1cccnc1)C[C@H](C(=O)N[C@@H]1[C@H](O)Cc2c1cccc2)Cc1ccccc1	240	Yes
436	Echoside E	OC(=O)C1OC(Oc2c(O)c(c3ccccc3)c3c(c2c2ccccc2)n(C)c(=O)s3)C(C(C1O)O)O	241	No
437	Echoside A	COC(=O)C1OC(Oc2c(cc(c(c2O)c2ccccc2)O)c2ccccc2)C(C(C1O)O)O	241	No
438	Echoside D	OC(=O)C1OC(Oc2c(c3ccccc3)c3ncsc3c(c2O)c2ccccc2)C(C(C1O)O)O	241	No
439	Echoside C	OC(=O)C1OC(Oc2c(cc(c(c2O)c2ccccc2)O)c2ccccc2)C(C(C1O)O)O	241	Yes
440	Echoside B	COc1c(cc(c(c1O)c1ccccc1)OC1OC(C(=O)O)C(C(C1O)O)O)c1ccccc1	241	No
441	Strepantibin E	OC[C@H]1O[C@@H](Oc2c(c3ccccc3)c(OC)cc(c2O)c2ccccc2)[C@@H]([C@H]([C@@H]1O)O)O	241	No
442	Strepantibin D	OC[C@H]1O[C@@H](Oc2c(cc(c(c2O)c2ccccc2)OC)c2ccccc2)[C@@H]([C@H]([C@@H]1O)O)O	241	No
443	Streptochlorin	Clc1ncoc1c1c[nH]c2c1cccc2	242	Yes
444	9-(4-Aminophenyl)-3,7-dihydroxy-2,4,6-trimethyl-9-oxo-nonanoic acid	OC(C(CC(C(C(C(=O)O)O)C)O)C)C)CC(=O)c1ccc(cc1)N	243	Yes
445	(2E)-11-(4-Aminophenyl)-5,9-dihydroxy-4,6,8-trimethyl-11-oxo-undec-2-enoic Acid	CC(C(CC(=O)c1ccc(cc1)N)O)CC(C(C(/C=C/C(=O)O)O)C)O)C	243	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
446	(E)-4-[(2S,3R,5R,6S)-6-[2-(4-Aminophenyl)-2-oxoethyl]-3,5-dimethyloxan-2-yl]pent-2-enoic acid	OC(=O)/C=C/C([C@H]1O[C@@H](CC(=O)c2ccc(cc2)N)[C@@H](C[C@H]1C)C)C	244	Yes
447	2-[(2S,3R,5R,6S)-6-[2-(4-Aminophenyl)-2-oxo-ethyl]-3,5-dimethyl-tetrahydropyran-2-yl]propanoic acid	OC(=O)C([C@H]1O[C@@H](CC(=O)c2ccc(cc2)N)[C@@H](C[C@H]1C)C)C	244	No
448	Pinocembrin chalcone	Oc1cc(O)c(c(c1)O)C(=O)/C=C/c1ccccc1	245	Yes
449	Anthracimycin	CC1=CC[C@H]2[C@H](C1)C=C[C@H]1[C@@H]2/C(=C/C(=O)[C@@H](C)C(=O)O[C@@H](/C=C/C=C\[C@H]1C)C)/O	246	Yes
450	Anthracimycin B	OC1CC(=O)O[C@H](C)/C=C/C=C\[C@@H]([C@@H]2[C@H](C(=O)C1)[C@H]1CC=C(C[C@@H]1C=C2)C)C	247	Yes
451	Anthracimycin BII-2619	OC1CC(=O)O[C@H](C)/C=C/C=C\[C@@H]([C@@H]2[C@H](C(=O)C1)[C@@H]1[C@@H](C=C2)CC(=C[C@@H]1C)C)C	247	No
452	BE-24566B	Oc1cc(C)c2c(c1)OC1(OC2c2c(C1)cc1c(c2O)C(=O)c2c(C1(C)C)cc(cc2O)O)C	248	No
453	Tetarimycin A	Oc1cc(C)c2c(c1)C(=O)C1=C(C2=O)C(=O)c2c(C1(C)C)cc(cc2O)O	248	No
454	Tetarimycin B	OC1Cc2cc3c(c(c2C(C1)(C)O)O)C(=O)c1c(C3(C)C)cc(cc1O)O	248	Yes
455	Fipronil	N#Cc1nn(c(c1S(=O)C(F)(F)F)N)c1c(Cl)cc(cc1Cl)C(F)(F)F	249	Yes
456	Fipronil sulfone	N#Cc1nn(c(c1S(=O)(=O)C(F)(F)F)N)c1c(Cl)cc(cc1Cl)C(F)(F)F	249	No
457	CHEMBL373620	OCC1=C[C@H]2[C@H](CC[C@@]([C@H]2CC1=O)(C)O)C(C)C	250	Yes
458	Scopranone A	CCC(CC1=C(OC(C1=O)(O)CC)/C(=C/C)/CC)CC	251	Yes
459	Scopranone C	CCC(CC1=C(OC(C1=O)(O)C(O)C)C(=CC)CC)CC	251	No
460	Kandenol A	O=C1C=C(C)[C@H]2[C@@](C1)(C)C[C@H]([C@@H](C2)C(O)(C)C)O	252	Yes
461	1,6,11-Eudesmanetriol	C[C@@H]1CC[C@@H]([C@@]2([C@@H]1[C@H](O)[C@H](CC2)C(O)(C)C)C)O	253	Yes
462	Strepsesquitriol	C[C@H]1C[C@H]([C@@]23[C@]1(O)CC[C@@H](C2)C([C@]3(C)O)(C)C)O	253	No
463	Actinopolysporin B	COC(=O)/C(=C/C(CC(CC(CC(O)C)(O)C)C)C)/C	254	Yes
464	ZINC04026203	CC(C[C@@H]1NC(=O)[C@@H](NC1=O)Cc1ccccc1)C	255	No
465	cyclo(Phe-Phe)	O=C1N[C@@H](Cc2ccccc2)C(=O)N[C@H]1Cc1ccccc1	255	Yes
466	3-(1,3-Benzodioxol-5-ylmethyl)-6- isobutyl-2,5-diketopiperazine	CC(C[C@H]1NC(=O)[C@H](NC1=O)Cc1ccc2c(c1)OCO2)C	255	No
467	Piperafizine B	O=c1[nH]/c(=C\c2ccccc2)/c(=O)[nH]/c/1=C\c1ccccc1	255	No
468	Piperafizine A	O=c1/c(=C/c2ccccc2)/[nH]c(=O)/c(=C/c2ccccc2)/n1C	255	No
469	Cyclo-l-Trp-l-Phe	O=C1N[C@@H](Cc2ccccc2)C(=O)N[C@H]1Cc1c[nH]c2c1cccc2	255	No
470	3-((1H-indol-3-yl)methyl)-6-benzyl-1,4-dimethylpiperazine-2,5-dione	CN1C(=O)C(Cc2ccccc2)N(C(=O)C1Cc1c[nH]c2c1cccc2)C	256	No
471	Thaxtomin C	O=C1N[C@@H](Cc2ccccc2)C(=O)N([C@H]1Cc1c[nH]c2c1c(ccc2)[N+](=O)[O-])C	256	No
472	Thaxtomin D	CN1C(=O)[C@H](Cc2ccccc2)N(C(=O)[C@@H]1Cc1c[nH]c2c1c(ccc2)[N+](=O)[O-])C	256	Yes
473	Terezine D	CC(=CCc1cccc2c1[nH]cc2C[C@@H]1NC(=O)[C@@H](NC1=O)C)C	257	Yes
474	Gloeosporiocide	CC(CC(NC(=O)CNC(=O)CNC(=O)c1csc(n1)C(Cc1c[nH]c2c1cccc2)NC(=O)C(NC(=O)c1csc(n1)C(Cc1ccccc1)NC(=O)CNC(=O)c1cscn1)C)C)C	258	Yes
475	Galbonolide B	CC[C@@H]1OC(=O)[C@H](C)C(=O)C(O)(CO)C/C(=C/[C@H](CC(=C)/C=C/1\C)C)/C	259	No
476	Rustmicin	CO/C/1=C\[C@@H](C)CC(=C)/C=C(\C)/[C@@H](OC(=O)[C@@H](C(=O)C(C1)(O)CO)C)CC	259	No
477	Galbonolide E	CC[C@@H]1OC(=O)[C@H](C)C(=O)[C@](O)(CO)CC(=O)C[C@H](CC(=C)/C=C/1\C)C	259	No
478	Neorustmicin A	CC[C@@H]1OC(=O)[C@H](C)C(=O)[C@@](O)(CO)C/C(=C/[C@H](CC(=C)/C=C/1\C)C)/C	259	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
479	Leptolstatin	OC/C=C(/CC(C(C(C(=O)C(/C=C(/C=C/CC(/C=C(/CCC1CC=CC(=O)O1)\C)C)\C)C)C)O)C)\C	260	Yes
480	Reductoleptomycin A	OC/C=C(/CC(C(C(C(=O)C(/C=C(/C=C/CC(/C=C(/C=C/C1OC(=O)C=CC1C)\C)C)\C)C)C)O)C)\C	260	No
481	Christolane A	CC(C(=O)O)CNc1ccc(cc1Cl)C(=O)O	261	Yes
482	Elaiomycin K	CCCCCCCC/[N+](=N/[C@H](C(=O)O)CO)/O	262	Yes
483	Elaiomycin L	CCCCCCCC/[N+](=N/[C@H](C(=O)O)COC)/O	262	No
484	Verticilactam	O=C1CC(=O)NCC(C)/C=C/C=C\C=C(\[C@H]2[C@@H]3[C@H](C1)O[C@@H]1C3C(CC2)[C@@H](C[C@@H]1O)O)/C	263	Yes
485	Platensimycin	O=C(Nc1c(O)ccc(c1O)C(=O)O)CC[C@]1(C)C(=O)C=C[C@]23C1C1CC(C2)[C@@](O1)(C3)C	264	Yes
486	Platencin	O=C(Nc1c(O)ccc(c1O)C(=O)O)CC[C@]1(C)C(=O)C=C[C@]23C1CC(CC2)C(=C)C3	264	No
487	Platencin A1	O=C(Nc1c(O)ccc(c1O)C(=O)O)CCC1(C)C(=O)C=CC23C1CC(CC3O)C(=C)C2	264	No
488	Spirotoamide A	CC/C(=C\CCC(C[C@@H]([C@@H]1C[C@H](O)[C@@H]([C@@]2(O1)C[C@@H](O)[C@@H]([C@H](O2)C)C)C)C)(O)C)/C=C/C(=O)N	265	Yes
489	Spirotoamide C	OCC(CC([C@@H]1C[C@H](O)[C@@H]([C@@]2(O1)C[C@@H](O)[C@@H]([C@H](O2)C)C)C)C)CC/C=C(/C=C/C(=O)N)\CC	265	No
490	Spirotoamide B	CC/C(=C\C(CC(C[C@@H]([C@@H]1C[C@H](O)[C@@H]([C@@]2(O1)C[C@@H](O)[C@@H]([C@H](O2)C)C)C)C)O)/C=C/C(=O)N	265	No
491	Spirotoamide D	OCC(CC([C@H]1C[C@H](O)[C@@H]([C@@]2(O1)C[C@@H](O)[C@@H]([C@H](O2)C)C)C)C)CC/C=C(/C=C/C(=O)N)\CC	265	No
492	Chromopyrrolate	OC(=O)c1[nH]c(c(c1c1c[nH]c2c1cccc2)c1c[nH]c2c1cccc2)C(=O)O	266	Yes
493	Dichlorochromopyrrolic acid	OC(=O)c1[nH]c(c(c1c1c[nH]c2c1cccc2Cl)c1c[nH]c2c1cccc2Cl)C(=O)O	266	No
494	Dimethyl N1-methylchromopyrrolate	[nH]1cc(c2c1cccc2)c1c(n(C)c(C(=O)OC)c1c1c[nH]c2c1cccc2)C(=O)OC	267	No
495	Lycogarubin C	COC(=O)c1[nH]c(c(c1c1c[nH]c2c1cccc2)c1c[nH]c2c1cccc2)C(=O)OC	267	No
496	IDM G	COC(=O)C1NC(C(=C1c1c[nH]c2c1cccc2)c1c[nH]c2c1cccc2)C(=O)OC	267	Yes
497	SPM G	COC(=O)C1NC(C2=C1c1c3ccccc3[nH]c1[C@]12CN(c2c1cccc2)C)C(=O)OC	267	No
498	Lynamicin E	COC(=O)c1[nH]c(c(c1c1c[nH]c2c1cccc2)c1c[nH]c2c1cc(Cl)cc2)C(=O)OC	268	No
499	Lynamicin G	COC(=O)c1c(c2c[nH]c3c2cc(Cl)cc3)c(c(n1C)C(=O)OC)c1c[nH]c2c1cc(Cl)cc2	268	No
500	Lynamicin D	COC(=O)c1[nH]c(c(c1c1c[nH]c2c1cc(Cl)cc2)c1c[nH]c2c1cc(Cl)cc2)C(=O)OC	268	Yes
501	Lynamicin A	COC(=O)c1[nH]cc(c1c1c[nH]c2c1cc(Cl)cc2)c1c[nH]c2c1cc(Cl)cc2	268	No
502	Lynamicin F	COC(=O)c1n(C)cc(c1c1c[nH]c2c1cc(Cl)cc2)c1c[nH]c2c1cc(Cl)cc2	268	No
503	Azolemycin A	CC[C@@H]([C@@H](C(=O)OC)NC(=O)c1nc(oc1C)c1csc(n1)c1nc(oc1C)c1coc(n1)[C@H](C(C)C)NC(=O)/C(=N\O)/C(C)C)C	269	Yes
504	Azolemycin C	CO/N=C(\C(=O)N[C@H](c1occ(n1)c1nc(c(o1)C)c1scc(n1)c1nc(c(o1)C)C(=O)N[C@H](C(=O)OC)[C@H](CC)C)C(C)C)/C(C)C	269	No
505	Aurantizdicin	CCC(C1NC(=O)C(NC(=O)c2nc(oc2c2ccccc2)c2csc(n2)c2nc(c3nc(c4nc(CNC1=O)oc4)oc3)sc2)C(CC)C)C	270	No
506	Urukthapelstatin A	CC[C@@H]([C@H]1NC(=O)c2nc(oc2c2ccccc2)c2csc(n2)c2csc(n2)c2nc(c3nc(/C(=C/C)/NC(=O)[C@@H](NC1=O)C)oc3)oc2)C	270	No
507	Curacozole	CCC(C1NC(=O)C(NC(=O)c2nc(oc2c2ccccc2)c2csc(n2)c2nc(c3nc(c4nc(CNC1=O)oc4)oc3C)sc2)C(CC)C)C	270	No
508	Mechercharstatin	CC[C@@H]([C@H]1NC(=O)c2nc(oc2c2ccccc2)c2coc(n2)c2csc(n2)c2nc(c3nc(C(=C)NC(=O)[C@@H](NC1=O)C(C)C)oc3)oc2)C	270	Yes
509	YM-216391	CC[C@H]([C@H]1NC(=O)c2nc(oc2c2ccccc2)c2csc(n2)c2coc(n2)c2nc(c3nc(CNC(=O)[C@@H](NC1=O)C(C)C)oc3)oc2)C	270	No
510	Marthiapeptide A	CC[C@@H]([C@@H]1NC(=O)[C@@H](Cc2ccccc2)NC(=O)[C@@H]2CSC(=N2)c2csc(c3nc(c4nc([C@H](NC1=O)C)sc4)sc3)n2)C	271	Yes
511	Violapyrone Q	COc1cc(CCCC(C)C)oc(=O)c1C	272	No
512	Violapyrone R	COc1cc(CCCCC(C)C)oc(=O)c1C	272	Yes
513	Violapyrone T	CCC(CCCCc1cc(OC)c(c(=O)o1)C)C	272	No
514	CHEMBL3087380	COc1cc(CCCCC(O)(C)C)oc(=O)c1C	272	No
515	Violapyrone S	CCCCCCCc1cc(OC)c(c(=O)o1)C	272	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
516	Violapyrone H	CC(CCCCCc1cc(O)c(c(=O)o1)C)C	273	Yes
517	Violapyrone C	CC[C@@H](CCCCc1cc(O)c(c(=O)o1)C)C	273	No
518	Presuficidin A	CC(CCCCc1cc(O)c(c(=O)o1)C)C	273	No
519	Violapyrone I	CCCCCCCCc1cc(O)c(c(=O)o1)C	273	No
520	Violapyrone L	CC(C(CCCc1cc(O)c(c(=O)o1)C)O)C	273	No
521	Violapyrone M	CCC(CCCCc1cc(O)c(c(=O)o1)C)(O)C	273	No
522	CHEMBL3087386	Oc1cc(CCCCC(O)(C)C)oc(=O)c1C	273	No
523	Streptcytosine L	C[C@H]1O[C@H](CC[C@@H]1O)n1ccc(nc1=O)NC(=O)CC=C(C)C	274	Yes
524	40551-G	CCC(/C=C/C(=O)Nc1ccn(c(=O)n1)[C@H]1CC[C@@H]([C@H](O1)C)OC1C[C@H](O)[C@@H]([C@H](O1)C)N(C)C)C	275	Yes
525	Indolizomycin	C/C=C(/C=C/C=C/[C@H]1[C@@H]2C[C@@H]2[C@]2(N1CC[C@@H]1[C@H]2O1)O)\C	276	Yes
526	Cyclizidine G	OCC/C=C/C=C(/C[C@@H]1N2CCCC[C@@H]2[C@]([C@H]1O)(C)O)\C	277	Yes
527	Cyclizidine B	C/C(=C\[C@@H]1N2CCCC[C@@H]2[C@]([C@H]1O)(C)O)/C=C/C1CC1	278	Yes
528	Cyclizidine	C/C(=C\[C@@H]1N2CC[C@@H]3[C@H]([C@@H]2[C@]([C@H]1O)(C)O)O3)/C=C/C1CC1	278	No
529	19-Hydroxyl-24-methyl ester-N,N-dixiamycin	COC(=O)[C@]1(C)[C@@H](O)CC[C@]2([C@H]1CCc1c2cc2c(c1)n(c1c2cccc1)n1c2ccccc2c2c1cc1CC[C@@H]3[C@](c1c2)(C)CC[C@@H]([C@@]3(C)C(=O)O)O)C	279	Yes
530	Dixiamycin B	OC(=O)[C@]1(C)[C@@H](O)CC[C@]2([C@H]1CCc1c2cc2c(c1)n(c1c2cccc1)n1c2ccccc2c2c1cc1CC[C@@H]3[C@](c1c2)(C)CC[C@@H]([C@@]3(C)C(=O)O)O)C	279	No
531	Austradixanthone	OCc1cc(O)c2c(c1)oc1c(c2=O)c(C)cc(c1Oc1c(O)cc(c2c1oc1c(O)c(O)c(c(c1c2=O)OC)O)C)O	280	Yes
532	Cyanosporaside C	N#CCc1cc(Cl)c2c(c1)[C@@]1(OC3OC(C)C(C(=O)C3O)(C)OC(=O)C)[C@@H](O)C=CC1=C2	281	No
533	Cyanosporaside B	N#CCc1cc(Cl)c2c(c1)[C@@]1(OC3OC(C)C(C(=O)C3O)(C)O)[C@@H](O)C=CC1=C2	281	Yes
534	Cyanosporaside A	N#CCc1ccc2c(c1Cl)[C@@]1(OC3OC(C)C(C(=O)C3O)(C)O)[C@@H](O)C=CC1=C2	281	No
535	Cyanosporaside F	N#CCc1ccc2c(c1Cl)[C@@]1(O)[C@H](C=CC1=C2)OC1OC(C)C(CC1SCCNC(=O)C)O	282	Yes
536	Kobutimycin A	CC(=O)OC(C(/C=C\1/C=C(C2=NCCC3C12O3)C)OC(=O)C(C)C)C	283	Yes
537	Kobutimycin B	CCC(C(=O)OC(C(OC(=O)C)C)/C=C\1/C=C(C2=NCCC3C12O3)C)C	283	No
538	5OE+/-,10OE+/-,11-trihydroxyamorphan-3-one	O=C1C[C@H]2[C@@H]([C@@H]([C@H]1C)O)[C@H](CC[C@@]2(C)O)C(O)(C)C	284	Yes
539	5alpha,10alpha,11-Trihydroxyamorphan-3-one	O=C1C[C@H]2[C@@H]([C@@H](C1C)O)[C@H](CC[C@@]2(C)O)C(O)(C)C	284	No
540	(2alpha,4beta,5beta,7beta,10alpha)-2,5,11-Eudesmanetriol	O[C@H]1C[C@H](C)[C@@]2([C@](C1)(C)CC[C@H](C2)C(O)(C)C)O	284	No
541	(1alpha,4alpha,5beta,7alpha,10alpha)-1,5,11-Eudesmanetriol	C[C@@H]1CC[C@@H]([C@@]2([C@]1(O)C[C@H](CC2)C(O)(C)C)C)O	285	Yes
542	Fumonisin B2	CCCC[C@H]([C@H]([C@@H](OC(=O)C[C@H](C(=O)O)CC(=O)O)C[C@H](CCCCCC[C@H](C[C@@H]([C@@H](N)C)O)O)C)OC(=O)C[C@H](C(=O)O)CC(=O)O)C	286	Yes
543	Caerulomycin D	O/N=C/c1cc2OC3(O)C(Oc2c(n1)c1ccccn1)(C)OC(C(C3(C)O)(C)OC)(C)C	287	Yes
544	Heronamide E	C/C=C/C=C/C[C@H]1NC(=O)[C@H]2[C@H](C1)/C=C/C(=C/[C@@H]1[C@@H](/C(=C/C=C/2)/C)[C@H](O)[C@@H](C=C1)O)/C	288	Yes
545	Heronamide D	C/C=C/C=C/C[C@@H]1C[C@@H]([C@@H]2N1C(=O)[C@@H]1[C@H]2/C(=C/[C@H]2C=C[C@H]([C@H]([C@@H]2/C(=C/C=C\1)/C)O)O)/C)O	289	Yes
546	Ethyl iso-allocholate	CCOC(=O)CC[C@H]([C@H]1CC[C@@H]2[C@]1(C)[C@@H](O)C[C@H]1[C@H]2[C@H](O)C[C@H]2[C@]1(C)CC[C@H](C2)O)C	289	No
547	Antibiotic FR 900848	O=C1CCN(C(=O)N1)[C@@H]1O[C@@H]([C@H]([C@H]1O)O)CNC(=O)/C=C/C=C/[C@@H]1CC1C1CC1C1CC1C1C[C@H]1/C=C/[C@@H]1C[C@H]1C	290	Yes
548	3-Hydroxy-7-methoxy-K252c	COC1NC(=O)c2c1c1c(c3c2c2cc(O)ccc2[nH]3)[nH]c2c1cccc2	291	No
549	9-Hydroxy-K252c	Oc1ccc2c(c1)c1c3CNC(=O)c3c3c(c1[nH]2)[nH]c1c3cccc1	291	No
550	3-Hydroxy-K252c	Oc1ccc2c(c1)c1c3C(=O)NCc3c3c(c1[nH]2)[nH]c1c3cccc1	291	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
551	Staurosporine aglycone	O=C1NCc2c1c1c([nH]c3c1cccc3)c1c2c2ccccc2[nH]1	291	No
552	Arcyriaflavin A	O=c1[nH]c(=O)c2c1c1c3ccccc3[nH]c1c1c2c2ccccc2[nH]1	291	No
553	IDM F	O=C1N(C)[C@@](C2=C1[C@]1(C)c3ccccc3N([C@@H]1c1c2c2ccccc2[nH]1)C)(C)O	292	Yes
554	EM18	Oc1cc(=O)cc(o1)[C@H]1c2cccc(c2C(=O)C[C@@]1(C)O)O	293	Yes
555	Octoketide 4b	Oc1cc2OC(O)(Cc3oc(O)cc(=O)c3)CC(=O)c2c(c1)C	293	No
556	SEK34	O=c1cc(oc(c1)O)Cc1cccc2c1C(=O)CC(O2)(C)O	294	Yes
557	SEK34b	CC1CC(=O)c2c(O1)cccc2Cc1cc(=O)cc(o1)O	294	No
558	5,10-Dihydrophencomycin	COC(=O)c1cccc2c1[nH]c1cccc(c1[nH]2)C(=O)O	295	Yes
559	10T024A	OC(=O)Cn1c2cccc(c2[nH]c2c1cccc2)C(=O)O	295	No
560	Endophenazine C	CC(=CCc1cccc2c1[nH]c1c(cccc1n2C)C(=O)O)C	296	Yes
561	Endophenazine D	OC(=O)COC(=O)c1cccc2c1[nH]c1ccccc1[nH]2	296	No
562	Antartin	C[C@H]1C[C@H](C2=C(C([C@@H]3C[C@]12CC3)(C)C)C)Nc1ccccc1C(=O)O	297	Yes
563	Pravastatin	CC[C@@H](C(=O)O[C@H]1C[C@H](O)C=C2C1[C@@H](CC[C@H](C[C@H](CC(=O)O)O)O)[C@H](C=C2)C)C	298	Yes
564	Pulvomycin	COC1C(OC(C(/C=C/C=C/C=C/C(=O)C(C(C(C2C/C=C/C=C/C=C/C(O)C(=O)/C(=C\C=C/C(=C/C(/C(=C/CC(=O)O2)/C)O)/C)/C)C)O)C)O)C)OC(C(C1O)OC)C	299	Yes
565	FW-04-806	C[C@H]1C[C@@H](C)[C@H](Cc2cnco2)OC(=O)C(=C[C@H](C[C@H]([C@@H](OC(=O)C(=C1)C)Cc1cnco1)C)C)C	300	Yes
566	Conglobatin	C[C@@H]1C[C@H](C)[C@H](Cc2cnco2)OC(=O)/C(=C\[C@H](C[C@@H]([C@@H](OC(=O)/C(=C\1)/C)Cc1cnco1)C)C)/C	300	No
567	Cremimycin	CCCCCCC1CC(=O)CCCC(O)CC(=O)C2=C(O)C(CC2/C=C(/C=C/C=C/C(=O)N1)\C)OC1CC(OC)C(C(O1)C)O	301	Yes
568	Antibiotic WS5995A	COc1cc(C)cc2c1c1C(=O)c3cccc(c3C(=O)c1oc2=O)O	302	Yes
569	Antibiotic WS 5995B	COc1cc(C)cc(c1C1=CC(=O)c2c(C1=O)cccc2O)C(=O)O	302	No
570	Epothilone B	O=C1O[C@@H](CC2O[C@]2(C)CCC[C@@H]([C@@H]([C@H](C(=O)C([C@H](C1)O)(C)C)C)O)C)/C(=C/c1csc(n1)C)/C	303	Yes
571	Epothilone A	O=C1O[C@@H](C[C@@H]2O[C@@H]2CCC[C@@H]([C@@H]([C@H](C(=O)C([C@H](C1)O)(C)C)C)O)C)/C(=C/c1csc(n1)C)/C	303	No
572	Desoxyepothilone B	O=C1O[C@@H](C/C=C(/C)\CCC[C@@H]([C@@H]([C@H](C(=O)C([C@H](C1)O)(C)C)C)O)C)/C(=C/c1csc(n1)C)/C	304	Yes
573	Delaminomycin C	CCC(C(/C=C/C=C/C(CC1C=CC2C(C1(C)/C(=C/1\C(=O)CNC1=O)/O)C(C)CC(C2)C)O)C)O	305	Yes
574	Delaminomycin B	CCC(C(/C=C/C=C/C(CC1C=CC2C(C1(C)/C(=C\1/C(=O)NC(C1=O)OC)/O)C(C)CC(C2)C)O)C)O	305	No
575	Delaminomycin A	CCC(C(/C=C/C=C/C(CC1C=CC2C(C1(C)/C(=C\1/C(=O)NC(C1=O)O)/O)C(C)CC(C2)C)O)C)O	305	No
576	Actinoranone	COc1cc(OC)c2c(c1)[C@@H](CCC2=O)[C@@H](/C=C(/CC[C@@H]1C(=CC[C@H]2[C@@]1(C)CCCC2(C)C)C)\C)O	306	Yes
577	Distamycin	CC(COc1ccc(cc1Cn1nc(cc1C)NC(=O)c1ccc(cc1)CN1CCCC1)Cl)C	307	Yes
578	Physostigmine	CNC(=O)Oc1ccc2c(c1)[C@]1(C)CCN([C@@H]1N2C)C	308	Yes
579	FR-008-III	OC1CC(O)CC(=O)CCCC(=O)CC(=O)OC(C(CC(C(CC(=O)c2ccc(cc2)N)O)C)C)C(C)/C=C/C=C/C=C/C=C/C=C/C=C/C(CC2OC(CC(C1)O)(O)CC(O)C2C(=O)O)OC1O[C@H](C)[C@H]([C@@H]([C@@H]1O)N)O	309	Yes
580	CS103	OC1CC(=O)CCCC(O)CC(=O)OC(C(CC(C(CC(=O)c2ccc(cc2)N)O)C)C)C(C)/C=C/C=C/C=C/C=C/C=C/C=C/C(CC2OC(C(CC(C1)O)O)(O)CC(O)C2C)OC1O[C@H](C)[C@H]([C@@H]([C@@H]1O)N)O	310	Yes
581	Candicidin D	OC1CC(O)CC(=O)CCCC(=O)CC(=O)OC(C(CC(C(CC(=O)c2ccc(cc2)N)O)C)C)C(C)/C=C/C=C/C=C/C=C/C=C/C=C/C(CC(C(C(CC(=O)CC(C1)O)O)O)C(=O)O)O)O[C@@H]1OC(C)[C@H]([C@H](C1O)N)O	311	Yes
582	Trichomycin A	OC1CCCC(O)CC(O)CC2(O)CC(O)C(C(O2)CC(/C=C/C=C/C=C/C=C/C=C/C=C/C=C/C=C/C(C(OC(=O)CC(=O)CC(C1)O)C(CCC(CC(=O)c1ccc(cc1)N)O)C)C)O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@@H]1O)N)O)C(=O)O	312	Yes
583	(1S,3R,5Z,7Z,11S,13Z,15Z,17Z,19Z,21S,23R,24S,25R)-21-((3S,4R,5R,6S)-4-amino-tetrahydro-3,5-	C[C@H]1C/C=C/C=C/C=C/C=C/[C@H](C[C@H]2O[C@](C[C@@H](C/C=C/C=C/C(=O)O1)O)(O)C[C@H]([C@@H]2C)O)OC1O[C@@H](C)[C@@H]([C@H]([C@@H]1O)N)O	313	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	dihydroxy-6-methyl-2H-pyran-2-yloxy)-1,3,25-trihydroxy-11,24-dimethyl-10,27-dioxa-bicyclo[21.3.1]heptacosa-5,7,13,15,17,19-hexaen-9-one			
584	4,5-Desepoxy-12-decarboxy-12-methyl pimaricin	C[C@@H]1C/C=C/C=C/C=C/C=C/[C@@H](C[C@@H]2O[C@@](C[C@H](C/C=C/C=C/C(=O)O1)O)(O)C[C@@H]([C@H]2C)O)O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@@H]1O)N)O	313	Yes
585	2-Hydro-3-hydroxy-4,5-desepoxy-12-decarboxy-12-methyl pimaricin	O[C@H]1/C=C/C[C@H](O)C[C@]2(O)C[C@H](O)[C@H]([C@@H](O2)C[C@H](/C=C/C=C/C=C/C=C/C[C@H](OC(=O)C1)C)O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@@H]1O)N)O)C	313	No
586	(1S,3R,5Z,7S,11S,13Z,15Z,17Z,19Z,21S,23R,24S,25R)-21-((3S,4R,5R,6S)-4-amino-tetrahydro-3,5-dihydroxy-6-methyl-2H-pyran-2-yloxy)-1,3,7,25-tetrahydroxy-11,24-dimethyl-10,27-dioxa-bicyclo[21.3.1]heptacosa-5,13,15,17,19-pentaen-9-one	O[C@@H]1/C=C/C[C@@H](O)C[C@@]2(O)C[C@@H](O)[C@@H]([C@H](O2)C[C@@H](/C=C/C=C/C=C/C=C/C[C@@H](OC(=O)C1)C)OC1O[C@@H](C)[C@@H]([C@H]([C@@H]1O)N)O)C	313	No
587	2-Decarboxy-12-methyl pimaricin	C[C@@H]1C/C=C/C=C/C=C/C=C/C=C/[C@@H](C[C@@H]2O[C@@](C[C@H](C[C@@H]3[C@@H](/C=C/C(=O)O1)O3)O)(O)C[C@@H]([C@H]2C)O)O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@@H]1O)N)O	314	Yes
588	(1S,3R,5S,7S,8Z,12S,14Z,16Z,18Z,20Z,22S,24R,25S,26R)-22-{[(3S,4R,5R,6S)-4-amino-3,5-dihydroxy-6-methyloxan-2-yl]oxy}-1,3,26-trihydroxy-12,25-dimethyl-6,11,28-trioxatricyclo[22.3.1.0⁵,⁷]octacosa-8,14,16,18,20-pentaen-10-one	C[C@H]1C/C=C/C=C/C=C/C=C/[C@H](C[C@H]2O[C@](C[C@@H](C[C@H]3[C@H](/C=C/C(=O)O1)O3)O)(O)C[C@H]([C@@H]2C)O)OC1O[C@@H](C)[C@@H]([C@H]([C@@H]1O)N)O	314	No
589	4,5-de-Epoxynatamycin	CC1CCCCCCCCCC(OC2O[C@H](C)[C@H]([C@@H]([C@H]2O)N)O)CC2CC(CC(CCCCCC(=O)O1)O)(O)CC(C2C(=O)O)O	315	Yes
590	Rimocidin B	CCCC1C/C=C/C=C\C=C\C=C/C(OC2O[C@H](C)[C@H]([C@@H]([C@@H]2O)N)O)CC2OC(CC(CCC(=O)CC(C(C(=O)O1)CC)O)O)(O)CC(C2C(=O)N)O	316	Yes
591	Pyrisulfoxin A	COSc1c(OC)cc(nc1/C=N/O)c1ccccn1	317	Yes
592	Coprismycin B	O/N=C\c1nc(cc(c1SC)OC)c1ccccc1	317	No
593	Caerulomycin B	O/N=C/c1cc(OC)c(c(n1)c1ccccn1)O	317	No
594	Tuberine	OC(C1(C)CCC(O1)C(OC(=O)C)(C)C)COc1ccc(cc1)CCNC(=O)c1ccccc1	318	Yes
595	CHEMBL91194	CCCCC1=C(C)C(=O)[C@](C1=O)(C)CN1c2ccccc2[C@]2(C1OCC2)O	319	Yes
596	Piperazinomycin	Oc1ccc2cc1Oc1ccc(cc1)CC1NCC(C2)NC1	320	Yes
597	Argimycins PII	C/C(=C/C=C\1/C=Cc2c1cccn2)/SC[C@H](C(=O)O)NC(=O)C	321	Yes
598	Argimycin PI	C/C(=C\C=C/1\C=Cc2c1cccn2)/SC[C@@H](C(=O)O)NC(=O)C	321	No
599	C09245	Clc1ccc2c(c1)[nH]c1c2cc(s1)C(=O)N	322	Yes
600	Albocycline D	O=C1/C=C/[C@](C)(O)/C=C/[C@H](O)C(=C)C(CC[C@@H]([C@H](O1)C)C)O	323	No
601	Albocycline B	O=C1O[C@H](C)[C@@H](C)CC/C=C(/[C@H](/C=C/[C@@](C(C1)O)(C)O)O)\C	323	No
602	2,3-Dihydrocineromycin B	O=C1CC[C@](C)(O)/C=C/[C@H](O)/C(=C/CC[C@@H]([C@H](O1)C)C)/C	323	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
603	Oxycineromycin B	OCC1=CCCC(C)C(C)OC(=O)CCC(C=CC1O)(C)O	323	No
604	Cineromycin B	O=C1/C=C\[C@](C)(O)/C=C\[C@H](O)/C(=C\CC[C@@H]([C@H](O1)C)C)/C	323	No
605	7-O-Demethylalbocycline	O=C1/C=C/[C@](C)(O)/C=C/[C@H](O)/C(=C/CC[C@@H]([C@H](O1)C)C)/C	323	Yes
606	Platensimycin B4	OCC1OC(Oc2ccc(c(c2NC(=O)CCC(C(=O)/C=C\[C@]23C[C@H]4[C@@](C2)(C)O[C@H](C3C)C4)(C)C)O)C(=O)O)C(C(C1O)O)O	324	No
607	Platencin A14	OCC1OC(Oc2ccc(c(c2NC(=O)CCC(C(=O)/C=C\C23CCC(C(=C)C2)C[C@H]3O)(C)C)O)CO)C(C(C1O)O)O	324	Yes
608	Platencin A13	OCC1OC(Oc2ccc(c(c2NC(=O)CCC(C(=O)CCC23CCC(CC2)C(=C)C3)(C)C)O)CO)C(C(C1O)O)O	324	No
609	Platencin A9	OCC1OC(Oc2ccc(c(c2NC(=O)CCC(C(=O)/C=C\C23CCC(C(=C)C2)CC3O)(C)C)O)C(=O)SC)C(C(C1O)O)O	324	No
610	Platencin A10	OCC1OC(Oc2ccc(c(c2NC(=O)CCC(C(=O)/C=C\C23CCC(C(=C)C2)CC3O)(C)C)O)C(=O)OC)C(C(C1O)O)O	324	No
611	Platencin A15	OCC1OC(Oc2ccc(c(c2NC(=O)CCC(C(=O)/C=C\C23CCC(CC2)C(=C)[C@@H]3O)(C)C)O)CO)C(C(C1O)O)O	324	No
612	3-[2,5'-Diethyl-5'-(1-hydroxyethyl)-4-methyl-[2,2'-bioxolan]-5-yl]-6-hydroxy-9-(3-hydroxy-2-{4-[(methoxymethyl)amino]butanoyl}-4-methylphenyl)-5,7-dimethylnonan-4-one	COCNCCCC(=O)c1c(CCC(C(C(C(=O)C(C2OC(CC2C)(CC)C2CCC(O2)(CC)C(O)C)CC)C)O)C)ccc(c1O)C	325	No
613	iso-Lasalocid	CCC(C(=O)C(C(C(CCc1ccc(c(c1C(=O)O)O)C)C)O)C)C1OC(CC1C)(CC)C1CCC(O1)(CC)CC(O)C	325	No
614	Isolasalocid A	CC[C@@H](C(=O)[C@H]([C@H]([C@@H](CCc1ccc(c(c1C(=O)O)O)C)C)O)C)C1O[C@](C[C@@H]1C)(CC)C1CC[C@@](O1)(CC)[C@H](O)C	325	No
615	Lasalocid	CC[C@H](C(=O)[C@H]([C@H]([C@@H](CCc1ccc(c(c1C(=O)O)O)C)C)O)C)C1O[C@](C[C@@H]1C)(CC)C1CC[C@](C[C@@H](O1)C)(O)CC	325	No
616	Acetamide, N-[15-[2,5'-diethyloctahydro-5'-(1-hydroxyethyl)-4-methyl[2,2'-bifuran]-5-yl]-6,12-dihydroxy-11,13-dimethyl-4,8,14-trioxoheptadecyl]-	CNCCCC(=O)C(C(CC(=O)CCC(C(C(C(=O)C(C1OC(CC1C)(CC)C1CCC(O1)(CC)C(O)C)CC)C)O)C)O)C	325	No
617	Acetamide, N-[15-[5-ethyl-5-(5-ethyltetrahydro-5-hydroxy-6-methyl-2H-pyran-2-yl)tetrahydro-3-methyl-2-furanyl]-6,12-dihydroxy-11,13-dimethyl-4,8,14-trioxoheptadecyl]-	CCC(C1OC(CC1C)(CC)C1CCC(C(O1)C)(O)CC)C(=O)C(C(C(CCC(=O)CC(CC(=O)CCCNC(=O)C)O)C)O)C	325	No
618	Acetamide, N-[15-[5-ethyl-5-(5-ethyltetrahydro-5-hydroxy-6-methyl-2H-pyran-2-yl)tetrahydro-3-methyl-2-furanyl]-6,12-dihydroxy-5,11,13-trimethyl-4,8,14-trioxoheptadecyl]-	CCC(C1OC(CC1C)(CC)C1CCC(C(O1)C)(O)CC)C(=O)C(C(C(CCC(=O)CC(C(C(=O)CCCNC(=O)C)C)O)C)O)C	325	No
619	Acetamide, N-[4-[6-[7-[5-ethyl-5-(5-ethyltetrahydro-5-hydroxy-6-methyl-2H-pyran-2-yl)tetrahydro-3-methyl-2-furanyl]-4-hydroxy-3,5-dimethyl-6-oxononyl]-2-hydroxy-3-methylphenyl]-4-oxobutyl]-	CCC(C1OC(CC1C)(CC)C1CCC(C(O1)C)(O)CC)C(=O)C(C(C(CCc1ccc(c(c1C(=O)CCCNC(=O)C)O)C)C)O)C	325	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
620	Ansalactam A	CC(C[C@H]1C(=O)N[C@]23[C@@H]1[C@@H](C)C(=O)/C(=C/[C@H](C)/C=C(/C)\C=C(\C(=O)c1c(C(=O)C2)c(C3=O)cc(c1O)C)/C)/C)C	326	Yes
621	10-Deoxymethynolide	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@@H](C)C[C@H](C(=O)/C=C/[C@H]1C)C	327	Yes
622	3-Dehydro-10-deoxymethynolide	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@@H](C)C[C@H](C(=O)/C=C/[C@H]1C)C	327	No
623	Narbonolide	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O)[C@H](C[C@H](C(=O)/C=C/[C@H]1C)C)C	328	Yes
624	Dihydronarbonolide	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O)[C@H](C[C@H]([C@@H](/C=C/[C@H]1C)O)C)C	329	Yes
625	12-Deoxo-12-hydroxy-8-Omethyltetrangomycin	O=C1C[C@](C)(O)Cc2c1c1c(cc2)C(=O)c2c(C1O)cccc2O	330	No
626	2-[5-Hydroxy-1-(1-hydroxyethyl)-3-methyl-4,9-dioxobenzo[f]isoindol-2-yl]benzoic acid	CC(c1c2C(=O)c3cccc(c3C(=O)c2c(n1c1ccccc1C(=O)O)C)O)O	330	Yes
627	Bhimamycin H	CC(c1c2C(=O)c3cccc(c3C(=O)c2c(n1c1ccc(cc1)C(=O)O)C)O)O	330	No
628	Cangumycin C	C[C@@H]1CC(=O)C2=C(C1)CC[C@]13[C@]2(O1)C(=O)c1cccc(c1[C@@H]3O)O	331	Yes
629	SM 196A	COc1cccc2c1C(O)c1ccc3c(c1C2=O)C(O)CC(C3)(C)O	332	Yes
630	CHEMBL556717	N#Cc1ccc(cc1)C(=O)NCC[C@H](c1ccc(cc1)S(=O)(=O)C)c1ccc(cc1)F	333	Yes
631	Kendomycin	C[C@H]1CCC2OC([C@@H]([C@H]([C@H]2C)O)C)C2=C(O)C(=O)C(=C3C2=C[C@@]([C@H](C[C@@H](C/C(=C/1)/C)C)C)(O)O3)C	334	Yes
632	Makinolide B	COC1/C=C/C=C(\C)/CC(C)C(O)C(/C=C(/C=C(/C(=O)OC1C(C(C(C(=O)/C=C/C(C(C(C)C)O)C)C)O)C)\C)\C)C	335	Yes
633	Oxohygrolidin	CC[C@H]([C@@H](/C=C/C(=O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C(=C/C(=C/[C@@H](C)[C@H]([C@H](C/C(=C/C=C/[C@@H]1OC)/C)C)O)/C)/C)C)O)C)C)O	335	No
634	PD 118576	COC1/C=C/C=C(\C)/CC(C)C(O)C(/C=C(/C=C(\C(=O)OC1C(C(C(C(=O)/C=C/C(C(O)C)C)C)O)C)/OC)\C)C	336	No
635	23-O-Butyrylbafilomycin D	CCCC(=O)O[C@@H]([C@H](/C=C/C(=O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C(=C/C(=C/[C@@H](C)[C@H]([C@@H](C/C(=C/C=C/[C@@H]1OC)/C)C)O)/C)/OC)C)O)C)C(C)C	336	No
636	21,22-en-Bafilomycin D	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)O[C@@H]1[C@H]([C@H]([C@@H](C(=O)C/C=C(/[C@@H](C(C)C)O)\C)C)O)C)\OC)\C)C	336	No
637	Bafilomycin D	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@H](O)[C@@H](/C=C(/C=C(\C(=O)OC1[C@H]([C@H]([C@@H](C(=O)/C=C/[C@@H]([C@@H](C(C)C)O)C)C)O)C)/OC)\C)C	336	No
638	21,22-en-9-Hydroxybafilomycin D	CO[C@H]1/C=C/C=C(\C)/[C@@H](O)[C@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)O[C@@H]1[C@H]([C@H]([C@@H](C(=O)C/C=C(/[C@@H](C(C)C)O)\C)C)O)C)\OC)\C)C	336	No
639	9-Hydroxybafilomycin D	CO[C@H]1/C=C/C=C(\C)/C(O)[C@H](C)[C@@H](O)[C@@H](/C=C(/C=C(\C(=O)O[C@@H]1[C@H]([C@H]([C@@H](C(=O)/C=C/[C@@H]([C@@H](C(C)C)O)C)C)O)C)/OC)\C)C	336	No
640	Concanamycin G	C/C=C/C(C(/C=C/C(=O)[C@H]([C@@H]([C@@H](C1OC(=O)/C(=C\C(=C/[C@@H](C)[C@@H](O)[C@H]([C@H]([C@@H](C/C(=C\C=C/[C@@H]1OC)/C)C)O)C)\C)/OC)C)O)C)C)O	336	No
641	Bafiomycin A2	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@@H](O)[C@@H](/C=C(/C=C(\C(=O)OC1[C@H]([C@H]([C@@H]([C@]1(O)C[C@H](O)[C@H]([C@@H](O1)C(C)C)C)C)O)C)/OC)\C)C	336	No
642	Bafilomycin	CO[C@H]1C=C/C=C(/C)\C[C@@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)O[C@@H]1[C@H]([C@H]([C@@H]([C@@]1(O)C[C@@H](O)[C@@H]([C@H](O1)C(C)C)C)C)O)C)\OC)\C)C	336	Yes
643	24-Demethylbafilomycin A2	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)O[C@@H]1[C@H]([C@H]([C@@H]([C@@]1(OC)C[C@@H](O)[C@@H]([C@H](O1)CC)C)C)O)C)\OC)\C)C	336	No
644	Bafilomycin A2	COC1/C=C/C=C(\C)/CC(C)C(O)C(/C=C(/C=C(/C(=O)OC1C(C(C(C1(OC)CC(O)C(C(O1)C(C)C)C)C)O)C)\OC)\C)C	336	No
645	21-Deoxybafilomycin A1	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)O[C@@H]1[C@H]([C@H]([C@@H]([C@@]1(O)CC[C@@H]([C@H](O1)C(C)C)C)C)O)C)\OC)\C)C	336	No
646	21-Deoxybafilomycin A2	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)O[C@@H]1[C@H]([C@H]([C@@H]([C@@]1(OC)CC[C@@H]([C@H](O1)C(C)C)C)C)O)C)\OC)\C)C	336	No
647	Bafilomycin G	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)O[C@@H]1[C@H]([C@H]([C@@H]([C@@]1(O)C[C@@H](OC)[C@@H]([C@H](O1)C(C)C)C)C)O)C)\OC)\C)C	336	No
648	Bafilomycin A1	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)OC1[C@H]([C@H]([C@@H]([C@@]1(O)C[C@@H](O)[C@@H]([C@H](O1)C(C)C)C)C)O)C)\OC)\C)C	336	No
649	Bafiomycin C1	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@@H](O)[C@@H](/C=C(/C=C(\C(=O)OC1[C@H]([C@H]([C@@H]([C@]1(OC)C[C@H](O)[C@H]([C@@H](O1)C(C)C)C)C)O)C)/OC)\C)C	336	No
650	Bafilomycin L (BFL)	COC1/C=C/C=C(\C)/C[C@@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)OC1/C(=C/C(C1=CC=C(C(O1)C(C)C)C)C)/C)\C)\C)C	337	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
651	24-Demethylbafilomycin Z	CO[C@H]1/C=C/C=C(\C)/C[C@H](C)[C@H](O)[C@@H](/C=C(/C=C(/C(=O)O[C@@H]1[C@H](/C=C(/C1=CC=C([C@H](O1)CC)C)\C)C)\OC)\C)C	338	Yes
652	Benthocyanin C	N#C/C(=c\1/cc2n(C/C=C(/CCC=C(C)C)\C)c3ccccc3[nH]c2c(c1=O)C(=O)O)/c1ccccc1	339	Yes
653	Sespenine	O=C1CC2[C@@]3(C)CC[C@@H]([C@@]([C@@H]3CC[C@@]32C[C@H]1Nc1c3cccc1)(C)C(=O)O)O	340	No
654	Indosespene	C=C1CC[C@@H]2[C@]([C@H]1Cc1c[nH]c3c1cccc3)(C)CC[C@@H]([C@@]2(C)C(=O)O)O	340	Yes
655	Indosespenol	OC[C@]1(C)[C@@H](O)CC[C@]2([C@H]1CCC(=C)[C@@H]2Cc1c[nH]c2c1cccc2)C	340	No
656	Prexiamycin	O[C@H]1CC[C@]2([C@H]([C@]1(C)C(=O)O)CCC1=C2Cc2c(C1)[nH]c1c2cccc1)C	340	No
657	Salinazinone B	CC(=Cc1nc(cc(=O)o1)N1[C@@H](C)CCC1=O)C	341	Yes
658	Mycemycin B	COC(=O)c1cccc2c1NC(=O)c1c(O2)ccc(c1)Cl	342	Yes
659	Mycemycin A	COC(=O)c1cccc2c1NC(=O)c1c(O2)cccc1	342	No
660	Mycemycin H	O=C1Nc2c(cc(c(c2Oc2c1cccc2)C)Cl)C(=O)C	343	Yes
661	Mycemycin D	O=C1Nc2c(cc(c(c2Oc2c1cccc2)C)Cl)C(=O)N	343	No
662	Mycemycin E	Clc1ccc2c(c1)C(=O)Nc1c(O2)c(C)c(cc1C(=O)N)Cl	344	Yes
663	Mycemycin F	O=Cc1cc(Cl)c(c2c1NC(=O)c1c(O2)ccc(c1)Cl)C	344	No
664	Mycemycin C	COC(=O)c1cc(Cl)c(c2c1NC(=O)c1c(O2)ccc(c1)Cl)C	344	No
665	19-Methoxyxiamycin	COC1C[C@H]2[C@](C)(C(=O)O)[C@@H](O)CC[C@@]2(c2c1cc1[nH]c3c(c1c2)cccc3)C	345	No
666	19-Carbonylxiamycin	O[C@H]1CC[C@]2([C@H]([C@]1(C)C(=O)O)CC(=O)c1c2cc2c(c1)[nH]c1c2cccc1)C	345	No
667	Xiamycin C	O[C@H]1CC[C@]2([C@H]([C@]1(C)C(=O)O)C[C@@H](c1c2cc2c(c1)[nH]c1c2cccc1)O)C	345	No
668	Xiamycin A	O[C@H]1CC[C@]2([C@H]([C@]1(C)C(=O)O)CCc1c2cc2c(c1)[nH]c1c2cccc1)C	345	No
669	Oridamycin A	O[C@H]1CC[C@]2(C([C@@]1(C)C(=O)O)CCc1c2cc2c(c1)[nH]c1c2cccc1)C	345	No
670	Chloroxiamycin	O[C@H]1CC[C@]2([C@H]([C@]1(C)C(=O)O)CCc1c2cc2c(c1Cl)[nH]c1c2cccc1)C	345	Yes
671	Xiamycin E	COC(=O)[C@]1(C)[C@@H](O)CC[C@]2([C@H]1CC(=O)c1c2cc2c(c1)[nH]c1c2cccc1)C	345	No
672	Xiamycin D	COC(=O)[C@]1(C)[C@@H](O)CC[C@]2([C@H]1C[C@H](O)c1c2cc2c(c1)[nH]c1c2cccc1)C	345	No
673	Oxiamycin	OC(=O)[C@]1(C)[C@@H](O)CC[C@]2([C@H]1CCc1c(O2)cc2c(c1)[nH]c1c2cccc1)C	345	No
674	Flazin, methyl ester	OCc1ccc(o1)c1nc(cc2c1[nH]c1c2cccc1)C(=O)OC	346	Yes
675	Perlolyrine	OCc1ccc(o1)c1nccc2c1[nH]c1c2cccc1	346	No
676	(3R)-3,7-Dihydroxy-8-[2-(hydroxymethyl)-3-methoxybenzoyl]-3-methyl-1,2,3,4-tetrahydronaphthalen-1-one	COc1cccc(c1CO)C(=O)c1c(O)ccc2c1C(=O)C[C@](C2)(C)O	347	No
677	Elmenol C	CO[C@H]1O[C@H](c2c1c(OC)ccc2)c1c(O)ccc2c1C(=O)CC(C2)(C)O	347	No
678	Elmenol D	CO[C@@H]1O[C@H](c2c1c(OC)ccc2)c1c(O)ccc2c1C(=O)CC(C2)(C)O	347	Yes
679	Cangumycin F	OCc1c(O)cccc1C(=O)c1c(O)c(O)cc2c1C(=O)C[C@H](C2)C	348	Yes
680	Cangumycin E	OCc1c(O)cccc1C(=O)c1c(O)ccc2c1C(=O)C[C@H](C2)C	348	No
681	Tirandamycin C	C/C(=C\[C@H]([C@H]1O[C@@]2(C)O[C@@H]([C@@H]1C)CC=C2C)C)/C=C/C(=C\1/C(=O)CNC1=O)/O	349	No
682	Tirandamycin A	C/C(=C\[C@H]([C@H]1O[C@@]2(C)O[C@@H]([C@@H]1C)C(=O)[C@H]1[C@]2(C)O1)C)/C=C/C(=C\1/C(=O)CNC1=O)/O	349	No
683	Tirandamycin L	C/C(=C\[C@H]([C@H]1O[C@]2(C)O[C@H]([C@@H]1C)C(=O)C[C@H]2C)C)/C=C/C(=C\1/C(=O)CNC1=O)/O	349	Yes
684	octa-Valinomycin	CC1OC(=O)C(NC(=O)C(OC(=O)C(NC(=O)C(OC(=O)C(NC(=O)C(OC(=O)C(NC1=O)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C	350	Yes
685	Valinomycin	C[C@@H]1OC(=O)[C@H](NC(=O)[C@H](OC(=O)[C@@H](NC(=O)[C@H](C)OC(=O)[C@H](NC(=O)[C@H](OC(=O)[C@@H](NC(=O)[C@@H](OC(=O)[C@H](NC(=O)[C@H](OC(=O)[C@@H](NC1=O)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C	351	Yes
686	Carbazomycin G	COC1=C(C)C(c2c(C1=O)c1ccccc1[nH]2)(C)O	352	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
687	Carbazomycin H	COc1ccc2c(c1)c1C(=O)C(=C(C(c1[nH]2)(C)O)C)OC	352	No
688	Ansaseomycin A	CC(C/C/1=C\[C@@H]2C=C[C@H]3[C@]4([C@@H]2C(=O)c2c(C(=O)[C@@H](C=C[C@H]([C@@H](C1=O)C)O)C)c(O)c(c(c2C4=O)O)C)NC(=O)C3)C	353	Yes
689	Ansaseomycin B	CC(C/C/1=C\[C@@H]2C=C[C@H]3[C@]4([C@@H]2C(=O)c2c(C(=O)/C(=C/C[C@H]([C@@H](C1=O)C)O)/C)c(O)c(c(c2C4=O)O)C)NC(=O)C3)C	353	No
690	Mohangic acid E	OC[C@H]1O[C@@H](Nc2ccc(cc2)C(=O)C[C@H]([C@@H](C[C@H]([C@@H]([C@@H](/C=C/C=C/C=C/[C@@H](CC(=O)O)O)C)O)C)C)O)[C@@H]([C@H]([C@@H]1O)O)O	354	Yes
691	Hydrazidomycin D	CCCCCC/C=C\CCCCCCCCCC(=O)N(NC(=O)C)CCCCCC	355	Yes
692	Elaiomycin B	CCCCCCCC/C=C/CCCC/C=C\N(C(=O)CCCCCCCCC)NC(=O)COC	356	No
693	Hydrazidomycin A	CCCCCCCCCCCC/C=C\N(C(=O)CCCCCCCCC)NC(=O)COC	356	No
694	Elaiomycin C	CCCCCCCCCC(=O)N(NC(=O)COC)/C=C\CCCC/C=C/C/C=C/CCCCC	356	Yes
695	CP 78545	C=CCC(/C=C(/C(C(/C=C/CCC(C(C(C(C(C(C1OC(CCC1C)C(C(=O)O)C)C)O)C)O)C)O)C)O)\C)C	357	Yes
696	Nahuoic acid B	O[C@@H](C[C@@H]([C@H]([C@@H](C(C)C)O)C)O)C/C=C(/[C@H]1C(=C[C@@]2([C@H]([C@@H]1/C=C(/C(=O)O)\C)[C@H](C)[C@H]([C@H](C2)O)O)C)C)\C	358	No
697	Nahuoic acid A	O[C@H](C[C@H]([C@@H]([C@H](C(C)C)O)C)O)C/C=C(/[C@@H]1C(=C[C@]2([C@@H]([C@H]1/C=C(/C(=O)O)\C)[C@@H](C)[C@@H](C[C@H]2O)O)C)C)\C	358	No
698	Nahuoic acid C	O[C@@H](C[C@@H]([C@H]([C@@H](C(C)C)O)C)O)C/C=C(/[C@H]1C(=C[C@@]2([C@H]([C@@H]1/C=C(/C(=O)O)\C)[C@H](C)[C@H]([C@H]([C@@H]2O)O)O)C)C)\C	358	No
699	Nahuoic acid D	O[C@@H](C[C@@H](C[C@@H](C([C@H](C(C)C)O)C)O)O)C/C=C(/[C@H]1C(=C[C@@]2([C@H]([C@@H]1/C=C(/C(=O)O)\C)[C@H](C)[C@H]([C@H](C2)O)O)C)C)\C	358	No
700	Nahuoic acid E	O[C@@H](C[C@@H](C[C@@H](C([C@H](C(C)C)O)C)O)O)C/C=C(/[C@H]1C(=C[C@@]2([C@H]([C@@H]1/C=C(/C(=O)O)\C)[C@H](C)[C@H](C[C@H]2O)O)C)C)\C	358	Yes
701	Derivative	CCN(c1ccc2c(c1)oc(=O)c(c2)c1nnc(s1)c1ccccc1)CC	359	Yes
702	Antarlide B	C[C@H]1/C=C/C=C(\C)/[C@H](O)C/C=C\C=C\C=C/C=C(/C(=O)O[C@@H](C[C@H](CC1)O)[C@H]([C@H](c1cccc(c1)O)O)C)\C	360	No
703	Antarlide A	C[C@H]1/C=C/C=C(\C)/[C@H](O)C/C=C/C=C/C=C/C=C(/C(=O)O[C@@H](C[C@H](CC1)O)[C@H]([C@H](c1cccc(c1)O)O)C)\C	360	No
704	Antarlide G	C[C@H]1/C=C/C=C(\C)/[C@@H](O)C/C=C/C=C/C=C\C=C(\C(=O)OC(CC1)CC([C@@H]([C@H](c1ccc(c1)O)O)C)O)/C	360	No
705	Antarlide H	C[C@H]1/C=C/C=C(\C)/[C@@H](O)C/C=C/C=C\C=C\C=C(\C(=O)OC(CC1)CC([C@@H]([C@H](c1ccc(c1)O)O)C)O)/C	360	Yes
706	Antarlide E	C[C@H]1/C=C/C=C(\C)/[C@H](O)C/C=C/C=C/C=C\C=C(\C(=O)O[C@@H](C[C@H](CC1)O)[C@H]([C@H](c1cccc(c1)O)O)C)/C	361	Yes
707	Antarlide D	C[C@H]1/C=C/C=C(\C)/[C@H](O)C/C=C/C=C\C=C\C=C(\C(=O)O[C@@H](C[C@H](CC1)O)[C@H]([C@H](c1cccc(c1)O)O)C)/C	361	No
708	Antarlide F	C[C@H]1/C=C/C=C(\C)/[C@@H](O)C/C=C/C=C/C=C/C=C(\C(=O)O[C@@H](C[C@H](CC1)O)[C@@H]([C@H](c1cccc(c1)O)O)C)/C	361	No
709	Antarlide C	C[C@H]1/C=C/C=C(\C)/[C@H](O)C/C=C\C=C/C=C/C=C(/C(=O)O[C@@H](C[C@H](CC1)O)[C@H]([C@H](c1cccc(c1)O)O)C)\C	361	No
710	Methylsulochrin	COc1cc(OC)c(c(c1)C(=O)OC)C(=O)c1c(O)cc(cc1O)C	362	Yes
711	Metatricycloene	NC(=O)/C=C/C=C/C1C=CC2C3C1C(/C=C/C=C/C=C/C=C/C(=O)O)OC3C=C2	363	Yes
712	Alpiniamide C	C[C@@H](C(=O)NCC(=O)/C(=C/C(C(=O)O)C)/C)[C@H](/C(=C/CC)/C)O	364	Yes
713	L-Isoleucine, N-[[(1S,3aS,6R,7aS)-6-ethyl-2,3,3a,6,7,7a-hexahydro-1-hydroxy-1H-inden-4-yl]carbonyl]-	CC[C@@H]([C@@H](C(=O)O)NC(=O)C1=C[C@H](CC)C[C@H]2[C@@H]1CC[C@@H]2O)C	365	Yes
714	L-Isoleucine, N-[[(1R,3aS,6R,7aS)-6-ethyl-2,3,3a,6,7,7a-hexahydro-1-hydroxy-1H-inden-4-yl]carbonyl]-	CC[C@@H]([C@@H](C(=O)O)NC(=O)C1=C[C@H](CC)C[C@H]2[C@@H]1CC[C@H]2O)C	365	No
715	Coronatine	CC[C@H]1C=C(C(=O)N[C@]2(C[C@@H]2CC)C(=O)O)[C@@H]2[C@H](C1)C(=O)CC2	365	No
716	3-[(2E,8E,10E,16E,18E)-14-Ethyl-7,13-dihydroxy-2,16,18-	CCC(C(C/C=C/C=C/C(CCC/C=C(/C(=O)C1=C(O)C(NC1=O)CO)\C)O)O)C/C(=C/C(=C/C)/C)/C	366	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	trimethylicosa-2,8,10,16,18-pentaenoyl]-4-hydroxy-5-(hydroxymethyl)-2,5-dihydro-1H-pyrrol-2-one			
717	{4-[(2E,8E,10E,16E,18E)-14-Ethyl-7,13-dihydroxy-2,16,18-trimethylicosa-2,8,10,16,18-pentaenoyl]-3-hydroxy-5-oxo-2,5-dihydro-1H-pyrrol-2-yl}methyl acetate	CCC(C(C/C=C/C=C/C(CCC/C=C(/C(=O)C1=C(O)C(NC1=O)COC(=O)C)\C)O)O)C/C(=C/C(=C/C)/C)/C	366	No
718	3-[(2Z,7S,8E,10E,13R,14R,16E,18E)-14-Ethyl-7,13-dihydroxy-2,16,18-trimethylicosa-2,8,10,16,18-pentaenoyl]-4-hydroxy-5-methylidenepyrrolidin-2-one	CC[C@@H]([C@@H](C/C=C/C=C/[C@H](CCC/C=C(\C(=O)C1C(=O)NC(=C)C1O)/C)O)O)C/C(=C/C(=C/C)/C)/C	366	No
719	MX-1	O=Cc1cc(O)c2c(c1C(=O)O)OC1(C2)C(C)CCC2C1(C)CC(O)C(C2(C)C)O	367	Yes
720	SF2768 analogue 2	CC(CC(=O)NCC1CCC(C(O1)O)NC(=O)CC(C)C)C	368	Yes
721	Actinoquinoline A	OC[C@@H](NC(=O)c1nc2ccccc2cc1O)CC[C@H](CNC(=O)CC(C)C)O	369	Yes
722	Actinoquinoline B	CC(CC(=O)NC[C@H]1CC[C@@H]([C@@H](O1)O)NC(=O)c1nc2ccccc2cc1O)C	369	No
723	Chimonanthine	CN1CC[C@@]2([C@H]1Nc1c2cccc1)[C@@]12CCN([C@@H]1Nc1c2cccc1)C	370	Yes
724	Furaquinocin J	COC1=C(C)C(=O)c2c(C1=O)cc(c1c2O[C@@H]([C@]1(C)[C@@H](C/C=C(/C(=O)N)\C)O)C)O	371	No
725	Furaquinocin I	COC1=C(C)C(=O)c2c(C1=O)cc(c1c2O[C@@H]([C@]1(C)[C@@H](C/C=C(/C(=O)O)\C)O)C)O	371	No
726	Fumaquinone	COC1=C(C)C(=O)c2c(C1=O)cc(c(c2O)CC=C(C)C)O	371	No
727	Furaquinocin E	OC/C(=C/C=C/C1(C)C(C)Oc2c1c(O)cc1c2C(=O)C(=C(C1=O)OC)C)/C	371	No
728	Furaquinocin G	COC1=C(C)C(=O)c2c(C1=O)cc(c1c2OC(C1(C)C1CC=C(C(O1)O)C)C)O	371	No
729	Furaquinocin C	COC1=C(C)C(=O)c2c(C1=O)cc(c1c2OC(C1(C)CCC=C(C)C)C)O	371	No
730	NSC647943	COC1=C(C)C(=O)c2c(C1=O)cc1c(c2O)C(C(O1)C)(C)CCC=C(C)C	371	No
731	Furaquinocin H	OCC(=CCC(C1(C)C(C)Oc2c1c(O)cc1c2C(=O)C(=C(C1=O)OC)C)O)CO	371	No
732	Furaquinocin F	OC/C(=C/CCC1(C)C(C)Oc2c1c(O)cc1c2C(=O)C(=C(C1=O)OC)C)/C	371	No
733	Furaquinocin A	OC/C(=C/CC(C1(C)C(C)Oc2c1c(O)cc1c2C(=O)C(=C(C1=O)OC)C)O)/C	371	No
734	Furaquinocin D	COC1=C(C)C(=O)c2c(C1=O)cc(c1c2O[C@@H]([C@]1(C)[C@@H](CC=C(C)C)O)C)O	371	Yes
735	CHEMBL3092696	COC1=CC(=O)c2c(C1=O)cc(c1c2O[C@@H]([C@@]1(C)CCC1C(=C)CCCC1(C)C)C)O	371	No
736	CHEMBL3092699	OC[C@H]1Oc2c([C@@]1(C)CCC1C(=C)CCCC1(C)C)c(O)cc1c2C(=O)C=C(C1=O)OC	371	No
737	CHEMBL3092698	OC[C@H]1Oc2c([C@]1(C)CCC1C(=C)CCCC1(C)C)c(O)cc1c2C(=O)C=C(C1=O)OC	371	No
738	CHEMBL3092697	COC1=CC(=O)c2c(C1=O)cc(c1c2O[C@@H]([C@]1(C)CCC1C(=C)CCCC1(C)C)C)O	371	No
739	JBIR-136	CO[C@@H]1CC(=O)c2c([C@H]1O)cc(c1c2O[C@@H]([C@]1(C)[C@@H](CC=C(C)C)O)C)O	372	Yes
740	Actinonin	CCCCC[C@@H](C(=O)N[C@H](C(=O)N1CCC[C@H]1CO)C(C)C)CC(=O)NO	373	Yes
741	LL-Z 1272d	O=Cc1c(O)c(C/C=C(/CC[C@@]2(C)[C@H](C)CCC(=O)[C@@H]2C)\C)c(c(c1C)Cl)O	374	Yes
742	Ascochlorin	O=Cc1c(O)c(C/C=C(/C=C/[C@@]2(C)[C@H](C)CCC(=O)[C@@H]2C)\C)c(c(c1C)Cl)O	374	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
743	Pyrroindomycin A	CCC1CC2(C)C=C(C(=O)O)C(C3(C2)NC(=O)C(=C(C2(C(CC1O)C=CC1C2CCCC1O[C@@H]1CC[C@@H]([C@@H](O1)C)O[C@@H]1O[C@H](C)[C@H]([C@@](C1)(C)O)O[C@@H]1O[C@H](C)[C@@H]([C@@H](C1)OC(=O)c1[nH]c2c(c1)c1c([nH]2)cccc1)N)C)O)C3=O)C	375	Yes
744	Pyrroindomycin B	CCC1CC2(C)C=C(C(=O)O)C(CC32NC(=O)C(=C3O)C(=O)C2(C(CC1O)C=CC1C2CCCC1OC1OCC(C(C1)OC1OC(C)C(C(C1)(C)O)OC1CC(OC(=O)c2[nH]c3c(c2)c2c([nH]3)ccc(c2)Cl)C(C(O1)C)N)C)C)C	376	Yes
745	2-(3-Acetoxy-4,4,14-trimethylandrost-8-en-17-yl)-propanoic acid	CC(=O)OC1CC[C@]2(C(C1(C)C)CCC1=C2CC[C@]2([C@@]1(C)CCC2C(C(=O)O)C)C)C	377	Yes
746	Oxaloterpin E	C=C[C@@]1(C)CC=C2[C@H](C1)CC[C@H]1[C@@]2(C)CC[C@H](C1(C)C)OC(=O)N	378	Yes
747	Oxaloterpin D	C=C[C@@]1(C)CC=C2[C@H](C1)CC[C@H]1[C@@]2(C)CC[C@H](C1(C)C)OC(=O)C(=O)N	379	Yes
748	Oxaloterpin C	ONC(=O)C(=O)O[C@@H]1CC[C@@]2([C@@H](C1(C)C)CC[C@@H]1C2=CC[C@](C1)(C)C=C)C	379	No
749	Niizalactam C	C[C@@H]1/C=C/C=C/C=C(\C)/[C@H]2C=C[C@@H]3[C@H]([C@@H]2/C=C(/C=C/C(=O)CC(=O)NC1)\C)[C@@H](O)[C@@H]([C@@H](C3=O)O)O	380	Yes
750	Tetronasin	CO[C@H]([C@H]1C[C@@H]([C@@H](O1)[C@H](/C=C/[C@@H]1CC[C@H]([C@@H](O1)/C(=C/[C@H]1CCC[C@H]([C@@H]1[C@@H](/C(=C/1\C(=O)OCC1=O)/O)C)C)/CO)C)C)C)C	381	No
751	Tetronomycin	CO[C@@H]([C@@H]1CC[C@H](O1)C/C=C/[C@H]1CC[C@@H](C(O1)/C(=C/[C@@H]1CCC[C@@H](C1C(C(=O)C1=C(O)C(=C)OC1=O)C)C)/CO)C)C	381	No
752	Tetronasin sodium	CO[C@H]([C@H]1C[C@@H]([C@@H](O1)[C@H](/C=C/C1CC[C@H]([C@@H](O1)/C(=C/[C@H]1CCC[C@H]([C@@H]1[C@@H](C(=O)C1=C([O-])COC1=O)C)C)/CO)C)C)C)C.[Na+]	381	Yes
753	Lankamycin	CO[C@H]1C[C@@H](C)O[C@H]([C@@H]1O)O[C@H]1[C@@H](C)C[C@](C)(O)C(=O)[C@H](C)[C@@H](OC(=O)C)[C@H]([C@H](OC(=O)[C@@H]([C@H]([C@@H]1C)O[C@@H]1O[C@@H](C)[C@H]([C@](C1)(C)OC)OC(=O)C)C)[C@H]([C@@H](O)C)C)C	382	No
754	Lankavamycin	COC1CC(C)OC(C1O)O[C@H]1[C@@H](C)C[C@](C)(O)C(=O)[C@H](C)[C@@H](OC(=O)C)[C@H]([C@H](OC(=O)[C@@H]([C@H]([C@@H]1C)OC1OC(C)C(C(C1)(C)OC)OC(=O)C)C)C(C(O)C)C)C	382	Yes
755	15-Deoxylankamycin	COC1CC(C)OC(C1O)O[C@H]1[C@@H](C)C[C@](C)(O)C(=O)[C@H](C)[C@@H](OC(=O)C)[C@H]([C@H](OC(=O)[C@@H]([C@H]([C@@H]1C)OC1OC(C)C(C(C1)(C)OC)OC(=O)C)C)[C@H](CC)C)C	382	No
756	Kujimycin A	COC1CC(C)OC(C1O)OC1C(C)CC(C)(O)C(=O)C(C)C(OC(=O)C)C(C(OC(=O)C(C(C1C)OC1OC(C)C(C(C1)(C)OC)O)C)C(C(O)C)C)C	382	No
757	8,15-Dideoxylankamycin	COC1CC(C)OC(C1O)O[C@H]1[C@@H](C)C[C@@H](C)C(=O)[C@H](C)[C@@H](OC(=O)C)[C@H]([C@H](OC(=O)[C@@H]([C@H]([C@@H]1C)OC1OC(C)C(C(C1)(C)OC)OC(=O)C)C)[C@H](CC)C)C	382	No
758	8-Deoxylankamycin	CO[C@H]1C[C@@H](C)O[C@H]([C@@H]1O)O[C@H]1[C@@H](C)C[C@@H](C)C(=O)[C@H](C)[C@@H](OC(=O)C)[C@H](C(OC(=O)[C@@H]([C@H]([C@@H]1C)O[C@@H]1O[C@@H](C)[C@H]([C@](C1)(C)OC)OC(=O)C)C)[C@H]([C@@H](O)C)C)C	382	No
759	Ebelactone B	CC[C@H]([C@H]([C@@H](C(=O)[C@@H](/C=C(/C[C@@H](C1OC(=O)[C@H]1CC)C)\C)C)C)O)C	383	Yes
760	Ebelactone A	CCC(C(C(C(=O)C(/C=C(/CC(C1OC(=O)C1C)C)\C)C)C)O)C	383	No
761	6-Deoxyerythronolide A	CCC1OC(=O)C(C)C(O)C(C)C(O)C(CC(C(=O)C(C(C1(C)O)O)C)C)C	384	Yes
762	6-Deoxyerythronolide B	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O)[C@H](C[C@H](C(=O)[C@@H]([C@H]([C@H]1C)O)C)C)C	385	Yes
763	SCHEMBL14000791	CCC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O)[C@H](C[C@H](C(=O)[C@@H]([C@H]([C@H]1C)O)C)C)C	385	No
764	Nisamycin	OC(=O)/C=C/C=C/C=C/[C@@]1(O)C=C(NC(=O)/C=C/C=C/C2CCCCC2)C(=O)[C@H]2[C@@H]1O2	386	Yes
765	4-Hydroxyprotoasukamcyin	C/C=C/C=C/C=C/C(=O)NC1=C[C@@](O)(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)C2C(C1=O)O2	387	No
766	Alisamycin	O=C(NC1=CC(O)(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)C2C(C1=O)O2)/C=C/C=C/C1CCCCC1	387	No
767	Asukamycin I	CCCC/C=C/C=C/C=C\C(=O)NC1=CC(O)(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)C2C(C1=O)O2	387	No
768	Manumycin B	CCCC[C@H](/C=C(/C(=O)NC1=C[C@@](O)(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)[C@H]2[C@@H](C1=O)O2)\C)C	387	No
769	Manumycin A, Streptomyces Parvulus	CCCC[C@H](/C=C(/C=C(/C(=O)NC1=C[C@@](O)(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)[C@H]2C(C1=O)O2)\C)\C)C	387	No
770	Manumycin E	CC(CC/C=C/C=C/C=C/C(=O)NC1=CC(O)(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)C2C(C1=O)O2)C	387	No
771	Manumycin	CCCC[C@H](/C=C(/C=C(/C(=O)NC1=C[C@@](O)(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)[C@H]2[C@@H](C1=O)O2)\C)\C)C	387	No
772	Asukamycin	O=C(NC1=C[C@@](O)(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)[C@H]2[C@@H](C1=O)O2)/C=C/C=C/C=C/C1CCCCC1	387	Yes
773	Colabomycin A	C/C=C/C=C/C=C/C=C/C(=O)NC1=C[C@@](O)(/C=C/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)[C@H]2[C@@H](C1=O)O2	387	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
774	Manumycin G	CC(/C=C/C=C/C=C/C(=O)NC1=C[C@@](O)(/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)[C@H]2[C@@H](C1=O)O2)C	387	No
775	Colabomycin E	C/C=C/C=C\C=C\C=C\C=C\C(=O)NC1=CC(O)(/C=C/C=C/C=C/C=C/C(=O)NC2=C(O)CCC2=O)C2C(C1=O)O2	388	Yes
776	Salternamide A	OC(=O)CCCC[C@@]1(O)C=C(NC(=O)/C=C/[C@H](C[C@H](C=C(C)C)C)C)C(=O)C(=C1)Cl	389	Yes
777	Antibiotic U-62162	OC(=O)CCCCC1(O)C=C(NC(=O)/C=C/C(CC(C=C(C)C)C)C)C(=O)C2C1O2	389	No
778	Puupehenone	O=C1C=C2O[C@@]3(C)CC[C@@H]4[C@]([C@H]3C=C2C=C1O)(C)CCCC4(C)C	390	Yes
779	(7E)-7-Ethyl-4-hydroxy-7-undecene-3,6-dione	CCC/C=C(/C(=O)CC(C(=O)CC)O)\CC	390	No
780	2',5'-Dimethoxyflavone	COc1ccc(cc1c1cc(=O)c2c(o1)cccc2)OC	391	Yes
781	JS1	CCCC1CCC(O1)c1cc(OC)c(c(c1)OC)OC	392	Yes
782	4'-O-beta-D-Glucose piericidin A 10-O-alpha-D-glucose (1→6)-beta-D-glucoside	COc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)OC	393	Yes
783	5,7,4'-Trimethoxyflavone	COc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2OC)OC	393	No
784	5-Hydroxy-7,4'-dimethoxyflavanone	COc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2O)OC	393	No
785	Naringenin trimethyl ether	COc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2OC)OC	393	No
786	Genkwanin	COc1cc(O)c2c(c1)oc(cc2=O)c1ccc(cc1)O	394	No
787	4'-Hydroxy-5,7-dimethoxyflavanone	COc1cc2OC(CC(=O)c2c(c1)OC)c1ccc(cc1)O	394	No
788	Sakuranetin	COc1cc2O[C@@H](CC(=O)c2c(c1)O)c1ccc(cc1)O	394	Yes
789	Naphterpin C	O=C1C2=C(OC([C@@H]3C2=C[C@@](C)(O)CC3)(C)C)C(=O)c2c1cc(O)c(c2O)C	395	Yes
790	Naphterpin B	O=C1C2=C(OC([C@@H]3C2=C[C@](C)(O)CC3)(C)C)C(=O)c2c1cc(O)c(c2O)C	395	No
791	Naphterpin E	CC(=O)O[C@H]1CC2C(C[C@H]1C)C1=C(OC2(C)C)C(=O)c2c(C1=O)cc(c(c2O)C)O	395	No
792	Naphterpin D	C[C@@H]1CC2C3=C(OC(C2C[C@@H]1O)(C)C)C(=O)c1c(C3=O)cc(c(c1O)C)O	395	No
793	Debromomarinone	CC(=CCC[C@]1(C)OC2=C([C@@H]3[C@H]1CCC(=C3)C)C(=O)c1c(C2=O)c(O)cc(c1)O)C	395	No
794	Naphthgeranine B	OCC1=CC2C(CC1)C(C)(C)OC1=C2C(=O)c2c(C1=O)c(O)cc(c2)O	395	No
795	NSC640155	CC1=CC2C(CC1)C(C)(C)OC1=C2C(=O)c2c(C1=O)c(O)c(c(c2)O)C	395	No
796	Naphthablin B	CCC(C(=O)O[C@H]1C[C@H]2[C@@H](C[C@H]1C)C1=C(OC2(C)C)C(=O)c2c(C1=O)cc(c1c2C[C@H]2[C@]1(C)CO[C@@H]2O)O)C	396	No
797	Naphthablin	OCC(c1c(O)cc2c(c1O)C(=O)C1=C(C2=O)C2CC(C)C(CC2C(O1)(C)C)OC(=O)C(C)C)(C=C)C	396	No
798	Naphthablin C	O=C(C(C)C)O[C@H]1C[C@H]2[C@@H](C[C@H]1C)C1=C(OC2(C)C)C(=O)c2c(C1=O)cc(c1c2C[C@H]2[C@]1(C)CO[C@@H]2O)O	396	Yes
799	(2R,3R,4S,5S,6R)-2-(((2E,4R,5R,6E,8E,11E)-13-(4-Hydroxy-6-methoxy-3-methylpyridin-2-yl)-3,5,7,11-tetramethyltrideca-2,6,8,11-tetraen-4-yl)oxy)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol	OC[C@H]1O[C@@H](O[C@@H](/C(=C/C)/C)[C@@H](/C=C(/C=C/C/C(=C/Cc2[nH]c(OC)cc(=O)c2C)/C)\C)C)[C@@H]([C@H]([C@@H]1O)O)O	397	No
800	(2R,3R,4S,5S,6R)-2-(((2E,4R,5R,6E,8E,11E)-1-Hydroxy-13-(4-hydroxy-5,6-dimethoxy-3-methylpyridin-2-yl)-3,5,7,11-tetramethyltrideca-2,6,8,11-tetraen-4-yl)oxy)-6-	OC/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)\C)C)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)\C	397	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol			
801	Glucopiericidin A	OC[C@H]1O[C@@H](O[C@@H](/C(=C/C)/C)[C@@H](/C=C(/C=C/C/C(=C/Cc2[nH]c(OC)c(c(=O)c2C)OC)/C)\C)C)[C@@H]([C@H]([C@@H]1O)O)O	397	Yes
802	PM050511	C/C=C(/C(C(/C=C(/C=C/CC(/C=C/c1oc(OC)c(c(=O)c1C)C)C)\C)C)OC1OC(CO)C(C(C1O)O)O)\C	397	No
803	Glucopiericidinol A1	OC[C@H]1O[C@@H](OC(/C(=C/C)/C)C(/C=C(/C=C/CC(/C=C/c2[nH]c(OC)c(c(=O)c2C)OC)(O)C)\C)C)[C@@H]([C@H]([C@@H]1O)O)O	397	No
804	13-Hydroxyglucopiericidin A	OC/C=C(\[C@@H]([C@@H](/C=C(\C=C/C/C(=C\Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)/C)C)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)/C	397	No
805	PM060431	OCC1OC(OC(/C(=C/C)/C)C(/C=C(/C=C/CC(/C=C/c2oc(OC)c(c(=O)c2C)CC)C)\C)C)C(C(C1O)O)O	397	No
806	2-Hydroxymethyl-delta3, 4-glucopiericidin A	COC(/C(=C/C=C/C(=C/[C@H]([C@H](/C(=C/C)/C)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)C)/C)/C)Cc1nc(OC)c(c(c1C)O)OC	397	No
807	(11S,12R)-Piericidin C1 10-O-beta-D-glucoside	OC[C@H]1O[C@@H](O[C@@H]([C@@]2(C)O[C@@H]2C)[C@@H](/C=C(/C=C/C/C(=C/Cc2nc(OC)c(c(c2C)O)OC)/C)\C)C)[C@@H]([C@H]([C@@H]1O)O)O	397	No
808	7-Demethyl-13-hydroxyglucopiericidin A	OC/C=C(/[C@@H]([C@@H](/C=C/C=C/C/C(=C/Cc1nc(OC)c(c(c1C)O)OC)/C)C)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)\C	397	No
809	5-Hydroxy-6-hydroxymethyl glucopiericidin A	CO[C@@H]([C@H](C/C(=C/Cc1nc(OC)c(c(c1C)O)OC)/C)O)/C(=C/[C@H]([C@H](/C(=C/C)/C)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)C)/C	397	No
810	5-Hydroxy-6-hydroxymethyl-13-hydroxyglucopiericidin A	OC/C=C(/[C@@H]([C@@H](/C=C(/[C@H]([C@H](C/C(=C/Cc1nc(OC)c(c(c1C)O)OC)/C)O)OC)\C)C)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)\C	397	No
811	Phileucin	CCC(c1ncc([nH]c1=O)Cc1ccccc1)C	398	Yes
812	Benastatin A	CCCCCc1cc2ccc3c(c2c(c1C(=O)O)O)cc1c(c3O)C(=O)c2c(C1(C)C)cc(cc2O)O	399	Yes
813	Benastatin B	CCCCCc1cc2CCc3c(c2c(c1C(=O)O)O)cc1c(c3O)C(=O)c2c(C1(C)C)cc(cc2O)O	399	No
814	Benastatin C	CCCCCc1cc(O)c2c(c1)ccc1c2cc2c(c1O)C(=O)c1c(C2(C)C)cc(cc1O)O	399	No
815	Citreaglycon A	COC1(C)OC(=O)c2c(C1)cc1c(c2O)c2c(CC1)c(O)c1c(c2O)c(=O)c2c(o1)ccc(c2O)C(=O)O	400	Yes
816	Dehydrocitreaglycon A	COC1(C)OC(=O)c2c(C1)cc1c(c2O)c2c(CC1)cc1c(c2O)c(=O)c2c(o1)ccc(c2O)C(=O)O	400	No
817	Lagunapyrone E	CCCCCc1ccc(oc1=O)[C@@H](C(/C(=C/C/C/C=C(/C/C(=C/C(=C/C[C@H]([C@H]([C@@H](/C(=C/C)/C)O)C)O)/C)/C)\C)/C)O)C	401	No
818	Lagunapyrone C	CCCCc1ccc(oc1=O)C([C@@H](/C(=C/C/C=C(/C/C(=C/C(=C/C[C@H]([C@H]([C@@H](/C(=C/C)/C)O)C)O)/C)/C)\C)/C)O)C	401	Yes
819	Lagunapyrone D	CCCc1ccc(oc1=O)[C@@H](C(/C(=C/C/C=C(/C/C(=C/C(=C/C[C@H]([C@H]([C@@H](/C(=C/C)/C)O)C)O)/C)/C)\C)/C)O)C	401	No
820	Lagunapyrone A	C/C=C(/[C@H]([C@@H]([C@@H](C/C=C(/C=C(/C/C(=C/C/C=C(/[C@H](C(c1ccc(c(=O)o1)C)C)O)\C)/C)\C)\C)O)C)O)\C	401	No
821	Lagunapyrone B	CCCc1ccc(oc1=O)[C@@H]([C@@H](/C(=C/C/C=C(/C/C(=C/C(=C/C[C@H]([C@H]([C@@H](/C(=C/C)/C)O)C)O)/C)/C)\C)/C)O)C	401	No
822	Isoxanthohumol	COc1cc(O)c(c2c1C(=O)CC(O2)c1ccc(cc1)O)CC=C(C)C	402	Yes
823	6-Prenyl-4'-methoxy-5,7-dihydroxylflavanone	COc1ccc(cc1)[C@@H]1CC(=O)c2c(O1)cc(c(c2O)CC=C(C)C)O	403	Yes
824	(2"S)-5'-Lavandulyl-2'-methoxy-2,4,4',6'-tetrahydroxylchalcone	COc1cc(O)c(c(c1C(=O)/C=C/c1ccc(cc1O)O)O)C[C@@H](C(=C)C)CC=C(C)C	404	Yes
825	5'-Lavandulyl-4'-methoxy-2,4,2',6'-tetrahydroxylchalcone	COc1cc(O)c(c(c1C[C@@H](C(=C)C)CC=C(C)C)O)C(=O)/C=C/c1ccc(cc1O)O	404	No
826	(2S,2"S)-6-Lavandulyl-5,7,2',4'-tetrahydroxylflavanone	CC(=CC[C@H](C(=C)C)Cc1c(O)cc2c(c1O)C(=O)C[C@H](O2)c1ccc(cc1O)O)C	404	No
827	Benthocyanin A	c1ccccc1.C/C(=C\Cn1c2cc3c(cc2nc2c1cccc2C(=O)O)oc(=O)c3C)/CCC=C(C)C	405	Yes
828	Benthocyanin B	C/C(=C\Cn1c2ccccc2nc2c1cc1c(c2C(=O)O)oc(=O)c1C)/CCC=C(C)C	405	No
829	Piericidin B5 N-Oxide	CC/C=C(/C(C(/C=C(/C=C/C/C(=C/Cc1c(C)c(O)c(c([n+]1[O-])OC)OC)/C)\C)C)OC)\C	406	No
830	Piericidin C4	COc1nc(C/C=C(/C/C(=C/C(=C/C(C(C2(C)OC2C(C)C)O)C)/C)/C)\C)c(c(c1OC)O)C	406	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
831	2-((2E,5E,7E,9R,10R)-10-((2S,3S)-2,3-Dimethyloxiran-2-yl)-10-hydroxy-3,5,7,9-tetramethyldeca-2,5,7-trien-1-yl)-5,6-dimethoxy-3-methylpyridin-4-ol	COc1nc(C/C=C(/C/C(=C/C(=C/[C@H]([C@H]([C@]2(C)O[C@H]2C)O)C)/C)/C)\C)c(c(c1OC)O)C	406	No
832	Piericidin C6	CCC1OC1(C)C(C(/C=C(\C=C(\C/C(=C/Cc1nc(OC)c(c(c1C)O)OC)/C)/C)/C)C)O	406	No
833	Piericidin C5	CCC1OC1(C)C(C(/C=C(\C=C\C/C(=C/Cc1nc(OC)c(c(c1C)O)OC)/C)/C)C)O	406	No
834	11-Demethylpiericidin A	C/C=C/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1nc(OC)c(c(c1C)O)OC)/C)\C)C)O	406	No
835	(2E,5E,7E,11E,9R,10R,13R,19S)-13,19-Dihydroxyl-IT-143-A	COc1c(OC)nc(c(c1O)C)C/C=C(/C/C(=C/C(=C/[C@H]([C@H](/C(=C/[C@@]([C@H](O)C)(O)C)/C)O)C)/C)/C)\C	406	No
836	(2E,5E,7E,11E,9R,10R,13S,19R)-13,19-Dihydroxyl-IT-143-A	COc1c(OC)nc(c(c1O)C)C/C=C(/C/C(=C/C(=C/[C@H]([C@H](/C(=C/[C@]([C@@H](O)C)(O)C)/C)O)C)/C)/C)\C	406	No
837	Piericidin A3	COc1nc(C/C=C(/C/C=C/C(=C/C(C(/C(=C\C(C)C)/C)O)C)/C)\C)c(c(c1OC)O)C	406	No
838	2-((2E,5E,7E,9R,10R,11E)-10-Hydroxy-3,5,7,9,11-pentamethyltrideca-2,5,7,11-tetraen-1-yl)-5,6-dimethoxy-3-methylpyridin-4-ol	C/C=C(/[C@@H]([C@@H](/C=C(/C=C(/C/C(=C/Cc1nc(OC)c(c(c1C)O)OC)/C)\C)\C)C)O)\C	406	Yes
839	Spinosyn A	CC[C@H]1CCC[C@H](O[C@H]2CC[C@@H]([C@H](O2)C)N(C)C)[C@@H](C)C(=O)C2=C[C@@H]3[C@H]([C@@H]2CC(=O)O1)C=C[C@H]1[C@H]3C[C@@H](C1)O[C@@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1OC)OC)OC	407	Yes
840	Spinosyn B	CC[C@H]1CCC[C@H](O[C@H]2CC[C@@H]([C@H](O2)C)NC)[C@@H](C)C(=O)C2=C[C@@H]3[C@H]([C@@H]2CC(=O)O1)C=C[C@H]1[C@H]3C[C@@H](C1)O[C@@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1OC)OC)OC	407	No
841	Spinosad	CC[C@H]1CCCC(O[C@H]2CC[C@@H]([C@H](O2)C)N(C)C)[C@@H](C)C(=O)C2=C[C@@H]3[C@H]([C@@H]2CC(=O)O1)C=C[C@H]1[C@H]3C[C@@H](C1)O[C@@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1OC)OC)OC.CC[C@H]1CCCC(O[C@H]2CC[C@@H]([C@H](O2)C)N(C)C)[C@@H](C)C(=O)C2=C[C@@H]3[C@H]([C@@H]2CC(=O)O1)C=C(C)[C@H]1[C@H]3C[C@@H](C1)O[C@@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1OC)OC)OC	407	No
842	5-O-Desosaminylplatenolide	CCC1CC(C)C(=O)/C=C\C=C\CC(OC(=O)CC(C(C1OC1OC(C)CC(C1O)N(C)C)OC)O)C	408	Yes
843	Desosaminyl tylactone	CC[C@H]1C[C@@H](C)C(=O)/C=C/C(=C/[C@@H]([C@H](OC(=O)C[C@H]([C@@H]([C@H]1OC1OC(C)CC(C1O)N(C)C)C)O)CC)C)/C	409	Yes
844	D-Quinovosyl-tylactone	CC[C@H]1C[C@@H](C)C(=O)/C=C/C(=C/[C@@H]([C@H](OC(=O)C[C@H]([C@@H]([C@H]1OC1OC(C)C(C(C1O)O)O)C)O)CC)C)/C	409	No
845	Dihydropicromycin	CCC1OC(=O)C(C)C(=O)C(C)C(OC2OC(C)CC(C2O)N(C)C)C(CC(C(=O)CCC1(C)O)C)C	410	No
846	Narbomycin	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@H](C[C@H](C(=O)/C=C/[C@H]1C)C)C	410	No
847	Albomycetin	CCC1OC(=O)C(C)C(=O)C(C)C(OC2OC(C)CC(C2O)N(C)C)C(CC(C(=O)/C=C\C1(C)O)C)C	410	No
848	Dihydropikromycin	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O[C@H]2O[C@@H](C)C[C@H]([C@@H]2O)N(C)C)[C@H](C[C@H](C(=O)/C=C/[C@]1(C)O)C)C	410	Yes
849	Neopikromycin	C[C@H]1O[C@@H](O[C@H]2[C@@H](C)C[C@@H](C)C(=O)/C=C/[C@H]([C@H](OC(=O)[C@@H](C(=O)[C@@H]2C)C)[C@H](O)C)C)[C@@H]([C@H](C1)N(C)C)O	410	No
850	Novapikromycin	C[C@H]1O[C@@H](O[C@H]2[C@@H](C)C[C@@H](C)C(=O)/C=C/[C@]([C@H](OC(=O)[C@@H](C(=O)[C@@H]2C)C)[C@H](O)C)(C)O)[C@@H]([C@H](C1)N(C)C)O	410	No
851	3'-Demethylneomethymycin	CNC1CC(C)OC(C1O)O[C@H]1[C@@H](C)C[C@@H](C)C(=O)/C=C/[C@H]([C@H](OC(=O)[C@@H]1C)[C@H](O)C)C	411	Yes
852	Neomethymycin	C[C@H]1O[C@@H](O[C@H]2[C@@H](C)C[C@@H](C)C(=O)/C=C/[C@H]([C@H](OC(=O)[C@@H]2C)[C@H](O)C)C)[C@@H]([C@H](C1)N(C)C)O	411	No
853	3'-Demethylmethymycin	CNC1CC(C)OC(C1O)O[C@H]1[C@@H](C)C[C@@H](C)C(=O)/C=C/[C@]([C@H](OC(=O)[C@@H]1C)CC)(C)O	412	No
854	10-Deoxymethymycin	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@@H](C)C[C@H](C(=O)/C=C/[C@H]1C)C	412	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
855	Methymycin	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@@H](C)C[C@H](C(=O)/C=C/[C@]1(C)O)C	412	Yes
856	3'-Demethyldeoxymethymycin	CNC1CC(C)OC(C1O)O[C@H]1[C@@H](C)C[C@@H](C)C(=O)/C=C/[C@H]([C@H](OC(=O)[C@@H]1C)CC)C	412	No
857	Chimeramycin A	O=C[C@H]1C[C@@H](C)C(/C=C/C(=C/[C@@H]([C@H](OC(=O)C[C@H]([C@@H]([C@H]1O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@H]1O)N(C)C)O[C@@H]1O[C@@H](C)[C@@H]([C@](C1)(C)O)O)C)OC(=O)C)CC)C)/C)O[C@H]1CC[C@@H]([C@H](O1)C)N(C)C	413	Yes
858	Chimeramycin B	O=C[C@H]1C[C@@H](C)C(/C=C/C(=C/[C@@H]([C@H](OC(=O)C[C@H]([C@@H]([C@H]1O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@H]1O)N(C)C)O[C@@H]1O[C@@H](C)[C@@H]([C@](C1)(C)O)O)C)O)CC)C)/C)O[C@H]1CC[C@@H]([C@H](O1)C)N(C)C	413	No
859	Relomycin	OCCC1CC(C)C(=O)/C=C\C(=C\C(C(OC(=O)CC(C(C1OC1OC(C)C(C(C1O)N(C)C)OC1OC(C)C(C(C1)(C)O)O)C)O)CC)COC1OC(C)C(C(C1OC)OC)O)\C	414	Yes
860	Flurithromycin	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2O[C@@H](C)[C@@H]([C@](C2)(C)OC)O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C[C@](C(=O)[C@@H]([C@H]([C@]1(C)O)O)C)(C)F)(C)O	415	No
861	Auricin	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2O[C@@H](C)[C@@H]([C@](C2)(C)OC)O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C[C@H](CN([C@@H]([C@H]([C@]1(C)O)O)C)C)C)(C)O	415	No
862	Erythromycin	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2O[C@@H](C)[C@@H]([C@](C2)(C)OC)O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C[C@H](C(=O)[C@@H]([C@H]([C@]1(C)O)O)C)C)(C)O	415	Yes
863	Spectomycin B1	OC(=O)C=C(C1c2cc3ccc(c(c3c(c2C(=O)CC1(C)O)O)O)c1ccc2c(c1O)c(O)c1c(c2)C(C(=CC(=O)O)C)C(CC1=O)(C)O)C	416	Yes
864	Julichrome Q6.6	CC(=O)OC(C1c2cc3ccc(c(c3c(c2C(=O)CC1(C)O)O)O)c1ccc2c(c1O)c(O)c1c(c2)C(C(OC(=O)C)C)C(CC1=O)(C)O)C	416	No
865	Nivetetracyclate B	COC(=O)[C@@H]1c2cc3cc4[C@H](O)CCC(=O)c4c(c3c(c2CC[C@]1(O)CC)O)O	417	Yes
866	Nivetetracyclate A	COC(=O)[C@@H]1c2cc3c(O)c4C(=O)CC[C@H](c4cc3c(c2CC[C@]1(O)CC)O)O	418	Yes
867	Julichrome Q6	CC(=O)O[C@@H]([C@@H]1c2cc3cccc(c3c(c2C(=O)C[C@]1(C)O)O)O)C	419	No
868	12T061A	CC(=O)O[C@H]([C@H]1c2c(C(=O)C[C@@]1(C)O)c(O)c1c(c2O)cccc1O)C	419	Yes
869	12T061C	COc1cccc2c1c(O)c1C(=O)C[C@@]([C@H](c1c2O)[C@@H](OC(=O)C)C)(C)O	419	No
870	Chrymutasin	CO[C@@H]1[C@@H](O)[C@@H](O[C@H]2[C@@H](O[C@@H]([C@@H]([C@@H]2O)O)C)Oc2ccc3c2c2oc(=O)c4c5c2c(c3O)c(=N)c(=O)c5ccc4C)O[C@@H]([C@@H]1O)C	420	Yes
871	BE 12406B	O[C@H]1[C@@H](O[C@H]([C@@H]([C@H]1O)O)C)Oc1cc2c(c3c1c(O)ccc3)oc(=O)c1c2c(O)cc(c1)C	421	Yes
872	BE 12406A	COc1cc(C)cc2c1c1cc(O[C@@H]3O[C@@H](C)[C@@H]([C@H]([C@H]3O)O)O)c3c(c1oc2=O)cccc3O	421	No
873	(5R)-5-hydroxy-3-[[2-(4-hydroxyphenyl)ethyl]amino]-5-vinyl-2-cyclopenten-1-one	C=C[C@]1(O)CC(=CC1=O)NCCc1ccc(cc1)O	422	Yes
874	Formicapyridine B	COc1cc(C)c(c(c1)O)c1nc(C)cc2c1c(O)c1c(c2)C(C)(C)c2c(C1=O)c(O)cc(c2)O	423	No
875	Formicapyridine C	COc1cc(C)c(c(c1)OC)c1nc(C)cc2c1c(O)c1c(c2)C(C)(C)c2c(C1=O)c(O)cc(c2)O	423	No
876	Formicapyridine H	COc1cc(C)c(c(c1)O)c1nc(C)cc2c1c(O)c1c(c2)C(C)(C)c2c(C1=O)c(O)c(c(c2)O)Br	423	Yes
877	Formicapyridine I	COc1cc(C)c(c(c1)OC)c1nc(C)cc2c1c(O)c1c(c2)C(C)(C)c2c(C1=O)c(O)c(c(c2)O)Br	423	No
878	Formicapyridine G	Oc1cc(C)c(c(c1)O)c1nc(C)cc2c1c(O)c1c(c2)C(C)(C)c2c(C1=O)c(O)c(c(c2)O)Br	423	No
879	Formicapyridine A	Oc1cc(C)c(c(c1)O)c1nc(C)cc2c1c(O)c1c(c2)C(C)(C)c2c(C1=O)c(O)cc(c2)O	423	No
880	Bagremycin G	O=CNc1cc(ccc1O)C(=O)Oc1ccc(cc1)C=C	424	No
881	Bagremycin B	C=Cc1ccc(cc1)OC(=O)c1ccc(c(c1)NC(=O)C)O	424	No
882	Bagremycin D	C=Cc1ccc(cc1)OC(=O)c1ccc(c(c1S)N)O	424	No
883	Bagremycin E	C=Cc1ccc(cc1)OC(=O)c1ccc(cc1)O	424	Yes
884	Watasemycin	C[C@@H]1SC(=N[C@H]1[C@@H]1SC[C@](N1C)(C)C(=O)O)c1ccccc1O	425	Yes
885	4-Benzoxazolecarboxylic acid, 2-(5-chloro-2-hydroxyphenyl)-	Clc1ccc(c(c1)c1oc2c(n1)c(ccc2)C(=O)O)O	426	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
886	4-Benzoxazolecarboxylic acid, 2-(3-chloro-2-hydroxyphenyl)-	OC(=O)c1cccc2c1nc(o2)c1cccc(c1O)Cl	426	No
887	4-Benzoxazolecarboxylic acid, 2-(2-hydroxy-5-methylphenyl)-	Cc1ccc(c(c1)c1oc2c(n1)c(ccc2)C(=O)O)O	426	No
888	Caboxamycin	Oc1ccccc1c1oc2c(n1)c(ccc2)C(=O)O	426	Yes
889	4-Benzoxazolecarboxylic acid, 2-(2-hydroxy-5-methoxyphenyl)-	COc1ccc(c(c1)c1oc2c(n1)c(ccc2)C(=O)O)O	426	No
890	3'-Hydroxycaboxamycin	OC(=O)c1cccc2c1nc(o2)c1cccc(c1O)O	426	No
891	4-Benzoxazolecarboxylic acid, 2-(4-chloro-2-hydroxyphenyl)-	Clc1ccc(c(c1)O)c1oc2c(n1)c(ccc2)C(=O)O	426	No
892	4-Benzoxazolecarboxylic acid, 2-(2-hydroxy-4-methylphenyl)-	Cc1ccc(c(c1)O)c1oc2c(n1)c(ccc2)C(=O)O	426	No
893	O-Methylcaboxamycin	COC(=O)c1cccc2c1nc(o2)c1ccccc1O	427	Yes
894	4-Benzoxazolecarboxylic acid, 2-(2-chloro-6-hydroxyphenyl)-, methyl ester	COC(=O)c1cccc2c1nc(o2)c1c(O)cccc1Cl	427	No
895	4-Benzoxazolecarboxylic acid, 2-(3-hydroxy-2-pyridinyl)-, methyl ester	COC(=O)c1cccc2c1nc(o2)c1ncccc1O	427	No
896	4-Benzoxazolecarboxylic acid, 2-(2-hydroxy-4-methylphenyl)-, methyl ester	COC(=O)c1cccc2c1nc(o2)c1ccc(cc1O)C	427	No
897	5-Hydroxy-nataxazole	COC(=O)c1cccc2c1nc(o2)c1cccc2c1nc(o2)c1c(O)ccc(c1C)O	428	Yes
898	UK-1	COC(=O)c1cccc2c1nc(o2)c1cccc2c1nc(o2)c1ccccc1O	428	No
899	Antibiotic A 33853	Oc1cccc(c1NC(=O)c1ncccc1O)c1oc2c(n1)c(ccc2)C(=O)O	429	Yes
900	Benzoic acid, 4-[[(3-hydroxy-2-pyridinyl)carbonyl]amino]-, methyl ester	COC(=O)c1ccc(cc1)NC(=O)c1ncccc1O	430	Yes
901	Phenazinomycin	C/C(=C\Cn1c2ccccc2nc2c1cccc2=O)/CC[C@@H]1C(=C)CCCC1(C)C	431	Yes
902	Lavanducyanin	CC1=C(CCC(C1)(C)C)Cn1c2ccccc2nc2c1cccc2=O	431	No
903	Arylomycin A4	OCC(N(C(=O)CCCCCCCCCC(CC)C)C)C(=O)NC(C(=O)NCC(=O)N(C1C(=O)NC(C)C(=O)NC(Cc2cc(c3cc1ccc3O)c(O)cc2)C(=O)O)C)C	432	Yes
904	2-[2-(2-{2-[2-(N,10-Dimethyldodecanamido)-3-hydroxypropanamido]propanamido}-N-methylacetamido)-2-(4-hydroxyphenyl)acetamido]propanoic acid	CCC(CCCCCCCCC(=O)N(C(C(=O)NC(C(=O)NCC(=O)N(C(C(=O)NC(C(=O)O)C)c1ccc(cc1)O)C)C)CO)C)C	432	No
905	Bonnevillamide B	COc1c(Cl)cc(cc1Cl)/C=C(/C(=O)N[C@H](C(=O)N[C@H](C(=O)N1[C@H](C)[C@H](C[C@H]1C(=O)N[C@H](C(=O)N([C@H](C(=O)N1CCC[C@H]1C(=O)O)C(C)C)O)CC(C)C)O)CC(C)C)[C@H](O)C)\O	433	No
906	Bonnevillamide A	COC(=O)[C@H]1C[C@H](N1C(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H]1C[C@@H]([C@H](N1C(=O)[C@@H](NC(=O)[C@H]([C@H](O)C)NC(=O)C(=Cc1cc(Cl)c(c(c1)Cl)OC)O)CC(C)C)C)OC(=O)C)CC(C)C)O)C(C)C)C	433	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
907	Bonnevillamide C	COc1c(Cl)cc(cc1Cl)/C=C(/C(=O)N[C@H](C(=O)N[C@H](C(=O)N1[C@H](C)[C@H](C[C@H]1C(=O)N[C@H](C(=O)N([C@H](C(=O)N1CCC[C@H]1C(=O)O)C(C)C)O)CC(C)C)OC(=O)C)CC(C)C)[C@H](O)C)\O	433	Yes
908	Acyldepsipeptide 2	C[C@H]1CN2[C@@H](C1)C(=O)OC[C@H](NC(=O)[C@H](Cc1cc(F)cc(c1)F)NC(=O)CCC1CCCCC1)C(=O)N1CCC[C@H]1C(=O)N1[C@H](C(=O)N[C@H](C2=O)C)CCCC1	434	Yes
909	Acyldepsipeptide 4	CCCC/C=C/C(=O)N[C@H](C(=O)N[C@H]1COC(=O)[C@@H]2C[C@H](CN2C(=O)[C@H](C)NC(=O)[C@H]2N(C(=O)[C@H]3N(C1=O)CCC3)CCCC2)C)Cc1cc(F)cc(c1)F	434	No
910	ADEP1	C/C=C/C=C/C=C/C(=O)N[C@H](C(=O)N[C@H]1COC(=O)[C@@H]2CC(CN2C(=O)[C@H](C)NC(=O)[C@@H](N(C(=O)[C@@H]2N(C1=O)CCC2)C)C)C)Cc1ccccc1	435	No
911	A54556 Factor A	C/C=C/C=C/C=C/C(=O)N[C@H](C(=O)N[C@H]1COC(=O)[C@@H]2C[C@H](CN2C(=O)[C@H](C)NC(=O)[C@@H](N(C(=O)[C@H]2N(C1=O)CCC2)C)C)C)Cc1ccccc1	435	Yes
912	ADEP	C/C=C/C=C/C=C/C(=O)NC(C(=O)NC1COC(=O)C2CC(CN2C(=O)C(C)NC(=O)C(N(C(=O)C2N(C1=O)CCC2)C)C)C)Cc1ccccc1	435	No
913	Enopeptin A	CC1CN2C(C1)C(=O)OCC(NC(=O)C(Cc1ccccc1)NC(=O)/C=C\C=C\C=C\C=C\C=C/C(=O)NC1=C(O)CCC1=O)C(=O)N1CCCC1C(=O)N(C(C(=O)NC(C2=O)C)C)C	436	Yes
914	Kromycin	CC[C@H]1OC(=O)[C@H](C)C(=O)/C(=C\[C@H](C[C@H](C(=O)/C=C\[C@]1(C)O)C)C)/C	437	Yes
915	Formicamycin M	COc1cc(C)c(c(c1)OC)c1cc(OC)c(c2c1C(=O)[C@@]1([C@H](C2)C(C)(C)c2c(C1=O)c(O)cc(c2)O)O)Br	438	Yes
916	Penicisteroid C	O[C@H]1CC[C@]2(C(=C[C@@H](C3[C@@H]2[C@@H](O)C[C@]2([C@H]3C[C@@H]([C@@H]2[C@@H](/C=C/[C@H](C(C)C)C)C)OC(=O)C)C)O)C1)C	439	Yes
917	Sitosteryl 3-beta-D-glucoside	CC[C@@H](C(C)C)CC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC=C2[C@]1(C)CC[C@@H](C2)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)C	440	Yes
918	14-Hydroxycyclooctatin	OC[C@@H]1C[C@H]([C@@H]2[C@@H]1C[C@@]1(C)CC[C@](C1=CC[C@]2(C)O)(O)C(C)C)O	441	Yes
919	12alpha-Hydroxycyclooctatin	OC[C@@H]1C[C@H]([C@@H]2[C@@H]1C[C@@]1(C)[C@@H](O)C[C@@H](C1=CC[C@]2(C)O)C(C)C)O	442	Yes
920	12beta-Hydroxycyclooctatin	OC[C@@H]1C[C@H]([C@@H]2[C@@H]1C[C@@]1(C)[C@H](O)C[C@@H](C1=CC[C@]2(C)O)C(C)C)O	442	No
921	16,17-Dihydroxycyclooctatin	OCC([C@@H]1CC[C@@]2(C1=CC[C@@](C)(O)[C@@H]1[C@@H](C2)[C@@H](CC)C[C@@H]1O)C)CO	442	No
922	CHEBI:67808	OC[C@H]([C@H]1CC[C@]2(C1=CC[C@](C)(O)[C@H]1[C@H](C2)[C@H](CO)C[C@H]1O)C)C	442	No
923	Cyclooctatin	OCC1CC(C2C1CC1(C)CCC(C1=CCC2(C)O)C(C)C)O	443	Yes
924	Ergosta-8(9),22-diene-3beta,5alpha,6beta,7alpha-tetraol	O[C@H]1CC[C@]2([C@@](C1)(O)[C@H](O)[C@@H](C13C2(CC[C@]2(C3CC[C@@H]2[C@@H](/C=C/C(C(C)C)C)C)C)C1)O)C	444	No
925	Ananstrep A	OCC([C@H](/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1C2=C[C@H]([C@@]2([C@]1(C)CC[C@@H](C2)O)O)O)O)C)C	444	No
926	Ergosta-7,22-diene-3beta,5alpha,6beta-triol	O[C@H]1CC[C@]2([C@@](C1)(O)[C@H](O)C=C1[C@@H]2CC[C@]2([C@H]1CC[C@@H]2[C@@H](/C=C/[C@@H](C(C)C)C)C)C)C	444	No
927	Ergosta-8(14),22-diene-3beta,5alpha,6beta,7alpha-tetraol	O[C@H]1CC[C@]2([C@@](C1)(O)[C@H](O)[C@H](C1=C3[C@@](CC[C@H]21)(C)[C@H](CC3)[C@@H](/C=C/[C@@H](C(C)C)C)C)O)C	444	No
928	Ergosta-7,22-diene-3beta,5alpha,6alpha-triol	O[C@H]1CC[C@]2([C@@](C1)(O)[C@@H](O)C=C1[C@@H]2CC[C@]2([C@H]1CC[C@@H]2[C@@H](/C=C/[C@@H](C(C)C)C)C)C)C	444	Yes
929	Ergosta-7,22-diene-3beta,5α,6beta,9alpha-tetraol	O[C@H]1CC[C@]2([C@](C1)(C)[C@@H](O)C=C1[C@@]2(O)CC[C@]2(C1CC[C@@H]2[C@@H](/C=C/C(C(C)C)C)C)C)C	444	No
930	7-Prenylisatin	CC(=CCc1cccc2c1NC(=O)C2=O)C	445	No
931	(E)-6-(4-Hydroxy-3-methylbut-2-en-1-yl)indolin-2-one	OC/C(=C/Cc1ccc2c(c1)NC(=O)C2)/C	445	Yes
932	(Z)-6-(4-Hydroxy-3-methylbut-2-en-1-yl)indolin-2-one	OC/C(=C\Cc1ccc2c(c1)NC(=O)C2)/C	445	No
933	Vinylamycin	OCCC(C1OC(=O)C(NC(=O)C(C)NC(=O)C=CC(=C)NC1=O)C(C)C)C(CCCCCC)C	446	Yes
934	Rakicidin B	CC(CCCCCCCCCCCCC(C1OC(=O)C(NC(=O)CN(C(=O)/C=C\C(=C)NC(=O)C1C)C)C(C(=O)N)O)C)C	447	Yes
935	Rakicidin E	CC(CCCCCCCCCCCCCCC(C1OC(=O)C(NC(=O)N(C)C(=O)/C=C/C(=C)NC(=O)C1C)C(C(=O)N)O)C)C	447	No
936	Rakicidin A	CC(CCCCCCCCCCC(C1OC(=O)C(NC(=O)CN(C(=O)/C=C\C(=C)NC(=O)C1C)C)C(C(=O)N)O)C)C	447	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
937	Rakicidin C	CC(CC(CC(C1OC(=O)C(CCC(=O)N)NC(=O)CN(C(=O)/C=C/C(=C)NC(=O)C1C)C)C)C)C	448	Yes
938	Rakicidin F	CCC(CC(CC(C1OC(=O)C(CCC(=O)N)NC(=O)CN(C(=O)/C=C/C(=C)NC(=O)C1C)C)C)C)C	448	No
939	Herbimycin F	CO[C@H]1C[C@H](C)[C@@H](OC)C2=CC(CC3=C2O[C@@H]1[C@@H](C)/C=C(\C)/[C@H](OC(=O)N)[C@@H](OC)CC(=C)C[C@](C(=O)N3)(C)O)O	449	Yes
940	BE 18591	CCCCCCCCCCCCN/C=c/1\[nH]/c(=C\2/C=CC=N2)/cc1OC	450	Yes
941	Methylundecylprodiginine	COC1=CC(=NC1=Cc1ccc([nH]1)CCCCCCCCCC(C)C)c1ccc[nH]1	451	No
942	Undecylprodiginine	CCCCCCCCCCCc1ccc([nH]1)/C=C\1/N=C(C=C1OC)c1ccc[nH]1	451	No
943	Methyldodecylundecylprodiginine	COC1=CC(=N/C/1=C/c1ccc([nH]1)CCCCCCCCCC(C)C)c1ccc[nH]1	451	No
944	Methyldodecylprodiginine	COC1=CC(=NC1=Cc1ccc([nH]1)CCCCCCCCCCC(C)C)c1ccc[nH]1	451	No
945	Undecylprodigiosin	CCCCCCCCCCCc1ccc([nH]1)/C=C/1\N=C(C=C1OC)c1ccc[nH]1	451	Yes
946	Prodigiosin 25C	CCCCCCCCCCCc1ccc([nH]1)/C=c\1/[nH]/c(=C/2\C=CC=N2)/cc1OC	451	No
947	11-Methyldodecylprodiginine	COc1cc([nH]c1/C=C/1\C=CC(=N1)CCCCCCCCCCC(C)C)c1ccc[nH]1	451	No
948	Prodiginine	CCCCCCCCCCCc1ccc([nH]1)/C=C\1/C=CC(=N1)c1ccc[nH]1	451	No
949	Virginiamycin M	O=C1NC/C=C\C(=C/[C@@H](O)CC(=O)Cc2nc(C(=O)N3C(C(=O)O[C@@H]([C@@H](/C=C\1)C)C(C)C)CCC3)co2)\C	452	Yes
950	Ostreogrycin A	O=C1NC/C=C\C(=C/C(O)CC(=O)Cc2nc(C(=O)N3C(=CCC3)C(=O)OC(C(/C=C\1)C)C(C)C)co2)\C	453	Yes
951	16r-Dihydrovm1	O=C1NC/C=C\C(=C/[C@@H](O)C[C@@H](O)Cc2nc(C(=O)N3C(=CCC3)C(=O)O[C@@H]([C@@H](/C=C\1)C)C(C)C)co2)\C	453	No
952	Virginiamycin M1	O=C1NC/C=C\C(=C/[C@@H](O)CC(=O)Cc2nc(C(=O)N3C(=CCC3)C(=O)O[C@@H]([C@@H](/C=C\1)C)C(C)C)co2)\C	454	Yes
953	Xenocyloin B	CCC(C(=O)[C@@H](Cc1c[nH]c2c1cccc2)O)C	455	No
954	Xenocyloin D	CCC(C(=O)[C@@H](Cc1c[nH]c2c1cccc2)OC(=O)C)C	455	Yes
955	Xenocyloin C	CC(=O)O[C@@H](C(=O)C(C)C)Cc1c[nH]c2c1cccc2	455	No
956	Platenolide II	CCC1CC(C)C(O)/C=C\C=C\CC(OC(=O)CC(C(C1O)OC)O)C	456	Yes
957	Platenolide I	CC[C@H]1C[C@@H](C)C(=O)/C=C/C=C/C[C@H](OC(=O)C[C@H]([C@@H]([C@H]1O)OC)O)C	456	No
958	25-oxo-FD-892	C/C/1=C\[C@@H](C)[C@H](O)/C=C/CC/C=C/C[C@H](OC(=O)\C(=C1)\C)[C@H](C/C=C/C[C@@H]1OC(C)(O)[C@H]([C@@H]([C@@H]1C)O)C)C	457	Yes
959	FD 892	OC(C(C(C(C(O)C)C)O)C)CCC(C1C/C=C\C=C/CC/C=C\C(C(/C=C(\C=C(/C(=O)O1)\C)/C)C)O)C	458	Yes
960	25-O-methyl-FD-892	CO[C@H]([C@H]([C@@H]([C@@H]([C@H](C/C=C/C[C@@H]([C@@H]1C/C=C/CC/C=C/[C@H]([C@@H](/C=C(/C=C(/C(=O)O1)\C)\C)C)O)C)O)C)O)C)C	458	No
961	Desertomycin G	NCCCC(C(C1C/C=C/C(O)CC(O)CC(O)C(C)C(O)C(C)C(O)CC(O)CC(O)C(C)C(O)C(/C=C(/C(C(/C=C/C(C(/C=C/CCC(C(C(C(/C=C/C=C/C(=O)O1)C)O)C)O)C)O)C)O)\C)O[C@H]1C[C@H](CO)[C@H]([C@@H]([C@@H]1O)O)O)C)O	459	Yes
962	Desertomycin B	OC[C@H]1O[C@H](O[C@@H]2/C=C(/C)\[C@H](O)[C@@H](C)/C=C\[C@H](O)[C@@H](C)/C=C\CC[C@H](O)[C@H](C)[C@H](O)[C@@H](C)CC/C=C(/C)\C(=O)OC(C/C=C\[C@H](C[C@@H](C[C@H]([C@@H]([C@@H]([C@H]([C@H](C[C@H](C[C@@H](C[C@H]2O)C)O)O)C)O)O)O)O)O)O)O)[C@@H]([C@@H](CCCN=C(N)N)O)C)[C@H]([C@H]([C@@H]1O)O)O	460	Yes
963	Desertomycin	NCCCC(C(C1C/C=C\C(O)CC(O)CC(O)C(C)C(O)C(C)C(O)CC(O)CC(O)CC(O)C(/C=C(\C(C(/C=C\C(C(/C=C\CCC(C(C(C(CC/C=C\C(=O)O1)/C)C)O)C)O)C)O)C)O)C)O)/C)O[C@H]1O[C@@H](CO)[C@@H]([C@H]([C@H]1O)O)O)C)O	461	Yes
964	Stambomycin B	OC1CCCC(O)C(C)C(O)CCC(C)C(O)CC(O)CC(O)CCC(O)C(O)C(CCCCC(C)C)/C=C(\C)/C(O)CC(CCC(C(C(C/C=C/C=C(/C(C(C2OC(CC(=O)OC(/C=C/C(C1)O)C)(O)C(C)C(C2)O[C@@H]1O[C@H](C)[C@H](C([C@H]1O)N(C)C)O)C)O)\C)O)C)O)O	462	Yes
965	Stambomycin C	CC(CCCC1/C=C(\C)/C(O)CC(O)CCCC(O)C(C)C(O)C/C=C/C=C(\C)/C(O)C(C)C2CC(O[C@@H]3O[C@H](C)[C@H]([C@@H]([C@H]3O)N(C)C)O)C(C(O2)(O)CC(=O)OC(/C=C/C(CC(CCCC(C(C(CCC(C(CC(CC(CCC(C1O)O)O)O)O)C)O)C)O)O)C)C)C	463	Yes
966	Stambomycin D	CCCCCCC1/C=C(\C)/C(O)CC(O)CCCC(O)C(C)C(O)C/C=C/C=C(\C)/C(O)C(C)C2CC(O[C@@H]3O[C@H](C)[C@H](C([C@H]3O)N(C)C)O)C(C(O2)(O)CC(=O)OC(/C=C/C(CC(CCCC(C(C(CCC(C(CC(CC(CCC(C1O)O)O)O)O)C)O)C)O)O)O)C)C	464	Yes
967	Stambomycin A	CCC(CCCC1/C=C(\C)/C(O)CC(O)CCCC(O)C(C)C(O)C/C=C/C=C(\C)/C(O)C(C)C2CC(O[C@@H]3O[C@H](C)[C@H](C([C@H]3O)N(C)C)O)C(C(O2)(O)CC(=O)OC(/C=C/C(CC(CCCC(C(C(CCC(C(CC(CC(CCC(C1O)O)O)O)O)C)O)C)O)O)O)C)C	465	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
968	Oasomycin A	O=C1CCC(O1)CC1CC=CC(O)CC(O)CC(O)C(C)C(O)C(C)C(O)CC(O)CC(O)CC(O)C(O)C=C(C(C(C=CC(C(=CCCC(C(C(C(CCC=C(C(=O)O1)C)C)O)C)O)C)O)C)O)C	466	Yes
969	Dmdm IV	CCC1OC(=O)/C=C/C(C)C(OC2OC(C)C(C(C2O)N(C)C)O)C(C)CC(C(=O)CC/C=C\C1COC1OC(C)C(C(C1OC)OC)O)C	467	No
970	Aldgamycin M	CO[C@H]1[C@H](OC[C@H]2/C=C/CCC(=O)[C@H](C)C[C@@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2C)C)O[C@@H]2O[C@H](C)C[C@]3([C@H]2O)OC(=O)O[C@H]3C)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	No
971	Aldgamycin L	CO[C@H]1[C@H](OC[C@H]2/C=C/CCC(=O)[C@H](C)C[C@@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2C)C)O[C@@H]2O[C@H](C)C[C@]([C@H]2O)(O)[C@@H](O)C)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	No
972	Chalcomycin B	CCC(=O)OC1C(OC(CC1OC)C)O[C@@H]1[C@@H](C)/C=C/C(=O)O[C@H](C)[C@@H](COC2OC(C)C(C(C2OC)OC)O)C2[C@@H](/C=C/C(=O)[C@@](CC1C)(C)O)O2	467	No
973	Aldgamycin G	CO[C@H]1[C@H](OC[C@@H]2[C@@H](C)OC(=O)/C=C/[C@H](C)[C@@H](O[C@@H]3O[C@H](C)CC4([C@H]3O)OC(=O)O[C@H]4C)[C@H](C[C@H](C(=O)/C=C/[C@H]3[C@H]2O3)C)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	No
974	Aldgamycin P	CO[C@H]1[C@H](OCC2[C@@H](C)OC(=O)/C=C/[C@H](C)C(O[C@@H]3O[C@H](C)C[C@]4([C@H]3O)OC(=O)O[C@H]4C)[C@H](C[C@](C(=O)CC[C@H]3[C@H]2O3)(C)O)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	No
975	Aldgamycin E	CO[C@H]1[C@H](OCC2C(C)OC(=O)/C=C/C(C)C(O[C@@H]3O[C@H](C)C[C@]4([C@H]3O)OC(=O)O[C@H]4C)C(CC(C(=O)CCC3C2O3)C)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	No
976	Swalpamycin	CO[C@H]1[C@H](OC[C@H]2/C=C/C=C/C(=O)[C@H](C)C[C@@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2C)C)O[C@@H]2O[C@H](C)CC3([C@H]2O)OC(=O)O[C@H]3C)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	No
977	Chalcomycin E	CO[C@H]1C[C@@H](C)O[C@H]([C@@H]1O)O[C@@H]1[C@@H](C)/C=C/C(=O)O[C@H](C)[C@H](/C=C/C=C/C(=O)[C@@](C[C@@H]1C)(C)O)CO[C@@H]1O[C@H](C)[C@H]([C@H]([C@H]1OC)OC)O	467	No
978	Neutramycin E	COC1C(OCC2C(C)OC(=O)/C=C\C(C)C(CCC(C(=O)/C=C\C3C2O3)C)OC2OC(C)CC(C2O)O)OC(C(C1OC)O)C	467	No
979	Aldgamycin K	CO[C@H]1[C@H](OC[C@@H]2[C@@H](C)OC(=O)/C=C/[C@H](C)[C@@H](O[C@@H]3O[C@H](C)C[C@]([C@H]3O)(O)[C@@H](O)C)[C@H](C[C@H](C(=O)CC[C@H]3[C@H]2O3)C)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	No
980	Aldgamycin N	CO[C@H]1[C@H](OC[C@H]2/C=C/CCC(=O)[C@@](C)(O)C[C@@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2C)C)O[C@@H]2O[C@H](C)C[C@]([C@H]2O)(O)[C@@H](O)C)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	Yes
981	Aldgamycin O	CO[C@H]1[C@H](OC[C@H]2/C=C/C=C/C(=O)[C@@](C)(O)C[C@@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2C)C)O[C@@H]2O[C@H](C)C[C@]([C@H]2O)(O)[C@@H](O)C)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	No
982	Swalpamycin B	CO[C@H]1[C@H](OC[C@H]2/C=C/C=C/C(=O)[C@H](C)C[C@@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2C)C)O[C@@H]2O[C@H](C)C[C@]([C@H]2O)(O)[C@@H](O)C)C)O[C@@H]([C@H]([C@H]1OC)O)C	467	No
983	Chalcomycin	CO[C@H]1C[C@@H](C)O[C@H]([C@@H]1O)O[C@H]1[C@@H](C)/C=C/C(=O)O[C@H](C)[C@@H](CO[C@@H]2O[C@H](C)[C@H]([C@H]([C@H]2OC)OC)O)[C@H]2[C@H](/C=C/C(=O)[C@@](C[C@@H]1C)(C)O)O2	467	No
984	Dihydrochalcomycin	CO[C@@H]1C[C@H](C)O[C@@H]([C@H]1O)O[C@@H]1[C@H](C)/C=C/C(=O)O[C@@H](C)[C@H](CO[C@H]2O[C@@H](C)[C@@H]([C@@H]([C@@H]2OC)OC)O)[C@@H]2[C@@H](CCC(=O)[C@](C[C@H]1C)(C)O)O2	467	No
985	Acidiscalide	CO[C@H]1C[C@@H](C)O[C@H]([C@@H]1O)OC1C(C)/C=C/C(=O)C(C)/C=C(\C)/C(=O)C(C)C(O)CC(=O)OC(C(C(C/C=C/C(=O)C(CC1C)(C)O)O)C)C(C(O)C)C	468	Yes
986	(11E,13E)-7,16-Diethyl-4,6-dihydroxy-15-{[(5- hydroxy-3,4-dimethoxy-6-methyloxan-2-yl)oxy]methyl}-5,9,13-trimethyl-1-oxacyclohexadeca-11,13-diene-2,10-dione	CCC1OC(=O)CC(O)C(C)C(O)C(CC)CC(C(=O)/C=C/C(=C/C1COC1OC(C)C(C(C1OC)OC)O)/C)C	469	Yes
987	(11E,13E)-16-Ethyl-4,6,7-trihydroxy-15-{[(5- hydroxy-3,4-dimethoxy-6-methyloxan-2-yl)oxy]methyl}-5,9,13-trimethyl-1-oxacyclohexadeca-11,13-diene-2,10-dione	CCC1OC(=O)CC(O)C(C)C(O)C(O)CC(C(=O)/C=C/C(=C/C1COC1OC(C)C(C(C1OC)OC)O)/C)C	469	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
988	3-O-(alpha-L-Oleandrosyl)erythronolide B	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@H](OC)[C@H]([C@@H](O2)C)O)[C@H](C)[C@@H](O)[C@](C[C@H](C(=O)[C@@H]([C@H]([C@H]1C)O)C)C)(C)O	470	Yes
989	Cycloprodigiosin	COC1=CC(=N/C/1=C\c1[nH]c(c2c1C(C)CCC2)C)c1ccc[nH]1	471	Yes
990	Prodigiosin R2	COC1=CC(=NC1=C1c2[nH]c3cc2C(C1CCCCCCCC3)C(C)C)c1ccc[nH]1	471	No
991	Streptorubin B	CCCC[C@H]1CCCCCCc2cc1c([nH]2)/C=c/1\[nH]/c(=C\2/C=CC=N2)/cc1OC	472	No
992	NSC247562	CCCCC1CCCCCCc2c1cc([nH]2)/C=c/1\[nH]/c(=C/2\C=CC=N2)/cc1OC	472	No
993	Butylcycloheptylprodigiosin	CCCCC1CCCCCCc2c1cc([nH]2)C=c1[nH]/c(=C\2/C=CC=N2)/cc1OC	472	Yes
994	Prodigiosin R1	COc1c/c(=C/2\C=CC=N2)/[nH]/c/1=C\c1[nH]c2cc1C(CCCCCCCC2)CC(C)C	472	No
995	Metacycloprodigiosin	CC[C@@H]1CCCCCCCCc2cc1c([nH]2)/C=c/1\[nH]/c(=C\2/C=CC=N2)/cc1OC	472	No
996	BMCHP	CCCCC1CCCCCCc2cc1c([nH]2)/C=c/1\[nH]/c(=C\2/C=CC=N2)/cc1OC	472	No
997	Prodigiosin	CCCCCc1cc([nH]c1C)/C=c/1\[nH]/c(=C\2/C=CC=N2)/cc1OC	472	No
998	Blasticidin A	CCCCCCCCCCC(CC1(O)OC(CC(C(C(C(C(CC(CC(CC(CC(C(C(C(C(CC(C(C(C(CC(CC(/C=C(/C(=C/2\C(=O)CN(C2=O)C)/O)\C)C)C)O)O)C)O)O)C)O)C)O)O)O)O)O)O)O)O)C(C(C1O)O)O)O	473	Yes
999	Aflastatin A	CCCCCCCCC[C@H](C[C@]1(O)O[C@H](C[C@H]([C@@H]([C@H]([C@@H]([C@H](C[C@H](C[C@H](C[C@H]([C@@H]([C@H]([C@H]([C@H](C[C@H]([C@@H]([C@H]([C@H]([C@H]([C@@H]([C@@H]([C@H](C[C@@H](C[C@@H](/C=C(/C(=C/2\C(=O)N([C@@H](C2=O)C)C)/O)\C)C)C)O)O)C)O)C)O)O)C)O)O)O)O)O)O)O)O)[C@H]([C@@H]([C@@H]1O)O)O)O	474	Yes
1000	Vancoresmycin	OC(CC(C/C=C(/C(=C\1/C(=O)/C(=C/C(C)C)/N(C1=O)C)/O)\C)O)CCC(C(C(C(CCCC(C(C(/C(=C/C(C(=O)/C(=C/C(C(CC(CC(C(CCC(CC(CCC(C(C(C(C(C)C)O)C)O)C)O)O)C)OC1OC(C)C(C(C1O)N)O)O)O)/C)C)/C)O)C)O)O)C)O)C	475	Yes
1001	Dimeric dinactin	CCC1CC2CCC(O2)C(C)C(=O)OC(CC2OC(C(C(=O)O1)C)CC2)C	476	Yes
1002	Dimeric Nonactin	CC1CC2CCC(O2)C(C)C(=O)OC(CC2OC(C(C(=O)O1)C)CC2)C	476	No
1003	Bonactin	CCC(CC1CCC(O1)C(C(=O)OC(CC1CCC(O1)C(C(=O)O)C)C)C)O	477	Yes
1004	Feigrisolide C	CC[C@H](C[C@@H]1CC[C@@H](O)[C@@H](C)C(=O)O[C@H](C[C@@H]2O[C@H]([C@@H](C(=O)O1)C)CC2)C)O	478	Yes
1005	Pamamycin	CCC[C@H]1C[C@@H]2CC[C@@H](O2)[C@H](C)C(=O)O[C@H]([C@@H]([C@H]2O[C@@H]([C@H](C(=O)O1)C)CC2)C)[C@@H]([C@H]1CC[C@H](O1)C[C@H](N(C)C)CCC)C	479	Yes
1006	Pamamycin-607	CCC[C@H]1CC2CCC(O2)[C@H](C)C(=O)OC([C@@H](C2OC([C@H](C(=O)O1)C)CC2)C)[C@@H](C1CC[C@H](O1)C[C@H](N(C)C)CCC)C	479	No
1007	Nonactin	C[C@@H]1C[C@H]2CC[C@H](O2)[C@H](C)C(=O)O[C@@H](C)C[C@@H]2CC[C@@H](O2)[C@@H](C)C(=O)O[C@@H](C[C@@H]2O[C@H]([C@@H](C(=O)O[C@H](C[C@H]3O[C@@H]([C@H](C(=O)O1)C)CC3)C)C)CC2)C	480	Yes
1008	Monactin	CCC1CC2CCC(O2)C(C)C(=O)OC(C)CC2CCC(O2)C(C)C(=O)OC(CC2OC(C(C(=O)OC(CC3OC(C(C(=O)O1)C)CC3)C)C)CC2)C	481	Yes
1009	Tetranactin	CC[C@@H]1C[C@H]2CC[C@H](O2)[C@H](C)C(=O)O[C@@H](CC)C[C@@H]2CC[C@@H](O2)[C@@H](C)C(=O)O[C@@H](C[C@@H]2O[C@H]([C@@H](C(=O)O[C@H](C[C@H]3O[C@@H]([C@H](C(=O)O1)C)CC3)CC)C)CC2)CC	482	Yes
1010	Dinactin	CC[C@H]1CC2CCC(O2)[C@H](C)C(=O)O[C@H](C)CC2CCC(O2)[C@H](C)C(=O)O[C@H](CC2OC([C@@H](C(=O)O[C@@H](CC3OC([C@@H](C(=O)O1)C)CC3)C)C)CC2)CC	483	Yes
1011	Trinactin	CC[C@H]1C[C@@H]2CC[C@@H](O2)[C@@H](C)C(=O)O[C@H](CC)C[C@H]2CC[C@H](O2)[C@H](C)C(=O)O[C@H](C[C@H]2O[C@@H]([C@H](C(=O)O[C@@H](C[C@@H]3O[C@H]([C@@H](C(=O)O1)C)CC3)CC)C)CC2)C	484	Yes
1012	Efomycin L	CC[C@H]([C@H](O)C)/C=C/C(=O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H](C(=O)/C=C/[C@@H]([C@H](O)C)C)C)O)C)C)O)C	485	Yes
1013	Efomycin M	CC[C@H]([C@H](O)C)/C=C/C(=O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H](C(=O)/C=C/[C@@H]([C@H](O)C)CC)C)O)C)C)O)C	485	No
1014	Efomycin K	O=C([C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H](C(=O)/C=C/[C@@H]([C@H](O)C)C)C)O)C)C)O)C)/C=C/[C@@H]([C@H](O)C)C	485	No
1015	Hyaluromycin	COc1cc(O)c2c(c1O)C(=O)C1=C(C2=O)C[C@@]2(O1)CCc1c(O2)c(O)c2c(c1)cc(oc2=O)C(=O)NC1=C(O)CCC1=O	486	Yes
1016	Rubromycin CA1	COc1cc(O)c2c(c1O)C(=O)C1=C(C2=O)C[C@@]2(O1)CCc1c(O2)c(O)c2c(c1)cc(oc2=O)C(=O)O	487	Yes
1017	Collinomycin	COC(=O)c1cc2cc(CCc3cc4c(o3)C(=O)c3c(C4=O)c(OC)cc(c3O)OC)c(c(c2c(=O)o1)O)O	488	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1018	beta-Rubromycin	COC(=O)c1cc2cc3CC[C@@]4(Oc3c(c2c(=O)o1)O)CC1=C(O4)C(=O)c2c(C1=O)c(OC)cc(c2O)OC	489	Yes
1019	gamma-Rubromycin	COC(=O)c1cc2cc3CC[C@@]4(Oc3c(c2c(=O)o1)O)Cc1c(O4)c(O)c2c(c1O)C(=O)C=C(C2=O)OC	489	No
1020	Misakimycin	COC1=CC(=O)c2c(C1=O)cc(c(c2O)C)OC	490	Yes
1021	Lactomycin B	NCC[C@]([C@@H](C[C@H](/C=C\C=C/[C@@H]1CCC[C@@H](C1)O)O)O)(/C=C/[C@@H]1OC(=O)C=C[C@@H]1CC)O	491	No
1022	Lactomycin C	CC[C@H]1C=CC(=O)O[C@H]1/C=C/[C@]([C@@H](C[C@H](/C=C\C=C/[C@@H]1CCC[C@@H](C1)O)O)O)(O)C	491	No
1023	Lactomycin A	OCC[C@]([C@@H](C[C@H](/C=C\C=C/[C@@H]1CCC[C@@H](C1)O)O)O)(/C=C/[C@@H]1OC(=O)C=C[C@@H]1CC)O	491	Yes
1024	Campechic Acid B	C[C@H](C[C@@H](/C(=C/C(=O)[C@@H](C[C@@H](C[C@H](C[C@H](C(=O)O)C)C)C)C)/O)C)C/C=C/[C@H](C(CC1CCC(O1)(C)C1CCC(O1)(C)[C@H](O)C)O)C	492	No
1025	Campechic Acid A	CCC(C(=O)/C=C(/[C@H](C[C@H](C/C=C/[C@H](C(CC1CCC(O1)(C)C1CCC(O1)(C)[C@H](O)C)O)C)C)\O)C[C@@H](C[C@H](C[C@H](C(=O)O)C)C)C	492	Yes
1026	Ionomycin	C[C@@H](C[C@H](/C(=C/C(=O)[C@H](C[C@H](C[C@@H](CCC(=O)O)C)C)C)/O)C)C/C=C/[C@H]([C@H]([C@H]([C@H](C[C@@H]1CC[C@@](O1)(C)[C@H]1CC[C@@](O1)(C)[C@H](O)C)O)C)O)C	492	No
1027	Antibiotic X 14667B	COC(C(C1OC2(CCC(O2)(C)C2CCC(O2)(CC)C2OC(CC2C)C2OC(O)(COC(=O)NCCc3ccccc3)C(CC2C)C)CC(C1C)O)C)C(C(=O)O)C	493	Yes
1028	Antibiotic X-14667A	COC(C(C1OC2(CC[C@@](O2)(C)C2CC[C@@](O2)(C)C2OC(CC2C)C2O[C@@](O)(COC(=O)NCCc3ccccc3)C(CC2C)C)CC(C1C)O)C)C(C(=O)O)C	493	No
1029	29-O-Methylabierixin	COC1CC(CC(CCC(/C=C(/C(=O)O)\C)C)O)OC2(C1C)OC(CC2C)(C)C1CCC(O1)(C)C1OC(CC1C)C1OC(CO)(OC)C(CC1C)C	494	No
1030	Abierixin	COC[C@@H]1C[C@@H](C[C@@H](CC[C@@H](/C=C(/C(=O)O)\C)C)O)O[C@@]2([C@@H]1C)O[C@](C[C@H]2C)(C)[C@H]1CC[C@@](O1)(C)[C@@H]1O[C@H](C[C@@H]1C)[C@H]1O[C@@](O)(CO)[C@@H](C[C@@H]1C)C	494	No
1031	Grisorixin methyl ester	COC(=O)[C@@H](C1OC(CC[C@@H]1C)CC1C[C@@H](OC)[C@H]([C@]2(O1)O[C@](C[C@H]2C)(C)C1CC[C@@](O1)(C)C1OC(C[C@@H]1C)C1O[C@](C)(O)[C@H](C[C@@H]1C)C)C)C	494	No
1032	Desoxynigericin	CO[C@@H]1C[C@@H](C[C@H]2CC[C@@H](C(O2)C(C(=O)O)C)C)O[C@@]2([C@@H]1C)OC(CC2C)(C)C1CCC(O1)(C)C1OC(C[C@@H]1C)C1O[C@](C)(O)[C@@H](C[C@@H]1C)C	494	No
1033	Grisorixin	CO[C@@H]1C[C@@H](C[C@H]2CC[C@@H](C(O2)C(C(=O)O)C)C)O[C@@]2([C@@H]1C)OC(CC2C)(C)C1CCC(O1)(C)C1O[C@H](C[C@@H]1C)[C@H]1O[C@](C)(O)[C@@H](C[C@@H]1C)C	494	No
1034	F-01A	CO[C@@H]1C[C@@H](C[C@H]2CC[C@@H]([C@@H](O2)[C@H](C(=O)O)C)C)OC2([C@@H]1C)O[C@@](C[C@@H]2C)(C)[C@@H]1CC[C@](O1)(C)[C@@H]1O[C@H](C[C@@H]1C)[C@H]1O[C@](CO)(OC)[C@@H](C[C@@H]1C)C	494	No
1035	Nigericin	CO[C@@H]1C[C@@H](C[C@H]2CC[C@@H](C(O2)[C@H](C(=O)O)C)C)O[C@@]2([C@@H]1C)O[C@](C[C@H]2C)(C)C1CC[C@@](O1)(C)C1OC(C[C@@H]1C)C1O[C@@](O)(CO)[C@@H](C[C@@H]1C)C	494	Yes
1036	Epigrisorixin	CO[C@@H]1C[C@@H](C[C@H]2CC[C@@H]([C@@H](O2)[C@H](C(=O)O)C)C)O[C@@]2([C@@H]1C)O[C@](C[C@H]2C)(C)[C@H]1CC[C@@](O1)(C)[C@@H]1O[C@H](C[C@@H]1C)[C@H]1O[C@](C)(O)[C@H](C[C@@H]1C)C	494	No
1037	Octacyclomycin	COC1CCC(OC1C)OC1CC(OC1C1(C)CCC(O1)C1(C)CCC2(O1)CC(O)C(C(O2)C(C1OC(O)(CC(=O)O)C(C(C1OC)OC1CCC(C(O1)C)OC)C)C)C)C1OC(O)(CO)C(CC1C)C	495	Yes
1038	Moyukamycin	CO[C@H]1CC[C@@H](O[C@@H]1C)OC[C@@H]1CC[C@@H](OC21O[C@H](C[C@@H]2C)[C@H]1O[C@](C)(O)[C@@H](C[C@@H]1C)C)[C@]1(C)CCC2(O1)C[C@H](O)[C@H]([C@H](O2)[C@H](/C=C(/C(=O)/C(=C/[C@@H](C(=O)O)C)/C)\C)C)C	496	No
1039	3'-Hydroxydianemycin	CC/C=C(/C(=O)C(CC(C(=O)O)C)C)\C[C@@]1(C)COC2(C[C@@H]1O)CC[C@@](O2)(C)C1C[C@H](O[C@@H]2C[C@@H](O)[C@@H]([C@H](O2)C)OC)[C@H](C2(O1)OC(C[C@H]2C)C1O[C@@](O)(CO)[C@@H](C[C@@H]1C)C)C	496	No
1040	TM-531B	CC/C=C(/C(=O)C(CC(C(=O)O)C)C)\C[C@@]1(C)COC2(C[C@@H]1O)CC[C@@](O2)(C)C1C[C@H](O[C@@H]2CC[C@@H]([C@H](O2)C)O)[C@H](C2(O1)OC(C[C@H]2C)C1O[C@@](O)(CO)[C@@H](C[C@@H]1C)C)C	496	No
1041	A 130C	CO[C@H]1CC[C@@H](O[C@@H]1C)O[C@@H]1CC(O[C@]2([C@@H]1C)CC[C@@](O2)(C)C1CC[C@H](C2(O1)OC(C[C@@H]2C)C1O[C@@](O)(CO)[C@H](C[C@@H]1C)C)C)[C@H](/C=C(/C(=O)[C@@H](C[C@@H](C(=O)O)C)C)\C)C	496	No
1042	CP 80219	COC1CCC(OC1C)OC1C(C)C(OC(C1C)(O)CO)C1CC(C2(O1)OC(CCC2C)C1(C)CCC2(O1)CC(O)C(C(O2)C(/C=C(/C(=O)C(CC(C(=O)O)C)C)\C)C)C)C	496	No
1043	Endusamycin	CO[C@H]1CC[C@@H](O[C@@H]1C)O[C@@H]1C[C@@]2(O[C@]1(C)[C@H]1CC[C@H](C3(O1)O[C@H](C[C@@H]3C)[C@@H]1O[C@](O)(CO)[C@H](C[C@H]1C)C)C)C[C@H](O)[C@H]([C@H](O2)[C@H](/C=C(/C(=O)[C@@H](C[C@@H](C(=O)O)C)C)\C)C)C	496	No
1044	Lenoremycin	CO[C@H]1CC[C@@H](O[C@@H]1C)O[C@@H]1C[C@H](O[C@]2([C@@H]1C)CC[C@@](O2)(C)[C@H]1CC[C@H]([C@]2(O1)O[C@H](C[C@@H]2C)[C@H]1O[C@@](O)(CO)[C@@H](C[C@@H]1C)C)C)[C@H](/C=C(/C(=O)[C@@H](C[C@@H](C(=O)O)C)C)\C)C	496	No
1045	Lenoremycin sodium salt	[Na]OC(=O)[C@H](C[C@H](C(=O)/C(=C/[C@@H]([C@@H]1C[C@@H](OC2CCC(C(O2)C)OC)[C@H]([C@@]2(O1)CC[C@@](O2)(C)C1CC[C@H]([C@]2(O1)O[C@H](C[C@@H]2C)[C@H]1O[C@@](O)(CO)[C@@H](C[C@@H]1C)C)C)C)C)/C)C)C	496	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1046	Leuseramycin	COC1CCC(OC1C)OC1CC(OC2(C1C)OC(CC2C)C1OC(C)(O)C(CC1C)C)C1(C)CCC2(O1)CC(O)C(C(O2)C(/C=C(/C(=O)C(CC(C(=O)O)C)C)\C)C)C	496	No
1047	Nanchangmycin	CO[C@H]1CCC(O[C@@H]1C)O[C@H]1CC(O[C@@]2([C@@H]1C)OC(C[C@@H]2C)C1O[C@@](O)(CO)[C@@H](C[C@@H]1C)C)[C@]1(C)CC[C@@]2(O1)C[C@H](O)[C@H](C(O2)[C@H](/C=C(/C(=O)[C@@H](C[C@@H](C(=O)O)C)C)\C)C)C	496	Yes
1048	Antibiotic X 14931A	OCC1(O)OC(C(CC1C)C)C1CC(C2(O1)OC(CCC2C)C1(C)CCC2(O1)CC(O)C(C(O2)C(/C=C(/C(=O)C(CC(C(=O)O)C)C)\C)C)C)C	496	No
1049	26-Deoxylaidlomycin	CCC(=O)OC(C(C(=O)O)C)C(C1OC2(CCC(O2)(C)C2CCC(O2)(C)C2OC(CC2C)C2OC(C)(O)C(CC2C)C)CC(C1C)O)C	497	No
1050	Laidlomycin	CCC(=O)OC(C(C(=O)O)C)C(C1OC2(CCC(O2)(C)C2CCC(O2)(C)C2OC(CC2C)C2OC(O)(CO)C(CC2C)C)CC(C1C)O)C	497	No
1051	26-Deoxymonensin B	COC(C(C1OC2(CCC(O2)(C)C2CCC(O2)(C)C2OC(CC2C)C2OC(C)(O)C(CC2C)C)CC(C1C)O)C)C(C(=O)O)C	497	Yes
1052	3-O-Demethylmonensin B	OC[C@]1(O)OC(C2C[C@@H](C(O2)[C@]2(C)CCC(O2)[C@]2(C)CC[C@@]3(O2)C[C@H](O)[C@H](C(O3)[C@H]([C@H]([C@@H](C(=O)O)C)O)C)C)C)[C@H](C[C@H]1C)C	497	No
1053	Monensin	CO[C@@H]([C@H]([C@H]1O[C@@]2(CC[C@](O2)(C)[C@H]2CC[C@@](O2)(CC)[C@H]2O[C@@H](C[C@H]2C)[C@H]2O[C@@](O)(CO)[C@@H](C[C@@H]2C)C)C[C@@H]([C@H]1C)O)C)[C@H](C(=O)O)C	497	No
1054	Monensin B	COC(C(C1OC2(OCC(C2)(C)C2CCC(O2)(C)C2OC(CC2C)C2OC(O)(CO)C(CC2C)C)CC(C1C)O)C)C(C(=O)O)C	497	No
1055	26-Deoxymonensin A	COC(C(C1OC2(CCC(O2)(C)C2CCC(O2)(CC)C2OC(CC2C)C2OC(C)(O)C(CC2C)C)CC(C1C)O)C)C(C(=O)O)C	497	No
1056	Mutalomycin	COC1C(C)C(OC(C1C)(O)C(C(=O)O)C)C(C1OC2(CCC(O2)(C)C2CCC(O2)(C)C2OC(CC2C)C2OC(C)(O)C(CC2C)C)CC(C1C)O)C	497	No
1057	Arenaric acid	CO[C@@H]1C[C@@H](C[C@@H]2O[C@](O)([C@H](C(=O)O)O)[C@H]([C@@H]([C@@]2(C)OC)OC)C)O[C@@]2([C@@H]1C)O[C@]([C@@H]([C@H]2C)OC)(C)[C@H]1CC[C@H](O1)[C@H]1CC[C@@H](O1)[C@H]([C@H](/C=C(/C(=O)C)\C)C)O	498	No
1058	K-41	CO[C@@H]1C[C@@H](C[C@@H]2O[C@](O)([C@H](C(=O)O)O)[C@H]([C@@H]([C@@]2(C)OC)OC)C)O[C@@]2([C@@H]1C)O[C@]([C@@H]([C@H]2C)OC)(C)[C@H]1CC[C@H](O1)[C@H]1CC[C@@H](O1)[C@H]1O[C@](C)(O)[C@@H]([C@H]([C@@H]1C)O[C@H]1CC[C@@H]([C@H](O1)C)OC)C	498	Yes
1059	W341C	CCO[C@H]1[C@H](OC)[C@H](C)[C@@H](O[C@]1(O)[C@H](C(=O)O)C)CC1C[C@@H](OC)[C@H]([C@]2(O1)O[C@@H](C[C@H]2C)C1O[C@@H](CC1OC1CC[C@@H]([C@H](O1)C)OC)[C@H]1CC[C@@H](O1)[C@H]1O[C@](C)(O)[C@@H](C[C@@H]1C)C)C	498	No
1060	Antibiotic 6016	CO[C@@H]1C[C@@H](C[C@@H]2O[C@@](O)([C@H]([C@@H]([C@@H]2C)OC)C)[C@H](C(=O)O)O)O[C@@]2([C@@H]1C)O[C@](C[C@H]2C)(C)[C@@H]1O[C@@H](C[C@H]1OC1CC[C@@H]([C@H](O1)C)OC)[C@H]1CC[C@@H](O1)[C@H]1O[C@](C)(O)[C@@H](C[C@@H]1C)C	498	No
1061	(R)-2-((2S,3S,4S,5S,6S)-6-(((2R,3R,4R,5S,7S,9R,10R)-3,9-dimethoxy-2-((2S,2'R,5R,5'R)-5'-((2S,3S,4S,5R,6S)-6-methoxy-4-(((2R,5S,6R)-5-methoxy-6-methyltetrahydro-2H-pyran-2-yl)oxy)-3,5,6-trimethyltetrahydro-2H-pyran-2-yl)octahydro-[2,2'-bifuran]-5-yl)-2,4,10-trimethyl-1,6-dioxaspiro[4.5]decan-7-yl)methyl)-2-hydroxy-4,5-dimethoxy-3,5-dimethyltetrahydro-2H-pyran-2-yl)-2-hydroxyacetic acid	CO[C@@H]1C[C@@H](C[C@@H]2O[C@](O)([C@H](C(=O)O)O)[C@H]([C@@H]([C@@]2(C)OC)OC)C)O[C@@]2([C@@H]1C)O[C@]([C@@H]([C@H]2C)OC)(C)[C@H]1CC[C@H](O1)[C@H]1CC[C@@H](O1)[C@H]1O[C@](C)(OC)[C@@H]([C@H]([C@@H]1C)O[C@H]1CC[C@@H]([C@H](O1)C)OC)C	498	No
1062	CP 96797	COC1CC(CC2OC(O)(C(C(=O)O)O)C(C(C2(C)OC)OC)C)OC2(C1C)OC(CC2C)(C)C1CCC(O1)C1CCC(O1)C1OC(C)(O)C(C(C1C)OC1CCC(C(O1)C)OC)C	498	No
1063	Terrosamycin A	C[C@H]1C[C@@H](C)[C@](O[C@@H]1C[C@@]1(O)O[C@@H](C[C@H]2CC[C@@H]([C@H](O2)[C@H](C(=O)[O])C)C)[C@@H](C[C@@H]1C)C)(O)C[C@H]([C@H](C(=O)[C@@]([C@@H]1CC[C@@](O1)(C)[C@H]1CC[C@@]([C@@H](O1)C)(C)O)(O)C)C)O	499	Yes
1064	Terrosamycin B	CO[C@]1(O[C@H](C[C@@]2(OC)O[C@@H](C[C@H]3CC[C@@H]([C@H](O3)[C@H](C(=O)O)C)C)[C@@H](C[C@@H]2C)C)[C@H](C[C@H]1C)C)C[C@H]([C@H](C(=O)[C@@]([C@@H]1CC[C@@](O1)(C)[C@H]1CC[C@@]([C@@H](O1)C)(C)O)(O)C)C)O	499	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1065	Emericid	CO[C@H]1CC2(CC[C@@](O2)(C)C2CC[C@@](O2)(C)C2OC([C@@H]([C@@H]2C)OC)C2O[C@](C)(O)[C@@H]([C@H]([C@@H]2C)OC)C)OC([C@@H]1C)[C@H](C1O[C@](O)([C@@H]([C@H]([C@H]1C)OC)C)[C@@H](C(=O)O)C)C	500	Yes
1066	K 41B	COC1CC(CC2OC(O)(C(C(=O)O)O)C(C(C2(C)OC)CC)O)OC2(C1C)OC(C(C2C)OC1CCC(C(O1)C)OC)(C)C1CCC(O1)C1CCC(O1)C1OC(C)(O)C(C(C1C)OC1CCC(C(O1)C)OC)C	501	Yes
1067	Septamycin	CO[C@@H]1C[C@@H](C[C@@H]2O[C@](O)([C@H](C(=O)O)C)[C@@H]([C@@H]([C@@]2(C)O[C@H]2CC[C@@H]([C@H](O2)C)OC)OC)C)O[C@@]2([C@@H]1C)O[C@]([C@@H]([C@H]2C)OC)(C)C1CC[C@H](O1)[C@H]1CC[C@@H](O1)C1O[C@](C)(O)[C@@H](C[C@@H]1C)C	502	Yes
1068	Alborixin	CC[C@@H]1O[C@H](CC[C@@]1(C)O)[C@]1(C)C[C@H]([C@](O1)(O)[C@]1(C)CC[C@H](O1)[C@H]([C@]1(O)O[C@H](C[C@@]2(O)O[C@H](CC[C@@H]2C)[C@H]([C@@H](C[C@@H]2O[C@@H]([C@H](C[C@H]2C)C)[C@H](C(=O)O)C)O)C)[C@H](C[C@H]1C)C)O)C	503	Yes
1069	Duocarmycin Sa	COc1cc2cc([nH]c2c(c1OC)OC)C(=O)N1CC2[C@]3(C1=CC(=O)c1c3cc([nH]1)C(=O)OC)C2	504	Yes
1070	Chlorizidine A	Clc1cc2n(c1Cl)C(=O)c1c2cc(O)c(c1O)[C@@H]1CCc2n1c(Cl)c(c2)Cl	505	Yes
1071	Actinofuranone B	C/C=C(/C([C@@H](/C=C/C=C(/CC/C=C/C1=C(C)C(=O)C(O1)(C)O)\C)C)O)\C	506	No
1072	E-875	CC=C(C(C(C=CC=C(CCC(CC1=C(C)C(=O)C(O1)(C)O)O)C)C)O)C	506	No
1073	SCHEMBL14571373	C/C=C(/C(/C=C/C=C(/CCC(CC1=C(C)C(=O)C(O1)(C)O)O)\C)C)O)\C	506	No
1074	Actinofuranone A	C/C=C(/[C@@H]([C@@H](/C=C/C=C(/CC[C@H](CC1=C(C)C(=O)C(O1)(C)O)O)\C)C)O)\C	506	No
1075	5-[(5E,7E,11E)-2,10-Dihydroxy-9,11-dimethyl-5,7,11-tridecatrien-1-yl]-2-hydroxy-2-(1-hydroxyethyl)-4-methyl-3(2H)-furanone	C/C=C(/C(C(/C=C/C=C/CCC(CC1=C(C)C(=O)C(O1)(O)C(O)C)O)C)O)\C	506	No
1076	Actinofuranone E	CCC(/C=C(/[C@H]([C@@H](/C=C/C=C/CC[C@H](CC1=C(C)C(=O)C(O1)(O)C(O)C)O)C)O)\C)O	506	No
1077	Actinofuranone I	CC/C=C(/C(C(/C=C/C=C/CC[C@H](CC1=C(C)C(=O)C(O1)(O)C(O)C)O)(O)C)O)\C	506	No
1078	Actinofuranone D	CCC(/C=C(/[C@@H]([C@@H](/C=C/C=C/CC[C@H](CC1=C(C)C(=O)C(O1)(O)C(O)C)O)C)O)\C)O	506	No
1079	Actinofuranone H	CC/C=C(/[C@@H]([C@@H](/C=C/C=C/CC[C@H](CC1=C(C)C(=O)C(O1)(O)C(O)C)O)C)O)\C	506	No
1080	E-492	OC(CC1=C(C)C(=O)C(O1)(O)C(O)C)CCC=CC=CC(C(C(=C)C)O)C	506	Yes
1081	E-975	CC/C=C(/C(C(/C=C/C=C/CCC(CC1=C(C)C(=O)C(O1)(O)C(O)C)O)C)O)\C	506	No
1082	Actinofuranone F	CC(C/C=C(/[C@@H]([C@@H](/C=C/C=C/CC[C@H](CC1=C(C)C(=O)C(O1)(O)C(O)C)O)C)O)\C)O	506	No
1083	JBIR-108	CCC/C=C(/[C@@H]([C@@H](/C=C/C=C/CC[C@H](CC1=C(C)C(=O)C(O1)(O)C(O)C)O)C)O)\C	506	No
1084	Salinomycin	CC[C@H]([C@H]1O[C@]2(C=C[C@H]([C@@]3(O2)CC[C@@](O3)(C)[C@H]2CC[C@](C[C@@H](O2)C)(O)CC)O)[C@@H](C[C@@H]1C)C)C(=O)[C@H]([C@H]([C@@H]([C@@H]1O[C@H](CC[C@@H]1C)[C@H](C(=O)O)CC)C)O)C	507	Yes
1085	Deoxy(O-8)-salinomycin	CC[C@H]([C@H]1O[C@]2(C=CC[C@@]3(O2)CC[C@@](O3)(C)[C@H]2CC[C@](C[C@@H](O2)C)(O)CC)[C@@H](C[C@@H]1C)C)C(=O)[C@H]([C@H]([C@@H]([C@@H]1O[C@H](CC[C@@H]1C)[C@@H](C(=O)O)CC)C)O)C	508	Yes
1086	17-Epi-deoxy(O-8)-salinomycin	CC[C@H]([C@H]1O[C@@]2(C=CCC3(O2)CC[C@@](O3)(C)[C@H]2CC[C@](C[C@@H](O2)C)(O)CC)[C@@H](C[C@@H]1C)C)C(=O)[C@H]([C@H]([C@@H]([C@@H]1O[C@H](CC[C@@H]1C)C(C(=O)O)CC)C)O)C	508	No
1087	Ferensimycin A	CCC(C(=O)C(C(C(C1OC(O)(C(CC1C)C)C(C(=O)O)C)C)O)C)C1OC(CC1C)(C)C1(O)OC(CC1C)(CC)C(O)C	509	Yes
1088	Inostamycin	CCC[C@@H]([C@]1(CC)C[C@H]([C@](O1)(O)[C@]1(C)C[C@H](C(O1)[C@H](C(=O)[C@H]([C@@H]([C@H](C1O[C@](O)([C@H]([C@@H]([C@H]1CC)O)C)[C@@H](C(=O)O)CC)C)O)C)CC)C)C)O	509	No
1089	Noboritomycin B	CCOC(=O)C1OC(C[C@H]1O)C1(C)OC2(C([C@H]1OC)C)OC1(C=CC2O)O[C@@H]([C@H](C[C@H]1C)C)C(C(=O)[C@H](C([C@@H](CC(c1ccc(c(c1C(=O)O)O)CC)C)C)O)C)C	510	Yes
1090	6-Chloronoboritomycin	CCOC(=O)[C@H]1O[C@H](C[C@H]1O)[C@@]1(C)O[C@@]2([C@@H]([C@H]1OC)C)O[C@]1(C=C[C@H]2O)O[C@@H]([C@H](C[C@H]1C)C)[C@H](C(=O)[C@H]([C@H]([C@@H](C[C@@H](c1c(Cl)cc(c(c1C(=O)O)O)C)C)C)O)C)C	510	No
1091	Antibiotic X-14766A	CCOC(=O)C1OC(C[C@H]1O)[C@@]1(C)OC2([C@@H]([C@H]1OC)C)O[C@]1(C=C[C@H]2O)OC([C@H](C[C@H]1C)C)[C@H](C(=O)[C@H]([C@H]([C@@H](C[C@@H](c1c(Cl)cc(c(c1C(=O)O)O)C)C)C)O)C)C	511	No
1092	Noboritomycin	CCOC(=O)[C@H]1O[C@H](C[C@H]1O)[C@@]1(C)O[C@@]2([C@@H]([C@H]1OC)C)O[C@]1(C=C[C@H]2O)O[C@@H]([C@H](C[C@H]1C)C)[C@H](C(=O)[C@H]([C@H]([C@@H](C[C@@H](c1ccc(c(c1C(=O)O)O)C)C)C)O)C)C	511	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1093	Noboritomycin A	CCOC(=O)C1OC(C[C@H]1O)C1(C)OC2(C([C@H]1OC)C)OC1(C=CC2O)O[C@@H]([C@H](C[C@H]1C)C)C(C(=O)[C@H](C([C@@H](CC(c1ccc(c(c1C(=O)O)O)C)C)C)O)C)C	511	No
1094	Sekgranaticin	OC(=O)C[C@@H]1O[C@@H](C)[C@@]23[C@@H]([C@@H]1Oc1c2c(=O)oc(c1)Cc1cccc2c1c(=O)cc(o2)C)C(=O)c1c(C3=O)c(O)c2c(c1O)[C@H]1C[C@H]([C@]2(O)[C@H](O1)C)O	512	Yes
1095	MC 033	O[C@@H]1C[C@@H](O[C@H]2CCCC3C2C=CC2[C@@]3(C)C(=O)OC3=C(O)C4(OC3=O)C[C@@H](C)C(=CC4/C=C\CCCC2)C(=O)O)O[C@@H]([C@H]1O[C@@H]1C[C@@H](O)[C@@H]([C@H](O1)C)OC(=O)c1c(O)ccc(c1C)Cl)C	513	No
1096	MC 032	OC1[C@H](O[C@H]2CCCC3C2C=CC2[C@@]3(C)C(=O)OC3=C(O)C4(OC3=O)C[C@@H](C)C(=CC4/C=C\CCCC2)C(=O)O)O[C@@H]([C@H]([C@@H]1O)O[C@H]1C[C@@H](OC(=O)c2c(O)ccc(c2C)Cl)[C@@H]([C@H](O1)C)O)C	513	No
1097	MC-031	O[C@@H]1C[C@H](O[C@H]2CCCC3C2C=CC2[C@@]3(C)C(=O)OC3=C(O)C4(OC3=O)C[C@@H](C)C(=CC4/C=C\CCCC2)C(=O)O)O[C@@H]([C@H]1O[C@H]1C[C@@H](OC(=O)c2c(O)ccc(c2C)Cl)[C@@H]([C@H](O1)C)O)C	513	Yes
1098	MC 034	OC1[C@H](O[C@H]2CCCC3C2C=CC2[C@@]3(C)C(=O)OC3=C(O)C4(OC3=O)C[C@@H](C)C(=CC4/C=C\CCCC2)C(=O)O)O[C@@H]([C@H]([C@@H]1O)O[C@H]1C[C@@H](O)[C@@H]([C@H](O1)C)OC(=O)c1c(O)ccc(c1C)Cl)C	513	No
1099	Chlorothricin	COc1ccc(c(c1C(=O)O[C@@H]1C[C@H](O[C@H]2[C@H](O)C[C@@H](O[C@@H]2C)O[C@H]2CCC[C@@H]3[C@@H]2C=C[C@@H]2[C@@]3(C)C(=O)OC3=C(O)[C@]4(OC3=O)C[C@@H](C)C(=C[C@H]4/C=C/CCCC2)C(=O)O)O[C@@H]([C@H]1O)C)C)Cl	513	No
1100	Strepantibin B	O=C1C=C(c2ccccc2)C2=NC(OC2=C1c1ccccc1)(C)C	514	Yes
1101	Phosphatidylinositolmannoside	CCCCCCCCCCCCCCCC(=O)O[C@@H](COP(=O)(OC1C(OC2O[C@H](CO)[C@H]([C@@H]([C@@H]2O)O)O)C(O)C(C(C1OC1O[C@H](CO)[C@H]([C@@H]([C@@H]1O)O)O)O)O)O)COC(=O)CCCCCCCCCC(CCCCCCCC)C	515	Yes
1102	Rha-Rha-C10-C10	CCCCCCCC(OC1OC(C)[C@@H]([C@@H]([C@@H]1OC1OC(C)[C@@H]([C@@H]([C@@H]1O)O)O)O)O)CC(=O)OC(CC(=O)O)CCCCCCC	516	Yes
1103	Astolide A	CC[C@H]([C@H]([C@@H]([C@@H]([C@@H]([C@H]([C@@H]1OC(=O)C=CCC(O)CC(O)CCCC(O)CCC(C)[C@H](O)C(=O)[C@]2(O[C@@H](C[C@H](C[C@@H](C[C@@H](CCCC(C=C[C@H]1C)O)O)O)O)C[C@@H](O)[C@@H]2O)O)C)O)C)O)C)O[C@H]1O[C@H](C)[C@@H]([C@@](C1)(C)O)O[C@@H]1CC[C@H]([C@H](O1)C)OC(=O)[C@@H]([C@@H](c1ccc2c(c1)C(=O)C=C(C2=O)C)O[C@@H]1CC[C@H]([C@H](O1)C)O)C	517	Yes
1104	Astolide B	CC[C@@H]([C@@H]([C@H]([C@H]([C@H]([C@@H]([C@H]1OC(=O)C=CCC(O)CC(O)CCCC(O)CCC(C)[C@@H](O)C(=O)[C@@]2(O[C@H](C[C@@H](C[C@H](C[C@H](CCCC(C=C[C@@H]1C)O)O)O)O)C[C@H](O)[C@H]2O)O)C)O)C)O)C)O[C@@H]1O[C@@H](C)[C@H]([C@](C1)(C)O)O[C@H]1C[C@H](O)[C@@H]([C@@H](O1)C)OC(=O)[C@H]([C@H](c1ccc2c(c1)C(=O)C=C(C2=O)C)O[C@H]1CC[C@@H]([C@@H](O1)C)O)C	518	Yes
1105	PM100117	CCC(C(C(C(C(C(C1OC(=O)C=CCC(O)CC(O)CCCC(O)CCC(C)C(O)C(=O)C2(OC(CC(CC(CC(CCCC(C=CC1C)O)O)O)O)CC(O)C2)O)C)O)C)O)C)OC1OC(C)C(C(C1)(C)O)OC1CC(O)C(C(O1)C)OC(=O)C(C(c1ccc2c(c1)C(=O)C=C(C2=O)C)OC1CCC(C(O1)C)O)C	519	Yes
1106	PM100118	CCC(C(C(C(C(C(C1OC(=O)C=CCC(O)CC(O)CCCC(O)CCC(C)C(O)C(=O)C2(OC(CC(CC(CC(CCCC(C=CC1C)O)O)O)O)CC(O)C2)O)C)O)C)O)C)OC1OC(C)C(C(C1)(C)O)OC1CCC(C(O1)C)OC(=O)C(C(c1ccc2c(c1)C(=O)C=C(C2=O)C)OC1CCC(C(O1)C)O)C	520	Yes
1107	Fattiviracin A1	OCC1OC(OC(CCCCCCCCCCCCCCCC(O)C)CCCCCCCCCCCCCCCC2CC(=O)OCC3OC(OC(CC(=O)OCC4OC(O2)C(O)C(C4O)O)CCCCCCCCCCCCCC(OC2OC(CO)C(C(C2O)O)O)CCCCCC(O)C)C(C(C3O)O)O)C(C(C1O)O)O	521	Yes
1108	Fattiviracin FV-8	OC[C@H]1O[C@@H](OC(CCCCCC(O)C)CCCCCCCCCCCCCC2CC(=O)OCC3OC(OC(CC(=O)OCC4OC(O2)[C@@H](O)[C@@H]([C@H]4O)O)CCCCCCCCCCCC(O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O)O)O)CCCCCC(O)C)[C@@H]([C@H]([C@@H]3O)O)O)[C@@H]([C@H]([C@@H]1O)O)O	522	Yes
1109	Antibiotic T 23IX	CCCCC(=O)N[C@@H](CO[C@H]1C/C=C/C=C/C=C\[C@H](OC)CC(=O)Nc2c(c(CC/C=C(\[C@@H]([C@@H]1C)O)/C)cc(O)c2)O)C	523	No
1110	D-Alanine, N-(2-methyl-1-oxopropyl)-, (5R,6E,8E,10E,13S,14R,15R,16Z)-15,22,24-trihydroxy-5-methoxy-14,16-dimethyl-3-oxo-2-azabicyclo[18.3.1]tetracosa-1(24),6,8,10,16,20,22-heptaen-13-yl ester	CO[C@H]1/C=C/C=C/C=C/C[C@H](OC(=O)[C@H](NC(=O)C(C)C)C)[C@@H](C)[C@H](/C(=C/CCc2c(c(NC(=O)C1)cc(O)c2)O)/C)O	523	No
1111	D-Alanine, N-(3-methyl-1-oxobutyl)-, (5R,6E,8E,10E,13S,14R,15R,16Z)-15,22,24-trihydroxy-5-methoxy-	CO[C@H]1/C=C/C=C/C=C/C[C@H](OC(=O)[C@H](NC(=O)CC(C)C)C)[C@@H](C)[C@H](/C(=C/CCc2c(c(NC(=O)C1)cc(O)c2)O)/C)O	523	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	14,16-dimethyl-3-oxo-2-azabicyclo[18.3.1]tetracosa-1(24),6,8,10,16,20,22-heptaen-13-yl ester			
1112	Mycotrienin II	CO[C@H]1/C=C/C=C/C=C/C[C@H](OC(=O)[C@H](NC(=O)C2CCCCC2)C)[C@@H](C)[C@H](/C(=C/CCc2c(c(NC(=O)C1)cc(O)c2)O)/C)O	523	No
1113	Cytotrienin A	CO[C@H]1/C=C/C=C/C=C/C[C@H](OC(=O)C2(CC2)NC(=O)C2=CCCCC2)[C@H](C)[C@H](/C(=C\CCc2c(c(NC(=O)C1)cc(O)c2)O)/C)O	523	No
1114	Ansatrienin B	CO[C@H]1/C=C\C=C/C=C\C[C@H](OC(=O)[C@H](NC(=O)C2CCCCC2)C)[C@H](C)[C@H](/C(=C\CCc2c(c(NC(=O)C1)cc(O)c2)O)/C)O	523	No
1115	Trienomycin D	COC1/C=C/C=C/C=C\CC(OC(=O)C(NC(=O)C2=CCCCC2)C)C(C)C(/C(=C/CCc2cc(NC(=O)C1)cc(c2)O)/C)O	523	No
1116	D-Alanine, N-(2-methyl-1-oxopropyl)-, (5R,6E,8E,10E,13S,14R,15R,16Z)-15,22-dihydroxy-5-methoxy-14,16-dimethyl-3-oxo-2-azabicyclo[18.3.1]tetracosa-1(24),6,8,10,16,20,22-heptaen-13-yl ester	CO[C@H]1/C=C/C=C/C=C/C[C@H](OC(=O)[C@H](NC(=O)C(C)C)C)[C@@H](C)[C@H](/C(=C/CCc2cc(NC(=O)C1)cc(c2)O)/C)O	523	No
1117	Trienomycin B	CO[C@H]1/C=C/C=C/C=C/C[C@H](OC(=O)[C@H](NC(=O)CC(C)C)C)[C@H](C)[C@H](/C(=C\CCc2cc(NC(=O)C1)cc(c2)O)/C)O	523	No
1118	Trienomycin K	CCCC(=O)N[C@@H](C(=O)O[C@H]1CC=CC=CC=C[C@H](OC)CC(=O)Nc2cc(CCC=C([C@@H]([C@H]1C)O)C)cc(O)c2)C	523	No
1119	Trienomycin A	COC1/C=C/C=C/C=C\CC(OC(=O)C(NC(=O)C2CCCCC2)C)C(C)C(/C(=C/CCc2cc(NC(=O)C1)cc(c2)O)/C)O	523	No
1120	Thiazinotrienomycin E	COC1/C=C/C=C/C=C/CC(OC(=O)C(NC(=O)C2CCCCC2)C)C(C)C(/C(=C\CCc2c(c(NC(=O)C1)cc1NC(=O)CSc21)O)/C)O	523	No
1121	Benzoxazomycin	COC1CC(=O)N2C1C1/C=C\C=C\CC(OC(=O)C(NC(=O)C3CCCCC3)C)C(C)C(/C(=C/CCc3c(O1)c2cc(c3)O)/C)O	523	No
1122	D-Alanine, N-(2-methyl-1-oxopropyl)-, (3R,3aS,4S,16S,17R,18R)-2,3,3a,4-tetrahydro-8,18-dihydroxy-3-methoxy-17,19-dimethyl-1-oxo-4,6-[1,3,9]dodecatrieno-1H-pyrrolo[2,1-c][1,4]benzoxazin-16-yl ester	COC1CC(=O)N2C1C1/C=C\C=C\CC(OC(=O)C(NC(=O)C(C)C)C)C(C)C(/C(=C/CCc3c(O1)c2cc(c3)O)/C)O	523	No
1123	D-Alanine, N-(3-methyl-1-oxobutyl)-, (1R,12Z,14R,15R,16S,18E,20E,22S,22aS)-2,3,10,11,14,15,16,17,22,22a-decahydro-7,14-dihydroxy-1-methoxy-13,15-dimethyl-3-oxo-1H-22,5,9-(epoxymethyno)pyrrolo[1,2-a]azacycloeicosin-16-yl ester	COC1CC(=O)N2C1C1/C=C\C=C\CC(OC(=O)C(NC(=O)CC(C)C)C)C(C)C(/C(=C/CCc3c(O1)c2cc(c3)O)/C)O	523	Yes
1124	D-Alanine, N-(4-methyl-1-oxopentyl)-, (1R,12Z,14R,15R,16S,18E,20E,22S,22aS)-2,3,10,11,14,15,16,17,22,22a-decahydro-7,14-dihydroxy-1-methoxy-	COC1CC(=O)N2C1C1/C=C\C=C\CC(OC(=O)C(NC(=O)CCC(C)C)C)C(C)C(/C(=C/CCc3c(O1)c2cc(c3)O)/C)O	523	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	13,15-dimethyl-3-oxo-1H-22,5,9-(epoxymethyno)pyrrolo[1,2-a]azacycloeicosin-16-yl ester			
1125	Trienomycin E	CO[C@H]1/C=C\C=C/C=C\C[C@H](OC(=O)[C@H](NC(=O)CCC(C)C)C)[C@@H](C)[C@H](/C(=C\Cc2cc(NC(=O)C1)cc(c2)O)/C)O	523	No
1126	Quinotrierixin	COC1/C=C/C=C/C=C/CC(OC(=O)C(NC(=O)C2CCCCC2)C)C(C)C(/C(=C\CCC2=C(C(=O)C=C(NC(=O)C1)C2=O)SC)/C)O	524	Yes
1127	Trienomycin L	CO[C@H]1C=CC=CC=CC[C@H](O)[C@H](C)[C@H](C(=CCCc2cc(NC(=O)C1)cc(c2)O)C)OC(=O)[C@H](NC(=O)CC(C)C)C	525	Yes
1128	Trienomycin G	COC1/C=C\C=C/C=C\CC(O)C(C)C(/C(=C\CCc2cc(NC(=O)C1)cc(c2)O)/C)OC(=O)[C@H](NC(=O)C1CCCCC1)C	525	No
1129	Ansatrienin A3	COC1/C=C/C=C/C=C/CC(OC(=O)C(NC(=O)CC(C)C)C)C(C)C(/C(=C\CCC2=CC(=O)C=C(NC(=O)C1)C2=O)/C)O	526	No
1130	Antibiotic T 23VIII	CO[C@H]1/C=C/C=C/C=C/C[C@H](OC(=O)[C@H](NC(=O)CCC(C)C)C)[C@@H](C)[C@H](/C(=C/CCC2=CC(=O)C=C(NC(=O)C1)C2=O)/C)O	526	No
1131	D-Alanine, N-(2-methyl-1-oxopropyl)-, (5R,6E,8E,10E,13S,14R,15R,16Z)-15-hydroxy-5-methoxy-14,16-dimethyl-3,22,24-trioxo-2-azabicyclo[18.3.1]tetracosa-6,8,10,16,20,23-hexaen-13-yl ester	CO[C@H]1/C=C/C=C/C=C/C[C@H](OC(=O)[C@H](NC(=O)C(C)C)C)[C@@H](C)[C@H](/C(=C/CCC2=CC(=O)C=C(NC(=O)C1)C2=O)/C)O	526	No
1132	Ansatrienin A	COC1/C=C\C=C/C=C\CC(OC(=O)[C@H](NC(=O)C2CCCCC2)C)C(C)C(/C(=C\CCC2=CC(=O)C=C(NC(=O)C1)C2=O)/C)O	526	Yes
1133	Mycotrienin I	CO[C@H]1/C=C/C=C/C=C/C[C@H](OC(=O)[C@H](NC(=O)C2CCCCC2)C)[C@@H](C)[C@H](/C(=C/CCC2=CC(=O)C=C(NC(=O)C1)C2=O)/C)O	526	No
1134	Mycotrienol I	CO[C@H]1/C=C/C=C/C=C/C[C@@H](O)[C@H](C)[C@@H](/C(=C/CCC2=CC(=O)C=C(NC(=O)C1)C2=O)/C)O	527	Yes
1135	Isolauryl 5-hydroxyanthranilate	CC(CCCCCCCCCOC(=O)c1cc(O)ccc1N)C	528	No
1136	Isodecyl 5-hydroxyanthranilate	CC(CCCCCCCOC(=O)c1cc(O)ccc1N)C	528	No
1137	Isoundecyl 5-hydroxyanthranilate	CC(CCCCCCCCOC(=O)c1cc(O)ccc1N)C	528	Yes
1138	Protylonolide	CC[C@H]1OC(=O)C[C@@H](O)[C@H](C)[C@@H](O)[C@@H](CC)C[C@H](C(=O)/C=C/C(=C/[C@@H]1C)/C)C	529	Yes
1139	Pironetin	C/C=C/C[C@@H]([C@H]([C@H]([C@@H](C[C@H]1OC(=O)C=C[C@H]1CC)O)C)OC)C	530	Yes
1140	Prejadomycin 2-carboxylate	OC(=O)C1=C(C)CC2(C(C1=O)c1cc3cccc(c3c(c1C(=O)C2)O)O)O	531	Yes
1141	2,3-Dehydro-UWM6	CC1=CC(=O)[C@H]2[C@](C1)(O)CC(=O)c1c2cc2cccc(c2c1O)O	531	No
1142	Rishirilide C	CC(CC[C@@]1(O)c2cc3c(O)cccc3c(c2C(=O)[C@@H]([C@]1(O)C(=O)O)C)O)C	532	Yes
1143	Eurystatin B	CCC(CC/C=C/C(=O)NC1CCCNC(=O)C(NC(=O)C(=O)C(NC1=O)C)CC(C)C)C	533	Yes
1144	YM-51084	O=CC(NC(=O)[C@H](C(C)C)NC(=O)[C@H](Cc1ccc(cc1)O)NC(=O)CC(C)C)Cc1ccccc1	534	Yes
1145	YM-51085	OCC(NC(=O)[C@H](C(C)C)NC(=O)[C@H](Cc1ccc(cc1)O)NC(=O)CC(C)C)Cc1ccccc1	534	No
1146	Cystargamide B	CCCCCCCC1OC1C(=O)N[C@@H]1[C@H](C)OC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@H](NC(=O)[C@H](NC1=O)Cc1ccccc1)CCC(=O)O)Cc1c[nH]c2c1cc(O)cc2)c1ccc(cc1)O	535	Yes
1147	Bottromycin C2	COC(=O)CC(c1nccs1)NC(=O)C(C(c1ccccc1)C)NC(=O)C/N=C(/C1C(C)C(CN1C(=O)C(C(C)C)NC(=O)C(C(C)(C)C)NC(=O)/C=C/C(C)C)C)\N	536	Yes
1148	Bottromycin B2	COC(=O)CC(c1nccs1)NC(=O)C(C(c1ccccc1)C)NC(=O)C/N=C(/C1CCCN1C(=O)C(C(C)C)NC(=O)C(C(C)(C)C)NC(=O)/C=C/C(C)C)\N	536	No
1149	Ahpatinin C	CC(C[C@@H]([C@H](CC(=O)N[C@H](C(=O)N[C@H]([C@H](CC(=O)O)O)CC(C)C)C)O)NC(=O)[C@H](C(C)C)NC(=O)[C@H](C(C)C)NC(=O)CC(C)C)C	537	No
1150	Ahpatinin (I)Bu	CC(C[C@H]([C@@H](CC(=O)N[C@@H](C(=O)N[C@@H]([C@@H](CC(=O)O)O)Cc1ccccc1)C)O)NC(=O)[C@@H](C(C)C)NC(=O)[C@@H](C(C)C)NC(=O)C(C)C)C	537	Yes
1151	YF-044P-D	OC(=O)CC(C(NC(=O)C(NC(=O)CC(C(NC(=O)C(C(C)C)NC(=O)C(C(C)C)NC(=O)Cc1ccccc1)Cc1ccccc1)O)C)Cc1ccccc1)O	537	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1152	Ahpatinin G	COC(=O)CC(C(Cc1ccccc1)NC(=O)C(NC(=O)CC(C(Cc1ccccc1)NC(=O)C(C(C)C)NC(=O)C(C(C)C)NC(=O)CC(C)C)O)C)O	537	No
1153	Ahpatinin E	COC(=O)CC(C(Cc1ccccc1)NC(=O)C(NC(=O)CC(C(NC(=O)C(C(C)C)NC(=O)C(C(C)C)NC(=O)CC(C)C)CC(C)C)O)C)O	537	No
1154	Bottromycin A2	COC(=O)CC(c1nccs1)NC(=O)C(C(c1ccccc1)C)NC(=O)C(C(C)(C)C)N/C/1=N/CC(=O)N2CCC(C2C(=O)NC(C(=O)NC1C(C)(C)C)C(C)C)C	538	Yes
1155	Bingchamide B	CCC(C1NC(=O)C(CC(C)C)NC(=O)C(Cc2cocc2)N(C(=O)C(NC(=O)C(NC1=O)Cc1ccccc1)Cc1ccccc1)C)C	539	Yes
1156	Bingchamide A	CCC(C1NC(=O)C(CC(C)C)NC(=O)C(Cc2ccccc2)N(C(=O)C(NC(=O)C(NC1=O)Cc1ccccc1)Cc1ccccc1)C)C	539	No
1157	Linearmycin C	NCCCCC(CC(C/C=C/C(C/C=C/C(CC(CC(CC(C/C=C/C(CC(CC(CC(=O)C(C(C/C=C/C=C/C=C/C=C/C=C/C=C/C(C(C(C(/C=C/CC/C=C/C=C/C=C/C=C/C=C/C=C(/C(=O)O)\C)C)O)C)O)O)C)O)O)O)O)O)O)O)O)O)O)O)O)O	540	Yes
1158	Linearmycin B	NCCCC(CC(C/C=C/C(C/C=C/C(CC(CC(CC(C/C=C/C(CC(CC(CC(=O)C(C(C/C=C/C=C/C=C/C=C/C=C/C(C(C(C(/C=C/CC/C=C/C=C/C=C/C=C/C=C(/C(=O)O)\C)C)O)C)O)O)C)O)O)O)O)O)O)O)O)O	541	Yes
1159	Linearmycin A	NCCCC(CC(C/C=C/C(C/C=C/C(CC(CC(CC(C/C=C/C(CC(CC(CC(=O)C(C(C/C=C/C=C/C=C/C=C/C=C/C(C(C(C(/C=C/CC/C=C/C=C/C=C/C=C/C=C(/C(=O)O)\C)C)O)C)O)O)C)O)O)O)O)O)O)O)O)O	542	Yes
1160	Desulfoclethramycin	OC(CC(CC(=O)C(CCC=CC=CC=CC=CC=CC(C(C(C(C=CCCC=CC=CC=C(C(=O)O)C)C)O)C)O)C)O)C=CCC(CC(CC(C=CCC(CC(C=CCC(CC(CCCN=C(N)N)O)O)O)O)O)O)O	543	Yes
1161	Mediomycin B	NCCC[C@@H](C[C@@H](C/C=C/[C@H](C[C@@H](C/C=C/[C@H](C[C@@H](C[C@H](C/C=C/[C@H](C[C@H](CC(=O)C(C(C/C=C/C=C/C=C/C=C/C=C/C=C/C=C/[C@H]([C@@H]([C@H](C(/C=C/CC/C=C/C=C/C=C(/C(=O)O)\C)C)O)C)O)O)C)O)O)O)O)O)O)O)O)O	544	Yes
1162	CHEBI:80047	NCCCC(CC(C/C=C/C(CC(CC(CC(C/C=C/C(CC(CC(CC(=O)C(C(O[C@@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1O)O)O)C/C=C/C=C/C=C/C=C/C=C/C=C/C(C(C(C(/C=C/CC/C=C/C=C/C=C/C=C/C(=O)NC1=C(O)CCC1=O)C)O)C)O)C)O)O)O)O)O)O)O)O)O	545	Yes
1163	Clethramycin	OC(CC(CC(=O)C(C(OS(=O)(=O)O)C/C=C/C=C/C=C/C=C/C=C/C=C/C(C(C(C(/C=C/CC/C=C/C=C/C=C(/C(=O)O)\C)C)O)C)O)C)O)/C=C/CC(CC(CC(/C=C/CC(CC(/C=C/CC(CC(CCCN=C(N)N)O)O)O)O)O)O)O	546	Yes
1164	Mediomycin A	NCCCC(CC(C/C=C/C(CC(C/C=C/C(CC(CC(C/C=C/C(CC(CC(=O)C(C(OS(=O)(=O)O)C/C=C/C=C/C=C/C=C/C=C/C=C/C(C(C(C(/C=C/CC/C=C/C=C/C=C/C=C(/C(=O)O)\C)C)O)C)O)C)O)O)O)O)O)O)O)O)O	547	Yes
1165	Cyanosporaside D	N#CCc1cc(Cl)c2c(c1)[C@@]1(O)[C@H](C=CC1=C2)OC(=O)C	548	Yes
1166	Cyanosporaside E	N#CCc1cc(Cl)c2c(c1)[C@@]1(O)[C@@H](O)C=CC1=C2	548	No
1167	1,8-Dihydroxy-2-methyl-3-(4-methylpentanoyl)phenanthrene-9,10-dione	CC(CCC(=O)c1cc2c(c(c1C)O)C(=O)C(=O)c1c2cccc1O)C	549	Yes
1168	9,10-Phenanthrenedione, 3-acetyl-1,8-dihydroxy-2-methyl-	O=C1c2c(cc(c(c2O)C)C(=O)C)c2c(C1=O)c(O)ccc2	549	No
1169	Murayaquinone	CCCC(=O)c1cc2c(c(c1C)O)C(=O)C(=O)c1c2cccc1O	549	No
1170	4,7-Dihydroxy-3-methyl-2-(4-methyl-1-oxopentyl)-6H-dibenzo[b,d]pyran-6-one	CC(CCC(=O)c1cc2c(c(c1C)O)oc(=O)c1c2cccc1O)C	549	No
1171	Murayalactone	CCCC(=O)c1cc2c(c(c1C)O)c(=O)oc1c2cccc1O	549	No
1172	Dimyristoylcephalin	CCCCCCCCCCCCCC(=O)OCC(OC(=O)CCCCCCCCCCCCC)COP(=O)(OCCN)O	550	Yes
1173	Phosphatidylcholine	CCCCCCCCCCCCCCCCCC(=O)OC[C@@H](OC(=O)CCCCCCC/C=C\C/C=C\CCCCC)COP(=O)(OCC[N+](C)(C)C)[O-]	550	No
1174	Lagunamycin	CC1=C(C2=C(C(=O)C(=O)C(=[N+]=[N-])C2=O)NC1=O)/C(=C/C(C)CC(C)C)/C	551	Yes
1175	Foxicin A	CC(=C[C@@H](/C=C(/C(=O)NC1=CC(=O)C(=C(C1=O)NC(=O)C)O)\C)C)C	552	Yes
1176	Diazaquinomycin E	CCCCCc1cc(=O)[nH]c2c1c(=O)c1c(CCCCC)cc(=O)[nH]c1c2=O	553	No
1177	Diazaquinomycin C	CCCCCc1c(C)c(=O)[nH]c2c1c(=O)c1c(c2=O)[nH]c(=O)c(c1CCC)C	553	No
1178	Diazaquinomycin A	CCCc1c(C)c(=O)[nH]c2c1c(=O)c1c(c2=O)[nH]c(=O)c(c1CCC)C	553	No
1179	Diazaquinomycin F	CCCCCc1cc(=O)[nH]c2c1c(=O)c1c(c2=O)[nH]c(=O)c(c1CCC)C	553	No
1180	Diazaquinomycin G	CCCCCc1c(C)c(=O)[nH]c2c1c(=O)c1c(c2=O)[nH]c(=O)cc1CCC	553	No
1181	Diazaquinomycin D	CCCCCc1c(C)c(=O)[nH]c2c1c(=O)c1c(c2=O)[nH]c(=O)c(c1CCCCC)C	553	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1182	Naphthomycin N	O[C@@H]1/C=C/[C@H](C)[C@H](O)[C@@H](C)/C=C(/C)\C(=O)c2c3C(=O)C(=C(C(=O)c3cc(c2O)C)NC(=O)/C(=C\C=C/C=C\[C@@H]([C@H](CC(=O)/C(=C/C1)/C)O)C)/C)NCCSC1=C2NC(=O)/C(=C\C=C/C=C/[C@H](C)[C@@H](O)CC(=O)/C(=C/C[C@@H](/C=C/[C@@H]([C@@H]([C@H](/C=C(/C(=O)c3c(C1=O)c(C2=O)cc(c3O)C)\C)C)O)C)O)/C)/C	554	Yes
1183	Naphthomycin O	O[C@@H]1/C=C/[C@H](C)[C@@H](O)[C@@H](C)/C=C(\C)/C(=O)c2c3C(=O)C4=C(C(=O)c3cc(c2O)C)NC(=O)C(/C=C/C(=O)/C=C/[C@@H]([C@H](CC(=O)/C(=C/C1)/C)O)C)(S4)C	555	Yes
1184	Diastovaricin II	O[C@@H]1/C=C\[C@H](C)[C@H](O)[C@@H](C)/C=C(\C)/C(=O)c2c3C(=O)C(=C(C(=O)c3cc(c2O)C)NC(=O)/C=C\C=C\C=C/[C@@H]([C@H](CC(=O)/C(=C/C1)/C)O)C)SC[C@@H](C(=O)O)NC(=O)C	556	Yes
1185	Naphthomycin M	OC(=O)CSC1=C2NC(=O)/C(=C\C=C/C=C/[C@H](C)[C@@H](O)CC(=O)/C(=C/C[C@@H](/C=C/[C@@H]([C@@H]([C@H](/C=C(/C(=O)c3c(C1=O)c(C2=O)cc(c3O)C)\C)C)O)C)O)/C)/C	556	No
1186	Naphthomycin P	O[C@H]1/C=C/[C@@H](C)[C@H](O)[C@@H](C)/C=C(\C)/C(=O)c2c3C(=O)C(=C(C(=O)c3cc(c2O)C)NC(=O)/C(=C\C=C/[C@@H]([C@@H]([C@@H]([C@H](CC(=O)/C(=C/C1)/C)O)C)O)O)/C)O	557	Yes
1187	Naphthomycin L	O[C@@H]1/C=C/[C@H](C)[C@H](O)[C@@H](C)/C=C(\C)/C(=O)c2c3C(=O)C(=C(C(=O)c3cc(c2O)C)NC(=O)/C(=C\C=C/C=C/[C@@H]([C@H](CC(=O)/C(=C/C1)/C)O)C)/C)N	558	Yes
1188	Naphthomycin E	O[C@@H]1/C=C/[C@H](C)[C@H](O)[C@@H](C)/C=C(\C)/C(=O)c2c3C(=O)C=C(C(=O)c3cc(c2O)C)NC(=O)/C(=C\C=C/C=C/[C@@H]([C@H](CC(=O)/C(=C/C1)/C)O)C)/C	559	Yes
1189	Naphthoquinomycin A	COC1=C2NC(=O)/C=C/C=C\C=C\C(C)C(O)CC(=O)/C(=C/CC(/C=C/C(C(C(/C=C(\C(=O)c3c(C1=O)c(C2=O)cc(c3O)C)/C)C)O)C)O)/C	560	Yes
1190	Naphthomycin A	O[C@H]1/C=C/[C@@H](C)[C@H](O)[C@@H](C)/C=C(\C)/C(=O)c2c3C(=O)C(=C(C(=O)c3cc(c2O)C)NC(=O)/C(=C/C=C\C=C/[C@@H]([C@H](CC(=O)/C(=C\C1)/C)O)C)/C)Cl	561	Yes
1191	Naphthomycin Q	O[C@@H]1/C=C/[C@@H](C)[C@H](O)[C@@H](C)/C=C(\C)/C(=O)c2c3C(=O)C(=C(C(=O)c3cc(c2O)C)NC(=O)/C(=C\C=C/C=C/C(/C=C/C(=O)/C(=C/C1)/C)C)/C)Cl	561	No
1192	Naphthoquinomycin B	CSC1=C2NC(=O)/C=C/C=C\C=C\C(C)C(O)CC(=O)/C(=C/CC(/C=C/C(C(C(/C=C(\C(=O)c3c(C1=O)c(C2=O)cc(c3O)C)/C)C)O)C)O)/C	562	Yes
1193	Pyridomycin	CC/C(=C/1\OC(=O)C(C)C(O)C(NC(=O)C(C(OC1=O)C)NC(=O)c1ncccc1O)Cc1cccnc1)/C	563	Yes
1194	Erizomycin	CC/C(=C/1\OC(=O)[C@H](C)[C@@H](O)[C@@H](NC(=O)[C@H]([C@H](OC1=O)C)NC(=O)c1ncccc1O)Cc1cccnc1)/C	563	No
1195	Kitamycin C	CCCCC[C@H]1C(=O)O[C@H](C)[C@@H](C(=O)O[C@H]([C@@H]1O)C)NC(=O)c1cccc(c1O)NC=O	564	No
1196	Urauchmycin B	O=CNc1cccc(c1O)C(=O)N[C@@H]1C(=O)O[C@@H](C)[C@@H]([C@H](C(=O)O[C@@H]1C)CCC(C)C)O	564	No
1197	Kitamycin A	CCCCCC[C@H]1C(=O)O[C@H](C)[C@@H](C(=O)O[C@H]([C@@H]1O)C)NC(=O)c1cccc(c1O)NC=O	564	No
1198	Kitamycin B	O=CNc1cccc(c1O)C(=O)N[C@@H]1C(=O)O[C@@H](C)[C@@H]([C@H](C(=O)O[C@@H]1C)CCCC(C)C)O	564	No
1199	Antimycin A19	CCCCC[C@H]1C(=O)O[C@H](C)[C@@H](C(=O)O[C@H]([C@@H]1OC(=O)[C@H](C(C)C)C)C)NC(=O)c1cccc(c1O)NC=O	564	No
1200	Urauchimycin B	O=CNc1cccc(c1O)C(=O)NC1C(=O)OC(C)C(C(C(=O)OC1C)CCC(C)C)O	564	No
1201	Urauchimycin A	O=CNc1cccc(c1O)C(=O)NC1C(=O)OC(C)C(C(C(=O)OC1C)CC(CC)C)O	564	No
1202	Antimycin A4b	CCCC[C@H]1C(=O)O[C@H](C)[C@@H](C(=O)O[C@H]([C@@H]1OC(=O)CCC)C)NC(=O)c1cccc(c1O)NC=O	564	No
1203	Antimycin A17	CCCCCC1C(=O)OC(C)C(C(=O)OC(C1OC(=O)C(CC)C)C)NC(=O)c1cccc(c1O)NC=O	564	No
1204	5-Fluoroantimycin	CCCCCC[C@@H]1[C@@H](OC(=O)C(CC)C)[C@H](C)OC(=O)[C@H]([C@H](C1=O)C)NC(=O)c1cc(F)cc(c1O)NC=O	564	No
1205	Antimycin A2	CCCC(=O)OC1C(C)OC(=O)C(C(OC(=O)C1CCCCCC)C)NC(=O)c1cccc(c1O)NC=O	564	No
1206	UNII-3471OQ4074	CCCC[C@H]1C(=O)O[C@H](C)[C@@H](C(=O)O[C@H]([C@@H]1OC(=O)C(C)C)C)NC(=O)c1cccc(c1O)NC=O	564	No
1207	Antimycin A6a	O=CNc1cccc(c1O)C(=O)N[C@@H]1C(=O)O[C@@H](C)[C@@H]([C@H](C(=O)O[C@@H]1C)CC)OC(=O)C(C)C	564	No
1208	Antimycin A4	CCCCC1C(=O)OC(C)C(C(=O)OC(C1OC(=O)CCC)C)NC(=O)c1cccc(c1O)NC=O	564	No
1209	UNII-745M0KNN2Y	CCCCCC[C@H]1C(=O)O[C@H](C)[C@@H](C(=O)O[C@H]([C@@H]1OC(=O)C(C)C)C)NC(=O)c1cccc(c1O)NC=O	564	No
1210	Antimycin A8	O=CNc1cccc(c1O)C(=O)N[C@@H]1C(=O)O[C@@H](C)[C@@H]([C@H](C(=O)O[C@@H]1C)CCC(C)C)OC(=O)C(CC)C	564	Yes
1211	UNII-DPA68O75PF	O=CNc1cccc(c1O)C(=O)N[C@@H]1C(=O)O[C@@H](C)[C@@H]([C@H](C(=O)O[C@@H]1C)CCC(C)C)OC(=O)C(C)C	564	No
1212	Antimycin A9	CCCCC1C(=O)OC(C)C(C(=O)OC(C1OC(=O)Cc1ccccc1)C)NC(=O)c1cccc(c1O)NC=O	564	No
1213	Antimycin A1a	CCCCCC[C@H]1C(=O)O[C@H](C)[C@@H](C(=O)O[C@H]([C@@H]1OC(=O)[C@H](CC)C)C)NC(=O)c1cccc(c1O)NC=O	564	No
1214	Antimycin A18	CCCC[C@@H]1[C@H](COC(=O)[C@H]([C@H](OC1=O)C)NC(=O)c1cccc(c1O)NC=O)OC(=O)C	564	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1215	Neoantimycin B	CCCCCC[C@H]1C(=O)O[C@H](C)[C@@H](C(=O)O[C@H]([C@@H]1OC(=O)C(C)C)C)NC(=O)c1ccccc1	565	No
1216	(2R,3S,7R,8R)-3-(3-Acetamido-2-hydroxybenzamido)-2-methyl-4,9-dioxo-8-pentyl-1,5-dioxonan-7-yl 2-methylpropanoate	CCCCC[C@@H]1[C@H](COC(=O)[C@H]([C@H](OC1=O)C)NC(=O)c1cccc(c1O)NC(=O)C)OC(=O)C(C)C	565	Yes
1217	(2R,3S,7R,8R)-3-(3-Acetamido-2-hydroxybenzamido)-8-heptyl-2-methyl-4,9-dioxo-1,5-dioxonan-7-yl acetate	CCCCCCC[C@@H]1[C@H](COC(=O)[C@H]([C@H](OC1=O)C)NC(=O)c1cccc(c1O)NC(=O)C)OC(=O)C	565	No
1218	(2R,3S,7R,8R)-3-(3-Acetamido-2-hydroxybenzamido)-2-methyl-4,9-dioxo-8-pentyl-1,5-dioxonan-7-yl propanoate	CCCCC[C@@H]1[C@H](COC(=O)[C@H]([C@H](OC1=O)C)NC(=O)c1cccc(c1O)NC(=O)C)OC(=O)CC	565	No
1219	N-Acetyl-deformylantimycin A	CCCCCCC[C@@H]1[C@H](COC(=O)[C@H]([C@H](OC1=O)C)NC(=O)c1cccc(c1O)NC(=O)C)OC(=O)CC(CC)C	565	No
1220	Deformylantimycin A2a	CCC(CC(=O)O[C@H]1COC(=O)[C@H]([C@H](OC(=O)[C@@H]1CCC(C)C)C)NC(=O)c1cccc(c1O)NC(=O)C)C	565	No
1221	N-(15-Benzyl-10-butan-2-yl-3,7,13,13-tetramethyl-2,5,9,12,14-pentaoxo-1,4,8,11-tetraoxacyclopentadec-6-yl)benzamide	CCC(C1OC(=O)C(C)(C)C(=O)C(Cc2ccccc2)OC(=O)C(OC(=O)C(C(OC1=O)C)NC(=O)c1ccccc1)C)C	566	No
1222	Prunustatin	O=CNc1cccc(c1O)C(=O)NC1C(=O)OC(C)C(=O)OC(Cc2ccccc2)C(=O)C(C(=O)OC(C(=O)OC1C)C(CC)C)(C)C	566	No
1223	Neoantimycin A	O=CNc1cccc(c1O)C(=O)N[C@@H]1C(=O)O[C@@H](C(C)C)C(=O)O[C@H](Cc2ccccc2)[C@@H](C(C(=O)O[C@H](C(=O)O[C@@H]1C)[C@H](CC)C)(C)C)O	566	No
1224	Neoantimycin I	O=CNc1cccc(c1O)C(=O)N[C@@H]1C(=O)O[C@@H](C(C)C)C(=O)O[C@H](Cc2ccccc2)C(=O)C(C(=O)O[C@H](C(=O)O[C@@H]1C)C(C)C)(C)C	566	No
1225	Neoantimycin G	O=CNc1cccc(c1O)C(=O)NC1C(=O)OC([C@H](CC)C)C(=O)O[C@H](Cc2ccccc2)C(C(C(=O)O[C@H](C(=O)O[C@@H]1C)[C@H](CC)C)(C)C)O	566	No
1226	Neoantimycin F	O=CNc1cccc(c1O)C(=O)NC1C(=O)OC(C(C)C)C(=O)O[C@H](Cc2ccccc2)C(C(C(=O)O[C@H](C(=O)O[C@@H]1C)C(C)C)(C)C)O	566	No
1227	Neoantimycin H	O=CNc1cccc(c1O)C(=O)N[C@@H]1C(=O)O[C@@H](C(C)C)C(=O)O[C@H](Cc2ccccc2)C(=O)C(C(=O)O[C@H](C(=O)O[C@@H]1C)[C@H](CC)C)(C)C	566	Yes
1228	Neoantimycin	O=CNc1cccc(c1O)C(=O)NC1C(=O)O[C@@H](C(C)C)C(=O)O[C@@H](Cc2ccccc2)[C@H](C(C(=O)OC(C(=O)OC1C)[C@H](CC)C)(C)C)O	566	No
1229	Respirantin	O=CNc1cccc(c1O)C(=O)N[C@H]1[C@@H](C)OC(=O)[C@H](CC(C)C)OC(=O)C(C)(C)C(=O)[C@@H](NC(=O)[C@@H](OC(=O)[C@@H](OC1=O)C)C(CC)C)CC(C)C	567	Yes
1230	AGN-PC-077DQ0	O=CNc1cccc(c1O)C(=O)NC1C(=O)OC(C(CC)C)C(=O)OC(C(=O)C(C(=O)OC1C)C)CC(C)C	568	Yes
1231	Methyl geldanamycinate	CO[C@H]([C@@H]([C@H](/C=C(/[C@@H]([C@H](/C=C\C=C(\C(=O)OC)/C)OC)OC(=O)N)\C)C)O)C[C@@H](CC1=C(OC)C(=O)C=C(C1=O)N)C	569	Yes
1232	Geldanamycin F	CO[C@H]([C@@H]([C@H](/C=C(/[C@@H]([C@H](/C=C\C=C(\C(=O)O)/C)OC)OC(=O)N)\C)C)O)C[C@@H](CC1=C(OC)C(=O)C=C(C1=O)N)C	569	No
1233	Herbimycin G	CO[C@@H]1[C@@H](C)C=C(C)[C@H](OC(=O)N)[C@@H](OC)C=CC=C(C(=O)N[C@H]2C(=O)C(=C[C@@H](O)C2)[C@@H]([C@H](C[C@@H]1OC)C)OC)C	570	Yes
1234	17-O-Demethylgeldanamycin	CO[C@H]1C[C@H](C)CC2=C(O)C(=CC(=O)C2=O)NC(=O)/C(=C\C=C/[C@@H]([C@H](/C(=C\[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	571	Yes
1235	CHEMBL436384	CO[C@H]1C[C@H](C)CC2=C(O)C(=CC(=O)C2=O)NC(=O)/C(=C/C=C\[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	571	No
1236	4,5-Dihydro-17-O-demethylgeldanamycin	CO[C@H]1C[C@H](C)CC2=C(O)C(=CC(=O)C2=O)NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	571	No
1237	KOSN1631	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C=C(C2=O)NC(=O)/C(=C/C=C\C[C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)/C	572	No
1238	Geldanamycin	CO[C@@H]1C[C@H](C)CC2=C(OC)C(=O)C=C(C2=O)NC(=O)/C(=C/C=C\[C@H]([C@@H](/C(=C/[C@H]([C@@H]1O)C)/C)OC(=O)N)OC)/C	572	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1239	15-Hydroxygeldanamycin	CO[C@H]1C[C@H](C)[C@@H](O)C2=C(OC)C(=O)C=C(C2=O)NC(=O)/C(=C/C=C\[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	572	No
1240	CHEMBL340169	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C=C(C2=O)NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	572	Yes
1241	CHEMBL2087236	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C=C(C2=O)NC(=O)/C(=C/[C@@H](C[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)O)/C	572	No
1242	CHEMBL2087235	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C=C(C2=O)NC(=O)/C(=C/[C@H](C[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)O)/C	572	No
1243	KOSN-1633	CO[C@H]1C[C@H](C)C2O[C@@H]1[C@@H](C)/C=C(\C)/[C@H](OC(=O)N)[C@@H](OC)/C=C/C=C(\C(=O)NC1=CC(=O)C(=C2C1=O)OC)/C	573	Yes
1244	Geldanamycin B	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C(=O)C(=C2O)NC(=O)/C(=C/C=C\[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	574	Yes
1245	19-Hydroxy-4,5-dihydrogeldanamycin	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C(=C(C2=O)NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)O	574	No
1246	Geldanamycin D	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C(=O)C(=C2O)NC(=O)/C(=C/[C@@H](C[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)O)/C	575	Yes
1247	SCHEMBL141220	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C=C(C2=O)NC(=O)/C(=C/C=C\[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)C)/C	576	Yes
1248	Herbimycin B	COC1CC(C)CC2=CC(=O)C=C(C2=O)NC(=O)/C(=C/C=C/C(C(/C(=C\C(C1O)C)/C)OC(=O)N)OC)/C	577	Yes
1249	SCHEMBL10035841	CO[C@H]1C[C@H](C)CC2=C(CO)C(=O)C=C(C2=O)NC(=O)/C(=C/C=C\[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	578	Yes
1250	Herbimycin C	CO[C@@H]1C[C@H](C)[C@@H](OC)C2=CC(=O)C=C(C2=O)NC(=O)/C(=C/C=C\[C@H]([C@@H](/C(=C/[C@H]([C@@H]1O)C)/C)OC(=O)N)OC)/C	578	No
1251	Herbimycin A	CO[C@@H]1[C@@H](C)/C=C(\C)/[C@H](OC(=O)N)[C@@H](OC)/C=C\C=C(\C(=O)NC2=CC(=O)C=C([C@@H]([C@H](C[C@@H]1OC)C)OC)C2=O)/C	579	Yes
1252	CHEMBL2419114	CO[C@@H]1[C@@H](C)/C=C(\C)/[C@H](OC(=O)N)[C@@H](OC)/C=C\C=C(\C(=O)NC2=C(C(=CC(=O)C2=O)[C@@H]([C@H](C[C@@H]1OC)C)OC)O)/C	580	Yes
1253	19-S-Methylgeldanamycin	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C(=C(C2=O)NC(=O)/C(=C/C=C\[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)SC	581	Yes
1254	CHEMBL2375649	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C(=C(C2=O)NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)[C@@H](C(=O)C[C@H](O)C)OC	582	Yes
1255	CHEMBL2375650	CO[C@H]1C[C@H](C)CC2=C(OC)C(=O)C(=C(C2=O)NC(=O)/C(=C/C=C\[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)[C@@H](C(=O)C[C@H](O)C)OC	583	Yes
1256	Herbimycin	CO[C@@H]1[C@@H](C)/C=C(\C)/[C@H](OC(=O)N)[C@@H](OC)/C=C/C=C(/C(=O)NC2=CC(=O)C=C([C@@H]([C@H](C[C@@H]1OC)C)OC)C2=O)\C	584	Yes
1257	Hexanedioic acid, dioctyl ester	CCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCC	585	Yes
1258	Di(2-propylpentyl) ester	CCCC(COC(=O)CCCC(=O)OCC(CCC)CCC)CCC	586	Yes
1259	Octadecanoic acid, 2-hydroxy-1,3-propanediyl ester	CCCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCCCC)O	587	Yes
1260	A Factor	OC[C@@H]1COC(=O)C1C(=O)CCCCC(C)C	588	No
1261	AC1L35AK	OCC1COC(=O)C1C(CCCCC(C)C)O	588	No
1262	Factor I	OC[C@@H]1COC(=O)[C@H]1C(CCCCC(C)C)O	588	No
1263	SCB7	CCCCCCCC[C@H]([C@H]1[C@H](CO)COC1=O)O	588	No
1264	SCB3	CCC(CCCC[C@H]([C@H]1[C@H](CO)COC1=O)O)C	588	Yes
1265	Virginiamycin butanolide D	CCCCCCC(C1C(CO)COC1=O)O	588	No
1266	SCB1	OC[C@@H]1COC(=O)[C@H]1[C@@H](CCCCC(C)C)O	588	No
1267	SCB2	CCCCCCC[C@H]([C@H]1[C@H](CO)COC1=O)O	588	No
1268	SCB6	CCCCCC[C@H]([C@H]1[C@H](CO)COC1=O)O	588	No
1269	CHEMBL2419113	CO[C@@H]1[C@@H](C)/C=C(\C)/[C@H](OC(=O)N)[C@@H](OC)/C=C\C=C(\C(=O)Nc2c(c([C@@H]([C@H](C[C@@H]1OC)C)OC)cc1NC(=O)CSc21)O)/C	589	Yes
1270	Dihydro-herbimycin A	CO[C@@H]1[C@@H](C)/C=C(\C)/[C@H](OC(=O)N)[C@@H](OC)/C=C\C=C(\C(=O)Nc2c(c([C@@H]([C@H](C[C@@H]1OC)C)OC)cc(O)c2)O)/C	590	Yes
1271	17-Formyl-17-demethoxy-18-O,21-O-dihydrogeldanamycin	CO[C@H]1C[C@H](C)Cc2c(O)c(NC(=O)/C(=C/C=C\[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)cc(c2C=O)O	590	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1272	4,5-Dehydro-17-de-O-methyl-reblastatin	CO[C@H]1C[C@@H](C)Cc2c(O)c(NC(=O)/C(=C/C=C\[C@H]([C@@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)cc(c2O)O	590	No
1273	18-Acetamido-17-de-O-methyl-21-hydroxyreblastatin	CO[C@H]1C[C@@H](C)Cc2c(O)c(NC(=O)/C(=C/CC[C@H]([C@@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)cc(c2O)NC(=O)C	590	No
1274	18-Dehydroxy-17-demethoxy-21-fluororeblastatin	CO[C@H]1C[C@@H](C)Cc2cccc(c2F)NC(=O)/C(=C/CC[C@H]([C@@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	591	Yes
1275	WK-88-1	CO[C@H]1CC\C=C(C)\C(=O)Nc2cccc(C[C@@H](C)C[C@H](OC)[C@H](O)[C@@H](C)\C=C(C)\[C@@H]1OC(N)=O)c2	592	Yes
1276	17-Demethoxy-18-ethynylreblastatin	CO[C@H]1C[C@@H](C)Cc2cc(cc(c2)C#C)NC(=O)/C(=C/CC[C@H]([C@@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	592	No
1277	18-Dehydroxy-17-de-O-methyl-21-fluororeblastatin	CO[C@H]1C[C@@H](C)Cc2c(O)ccc(c2F)NC(=O)/C(=C/CC[C@H]([C@@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C	593	No
1278	17-Demethoxy-18-prop-2-ynylreblastatin	C#CCc1cc2cc(c1)C[C@H](C)C[C@H](OC)[C@H](O)[C@@H](C)/C=C(/[C@H]([C@@H](CC/C=C(/C(=O)N2)\C)OC)OC(=O)N)\C	593	No
1279	CHEMBL401784	CO[C@H]1C[C@H](C)Cc2cc(NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)cc(c2O)O	593	No
1280	18-Amino-4,5-dehydro-17-demethylreblastatin	CO[C@H]1C[C@@H](C)Cc2cc(NC(=O)/C(=C/C=C\[C@H]([C@@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)cc(c2O)N	593	No
1281	17-de-O-Methyl-18-ethynylreblastatin	CO[C@H]1C[C@@H](C)Cc2cc(NC(=O)/C(=C/CC[C@H]([C@@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)cc(c2O)C#C	593	Yes
1282	4,5-Dehydro-17-demethoxy-18-prop-2-ynylreblastatin	C#CCc1cc2NC(=O)/C(=C/C=C\[C@@H](OC)[C@@H](/C(=C/[C@@H]([C@H]([C@H](C[C@H](Cc(c1O)c2)C)OC)O)C)/C)OC(=O)N)/C	593	No
1283	17-de-O-Methyl-18-prop-2-ynylreblastatin	C#CCc1cc2NC(=O)/C(=C/CC[C@@H](OC)[C@@H](/C(=C/[C@@H]([C@H]([C@H](C[C@H](Cc(c1O)c2)C)OC)O)C)/C)OC(=O)N)/C	593	No
1284	18-Acetamido 4,5-dehydro-17-de-O-methylreblastatin	CO[C@H]1C[C@@H](C)Cc2cc(NC(=O)/C(=C/C=C\[C@H]([C@@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)cc(c2O)NC(=O)C	593	No
1285	Thiazinogeldanamycin	CO[C@@H]1C[C@@H](C)Cc2c(O)c(NC(=O)C(=CC=C[C@H]([C@@H](C(=C[C@H]([C@@H]1O)C)C)OC(=O)N)OC)C)c1c(c2OC)NC(=O)CS1	594	Yes
1286	4,5-Dihydrothiazinogeldanamycin	CO[C@H]1C[C@H](C)Cc2c(O)c(NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)c1c(c2OC)NC(=O)CS1	595	Yes
1287	Geldanamycin G	CO[C@H]([C@@H]([C@H](/C=C(/[C@@H]([C@H](/C=C\C=C(\C(=O)O)/C)OC)OC(=O)N)\C)C)O)C[C@@H](Cc1c(O)c(NC(=O)CO)c2c(c1OC)NC(=O)CS2)C	596	Yes
1288	Reblastatin	CO[C@H]1C[C@H](C)Cc2cc(NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)cc(c2OC)O	597	No
1289	Progeldanamycin	CO[C@H]1C[C@H](C)Cc2cc(O)cc(c2)NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/C([C@H]1O)C)/C)O)OC)/C	597	Yes
1290	SCHEMBL13009061	CO[C@H]1C[C@H](C)Cc2cc(O)cc(c2)NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)O)OC)/C	597	No
1291	Geldanamycin E	CO[C@H]1C[C@H](C)Cc2c(OC(=O)CO)c(NC(=O)/C(=C/C=C\[C@@H]([C@H](/C(=C/[C@@H]([C@H]1O)C)/C)OC(=O)N)OC)/C)cc(c2OC)O	598	Yes
1292	18,21-Didehydro-18,21-dideoxo-18,21-dihydroxygeldanamycin	CO[C@H]1C[C@H](C)Cc2c(O)c(NC(=O)C(=CC=C[C@@H]([C@H](C(=C[C@@H]([C@H]1O)C)C)OC(=O)N)OC)C)cc(c2OC)O	599	Yes
1293	Streptoglyceride B	C/C=C/C=C/C=C/[C@]12OCC[C@H]3[C@@H]2[C@](CO1)(O)CO3	600	Yes
1294	Streptoglyceride A	C/C=C/C=C/CC[C@]12OCC[C@H]3[C@@H]2[C@](CO1)(O)CO3	600	No
1295	Piericidin B1 N-oxide	C/C=C(\[C@H]([C@H](/C=C(\C=C/C/C(=C\Cc1n(O)c(OC)c(c(=O)c1C)OC)/C)/C)C)OC)/C	601	No
1296	Piericidin E1	C/C=C(/[C@@H]([C@@H](/C=C(/C=C/CC1(C)OC1Cc1[nH]c(OC)cc(=O)c1C)\C)C)O)\C	601	No
1297	Piericidin B1	C/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)\C)C)OC)\C	601	No
1298	Piericidin B5	CC/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)\C)C)OC)\C	601	No
1299	Piericidin F	CO[C@@H](/C(=C/C)/C)[C@@H](/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)cc(=O)c1C)/C)\C)C	601	No
1300	Mer-A2026B	C/C=C(/C(C(/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)cc(=O)c1C)/C)\C)C)O)\C	601	No
1301	Piericidin A5	CC/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)\C)C)O)\C	601	No
1302	Piericidin A	C/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)\C)C)O)\C	601	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1303	Demethylpiericidin A1	C/C=C(/[C@@H](C/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)\C)O)\C	601	No
1304	7-Demethylpiericidin A1	C/C=C(/[C@@H]([C@@H](/C=C/C=C/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)C)O)\C	601	No
1305	Piericidin C7	C/C=C(/[C@@H]1O[C@@]1(C)[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)\C)C)O)\C	601	No
1306	Piericidin C3	COc1[nH]c(C/C=C(/C/C=C/C(=C/C(C(C2(C)OC2C(C)C)O)C)/C)\C)c(c(=O)c1OC)C	601	No
1307	Piericidin C1	COc1[nH]c(C/C=C(/C/C=C/C(=C/C(C(C2(C)OC2C)O)C)/C)\C)c(c(=O)c1OC)C	601	No
1308	Piericidin G	COC(C1(C)OC1C)C(/C=C(/C=C/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)\C)C	601	No
1309	Piericidin C8	C/C=C(/[C@@H]1O[C@@]1(C)[C@@H]([C@@H](/C=C(/C=C(/C/C(=C/Cc1[nH]c(OC)c(c(=O)c1C)OC)/C)\C)\C)C)O)\C	601	No
1310	2-((2E,5E,7E,9R,10R)-10-((2S,3S)-2,3-Dimethyloxiran-2-yl)-10-hydroxy-3,7,9-trimethyldeca-2,5,7-trien-1-yl)-5,6-dimethoxy-3-methylpyridin-4-ol	COc1[nH]c(C/C=C(/C/C=C/C(=C/[C@H]([C@H]([C@]2(C)O[C@H]2C)O)C)/C)\C)c(c(=O)c1OC)C	601	No
1311	CHEBI:69899	C/C=C(/C(C(/C=C(/C=C/CC(/C=C/c1oc(OC)c(c(=O)c1C)CC)C)\C)C)O)\C	601	No
1312	PM050463	C/C=C(/C(C(/C=C(/C=C/CC(/C=C/c1oc(OC)c(c(=O)c1C)C)C)\C)C)O)\C	601	No
1313	Actinopyrone B	C/C=C(/C(C(/C=C(/C=C/C/C(=C/Cc1oc(OC)cc(=O)c1C)/C)\C)C)O)\C	601	No
1314	Actinopyrone A	C/C=C(/C(C(/C=C(/C=C/C/C(=C/Cc1oc(OC)c(c(=O)c1C)C)/C)\C)C)O)\C	601	No
1315	Actinopyrone C	C/C=C(/C(C(/C=C(/C=C/C/C(=C/Cc1oc(OC)c(c(=O)c1C)CC)/C)\C)C)O)\C	601	No
1316	Ferroverdin B	O/C=C\c1ccc(cc1)OC(=O)C1=C/C(=N/O)/C(=O)C=C1	602	Yes
1317	Ferroverdin C	O/N=C\1/C=C(C=CC1=O)C(=O)Oc1ccc(cc1)/C=C\C(=O)O	602	No
1318	Elaiomycin F	CCCCCCCC[N+](=N[C@@H](COC)[C@H](C)O)[O-]	603	Yes
1319	Elaiomycin	CCCCCC/C=C\\[N+](=N[C@@H](COC)[C@H](C)O)[O-]	603	No
1320	Serofendic acid	CS(=O)C[C@H]1[C@H]2CC[C@@]3([C@@H]1O)[C@@H](C2)[C@]1(C)CCC[C@@]([C@H]1CC3)(C)C(=O)O	604	Yes
1321	Jietacine A	CC(C)CCCCCC(=O)CCCCCCCN=[N+](C=C)[O-]	605	Yes
1322	Jietacin B	C=C[N+](=NCCCCCCCC(=O)CCCCCCC(C)C)[O-]	605	No
1323	JBIR-120	CCC(c1cncc2c1C(=O)CC2)Nc1ccccc1C(=O)O	606	Yes
1324	N-[[3,4-Dihydro-3S-hydroxy-2S-methyl-2-(4'R-methyl-3'S-pentenyl)-2H-1-benzopyran-6-yl]carbonyl]-threonine	CC(=CCC[C@]1(C)Oc2ccc(cc2C[C@@H]1O)C(=O)NC(C(=O)O)[C@H](O)C)C	607	Yes
1325	Xiamenmycin D	COC(=O)[C@H]([C@H](O)C)NC(=O)c1ccc2c(c1)C[C@@H]([C@](O2)(C)CCC=C(C)C)O	607	No
1326	Xiamenmycin	CC(=CCC[C@]1(C)Oc2ccc(cc2C[C@@H]1O)C(=O)N[C@H](C(=O)O)[C@H](O)C)C	607	No
1327	4,25-Diethyl-4,25-demethyl-milbemycin beta3	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](C2)C/C=C(\C)/C[C@@H](C)/C=C/C=C(/c2c(C(=O)C1)cc(CC)c(c2)O)\C	608	Yes
1328	27-Formaldehyde-milbemycin beta14	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](C2)C/C=C(\C)/C[C@@H](C)/C=C/C=C(/c2c(C(=O)C1)cc(CC)c(c2)O)\CO	608	No
1329	Neo-actinomycin A	OC(=O)CCc1oc2c(n1)c(C(=O)N[C@@H]1[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C(=O)[C@H]3N(C(=O)[C@H](NC1=O)C(C)C)CCC3)C)c1c(c2C)Oc2c(N1)c(ccc2C)C(=O)N[C@H]1[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C(=O)[C@@H]2N(C(=O)[C@H](NC1=O)C(C)C)CCC2)C	609	Yes
1330	Neo-actinomycin B	Cc1oc2c(n1)c(C(=O)N[C@@H]1[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C(=O)[C@H]3N(C(=O)[C@H](NC1=O)C(C)C)CCC3)C)c1c(c2C)Oc2c(N1)c(ccc2C)C(=O)N[C@H]1[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C(=O)[C@@H]2N(C(=O)[C@H](NC1=O)C(C)C)CCC2)C	610	Yes
1331	Demethoxy-ohmyungsamycin A	CNC(C(=O)NC(C(=O)NC1C(C)OC(=O)C(CC(=O)C(NC(=O)C(NC(=O)C(Cc2c[nH]c3c2cccc3)N(C)C(=O)C(N(C(=O)C(NC(=O)C(N(C(=O)C(NC(=O)C(N(C1=O)C)C(O)C)C(C)C)C)CC(C)C)C(C)C)C)C(C)C)C(c1ccccc1)O)C(C)C)C(C)C)C(C)C	611	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1332	Dehydroxy-ohmyungsamycin A	CNC(C(=O)NC(C(=O)NC1C(C)OC(=O)C(CC(=O)C(Cc2ccccc2)NC(=O)C(NC(=O)C(Cc2c[nH]c3c2c(OC)ccc3)N(C)C(=O)C(N(C(=O)C(NC(=O)C(N(C(=O)C(NC(=O)C(N(C1=O)C)C(O)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C	612	Yes
1333	Ohmyungsamycin A	CN[C@H](C(=O)N[C@H](C(=O)N[C@H]1[C@@H](C)OC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](Cc2c[nH]c3c2c(OC)ccc3)N(C)C(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H](N(C1=O)C)[C@H](O)C)C(C)C)C)CC(C)C)C(C)C)C(C)C)[C@@H](c1ccccc1)O)C(C)C)C(C)C)C(C)C	613	Yes
1334	Ecumicin	CC[C@H]([C@H](N(C(=O)[C@H](C(C)C)NC(=O)[C@@H](N(C)C)C(C)C)C)C(=O)N[C@H]1[C@@H](C)OC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](Cc2c[nH]c3c2c(OC)ccc3)N(C)C(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H](N(C1=O)C)[C@H](O)C)C(C)C)C)CC(C)C)C(C)C)C(C)C)C(C)C)C(C)C)[C@@H](c1ccccc1)O)C(C)C	614	Yes
1335	Ohmyungsamycin B	COc1cccc2c1c(c[nH]2)C[C@H]1C(=O)N[C@@H](C(C)C)C(=O)N[C@H](C(=O)N[C@@H](C(C)C)C(=O)O[C@H](C)[C@H](NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N(C)C)C(C)C)C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N1C)C(C)C)C)C(C)C)CC(C)C)C)C(C)C)[C@H](O)C)C)[C@@H](c1ccccc1)O	615	Yes
1336	Hangtaimycin	C/C=C/C=C\C(=O)NC(C=C(C(=O)NC(C1CC(=CC(=O)O1)CCC/C=C/C=C\C(=O)NC(=C)C(=O)NC(C(=O)N1C(=O)[C@@H](Cc2c[nH]c3c2cccc3)N(C(=O)/C/1=C/C)C)C(OC)C)O)C)C	616	Yes
1337	Surfactin	CC(CCCCCCCCC[C@@H]1CC(=O)N[C@@H](CCC(=O)O)C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](CC(C)C)C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)O1)CC(C)C)CC(C)C)CC(=O)O)C(C)C)C	617	Yes
1338	Ilamycin F	C/C=C/C[C@@H]1NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C[C@@H](C(=O)O)C)N(C)C(=O)[C@H](C)NC(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC1=O)Cc1cn(c2c1cccc2)C(C=C)(C)C)C)CC(C)C)Cc1ccc(c(c1)[N+](=O)[O-])O	618	Yes
1339	Ilamycin B1	C/C=C/C[C@@H]1NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC(C)C)N(C)C(=O)[C@H](C)NC(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC1=O)Cc1cn(c2c1cccc2)C(C=C)(C)C)C)CC(C)C)Cc1ccc(c(c1)[N+](=O)[O-])O	619	Yes
1340	Ilamycin E	C/C=C/C[C@@H]1NC(=O)[C@H](CC(C)C)N2[C@@H](O)[C@@H](C)C[C@@H](C2=O)N(C)C(=O)[C@H](C)NC(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC1=O)Cc1cn(c2c1cccc2)C(C=C)(C)C)C)CC(C)C)Cc1ccc(c(c1)[N+](=O)[O-])O	620	Yes
1341	Ilamycin E1	C/C=C/C[C@@H]1NC(=O)[C@H](CC(C)C)N2[C@H](O)[C@@H](C)C[C@@H](C2=O)N(C)C(=O)[C@H](C)NC(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC1=O)Cc1cn(c2c1cccc2)C(C=C)(C)C)C)CC(C)C)Cc1ccc(c(c1)[N+](=O)[O-])O	621	Yes
1342	Octaminomycin A	CCC(=O)N[C@H]1[C@@H](C)OC(=O)[C@@H]2CCCN2C(=O)[C@H](Cc2ccc(cc2)O)N(C)C(=O)[C@H](CC(C)C)NC(=O)[C@H]2N(C(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC1=O)Cc1ccccc1)CC(C)C)C(C)C)CCC2	622	Yes
1343	Octaminomycin B	CC(C[C@@H]1NC(=O)[C@@H]2CCCN2C(=O)[C@@H](NC(=O)[C@@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@H]([C@H](OC(=O)[C@H]2N(C(=O)[C@@H](N(C1=O)C)Cc1ccc(cc1)O)CCC2)C)NC(=O)C)Cc1ccccc1)C(C)C)C	623	Yes
1344	Hormaomycin	CC=CC1CN2C(C1)C(=O)OC(C)C(NC(=O)C(NC(=O)c1ccc(n1O)Cl)CC1CC1N(=O)=O)C(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C2=O)C(CC)C)C(c1ccccc1)C)CC1CC1N(=O)=O)C(c1ccccc1)C	624	Yes
1345	Surugamide A	NCCCC[C@@H]1NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC1=O)[C@H](CC)C)Cc1ccccc1)CC(C)C)[C@H](CC)C)[C@H](CC)C)[C@@H](CC)C	625	No
1346	Surugamide B	NCCCC[C@@H]1NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC1=O)[C@H](CC)C)Cc1ccccc1)CC(C)C)[C@H](CC)C)[C@H](CC)C)C(C)C	625	No
1347	Surugamide C	NCCCC[C@@H]1NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC1=O)C(C)C)Cc1ccccc1)CC(C)C)[C@H](CC)C)[C@H](CC)C)[C@@H](CC)C	625	No
1348	Surugamide E	NCCCC[C@@H]1NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC1=O)[C@H](CC)C)Cc1ccccc1)CC(C)C)C(C)C)[C@H](CC)C)[C@@H](CC)C	625	Yes
1349	Acyl-surugamide A	CCCC(=O)NCCCC[C@@H]1NC(=O)C(NC(=O)C(NC(=O)[C@@H](C)NC(=O)C(NC(=O)[C@H](NC(=O)[C@H](NC(=O)[C@@H](NC1=O)[C@H](CC)C)Cc1ccccc1)CC(C)C)C(CC)C)C(CC)C)C(CC)C	625	No
1350	Surugamide D	NCCCC[C@@H]1NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](C)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC1=O)[C@H](CC)C)Cc1ccccc1)CC(C)C)[C@H](CC)C)C(C)C)[C@@H](CC)C	626	Yes
1351	Champacyclin	NCCCC[C@@H]1NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](Cc2ccccc2)NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@H](NC1=O)[C@H](CC)C)C)[C@H](CC)C)CC(C)C)[C@H](CC)C)[C@H](CC)C	627	Yes
1352	Cyclomarin D	OC[C@@H](C[C@@H]1NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](CC(C)C)N(C(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC1=O)C)[C@@H](c1ccccc1)OC)C(C)C)C)[C@@H](C=C(C)C)C)[C@@H](c1cn(c2c1cccc2)C(C=C)(C)C)O)C	628	Yes
1353	Desoxyclomarin C	OC[C@@H](C[C@H]1C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](C(C)C)C(=O)N([C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N1C)Cc1cn(c2c1cccc2)C(C=C)(C)C)[C@H](C=C(C)C)C)CC(C)C)C)[C@@H](c1ccccc1)OC)C	629	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1354	Cyclomarin C	OC[C@@H](C[C@H]1C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@@H](C(C)C)C(=O)N([C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N1C)[C@@H](c1cn(c2c1cccc2)C(C=C)(C)C)O)[C@@H](C=C(C)C)C)CC(C)C)C)[C@@H](c1ccccc1)OC)C	630	Yes
1355	Hygrocin A	CCC1/C=C/[C@H](O)[C@H](C)OC(=O)/C(=C\CC(=O)NC2=CC(=O)c3c(C(=O)CC1)c(O)c(C)cc3C2=O)/C	631	Yes
1356	Divergolide T	CC[C@H]1/C=C/C[C@H](CC(C)C)OC(=O)C(=C[C@@H]2[C@]3(c4c(c(C(=O)CC1)c(O)c(c4)C)C(=O)C=C3NC2=O)O)C	632	No
1357	Divergolide V	CC[C@H]1/C=C/C[C@H](CC(C)C)OC(=O)C(=C[C@H]2[C@]3(c4c(c(C(=O)CC1)c(O)c(c4)C)C(=O)C=C3NC2=O)O)C	632	No
1358	Divergolide U	CC[C@H]1/C=C/C(O)[C@H](CC(C)C)OC(=O)C(=C[C@@H]2[C@]3(c4c(c(C(=O)CC1)c(O)c(c4)C)C(=O)C=C3NC2=O)O)C	632	No
1359	Hygrocin E	CC[C@@H]1/C=C/[C@H](C)[C@H](C)OC(=O)C(=C[C@H]2[C@]3(c4c(c(C(=O)CC1)c(O)c(C)c4)C(=O)C=C3NC2=O)O)C	632	No
1360	Hygrocin D	CC[C@@H]1/C=C/[C@H](C)[C@H](C)OC(=O)/C(=C\[C@H]2[C@]3(c4c(c(C(=O)CC1)c(O)c(C)c4)C(=O)C=C3NC2=O)O)/C	632	No
1361	Hygrocin C	CCC1/C=C\C(O)C(C)OC(=O)C(=O)/C(=C\[C@@H]2[C@]3(c4c(c(C(=O)CC1)c(O)c(C)c4)C(=O)C=C3NC2=O)O)/C	632	No
1362	Divergolide D	CC[C@H]1/C=C\[C@H](OC(=O)/C(=C\[C@H]2[C@]3(c4c(c(C(=O)CC1)c(O)c(C)c4)C(=O)C=C3NC2=O)O)/C)[C@H](C=C(C)C)O	632	No
1363	Hygrocin F	CC[C@@H]1/C=C/[C@@H](OC(=O)C(=C[C@@H]2[C@]3(c4c(c(C(=O)CC1)c(O)c(C)c4)C(=O)C=C3NC2=O)O)C)C(O)C	632	Yes
1364	Hygrocin G	CCC1/C=C/[C@@H](OC(=O)[C@@]2(C)C=CC(=O)NC3=C2C(=O)c2c(C(=O)CC1)c(O)c(cc2C3=O)C)C(O)C	633	Yes
1365	Hygrocin B	CCC1/C=C/[C@H](O)[C@H](C)OC(=O)[C@@]2(C3=C(C(=O)c4c(c(C(=O)CC1)c(O)c(c4)C)C3=O)NC(=O)C=C2)C	633	No
1366	Benzastatin E	COC[C@]([C@@H]1Cc2c(N1)ccc(c2)C(=O)N)(CCC(=C(C)C)C)O	634	Yes
1367	Benzastatin D	COC[C@@]1(CCC(=C(C)C)C)Nc2ccc(cc2C[C@H]1O)C(=O)N	634	No
1368	Benzastatin F	CC(=C(CCC([C@H]1Cc2c(N1)ccc(c2)C(=O)N)(O)C)C)C	634	No
1369	A-503451 B	COC[C@@]([C@H]1Cc2c(N1)ccc(c2)C(=O)O)(CCC(=C(C)C)C)O	635	Yes
1370	7-Hydroxyl-O-demethylbenzastatin D	OC[C@@]1(CCC(=C(C)C)C)Nc2ccc(cc2C[C@H]1O)C(=O)O	635	No
1371	A-503451 D	COC[C@@]1(CCC(=C(C)C)C)Nc2ccc(cc2C[C@H]1O)C(=O)O	635	No
1372	7-Hydroxyl benzastatin F	CC(=C(CC[C@]([C@H]1Cc2c(N1)ccc(c2)C(=O)O)(O)C)C)C	635	No
1373	Ent-DDHK	OC(=O)C[C@@H]1O[C@@H](C)c2c(C1)cc1c(c2O)c(O)ccc1	636	No
1374	T3HN	OC(=O)C[C@H]1O[C@H](C)c2c(C1)c(O)c1c(c2O)c(O)ccc1	636	Yes
1375	Epi-DDHK	OC(=O)C[C@H]1O[C@@H](C)c2c(C1)cc1c(c2O)c(O)ccc1	636	No
1376	DHK-OH	OC(=O)C[C@H]1O[C@H](C)c2c(C1)c(O)c1c(c2O)c(O)ccc1O	636	No
1377	DDHK	OC(=O)C[C@@H]1CC2=C([C@H](O1)C)C(=O)c1c(C2)cccc1O	636	No
1378	Nanaomycin alphaA	COC(=O)C[C@@H]1O[C@@H](C)C2=C(C1)C(=O)c1c(C2=O)c(O)ccc1	636	No
1379	Deoxyfrenolicin	CCC[C@H]1O[C@H](CC(=O)O)CC2=C1C(=O)c1c(C2=O)cccc1O	636	No
1380	Phenalinolactone D	COC1CCC(OC1C)OCC1(COC(=O)c2[nH]ccc2)C(OC(=O)C)CC(C2(C1CCC1(C2CC=C(C1C1=C(O)C(=O)OC1O)C)C)C)C	637	Yes
1381	Phenalinolactone B	COC1CCC(OC1C)OCC1(COC(=O)c2[nH]ccc2)C(OC(=O)C)CC(C2(C1CCC1(C2CC=C(C1C1=C(O)C(=O)OC1O)C)C)C)O	638	Yes
1382	Phenalinolactone A	COC1CCC(OC1C)OC[C@]1(COC(=O)c2ccc([nH]2)C)[C@H](OC(=O)C)C[C@@H]([C@@]2(C1CC[C@@]1([C@H]2CC=C([C@H]1C1=C(O)C(=O)OC1O)C)C)C)O	638	No
1383	Phenalinolactone C	COCc1ccc([nH]1)C(=O)OC[C@@]1(CO[C@H]2CC[C@H]([C@@H](O2)C)OC)[C@H](OC(=O)C)C[C@@H]([C@@]2([C@@H]1CC[C@@]1([C@H]2CC=C([C@H]1C1=C(O)C(=O)OC1O)C)C)C)O	638	No
1384	Zoumbericin A	COc1cc(oc(=O)c1)Cc1cccc(c1C(=O)c1ccccc1)O	639	Yes
1385	Ruthmycin	CCC[C@H]1O[C@H](CC(=O)O)C=C2[C@@]31CC(=O)C[C@@]2(c1c(C3=O)c(O)ccc1)O	640	Yes
1386	Actinorhodin	OC(=O)C[C@H]1O[C@H](C)c2c(C1)c(O)c1c(c2O)C(=O)C(=CC1=O)C1=CC(=O)c2c(C1=O)c(O)c1c(c2O)C[C@H](O[C@@H]1C)CC(=O)O	641	Yes
1387	Actionorhodin	OC(=O)C[C@@H]1O[C@H](C)C2=C(C1)C(=O)c1c(C2=O)c(O)c(cc1O)c1cc(O)c2c(c1O)C(=O)C1=C(C2=O)C[C@@H](O[C@@H]1C)CC(=O)O	641	No
1388	7-Demethyl-glucopiericidin A	OC[C@H]1O[C@H](OC[C@H]2O[C@@H](O[C@@H](/C(=C/C)/C)[C@@H](/C=C/C=C/C/C(=C/Cc3[nH]c(OC)c(c(=O)c3C)OC)/C)C)[C@@H]([C@H]([C@@H]2O)O)O)[C@@H]([C@H]([C@H]1O)O)O	642	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1389	Glucopiericidinol A3	OC[C@H]1O[C@H](OC[C@H]2O[C@@H](O[C@@H](C(=CC)C)[C@@H](C=C(C=CCC(=CCc3[nH]c(OC)c(c(=O)c3C)OC)C)C)C)[C@@H]([C@H]([C@@H]2O)O)O)[C@@H]([C@H]([C@H]1O)O)O	642	No
1390	BE-14324-113	OCC1OC(OCC2OC(OC(/C(=C/C)/C)[C@@H](/C=C(/C=C/CC(/C=C/c3nc(OC)c(c(c3C)O)OC)(O)C)\C)C(C(C2O)O)O)C(C(C1O)O)O	642	No
1391	(2R,3R,4S,5S,6R)-2-(((2E,4R,5R,6E,8E,11E)-13-(4-Hydroxy-5,6-dimethoxy-3-methylpyridin-2-yl)-3,5,7,11-tetramethyltrideca-2,6,8,11-tetraen-4-yl)oxy)-6-((((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)methyl)tetrahydro-2H-pyran-3,4,5-triol	OC[C@H]1O[C@H](OC[C@H]2O[C@@H](O[C@@H](/C(=C/C)/C)[C@@H](/C=C(/C=C/C/C(=C/Cc3nc(OC)c(c(c3C)O)OC)/C)\C)C)[C@@H]([C@H]([C@@H]2O)O)O)[C@@H]([C@H]([C@@H]1O)O)O	642	Yes
1392	13-Hydroxypiericidin A 10-O-alpha-D-galactose (1→6)-beta-D-glucoside	OC/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1nc(OC)c(c(c1C)O)OC)/C)\C)C)O[C@@H]1O[C@H](CO[C@H]2O[C@H](CO)[C@@H]([C@@H]([C@H]2O)O)O)[C@H]([C@@H]([C@H]1O)O)O)\C	642	No
1393	13-Hydroxypiericidin A 10-O-alpha-D-glucose (1→6)-beta-D-glucoside	OC/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1nc(OC)c(c(c1C)O)OC)/C)\C)C)O[C@@H]1O[C@H](CO[C@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O)O)O)[C@H]([C@@H]([C@H]1O)O)O)\C	642	No
1394	(2R,3R,4S,5S,6R)-2-(((2E,4R,5R,6E,8E,11E)-13-(4-Hydroxy-5,6-dimethoxy-3-methylpyridin-2-yl)-3,5,7,11-tetramethyltrideca-2,6,8,11-tetraen-4-yl)oxy)-6-((((2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)methyl)tetrahydro-2H-pyran-3,4,5-triol	OC[C@H]1O[C@H](OC[C@H]2O[C@@H](O[C@@H](/C(=C/C)/C)[C@@H](/C=C(/C=C/C/C(=C/Cc3nc(OC)c(c(c3C)O)OC)/C)\C)C)[C@@H]([C@H]([C@@H]2O)O)O)[C@@H]([C@H]([C@H]1O)O)O	642	No
1395	4'-O-beta-D-Glucose 13-hydroxyglucopiericidin A	OC/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1nc(OC)c(c(c1C)O[C@H]1O[C@H](CO)[C@H](C([C@H]1O)O)O)OC)/C)\C)C)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)\C	643	Yes
1396	4'-O-beta-D-Glucose glucopiericidin A	C/C=C(/[C@@H]([C@@H](/C=C(/C=C/C/C(=C/Cc1nc(OC)c(c(c1C)O[C@H]1O[C@H](CO)[C@H](C([C@H]1O)O)O)OC)/C)\C)C)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)\C	643	No
1397	3'-Deoxytalopiericidin A1	C/C=C(\[C@@H]([C@@H](/C=C(\C=C/C/C(=C\Cc1nc(OC)c(c(c1C)O[C@@H]1O[C@H](C)[C@@H]([C@@H]([C@@H]1O)O)O)OC)/C)/C)C)O)/C	644	Yes
1398	Glucopiericidin B	OCC1OC(Oc2c(C)c(C/C=C(/C/C=C/C(=C/C(C(/C(=C/C)/C)C)O)C)/C)\C)nc(c2OC)OC)C(C(C1O)O)O	644	No
1399	3'-Rhamnopiericidin A1	C/C=C(\[C@@H]([C@@H](/C=C(\C=C/C/C(=C/Cc1nc(OC)c(c(c1C)O[C@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1O)O)O)OC)/C)/C)C)O)/C	644	No
1400	Awamycin	COC(=O)C1C(O)C(C)C(O)C(C)/C=C(/C)\C(=O)c2c(OC)c(C)c(c3c2C(=O)C(=C(NC(=O)/C(=C\C=C\C(C(C(C1O)C)O)C)/C)C3=O)SC)O	645	Yes
1401	Incednine	CN[C@H]1[C@@H](OC[C@H]([C@@H]1O)O[C@H]1CC[C@@H]([C@H](O1)C)NC)O[C@H]1/C=C\C=C\C(=C\C=C\C(=C\C[C@@H](NC(=O)/C(=C/C(=C/C=C/C=C/[C@@]1(C)O)/C)/OC)C)\C)\C	646	Yes
1402	SIP-B1	CC[C@@H](C/C/1=C\C(=C\C=C\C=C\[C@@](C)(O)C(/C=C\C=C\C(=C\[C@@H](CNC1=O)C)\C)\C)OC1OCC([C@@H](C1N)O)OC1COC([C@@H](C1O)O)C)\C)C	647	No
1403	SIP-C	C/C/1=C\C=C\C(=C\[C@H](C)CNC(=O)/C(=C/C(=C/C=C/C=C/[C@@](C(/C=C\C=C1)OC1OCC([C@@H](C1N)O)OC1OC(C)C([C@](C1)(C)O)N(C)C)(C)O)/C)/CC(C)C)\C	647	Yes
1404	SIP-A1	C/C/1=C\C=C\C(=C\[C@H](C)CNC(=O)/C(=C/C(=C/C=C/C=C/[C@@](C(/C=C\C=C1)OC1OCC([C@@H](C1N)O)OC1COC([C@@H](C1O)O)C)(C)O)/C)/CC(C)C)\C	647	No
1405	SIP-A2b	C/C/1=C\C=C\C(=C\[C@H](C)CNC(=O)/C(=C/C(=C/C=C/C=C/[C@@](C(/C=C\C=C1)OC1OCC([C@@H](C1N)O)OC1OC(C)C([C@](C1)(C)O)O)(C)O)/C)/CC(C)C)\C	647	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1406	SIP-B3	CC[C@@H](C/C/1=C\C(=C\C=C\C=C\[C@@](C)(O)C(/C=C\C=C\C(=C\C=C\C(=C\[C@@H](CNC1=O)C)\C)\C)OC1OCC([C@@H](C1N)O)OC1OC(C)C[C@@H](C1)N(C)C)\C)C	647	No
1407	SIP-A3	CC1OC(OC2COC(C([C@H]2O)N)OC2/C=C\C=C\C(=C\C=C\C(=C\[C@H](C)CNC(=O)/C(=C/C(=C/C=C/C=C/[C@@]2(C)O)/C)/CC(C)C)\C)\C)C[C@H](C1)N(C)C	647	No
1408	SIP-A2	C/C/1=C\C=C\C(=C\[C@H](C)CNC(=O)/C(=C/C(=C/C=C/C=C/[C@@](C(/C=C\C=C1)OC1OCC([C@@H](C1N)O)OC1C[C@@H](O)C(C(O1)C)O)(C)O)/C)/CC(C)C)\C	647	No
1409	dOHSipA	C/C/1=C\C=C\C(=C\C[C@H](C)NC(=O)/C(=C\C(=C\C=C\C=C\[C@@H]([C@H](/C=C\C=C1)O[C@@H]1OC[C@H]([C@@H]([C@H]1N)O)O[C@@H]1O[C@H](C)[C@H]([C@](C1)(C)O)N(C)C)C)\C)/CC(C)C)\C	647	No
1410	SIP-D	CC[C@@H](C/C/1=C\C(=C\C=C\C=C\[C@@](C)(O)C(/C=C\C=C\C(=C\C=C\C(=C\[C@@H](CNC1=O)C)\C)\C)OC1OCC([C@@H](C1N)O)OC1OC(C)C([C@](C1)(C)O)N(C)C)\C)C	647	No
1411	dNHSipA	C/C/1=C\C=C\C(=C\C[C@H](C)NC(=O)/C(=C\C(=C\C=C\C=C\[C@@]([C@H](/C=C\C=C1)O[C@@H]1OC[C@H]([C@@H]([C@H]1N)O)O[C@@H]1O[C@H](C)C(=O)[C@](C1)(C)O)(C)O)\C)/CC(C)C)\C	647	No
1412	dSipA	C/C/1=C\C=C\C(=C\C[C@H](C)NC(=O)/C(=C\C(=C\C=C\C=C\[C@@]([C@H](/C=C\C=C1)O[C@@H]1OC[C@H]([C@@H]([C@H]1N)O)O[C@H]1C[C@@H](O)[C@@H]([C@H](O1)C)N(C)C)(C)O)\C)/CC(C)C)\C	648	Yes
1413	Sipanmycin A	C/C/1=C\C=C\C(=C\C[C@@H](C)NC(=O)/C(=C/C(=C/C=C/C=C/[C@]([C@@H](/C=C\C=C1)O[C@H]1OC[C@@H]([C@H]([C@@H]1N)O)O[C@@H]1CC[C@H]([C@@H](O1)C)N(C)C)(C)O)/C)/CC(C)C)\C	648	No
1414	Sipanmycin B	CC[C@@H](C/C/1=C\C(=C\C=C\C=C\[C@@](C)(O)[C@H](/C=C\C=C\C(=C\C=C\C(=C\C[C@@H](NC1=O)C)\C)\C)O[C@@H]1OC[C@H]([C@@H]([C@H]1N)O)O[C@@H]1O[C@H](C)[C@H]([C@](C1)(C)O)N(C)C)\C)C	648	No
1415	3'-O-Demethylsilvalactam	C/C/1=C\C=C\C(=C\C[C@H](C)NC(=O)/C(=C\C(=C\C=C\C=C\[C@@]([C@H](/C=C\C=C1)O[C@@H]1OC[C@H]([C@@H]([C@H]1N)O)O)(C)O)\C)/CC(C)C)\C	648	No
1416	Silvalactam	CO[C@H]1[C@H](O)COC(C1N)OC1/C=C\C=C\C(=C\C=C\C(=C\CC(NC(=O)/C(=C/C(=C/C=C/C=C/C1(C)O)/C)/CC(C)C)C)\C)\C	648	No
1417	AgB+S1	CC[C@@H](C/C/1=C/C(=C/C=C/C=C/[C@@](C)(O)[C@H](/C=C\C=C\C(=C\C=C\C(=C\C[C@@H](NC1=O)C)\C)\C)O[C@@H]1OC[C@H]([C@@H]([C@H]1N)O)O)/C)C	648	No
1418	Auroramycin	C/C/1=C\C=C\C(=C\C[C@H](C)NC(=O)/C(=C/C(=C/C=C/C=C/[C@@]([C@H](/C=C/C=C1)O[C@@H]1OC[C@H]([C@@H]([C@H]1N)O)O[C@@H]1O[C@H](C)[C@H]([C@](C1)(C)O)N(C)C)(C)O)/C)/CC(C)C)\C	648	No
1419	dSipB	CC[C@@H](C/C/1=C/C(=C/C=C/C=C/[C@@](C)(O)[C@H](/C=C\C=C\C(=C\C=C\C(=C\C[C@@H](NC1=O)C)\C)\C)O[C@@H]1OC[C@H]([C@@H]([C@H]1N)O)O[C@H]1C[C@@H](O)[C@@H]([C@H](O1)C)N(C)C)/C)C	648	No
1420	Heronamide F	C/C=C/C=C/C[C@@H]1C/C=C/C=C(\C)/C=C/C=C\[C@H]([C@H](/C=C(/C=C/C=C/C(=O)N1)\C)O)O	649	Yes
1421	Bombyxamycin A	C[C@@H]1/C=C\C=C\C=C/C=C\C=C\C(=O)C[C@@H](C/C=C(\C=C\C=C/C=C\C(=O)NC1)/C)O	650	Yes
1422	(3Z,5E,7Z,9Z,12R,13E,15E,17Z,19Z,21Z,23R)-12- Hydroxy-23-methyl-1-azacyclotetracosa-3,5,7,9,13,15,17,19,21-nonaen-2-one	C[C@@H]1/C=C\C=C/C=C\C=C\C=C\[C@H](O)C/C=C\C=C/C=C/C=C\C(=O)NC1	651	Yes
1423	Cyclamenol A	CC1/C=C/C=C/C=C\C=C\C(O)C/C=C/C=C/C=C/C(=O)NC1	651	No
1424	Bafilomycin A	COC1C=CC=C(C)CC(C)C(O)C(C(=CC=C(C(=O)OC1C(C(C(C1(O)CC(O)C(C(O1)C(C)C)C)C)O)C)OC)C)C	652	Yes
1425	Concanamycin B	C/C=C/[C@H]1O[C@](O)(C[C@H]([C@@H]1C)O[C@H]1C[C@@H](O)[C@@H]([C@H](O1)C)OC(=O)N)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C(=C/C(=C/[C@@H](C)[C@@H](O)[C@H]([C@H]([C@@H](C/C(=C/C=C/[C@@H]1OC)/C)C)O)C)/C)/OC)C)O)C	653	Yes
1426	Concanamycin D	C/C=C/C1OC(O)(CC(C1C)O[C@@H]1C[C@@H](O)[C@@H]([C@H](O1)C)O)C(C(C(C1OC(=O)/C(=C\C(=C/C(C)C(O)C(C(C(C/C(=C\C=C/C1OC)/C)C)O)C)\C)/OC)C)O)C	653	No
1427	Concanamycin E	C/C=C/C1OC(O)(CC(C1C)OC1CC(O)C(C(O1)C)OC(=O)N)C(C(C(C1OC(=O)/C(=C/C(=C/C(C)C(O)CC(C(C/C(=C/C=C/C1OC)/C)C)O)/C)/OC)C)O)C	654	No
1428	Viranamycin B	COC1/C=C/C=C(\C)/CC(C)C(O)C(CC)C(C(/C=C(/C=C(/C(=O)OC1C(C(C(C1(O)CC(OC2CC(O)C(C(O2)C)OC(=O)N)C(C(O1)C)C)C)O)C)\OC)\C)C)O	654	No
1429	Concanamycin F	C/C=C/[C@H]1O[C@](O)(C[C@H]([C@@H]1C)O)[C@H]([C@@H]([C@@H](C1OC(=O)/C(=C\C(=C\[C@@H](C)[C@@H](O)[C@H]([C@H]([C@@H](C/C(=C/C=C/[C@@H]1OC)/C)C)O)CC)\C)/OC)C)O)C	654	No
1430	Concanamycin	C/C=C/[C@H]1O[C@](O)(C[C@H]([C@@H]1C)O)[C@H]([C@@H]([C@@H](C1OC(=O)/C(=C/C(=C/[C@@H](C)[C@@H](O)[C@H]([C@H]([C@@H](C/C(=C/C=C/[C@@H]1OC)/C)C)O)CC)/C)/OC)C)O)C	654	No
1431	Concanamycin C	C/C=C/C1OC(O)(CC(C1C)O[C@@H]1C[C@@H](O)[C@@H]([C@H](O1)C)O)C(C(C(C1OC(=O)/C(=C\C(=C/C(C)C(O)C(C(C(C/C(=C\C=C/C1OC)/C)C)O)CC)\C)/OC)C)O)C	654	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1432	Concanamycin A	C/C=C/[C@H]1O[C@](O)(C[C@H]([C@@H]1C)O[C@H]1C[C@@H](O)[C@@H]([C@H](O1)C)OC(=O)N)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C(=C/C(=C/[C@@H](C)[C@@H](O)[C@H]([C@H]([C@@H](C/C(=C/C=C/[C@@H]1OC)/C)C)O)CC)/C)/OC)C)O)C	655	Yes
1433	Linearolide A	COC1CC/C=C(\C)/C=C/C(OC2CC(NC(=O)C)C(C(O2)C)O)C(C)CC(C2OC(C(C(=O)OC1/C=C/C(=C/C(C(O)C)C)/C)C)(O)C(OC)C(C2C)O)OC	656	Yes
1434	5,6-Dihydro-kirromycin	C/C=C\C=C\C1OC(O)([C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H](C2OC([C@@H]([C@@H]2O)O)/C=C/C=C/C=C(/C(=O)C2=C(O)CCNC2=O)\C)C)OC)\C)CC)C(C(C1(C)C)O)O	657	Yes
1435	Kirrothricin	C/C=C\C=C\[C@@H]1O[C@@](O)(C[C@@H](C1(C)C)O)C(C(=O)NC/C=C/C=C(/C(C(C(C(/C=C/C=C/C=C/C=C(/C(=C\1/C(=O)CCN(C1=O)C)/O)\C)O)O)C)OC)\C)CC	657	No
1436	20-O-Demethyl-kirromycin	C/C=C\C=C\C1OC(O)([C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H](C2OC([C@@H]([C@@H]2O)O)/C=C/C=C/C=C(/C(=O)C2=C(O)CCNC2=O)\C)C)O)\C)CC)C(C(C1(C)C)O)O	657	No
1437	Kirromycin B	C/C=C/C=C/[C@@H]1O[C@](O)([C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H]([C@@H]2O[C@@H]([C@@H]([C@@H]2O)O)/C=C/C=C/C=C(/C(=O)c2c(O)cc[nH]c2=O)\C)C)OC)\C)CC)[C@@H]([C@@H](C1(C)C)O)O	657	No
1438	30-Hydroxy-5,6-dehydro- 1-N-demethyl-16-deoxy-kirrothricin	C/C=C\C=C\C1OC(O)([C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H](C(/C=C/C=C/C=C/C=C(/C(=O)c2c(O)cc[nH]c2=O)\C)O)C)OC)\C)CC)C(C(C1(C)C)O)O	657	No
1439	30-Deoxy-kirromycin	C/C=C\C=C\C1OC(O)(CC(C1(C)C)O)[C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H](C1OC([C@@H]([C@@H]1O)O)/C=C/C=C/C=C(/C(=O)C1=C(O)CCNC1=O)\C)C)OC)\C)CC	657	No
1440	Kirromycin	C/C=C\C=C\[C@@H]1O[C@](O)([C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H]([C@@H]2O[C@@H]([C@@H]([C@@H]2O)O)/C=C/C=C/C=C(/C(=O)c2c(O)cc[nH]c2=O)\C)C)OC)\C)CC)[C@@H]([C@@H](C1(C)C)O)O	657	No
1441	Factumycin	C/C=C\C=C\[C@@H]1O[C@@](O)(C[C@@H](C1(C)C)O)C(C(=O)NC/C=C/C=C(\[C@@H]([C@H](C([C@H](/C=C\C=C\C=C\C=C(\C(=O)c1c(O)ccn(c1=O)C)/C)O)O)C)OC)/C)CC	657	No
1442	Aurodox	C/C=C\C=C\[C@@H]1O[C@](O)([C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H](C2O[C@@H]([C@@H]([C@@H]2O)O)/C=C/C=C/C=C(/C(=C\2/C(=O)C=CN(C2=O)C)/O)\C)C)OC)\C)CC)[C@@H]([C@@H](C1(C)C)O)O	657	No
1443	Kirromycin C	C/C=C\C=C\[C@@H]1O[C@@](O)(C[C@@H](C1(C)C)O)[C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H]([C@@H]1O[C@@H]([C@@H]([C@@H]1O)O)/C=C/C=C/C=C(/C(=O)c1c(O)cc[nH]c1=O)\C)C)OC)\C)CC	657	No
1444	Mocimycin	C/C=C/C=C/[C@@H]1O[C@@](O)([C@@H]([C@@H](C1(C)C)O)O)[C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H](C1O[C@@H]([C@@H]([C@@H]1O)O)/C=C/C=C/C=C(/C(=C/1\C(=O)NC=CC1=O)/O)\C)C)OC)\C)CC	657	No
1445	Efrotomycin	C/C=C/C=C/C1OC(O)(C(C(=O)NC/C=C/C=C(/C(C(C2OC(C(C2O)O)/C=C/C=C/C=C(/C(=C\2/C(=O)C=CN(C2=O)C)/O)\C)C)OC)\C)CC)C(C(C1(C)C)OC1OC(C)C(C(C1O)OC)OC1OC(C)C(C(C1OC)O)OC)O	658	Yes
1446	Bisoxazolomycin	CO[C@H]([C@]1(O)[C@@H](C)C(=O)N([C@]1(COC(=O)[C@@]1(CO)N(C)C(=O)[C@@H]([C@@]1(O)[C@H](C[C@H]([C@H](C=CC=CCNC(=O)C([C@@H](C(=CC=CC=CCc1cnco1)C)O)(C)C)O)C)C)C(=O)O)C)C[C@H]([C@H](C=CC=CCNC(=O)C([C@@H](C(=CC=CC=CCc1cnco1)C)O)(C)C)O)C	659	Yes
1447	Lajollamycin	COC(C1(O)C(C)C(=O)N(C21C(C)OC2=O)C)CC(C(/C=C/C=C/CNC(=O)C(C(/C(=C\C=C/C=C/C(=C(/[N+](=O)[O-])\C)/C)/C)O)(C)C)O)C	660	No
1448	Triedimycin B	COC(C1(O)C(C)C(=O)N(C21C(C)OC2=O)C)CC(C(/C=C/C=C/CNC(=O)C(C(/C(=C/C=C/C=C/Cc1cnc(o1)C)/C)O)(C)C)O)C	660	No
1449	Triedimycin A	COCC1OC(=O)C21N(C)C(=O)C(C2(O)C(CC(C(/C=C/C=C/CNC(=O)C(C(/C(=C\C=C/C=C/Cc1cnc(o1)C)/C)O)(C)C)O)C)OC)C	660	No
1450	Oxazolomycin A	CO[C@H]([C@]1(O)[C@@H](C)C(=O)N([C@]21COC2=O)C)C[C@H]([C@H](/C=C/C=C/CNC(=O)C([C@@H](/C(=C\C=C/C=C/Cc1ocnc1)/C)O)(C)C)O)C	660	No
1451	Lajollamycin D	CO[C@H]([C@]1(O)[C@@H](C)C(=O)N([C@]21[C@@H](C)OC2=O)C)C[C@H]([C@H](/C=C/C=C/CNC(=O)C([C@@H](/C(=C\C=C\C=C\C(=C(\N(=O)=O)/C)\C)/C)O)(C)C)O)C	660	No
1452	Lajollamycin B	CO[C@@H]([C@]1(O)[C@@H](C)C(=O)N([C@]21COC2=O)C)C[C@@H]([C@@H](/C=C/C=C/CNC(=O)C([C@H](/C(=C/C=C/C=C/C=C(/N(=O)=O)\C)/C)/C)O)(C)C)O)C	660	No
1453	Lajollamycin C	CO[C@@H]([C@]1(O)[C@@H](C)C(=O)N([C@]21[C@@H](C)OC2=O)C)C[C@@H]([C@@H](/C=C/C=C/CNC(=O)C([C@H](/C(=C/C=C/C=C/C=C(/N(=O)=O)\C)/C)/C)O)(C)C)O)C	660	No
1454	Curromycin B	COC(C1(O)C(C)C(=O)N(C21C(C)OC2=O)C)CC(C(/C=C/C=C/CNC(=O)C(C(/C(=C\C=C/C=C/Cc1cnc(o1)C)/C)O)(C)C)O)C	660	No
1455	Diffusomycin	CO[C@H]([C@]1(O)[C@@H](C)C(=O)N(C21COC2=O)C)C[C@H](C(/C=C/C=C/CNC(=O)C(C(/C(=C\C=C/C=C/Cc1ocnc1)/C)O)(C)C)O)C	660	Yes
1456	Osmanicin	O=C1O[C@H]2[C@H]3N1CC[C@@H]1C3=C([C@@H]2O)[C@@H](C)[C@@H]([C@]21C=CC1=C2C(=O)CCN1)C	661	Yes
1457	Tetrapetalone B	CC(=O)O[C@@H]([C@]12C=C(C)[C@H]3[C@]4(C(=CC(=O)C=C4[C@H]([C@@H]3C)O[C@H]3CC[C@@H](C(O3)C)O)N2C(=O)C(=C1O)C)O)C	662	Yes
1458	Tetrapetalone A	CC[C@]12C=C(C)[C@H]3[C@]4(C(=CC(=O)C=C4[C@H]([C@@H]3C)O[C@H]3CC[C@H]([C@H](O3)C)O)N2C(=O)C(=C1O)C)O	662	No
1459	2,18-seco-Lankacidinol A	O[C@@H]1/C=C/C(=C/C(NC(=O)[C@@H](O)C)OC2=C(C)C(=O)O[C@H](C[C@@H](/C=C/C(=C/C1)/C)O)[C@H]2C)/C	663	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1460	Lankacidinol	O[C@@H]1/C=C/C(=C/[C@@H](NC(=O)[C@@H](O)C)[C@]2(C)C(=O)O[C@H](C[C@@H](/C=C/C(=C/C1)/C)O)[C@H](C2=O)C)/C	663	No
1461	Lankacidin	O[C@@H]1/C=C/C(=C/[C@@H](NC(=O)C(=O)C)[C@]2(C)C(=O)O[C@H](C[C@@H](/C=C/C(=C/C1)/C)O)[C@H](C2=O)C)/C	663	No
1462	iso-Lankacidinol	O[C@@H]1/C=C\C(=C/[C@@H](NC(=O)[C@@H](O)C)[C@]2(C)C(=O)O[C@@H](C[C@@H](/C=C\C(=C/C1)\C)O)[C@H](C2=O)C)\C	663	Yes
1463	Lankacidinol A	O[C@@H]1/C=C/C(=C\C(NC(=O)[C@H](O)C)[C@]2(C)C(=O)O[C@H](C[C@@H](/C=C\C(=C/C1)\C)OC(=O)C)[C@H](C2=O)C)/C	664	No
1464	Sedecamycin	OC1/C=C/C(=C/C(NC(=O)C(=O)C)C2(C)C(=O)OC(CC(/C=C/C(=C/C1)/C)OC(=O)C)C(C2=O)C)/C	664	Yes
1465	Lankacidin C 14-propionate	CCC(=O)OC1/C=C\C(=C/CC(O)/C=C\C(=C/C(C2(C(=O)OC(C1)C(C)C2=O)C)NC(=O)C(=O)C)\C)\C	664	No
1466	O-beta-Kijanosyl-(1→17)-kijanolide	COC(=O)N[C@H]1[C@@H](C)O[C@H](C[C@]1(C)N(=O)=O)O[C@H]1C/C=C(\C)/[C@@H]2C=C[C@H]3[C@H]([C@]2(C)C(=O)C2=C([C@]4([C@H](/C=C/1\C)C=C(CO)[C@@H](C4)C)OC2=O)O)[C@@H](C)C[C@@H]([C@@H]3O)C	665	Yes
1467	Phenelfamycin B	C/C=C/C=C/C1OC(O)(C(C(=O)NC/C=C/C=C(/C(C(C2OC(C(C2)O)/C=C/C=C/C=C/C(=O)O)C)OC)\C)COC2CC(OC)OC(C2O)C)C(C(C1(C)C)OC(=O)Cc1ccccc1)O	666	No
1468	Phenelfamycin A	C/C=C/C=C/C1OC(O)(C(C(=O)NC/C=C/C=C(/C(C(C2OC(C(C2)O)/C=C/C=C/C=C/C(=O)O)C)OC)\C)COC2CC(OC)OC(C2O)C)C(C(C1(C)C)O)OC(=O)Cc1ccccc1	666	No
1469	Unphenelfamycin	C/C=C/C=C/C1OC(O)(C(C(=O)NC/C=C/C=C(/C(C(C2OC(C(C2)O)/C=C/C=C/C=C/C(=O)O)C)OC)\C)COC2CC(OC)OC(C2O)C)C(C(C1(C)C)O)O	666	Yes
1470	L 681217	C/C=C/C=C/C1OC(O)(CC(C1(C)O)O)O)C(C(=O)NC/C=C/C=C(/C(C(C1OC(C(C1)O)/C=C/C=C/C=C/C(=O)O)C)OC)\C)CC	666	No
1471	Demethyl-L-681,217	C/C=C\C=C\[C@@H]1O[C@@](O)(C[C@@H](C1(C)O)O)[C@@H](C(=O)NC/C=C/C=C(/[C@H]([C@H]([C@@H]1O[C@@H]([C@@H](C1)O)/C=C/C=C/C=C/C(=O)O)C)OC)\C)C	666	No
1472	Phenelfamycin C	C/C=C/C=C/C1OC(O)(C(C(=O)NC/C=C/C=C(/C(C(C2OC(C(C2)O)/C=C/C=C/C=C/C(=O)O)C)OC)\C)COC2CC(OC)C(C(O2)C)OC2CC(OC)C(C(O2)C)O)C(C(C1(C)C)O)OC(=O)Cc1ccccc1	667	Yes
1473	Phenelfamycin E	C/C=C\C=C\[C@@H]1O[C@](O)(C(C(=O)NC/C=C/C=C(/C([C@H](C2O[C@@H]([C@@H](C2)O)/C=C/C=C/C=C/C(=O)O)C)OC)\C)CO[C@@H]2C[C@@H](OC)C([C@H](O2)C)O[C@H]2C[C@H](OC)[C@@H]([C@H](O2)C)O[C@@H]2C[C@@H](OC)[C@H]([C@H](O2)C)O)[C@@H]([C@@H](C1(C)C)O)OC(=O)Cc1ccccc1	668	Yes
1474	Phenelfamycin F	C/C=C/C=C/C1OC(O)(C(C(=O)NC/C=C/C=C(/C(C(C2OC(C(C2)O)/C=C/C=C/C=C/C(=O)O)C)OC)\C)COC2CC(OC)C(C(O2)C)OC2CC(OC)C(C(O2)C)OC2CC(OC)C(C(O2)C)O)C(C(C1(C)C)OC(=O)Cc1ccccc1)O	669	Yes
1475	9-DeoxoFK506	CCC[C@H]1/C=C(\C)/C[C@@H](C)C[C@H](OC)C2O[C@@](O)(CC(=O)N3C[C@H](C(=O)OC([C@@H]([C@@H](CC1=O)O)C)/C(=C/[C@@H]1CC[C@H]([C@@H](C1)OC)O)/C)CCC3)[C@@H](C[C@@H]2OC)C	670	Yes
1476	Tsukubamycin B	CCC[C@@H]1/C=C(\C)/C[C@H](C)C[C@H](OC)[C@H]2O[C@](O)([C@@H](C[C@H]2OC)C)C(=O)C(=O)N2[C@H](C(=O)O[C@@H]([C@@H]([C@H](CC1=O)O)C)/C(=C/[C@@H]1CC[C@H]([C@H](C1)OC)O)/C)CCCC2	671	No
1477	Tacrolimus	C=CC[C@@H]1/C=C(\C)/C[C@H](C)C[C@H](OC)[C@H]2O[C@](O)([C@@H](C[C@@H]2OC)C)C(=O)C(=O)N2[C@H](C(=O)O[C@@H]([C@@H]([C@H](CC1=O)O)C)/C(=C/[C@@H]1CC[C@H]([C@@H](C1)OC)O)/C)CCCC2	671	Yes
1478	32-Dehydroxy-FK506	C=CC[C@@H]1/C=C(\C)/C[C@H](C)C[C@H](OC)[C@H]2O[C@](O)([C@@H](C[C@@H]2OC)C)C(=O)C(=O)N2[C@H](C(=O)O[C@@H]([C@@H]([C@H](CC1=O)O)C)/C(=C/[C@@H]1CCC[C@@H](C1)OC)/C)CCCC2	671	No
1479	36-Methyl-Fk506	CO[C@@H]1C[C@@H](CC[C@H]1O)/C=C(/[C@H]1OC(=O)[C@@H]2CCCCN2C(=O)C(=O)[C@]2(O)O[C@H]([C@H](C[C@@H](C/C(=C\[C@H](C(=O)C[C@@H]([C@H]1C)O)CC(=C)C)/C)C)OC)[C@H](C[C@H]2C)OC)\C	671	No
1480	31-O-Demethyl-FK506	C=CCC1/C=C(\C)/CC(C)CC(OC)C2OC(O)(C(CC2OC)C)C(=O)C(=O)N2C(C(=O)OC(C(C(CC1=O)O)C)/C(=C/C1CCC(C(C1)O)O)/C)CCCC2	671	No
1481	FK520	CC[C@@H]1/C=C(\C)/C[C@H](C)C[C@H](OC)[C@H]2O[C@](O)([C@@H](C[C@@H]2OC)C)C(=O)C(=O)N2[C@H](C(=O)O[C@@H]([C@@H]([C@H](CC1=O)O)C)/C(=C/[C@@H]1CC[C@H]([C@@H](C1)OC)O)/C)CCCC2	671	No
1482	9-Deoxo-31-O-demethylFK506	C[C@@H]1C[C@@H]([C@@H]2[C@H](C[C@H]([C@@](O2)(CC(=O)N3CCCC[C@H]3C(=O)O[C@@H]([C@@H]([C@H](CC(=O)[C@@H](/C=C(\\C1)/C)CC=C)O)C)/C(=C/[C@@H]4CC[C@H]([C@@H](C4)O)O)/C)O)C)OC)OC	672	Yes
1483	9-Hydroxy-31-O-demethylFK506	C=CC[C@H]1/C=C(\C)/C[C@H](C)C[C@H](OC)[C@H]2O[C@](O)([C@@H](C[C@@H]2OC)C)C(C(=O)N2[C@H](C(=O)OC([C@@H]([C@H](CC1=O)O)C)/C(=C/[C@H]1CC[C@H]([C@@H](C1)O)O)/C)CCCC2)O	673	No
1484	FR900525	C=CC[C@@H]1/C=C(\C)/C[C@H](C)[C@H](OC)[C@H]2O[C@](O)([C@@H](C[C@@H]2OC)C)C(=O)C(=O)N2[C@H](C(=O)O[C@@H]([C@@H]([C@H](CC1=O)O)C)/C(=C/[C@@H]1CC[C@H]([C@@H](C1)OC)O)/C)CCC2	673	No
1485	9-HydroxyFK506	C=CC[C@H]1/C=C(\C)/C[C@H](C)C[C@H](OC)[C@H]2O[C@](O)([C@@H](C[C@@H]2OC)C)C(C(=O)N2[C@H](C(=O)OC([C@@H]([C@H](CC1=O)O)C)/C(=C/[C@H]1CC[C@H](C(C1)OC)O)/C)CCCC2)O	673	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1486	Homorapamycin A	CO[C@@H]1C[C@@H](CC[C@H]1O)C[C@H]([C@H]1OC(=O)C2CCCCN2C(=O)C(=O)[C@]2(O)O[C@@H](CC[C@H]2CC)C[C@H](OC)/C(=C/C=C/C=C/[C@H](C[C@H](C(=O)[C@@H]([C@@H](/C(=C/[C@H](C(=O)C1)C)/C)O)OC)C)C)/C)C
1487	Homorapamycin B	CC[C@@H]1/C=C/C=C/C=C(\C)/[C@@H](OC)C[C@@H]2CC[C@H]([C@](O2)(O)C(=O)C(=O)N2C(C(=O)O[C@@H](CC(=O)[C@@H](/C=C(/[C@H]([C@H](C(=O)[C@@H](C1)C)OC)O)\C)C)[C@@H](C[C@@H]1CC[C@H]([C@@H](C1)OC)O)C)CCCC2)C
1488	SCHEMBL7943587	CC/C/1=C/CC(OC(=O)C2CCCCN2C(=O)C(=O)C2(O)OC(CCC2C)CC(C(C(CC(CC(/C(=C\C(CC(C1O)C)C)/C)O)O)O)C)O)/C(=C/C(C(O)C)C)/C
1489	SCHEMBL8282790	CC/C/1=C/CC(OC(=O)C2CCCN2C(=O)C(=O)C2(O)OC(CCC2C)CC(C(C(CC(CC(/C(=C\C(CC(C1O)C)C)/C)O)O)O)C)O)/C(=C/C(C(O)C)C)/C	676	No
1490	BC325	CO[C@H]1C[C@@H]2CC[C@H]([C@](O2)(O)C(=O)C(=O)N2CCCC[C@H]2C(=O)O[C@@H](CC(=O)[C@@H](/C=C(/[C@H](CC(=O)[C@@H](C[C@@H](/C=C/C=C/C=C/1\C)C)C)O)\C)C)[C@@H](Cc1cccc(c1)O)C)C	677	Yes
1491	Demethoxyrapamycin	COC1CC(CCC1O)CC(C1OC(=O)C2CCCCN2C(=O)C(=O)C2(O)OC(CCC2C)CC(OC)/C(=C/C=C/C=C\C(CC(C(=O)CC(/C(=C/C(C(=O)C1)C)/C)O)C)C)/C)C	677	No
1492	BRN 4225908	C=CCC1/C=C(/C)\CC(C)CC(OC)C2OC(O)(C(CC2OC)C)C(=O)C(=O)N2C(C(=O)OC(C(C(CC1=O)O)C)/C(=C/C1CCC(C(C1)OC)O)/C)CCC2	678	Yes
1493	Rapamycin	CO[C@@H]1C[C@@H](CC[C@H]1O)C[C@H](C1OC(=O)C2CCCCN2C(=O)C(=O)[C@]2(O)OC(CC[C@H]2C)C[C@H](OC)/C(=C/C=C/C=C\[C@H](C[C@H](C(=O)[C@@H]([C@@H](/C(=C/[C@H](C(=O)C1)C)/C)O)OC)C)C)/C)C	679	Yes
1494	Homorapamycin C	CO[C@@H]1C[C@@H](CC[C@H]1O)C[C@H]([C@H]1OC(=O)C2CCCCN2C(=O)C(=O)[C@]2(O)O[C@@H](CC[C@H]2C)C[C@H](OC)/C(=C/C=C/C=C/[C@H](C[C@H](C(=O)[C@@H]([C@@H](/C(=C/[C@H](C(=O)C1)CC)/C)O)OC)C)C)/C)C	680	Yes
1495	FR 900523	CO[C@@H]1C[C@@H](CC[C@H]1O)/C=C(/[C@H]1OC(=O)C2CCCCN2C(=O)C(=O)[C@]2(O)OC([C@H](C[C@H](C/C(=C/[C@H](C(=O)C[C@@H]([C@H]1C)O)C)/C)C)OC)[C@H](C[C@H]2C)OC)\C	681	Yes
1496	L-156,586	O[C@H]1/C=C/C=C(/C)\C=N\C=N\C(=O)/C=C/C(=C)[C@@H](OC(=O)C2=CCCC32N2C(C1)OCC2C3O)C(C)C	682	Yes
1497	Cinnabaramide A	C[C@]12OC(=O)[C@@]2(NC(=O)[C@@H]1CCCCCC)[C@H](C1CCCC=C1)O	683	Yes
1498	5'-Epi-SPA-6952A	CCC(CC1CCCC2(O1)CC1OC(=O)/C=C/C(C)(O)C(O)C(C)C(O)C(OC3CCC(C(O3)C)N(C)C)C(O)C(CCCCC/C=C/C3=C(CC(O2)C1C)OC(C3)(C)C)(C)O)O	684	Yes
1499	Ossamycin	CC[C@H](C[C@H]1CCC[C@]2(O1)C[C@@H]1OC(=O)/C=C/[C@@](C)(O)[C@@H](O)[C@H](C)[C@@H](O)[C@H](OC3CCC(C(O3)C)N(C)C)[C@@H](O)[C@](CCCCC/C=C/[C@H]3[C@@](C[C@H](O2)[C@H]1C)(O)OC(C3)(C)C)(C)O)O	685	Yes
1500	NK 154183B	CCC(CC1CCCC2(O1)CC1OC(=O)/C=C/C(C)(O)C(O)C(C)C(O)C(OC3CCC(C(O3)C)N(C)C)C(O)C(CCCCC/C=C/C3C(CC(O2)C1C)(O)OC(C3)(C)C)(C)O)O	685	No
1501	Yokonolide B	CCC(CC1CCCC2(O1)CC1OC(=O)C=CC(C)(O)C(O)C(C)C(O)C(OC3CC(O)C(C(O3)C)N(C)C)C(C(CCCC=CC3(C(CC(O2)C1C)OC(O)C(C3)C)C)C)O)O	686	Yes
1502	A82548A	CC[C@H](C[C@H]1CCC[C@]2(O1)C[C@@H]1OC(=O)/C=C/[C@@](C)(O)[C@@H](O)[C@H](C)[C@@H](O)[C@H](O[C@H]3C[C@H](O)[C@@H]([C@@H](O3)C)N(C)C)[C@H]([C@H](CCC/C=C/[C@H]3[C@H](C[C@H](O2)[C@H]1C)OC(O)[C@H](C3)C)C)O)O	687	Yes
1503	Yokonolide A	OC[C@H](C[C@@H]1/C=C/CCC[C@H](C)[C@@H](O)[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)N(C)C)[C@H](O)[C@H](C)[C@@H]([C@](/C=C\C(=O)O[C@H]2[C@H]([C@H](C[C@@H]1O)O[C@]1(CCC[C@@H](O1)C[C@H](CC)O)[C@@H]2C)C)(C)O)O)C	688	Yes
1504	NK 154183A	CCC(CC1CCCC2(O1)CC1OC(=O)/C=C/C(C)(O)C(O)C(C)C(O)C(O)C(O)C(CCCCC/C=C/C3C(CC(O2)C1C)(O)OC(C3)(C)C)(C)O)O	689	Yes
1505	Cytovaricin	CC[C@H](C[C@@H]1O[C@@]2(CC[C@@H]1C)CC1OC(=O)/C=C/[C@@](C)(O)[C@@H](O)[C@@H](C)[C@@H](O)[C@H](O[C@H]3C[C@H](OC)[C@@H]([C@H](O3)C)O)[C@H]([C@](CCC/C=C/C3[C@@](CC(O2)[C@H]1C)(O)OC[C@H](C3)C)(C)O)O)O	690	Yes
1506	Phthoramycin	CC[C@H](C[C@@H]1O[C@@]2(CC[C@@H]1C)C[C@@H]1OC(=O)/C=C/[C@@](C)(O)[C@@H](O)[C@H](C)[C@@H](O)C[C@H]([C@](CCC/C=C/[C@H]3[C@@](C[C@H](O2)[C@H]1C)(O)OC[C@H](C3)C)(C)O)O)O	691	Yes
1507	Ushikulide A	CCC(CC1OC2(CCC1C)CC1OC(=O)/C=C/C(C)C(O)C(C)C(O)CC(C(CCC/C=C/C(C(=O)CC(O2)C1C)CC(C)C)(C)O)O)O	692	Yes
1508	Ushikulides A	CC[C@H](C[C@@H]1O[C@@]2(CC[C@@H]1C)C[C@@H]1OC(=O)/C=C/[C@H](C)[C@@H](O)[C@H](C)[C@@H](O)C[C@H]([C@H](CCC/C=C/[C@@H](C(=O)C[C@H](O2)[C@H]1C)CC(C)C)C)O)O	692	No
1509	Ushikulide B	CCC(CC1OC2(CCC1C)CC1OC(=O)/C=C/C(C)C(O)C(C)C(O)CC(C(CCCC/C=C(/C(=O)CC(O2)C1C)\CC(C)C)(C)O)O)O	692	No
1510	Dunaimycin	CC[C@H](C[C@H]1CCC[C@]2(O1)C[C@@H]1OC(=O)/C=C/[C@@](C)(O)[C@@H](O)[C@H](C)[C@@H](O)C[C@@H](O)[C@](CCCCC/C=C/[C@@H](C(=O)C[C@H](O2)[C@H]1C)CC(C)C)(C)O)O	692	No
1511	YO-001A	CCC(CC1OC2(CCC1C)CC1CC(O2)CCC(CC)/C=C/C=C/CCCC(C(CC(CC(C(C(C(/C=C/C(=O)O1)CC)O)C)O)O)O)(C)O)O	692	No
1512	Ushikulides B	CC[C@H](C[C@@H]1O[C@@]2(CC[C@@H]1C)C[C@@H]1OC(=O)/C=C/[C@H](C)[C@@H](O)[C@H](C)[C@@H](O)C[C@@H](O)[C@H](CCCCC/C=C/[C@@H](C(=O)C[C@H](O2)[C@H]1C)CC(C)C)C)O	693	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1513	Oligomycin F	CCC(CC1OC2(CCC1C)OC1CC[C@H](CC)/C=C\C=C/C[C@@H](C)[C@@H](O)[C@@](C)(O)C(=O)[C@H]([C@H]([C@H](C(=O)[C@H]([C@@H]([C@H](/C=C/C(=O)OC(C2C)[C@H]1C)C)O)C)C)O)C)O	694	No
1514	Oligomycin	CC[C@H]1/C=C\C=C\C[C@H](C)[C@@H](O)[C@](C)(O)C(=O)[C@H](C)[C@@H](O)C(C)C(=O)[C@@H]([C@@H]([C@H](/C=C/C(=O)OC2C([C@H](CC1)O[C@@]1(CC[C@H]([C@H](O1)CC(O)C)C)[C@@H]2C)C)C)O)C	694	Yes
1515	Oligomycin A	CC[C@@H]1/C=C/C=C/C[C@H](C)[C@@H](O)[C@](C)(O)C(=O)[C@H](C)[C@@H](O)[C@H](C)C(=O)[C@@H]([C@H]([C@@H](/C=C/C(=O)OC2[C@H](C(CC1)O[C@@]1(CC[C@H]([C@H](O1)C[C@@H](O)C)C)[C@@H]2C)C)C)O)C	694	No
1516	Oligomycin SC-II	CCC1/C=C/C=C/CC(C)C(O)C(C)(O)C(=O)CC(O)C(C)C(C(C(C(/C=C/C(=O)OC2C(C(CC1)OC1(CCC(C(O1)CC(O)C)C)C2C)C)C)O)C)O	695	Yes
1517	Oligomycin B	CC[C@@H]1/C=C/C=C/C[C@H](C)[C@@H](O)[C@](C)(O)C(=O)[C@H](C)[C@@H](O)[C@H](C)C(=O)[C@@H]([C@H]([C@@H](/C=C/C(=O)OC2[C@H](C(CC1)O[C@]1(O[C@H](C[C@@H](O)C)[C@@H](CC1=O)C)[C@@H]2C)C)C)O)C	696	Yes
1518	Oligomycin E	CC[C@H]1/C=C/C=C/C[C@@H](C)[C@H](O)[C@@](C)(O)C(=O)[C@@H](C)[C@H](O)[C@@H](C)C(=O)[C@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2[C@@H]([C@H](CC1)O[C@@]1(O[C@@H](C[C@H](O)C)[C@H](CC1=O)C)[C@]2(C)O)C)C)O)C	697	Yes
1519	21-Hydroxy-oligomycin A	CC[C@H]1/C=C/C=C/C[C@@H](C)[C@H](O)[C@@](C)(O)C(=O)[C@@H](C)[C@H](O)[C@@H](C)C(=O)[C@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2[C@@H]([C@H](C[C@H]1O)O[C@@]1(O[C@@H](C[C@H](O)C)[C@H](CC1=O)C)[C@H]2C)C)C)O)C	697	No
1520	Rutamycin B	CC[C@@H]1/C=C/C=C/C[C@H](C)[C@@H](O)[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@H](C)C(=O)[C@@H]([C@H]([C@@H](/C=C/C(=O)O[C@H]2[C@H]([C@@H](CC1)O[C@@]1(CC[C@H]([C@H](O1)C[C@@H](O)C)C)C2)C)C)O)C	698	Yes
1521	44-Homooligomycin A	CCC1/C=C\C=C/CC(C)C(O)C(C)(O)C(=O)C(C)C(O)C(C)C(=O)C(C(C(/C=C/C(=O)OC2C(C(CC1)OC1(CCC(C(O1)CC(O)C)C)C2CC)C)C)O)C	698	No
1522	Oligomycin C	CC[C@@H]1/C=C/C=C/C[C@H](C)[C@@H](O)[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@H](C)C(=O)[C@@H]([C@H]([C@@H](/C=C/C(=O)O[C@H]2[C@H]([C@@H](CC1)O[C@@]1(CC[C@H]([C@H](O1)C[C@@H](O)C)C)[C@@H]2C)C)C)O)C	699	No
1523	Rutamycin A	CC[C@H]1/C=C/C=C/C[C@@H](C)[C@H](O)[C@@](C)(O)C(=O)[C@@H](C)[C@H](O)[C@@H](C)C(=O)[C@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2[C@@H]([C@H](CC1)O[C@]1(CC[C@@H]([C@@H](O1)C[C@H](O)C)C)C2)C)C)O)C	699	No
1524	Oligomycin D	CC[C@@H]1/C=C/C=C/C[C@H](C)[C@@H](O)[C@](C)(O)C(=O)[C@H](C)[C@@H](O)[C@H](C)C(=O)[C@@H]([C@H]([C@@H](/C=C/C(=O)OC2[C@H](C(CC1)O[C@@]1(CC[C@H]([C@H](O1)C[C@@H](O)C)C)C2)C)C)O)C	699	Yes
1525	21-Hydroxyoligomycin C	CC[C@H]1/C=C/C=C/C[C@@H](C)[C@H](O)[C@H](C)C(=O)[C@@H](C)[C@H](O)[C@@H](C)C(=O)[C@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2[C@@H]([C@H](C[C@H]1O)O[C@@]1(O[C@@H](C[C@H](O)C)[C@H](CC1=O)C)[C@H]2C)C)C)O)C	700	Yes
1526	40-Hydroxy-oligomycin B	CC[C@H]1/C=C/C=C/C[C@@H](CO)[C@H](O)[C@@](C)(O)C(=O)[C@@H](C)[C@H](O)[C@@H](C)C(=O)[C@H]([C@@H]([C@H](/C=C/C(=O)O[C@@H]2[C@@H]([C@H](CC1)O[C@@]1(O[C@@H](C[C@H](O)C)[C@H](CC1=O)C)[C@H]2C)C)C)O)C	701	Yes
1527	44-Homooligomycin B	CC[C@H]1/C=C\C=C/C[C@@H](C)[C@H](O)[C@@](C)(O)C(=O)[C@@H](C)[C@H](O)[C@@H](C)C(=O)[C@H]([C@@H]([C@H](/C=C/C(=O)OC2C(C(CC1)O[C@@]1(O[C@@H](C[C@H](O)C)[C@H](CC1=O)C)[C@H]2CC)C)C)O)C	702	Yes
1528	Maclafungin	OCCCC1C2OC(=O)/C=C/C(CC)C(O)C(C)C(O)CC(OC)CC(C(C(CC/C=C/C=C/C(CCC1OC1(C2)CCC(C(O1)CC(C(O)C)O)C)CC)O)C)O	703	Yes
1529	JBIR-139	CCC(C(C(C(C(C(C1C/C=C/C=C/C(O)CC(O)C(C)C(O)CC(OC2O[C@H](CO)[C@@H]([C@@H]([C@H]2NC(=O)C)O)O)C(C)C2CC(O)C(C(O2)(CC(C(CCC(CC(C/C=C/C=C/C(=O)O1)O)O)C)O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@H]1O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@H]1O)O)O)O[C@H]1C[C@@H](O)[C@@H]([C@H](O1)C)O)O)O)C)O)C)O)C)O[C@H]1CC[C@@H]([C@H](O1)C)O[C@H]1CC[C@@H]([C@H](O1)C)O	704	Yes
1530	JBIR-129	CCC(C(C(C(C(C(C1C/C=C/C=C/C(O)CC(O)C(C)C(O)CC(O)C(C)C2CC(O)C(C(O2)(CC(C(CCC(CC(C/C=C/C=C/C(=O)O1)O)O)C)O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@H]1O)O)O)O[C@H]1C[C@@H](O)[C@@H]([C@H](O1)C)O)O)O)C)O)C)O)C)O[C@H]1CC[C@@H]([C@H](O1)C)O[C@H]1CC[C@@H]([C@H](O1)C)O	705	Yes
1531	CHEMBL3086647	CC[C@@H]1[C@@H](C)OC(=C[C@H]1O[C@H]1C[C@H](O)[C@@H]([C@@H](O1)C)O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H]([C@@]1(O)C[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)CC)C)O)C)C)O)C	706	Yes
1532	2,2'-Dimethyl-11,11'-O,O-dimethylelaiophylin	CC[C@H]1[C@H](OC2C[C@H](O)[C@@H]([C@@H](O2)C)O)C[C@](O[C@@H]1C)(OC)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C(=C/C=C/[C@H](C)[C@H](OC(=O)/C(=C/C=C/[C@@H]1C)/C)[C@H]([C@H]([C@@H]([C@@]1(OC)C[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)CC)C)O)C)/C)C)O)C	707	Yes
1533	2-Methylelaiophylin	CC[C@H]1[C@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)C[C@](O[C@@H]1C)(O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C(=C/C=C/[C@@H]1C)/C)[C@H]([C@H]([C@@H]([C@@]1(O)C[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)CC)C)O)C)C)O)C	708	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1534	11,11'-O-Dimethyl-14'-deethyl-14'-methylelaiophylin	CC[C@@H]1[C@H](O[C@](C[C@H]1O[C@H]2C[C@@H]([C@@H]([C@@H](O2)C)O)O)([C@@H](C)[C@@H]([C@H](C)[C@@H]3[C@H](/C=C/C=C/C(=O)O[C@@H]([C@H](/C=C/C=C/C(=O)O3)C)[C@@H](C)[C@H]([C@H](C)[C@]4(C[C@H]([C@@H]([C@H](O4)C)C)O[C@H]5C[C@@H]([C@@H]([C@@H](O5)C)O)O)OC)O)C)O)OC)C	709	Yes
1535	2,2'-Dimethylelaiophylin	CC[C@H]1[C@H](OC2C[C@H](O)[C@@H]([C@@H](O2)C)O)C[C@](O[C@@H]1C)(O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C(=C/C=C/[C@H](C)[C@H](OC(=O)/C(=C/C=C/[C@@H]1C)/C)[C@H]([C@H]([C@@H]([C@@]1(O)C[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)CC)C)O)C)/C)C)O)C	710	Yes
1536	2-Methyl-11,11'-O-dimethylelaiophylin	CC[C@H]1[C@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)C[C@](O[C@@H]1C)(OC)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C(=C/C=C/[C@@H]1C)/C)[C@H]([C@H]([C@@H]([C@@]1(OC)C[C@@H](OC2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)CC)C)O)C)C)O)C	711	Yes
1537	11,11'-O-Dimethylelaiophylin	CC[C@H]1[C@H](O[C@H]2C[C@H](C)[C@@H]([C@@H](O2)C)C)C[C@](O[C@@H]1C)(OC)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H]([C@@]1(OC)C[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)CC)C)O)C)C)O)C	712	Yes
1538	11-O-Methylelaiophylin	CC[C@H]1[C@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)C[C@](O[C@@H]1C)(O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H]([C@@]1(OC)C[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)CC)C)O)C)C)O)C	713	Yes
1539	Efomycin G	CC[C@H]1[C@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)C[C@](O[C@@H]1C)(O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H]([C@@]1(O)C[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)C)C)O)C)C)O)C	714	Yes
1540	11-O-Monomethylelaiophylin	CC[C@H]1[C@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)O)O)C[C@](O[C@@H]1C)(O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H]([C@@]1(OC)C[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)CC)C)O)C)C)O)C	715	Yes
1541	Efomycin A	CCC1C(OC2CC(O)C(C(O2)C)O)CC(OC1C)(O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H](C1(O)CC(OC2CC(OC)C(C(O2)C)O)C(C(O1)C)CC)C)O)C)C)O)C	716	Yes
1542	Halichoblelide D	CC[C@H]1[C@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)C[C@](O[C@@H]1C)(O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)[C@H](OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H]([C@@]1(O)C[C@@H](OC)[C@@H]([C@H](O1)C)CC)C)O)C)C)O)C	717	Yes
1543	Elaiophylin	CC[C@H]1[C@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)C[C@](O[C@@H]1C)(O)[C@H]([C@@H]([C@@H]([C@H]1OC(=O)/C=C/C=C/[C@H](C)C(OC(=O)/C=C/C=C/[C@@H]1C)[C@H]([C@H]([C@@H]([C@@]1(O)C[C@@H](O[C@H]2C[C@H](O)[C@@H]([C@@H](O2)C)O)[C@@H]([C@H](O1)C)CC)C)O)C)C)O)C	718	Yes
1544	Albonoursin	CC(/C=c/1\[nH]c(=O)/c(=C/c2ccccc2)/[nH]c1=O)C	719	No
1545	(3Z,6S)-3-Benzylidene-6-(2S-but-2-yl)piperazine-2,5-dione	CC[C@@H]([C@@H]1NC(=O)/C(=C/c2ccccc2)/NC1=O)C	719	No
1546	(6R,3Z)-3-benzylidene-6-isobutyl-1-methylpiperazine-2,5-dione	CC(C[C@@H]1C(=O)N/C(=C\c2ccccc2)/C(=O)N1C)C	719	No
1547	(3E,6E)-3-Benzylidene-1-methyl-6-(2-methylpropylidene)piperazine-2,5-dione	CC(/C=c/1\c(=O)[nH]/c(=C/c2ccccc2)/c(=O)n1C)C	719	No
1548	(3Z,6E)-3-(4-Hydroxybenzylidene)-1-methyl-6-(2-methylpropylidene)piperazine-2,5-dione	CC(C=c1c(=O)[nH]c(=Cc2ccccc2)c(=O)n1C)C	719	No
1549	1-N-Methylalbonoursin	CC(/C=c/1\c(=O)[nH]/c(=C\c2ccccc2)/c(=O)n1C)C	719	Yes
1550	(3E,6Z)-6-Benzylidene-1-methyl-3-(2-methylpropylidene)piperazine-2,5-dione	CC(/C=c\1/[nH]c(=O)/c(=C/c2ccccc2)/n(c1=O)C)C	719	No
1551	(3Z,6E)-1-N-Methyl-3-benzylidene-6-(methyl-3-hydroxypropylidene)piperazine-2,5-dione	CC(C/C=c/1\c(=O)[nH]/c(=C\c2ccccc2)/c(=O)n1C)O	720	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1552	Tryptophan-dehydrobutyrine diketopiperazine	C/C=C/1\NC(=O)C(N(C1=O)C)Cc1c[nH]c2c1cccc2	721	Yes
1553	Jadomycin hydroxy-4AMBA	Cc1cc(O)c2c(c1)[C@H](O)N(C1=C2C(=O)c2cccc(c2C1=O)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O)Cc1ccc(cc1)C(=O)O	722	No
1554	3a-O-Methyljadomycin 4AMBA	CO[C@@H]1N(Cc2ccc(cc2)C(=O)O)C2=C(c3c1cc(C)cc3O)C(=O)c1c(C2=O)c(ccc1)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O	722	No
1555	3a-O-Methyljadomycin 3AMBA	CO[C@@H]1N(Cc2cccc(c2)C(=O)O)C2=C(c3c1cc(C)cc3O)C(=O)c1c(C2=O)c(ccc1)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O	722	No
1556	Jadomycin acetate-3AMBA	OC(=O)C[C@@H]1N(Cc2cccc(c2)C(=O)O)C2=C(c3c1cc(C)cc3O)C(=O)c1c(C2=O)c(ccc1)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O	722	No
1557	Jadomycin acetate-4AMBA	OC(=O)C[C@@H]1N(Cc2ccc(cc2)C(=O)O)C2=C(c3c1cc(C)cc3O)C(=O)c1c(C2=O)c(ccc1)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O	722	No
1558	Jadomycin pyruvate-4AMBA	Cc1cc(O)c2c(c1)[C@H](CC(=O)C(=O)O)N(C1=C2C(=O)c2cccc(c2C1=O)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O)Cc1ccc(cc1)C(=O)O	722	No
1559	Jadomycin DNV	CCC[C@@H]1C(=O)OC2N1C1=C(C(=O)c3c(C1=O)c(ccc3)OC1CC(O)C(C(O1)C)O)c1c2cc(cc1O)C	722	No
1560	D-Olivosyl-jadomycin-His	Cc1cc(O)c2c(c1)C1OC(=O)[C@@H](N1C1=C2C(=O)c2cccc(c2C1=O)OC1CC(O)C(C(O1)C)O)CCc1[nH]cnc1	722	No
1561	Jadomycin SPhG	Cc1cc(O)c2c(c1)C1OC(=O)[C@@H](N1C1=C2C(=O)c2cccc(c2C1=O)OC1CC(O)C(C(O1)C)O)c1ccccc1	722	No
1562	4-Keto-6-deoxy-D-glucosyl-jadomycin A	CCC(C[C@H]1C(=O)OC2N1C1=C(C(=O)c3c(C1=O)c(ccc3)OC1OC(C)C(=O)C(C1O)O)c1c2cc(cc1O)C)C	722	No
1563	Jadomycin TFAL	Cc1cc(O)c2c(c1)C1OC(=O)[C@@H](N1C1=C2C(=O)c2c(C1=O)c(ccc2)O[C@H]1C[C@H](O)[C@H](C(O1)C)O)CCCCNC(=O)C(F)(F)F	722	No
1564	D-Olivosyl-jadomycin A	CCC(C[C@H]1C(=O)OC2N1C1=C(C(=O)c3c(C1=O)c(ccc3)OC1CC(O)C(C(O1)C)O)c1c2cc(cc1O)C)C	722	No
1565	Jadomycin L	CC(C[C@H]1C(=O)OC2N1C1=C(C(=O)c3c(C1=O)c(ccc3)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O)c1c2cc(cc1O)C)C	722	No
1566	6-Deoxy-D-glucosyl-jadomycin A	CCC(C[C@H]1C(=O)OC2N1C1=C(C(=O)c3c(C1=O)c(ccc3)OC1OC(C)C(C(C1O)O)O)c1c2cc(cc1O)C)C	722	No
1567	Jadomycin B	CC[C@@H]([C@H]1C(=O)O[C@@H]2N1C1=C(C(=O)c3c(C1=O)c(ccc3)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O)c1c2cc(cc1O)C)C	722	No
1568	D-Olivosyl-jadomycin-Trp	Cc1cc(O)c2c(c1)C1OC(=O)[C@@H](N1C1=C2C(=O)c2c(C1=O)c(ccc2)OC1CC(O)C(C(O1)C)O)CCc1c[nH]c2c1cccc2	722	No
1569	D-Olivosyl-jadomycin-Leu	CC(CC[C@H]1C(=O)OC2N1C1=C(C(=O)c3c(C1=O)c(ccc3)OC1CC(O)C(C(O1)C)O)c1c2cc(cc1O)C)C	722	Yes
1570	D-Olivosyl-jadomycin-Met	CSCCC[C@H]1C(=O)OC2N1C1=C(C(=O)c3c(C1=O)c(ccc3)OC1CC(O)C(C(O1)C)O)c1c2cc(cc1O)C	722	No
1571	D-Olivosyl-jadomycin-Phe	Cc1cc(O)c2c(c1)C1OC(=O)[C@@H](N1C1=C2C(=O)c2cccc(c2C1=O)OC1CC(O)C(C(O1)C)O)CCc1ccccc1	722	No
1572	D-Olivosyl-jadomycin-Tyr	Cc1cc(O)c2c(c1)C1OC(=O)[C@@H](N1C1=C2C(=O)c2c(C1=O)c(ccc2)OC1CC(O)C(C(O1)C)O)CCc1ccc(cc1)O	722	No
1573	Jadomycin F	Cc1cc(O)c2c(c1)[C@@H]1OC(=O)[C@@H](N1C1=C2C(=O)c2cccc(c2C1=O)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O)Cc1ccccc1	722	No
1574	D-Olivosyl-jadomycin-Val	CC(C[C@H]1C(=O)OC2N1C1=C(C(=O)c3c(C1=O)c(ccc3)OC1CC(O)C(C(O1)C)O)c1c2cc(cc1O)C)C	722	No
1575	2,6-Dideoxy-L-erythro-4-hexulosyl-jadomycin	CCC(C[C@H]1C(=O)OC2N1C1=C(C(=O)c3c(C1=O)c(ccc3)OC1CC(O)C(=O)C(O1)C)c1c2cc(cc1O)C)C	722	No
1576	Jadomycin 3AMBA-lactam	Cc1cc(O)c2c(c1)c(=O)n(c1c2C(=O)c2cccc(c2C1=O)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O)Cc1cccc(c1)C(=O)O	722	No
1577	Jadomycin 4AMBA-lactam	Cc1cc(O)c2c(c1)c(=O)n(c1c2C(=O)c2cccc(c2C1=O)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O)Cc1ccc(cc1)C(=O)O	722	No
1578	Jadomycin TFAL lactam	Cc1cc(O)c2c(c1)c(=O)n(c1c2C(=O)c2cccc(c2C1=O)O[C@H]1C[C@H](O)[C@H](C(O1)C)O)[C@H](C(=O)O)CCCCNC(=O)C(F)(F)F	722	No
1579	Jadomycin A	CC[C@@H]([C@H]1C(=O)O[C@@H]2N1C1=C(c3c2cc(C)cc3O)C(=O)c2c(C1=O)c(O)ccc2)C	723	Yes
1580	Jadomycin	CCC([C@H]1C(=O)O[C@@H]2N1C1=C(c3c2cc(C)cc3O)C(=O)c2c(C1=O)c(O)ccc2)C	723	No
1581	Ellagic acid	Oc1cc2c(=O)oc3c4c2c(c1O)oc(=O)c4cc(c3O)O	724	Yes
1582	Defucogilvocarcin V	COc1cc(C=C)cc2c1c1cc(OC)c3c(c1oc2=O)cccc3O	725	Yes
1583	2-(2-Methyl-4-oxochromen-5-yl)acetic acid	OC(=O)Cc1cccc2c1c(=O)cc(o2)C	726	Yes
1584	Phaeochromycin E	CCCc1cc(=O)c2c(o1)cccc2CC(=O)O	726	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1585	Phaeochromycin I	O[C@@H](CC(=O)O)CC(=O)Cc1cccc2c1c(=O)cc(o2)C	727	Yes
1586	Phaeochromycin H	CC(CC(=O)Cc1cccc2c1c(=O)cc(o2)C)O	727	No
1587	23-Valine demalonylazalomycin F5a ester	CN/C(=N\C)/NCCC/C=C/CCC[C@@H]([C@@H]1OC(=O)/C(=C\C=C\[C@H](C)[C@@H](O)C[C@H](O)[C@@H](C)[C@H](O)CC[C@H](C)[C@@H](O)C[C@]2(O[C@@H](C[C@H](C[C@@H](C[C@H](C[C@@H](/C(=C/C=C/[C@H]1C)/C)O)O)O)OC(=O)C(C(C)C)N)C[C@@H](O)[C@@H]2O)O)/C)C	728	Yes
1588	23-(9-Methyl)decanoic acid demalonylazalomycin F4a ester	CN/C(=N\C)/NCCC/C=C/CCC[C@@H]([C@@H]1OC(=O)/C(=C\C=C\[C@@H](C)[C@@H](O)C[C@@H](O)[C@H](C)[C@H](O)CC[C@H](C)[C@@H](O)C[C@]2(O[C@@H](C[C@@H](C[C@H](C[C@@H](C[C@H](/C(=C/C=C/[C@H]1C)/C)O)O)O)OC(=O)CCCCCCCCC(C)C)C[C@@H](O)[C@@H]2O)O)/C)C	729	Yes
1589	Kanchanamycin C	OC1CC(O)CC(OC(=O)CC(=O)O)CC2CC(O)C(C(O2)(O)CC(O)C(C)CCC(O)C(C)C(O)CC(C(/C=C\C=C/C(=O)OC(C(/C=C\C=C(/C(C1)O)\C)C)C(CCC/C=C/CCCNC(=N)N)C)C)O)O	730	Yes
1590	23-(6-Methyl)heptanoic acid demalonylazalomycin F4a ester	C/N=C(/NCCC/C=C/CCC[C@@H]([C@@H]1OC(=O)/C(=C\C=C\[C@@H](C)[C@@H](O)C[C@@H](O)[C@H](C)[C@H](O)CC[C@H](C)[C@@H](O)C[C@]2(O[C@@H](C[C@@H](C[C@H](C[C@@H](C[C@H](/C(=C/C=C/[C@H]1C)/C)O)O)O)OC(=O)CCCCC(C)C)C[C@@H](O)[C@@H]2O)O)/C)C)\N	731	Yes
1591	Neocopiamycin A	CC(CC(C1OC(=O)/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(C(C(/C=C\C1C)O)C)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)C)CCC/C=C/CCCN=C(N)N	732	Yes
1592	Azalomycin F4a	CN=C(NCCC/C=C/CCC[C@@H]([C@@H]1OC(=O)/C(=C/C=C/[C@H](C)[C@@H](O)C[C@H](O)[C@@H](C)[C@H](O)CC[C@H](C)[C@@H](O)C[C@]2(O[C@@H](C[C@H](C[C@@H](C[C@H](C[C@@H](/C(=C/C=C/[C@H]1C)/C)O)O)O)OC(=O)CC(=O)O)C[C@@H](O)[C@@H]2O)O)/C)C)N	733	Yes
1593	Shurimycin B	CN/C(=N\C)/NCCC/C=C/CCCC(C1OC(=O)/C=C\C=C\C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(C(C(/C(=C/C=C/C1C)/C)O)C)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)C	734	Yes
1594	Azalomycin F	OC1CC(O)CC(OC(=O)CC(=O)O)CC2CC(O)C(C(O2)(O)CC(O)C(C)CCC(O)C(C)C(O)CC(C(/C=C/C=C(/C(=O)OC(C(/C=C/C=C(/C(C1)O)\C)C)C(CCC/C=C/CCCN=C(N)N)C)\C)C)O)O	735	Yes
1595	Azalomycin RS-22A	OC1CC(O)CC(OC(=O)CC(=O)O)CC2CC(O)C(C(O2)(O)CC(O)C(C)CCC(O)C(C)C(O)CC(C(/C=C/C=C/C(=O)OC(C(/C=C/C=C(/C(C1)O)\C)C)C(CCC/C=C/CCCN=C(N)N)C)C)O)O	736	Yes
1596	Kanchanamycin A	OC1CC(O)CC(OC(=O)CC(=O)O)CC2CC(O)C(C(O2)(O)CC(O)C(C)CCC(O)C(C)C(O)CC(C(/C=C/C=C\C(=O)OC(C(/C=C/C=C(/C(C1)O)\C)C)C(CCC/C=C/CCCNC(=O)N)C)C)O)O	737	Yes
1597	Rs-22C	CN/C(=N\C)/NCCC/C=C/CCCC(C1OC(=O)/C=C/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(CC(/C(=C/C=C/C1C)/C)O)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)C	738	Yes
1598	Azalomycin F4	C/N=C(/NCCC/C=C/CCCC(C1OC(=O)/C(=C/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(/C(=C\C=C\C1C)/C)O)O)OC(=O)CC(=O)O)O)CC(O)C2O)O)/C)C)\N	739	Yes
1599	RS-22 B	C/N=C(/NCCC/C=C/CCCC(C1OC(=O)/C=C/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(CC(/C(=C/C=C/C1C)/C)O)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)C)\N	740	Yes
1600	23-(6-Methyl)heptanoic acid demalonylazalomycin F3a ester	CC(CCCCC(=O)O[C@@H]1C[C@@H](O)C[C@H](O)C[C@@H](O)/C(=C/C=C/[C@@H](C)[C@@H](OC(=O)/C(=C\C=C\[C@H]([C@H](C[C@H]([C@@H]([C@@H](CC[C@@H]([C@H](C[C@]2(O[C@@H](C1)C[C@@H](O)[C@@H]2O)O)O)C)O)C)O)O)C)/C)[C@H](CCC/C=C/CCCNC(=N)N)C)/C)C	741	Yes
1601	UNII-ZUD60NKS1C	O[C@@H]1C[C@@H](O)C[C@H](OC(=O)CC(=O)O)C[C@H]2C[C@@H](O)[C@@H]([C@@](O2)(O)C[C@H](O)[C@@H](C)CC[C@@H](O)[C@H](C)[C@@H](O)C[C@@H]([C@H](/C=C/C=C(/C(=O)O[C@H]([C@@H](/C=C/C=C(/[C@H](C1)O)\C)C)[C@H](CCC/C=C/CCCN=C(N)N)C)\C)C)O)O	742	Yes
1602	Kanchanamycin D	COC12OC(CC(CC(O)CC(O)CC(O)/C(=C\C=C/C(C)C(OC(=O)/C=C\C=C/C(C(CC(C(CCC(C(C1)O)C)O)C)O)O)O)C)C(CCC/C=C/CCCNC(=O)N)C)/C)OC(=O)CC(=O)O)CC(C2O)O	743	Yes
1603	23-(10-Methyl)undecanoic acid demalony lazalomycin F4a ester	CN/C(=N\C)/NCCC/C=C/CCC[C@@H]([C@@H]1OC(=O)/C(=C\C=C\[C@@H](C)[C@@H](O)C[C@@H](O)[C@H](C)[C@H](O)CC[C@H](C)[C@@H](O)C[C@]2(O[C@@H](C[C@@H](C[C@H](C[C@@H](C[C@H](/C(=C/C=C/[C@H]1C)/C)O)O)O)OC(=O)CCCCCCCCCC(C)C)C[C@@H](O)[C@@H]2O)O)/C)C	744	Yes
1604	23-(6-Methyl)heptanoic acid demalonylazalomycin F5a ester	CN/C(=N\C)/NCCC/C=C/CCC[C@@H]([C@@H]1OC(=O)/C(=C\C=C\[C@@H](C)[C@@H](O)C[C@@H](O)[C@H](C)[C@H](O)CC[C@H](C)[C@@H](O)C[C@]2(O[C@@H](C[C@@H](C[C@H](C[C@@H](C[C@H](/C(=C/C=C/[C@H]1C)/C)O)O)O)OC(=O)CCCCC(C)C)C[C@@H](O)[C@@H]2O)O)/C)C	745	Yes
1605	Copiamycin	C/N=C(/NCCC/C=C/CCCC(CC(C1OC(=O)/C=C\C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(C(/C=C\C1C)O)C)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)C)C)\N	746	Yes
1606	UNII-H7Q3DUM9N6	CNC(=NC)NCCC/C=C/CCC[C@@H]([C@@H]1OC(=O)/C(=C/C=C/[C@H](C)[C@@H](O)C[C@H](O)[C@@H](C)[C@H](O)CC[C@H](C)[C@@H](O)C[C@]2(O[C@@H](C[C@H](C[C@@H](C[C@H](C[C@@H](/C(=C/C=C/[C@H]1C)/C)O)O)O)OC(=O)CC(=O)O)C[C@@H](O)[C@@H]2O)O)/C)C	747	Yes
1607	Malolactomycin C	C/N=C(/NCCCCC/C=C(/CC(C1OC(=O)C(C)C(O)/C(=C\CC(O)C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(CC(C(C(/C=C/C=C\C1C)O)C)O)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)/C)C)\C)\N	748	Yes
1608	Niphimycin	C/N=C(/NCCC/C=C/CCC[C@@H](C[C@@H](C1OC(=O)C(C)C(O)/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(C(C(/C=C/C=C/C1C)O)C)O)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)C)C)\N	749	Yes
1609	17-O-Methylniphimycin	CN=C(NCCC/C=C/CCC[C@@H](C[C@@H]([C@H]1OC(=O)[C@H](C)[C@H](O)/C=C/[C@H](C)[C@H](O)C[C@H](O)[C@H](C)[C@@H](O)CC[C@H](C)[C@H](O)C[C@@]2(O[C@H](C[C@H](C[C@@	750	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
		H](C[C@H]([C@@H]([C@@H](/C=C/C=C/[C@@H]1C)O)C)O)O)OC(=O)CC(=O)O)C[C@H](O)[C@H]2O)OC)C)C)N		
1610	19-O-Malonylniphimycin	CN=C(NCCC/C=C/CCCC(CC(C1OC(=O)C(C)C(O)CCC(C)C(O)C(C)C(O)C(C)C(O)CCCC(O)CC2(OC(CC(CC(CC(C(C(/C=C\C=C\C1C)O)C)O)O)OC(=O)CC(=O)O)CC(OC(=O)CC(=O)O)C2O)O)C)C)N	751	Yes
1611	Guanidylfungin A	CN=C(NCCCCC/C=C(/CC(C1OC(=O)C(C)C(O)/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(C(C(/C(=C/CCC1C)/C)O)C)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)C)\C)N	752	Yes
1612	Niphimycin C	CN=C(NCCC/C=C/CCC[C@@H](C[C@@H]([C@H]1OC(=O)[C@H](C)[C@H](O)/C=C/[C@H](C)[C@H](O)C[C@H](O)[C@H](C)[C@@H](O)CC[C@H](C)[C@H](O)C[C@@]2(O[C@H](C[C@H](C[C@@H](C[C@H]([C@@H]([C@@H](/C=C/C=C/[C@@H]1C)O)C)O)OC(=O)CC(=O)O)O)C[C@H](O)[C@H]2O)O)C)C)N	753	Yes
1613	Niphimycin D	CN=C(NCCC/C=C/CCC[C@@H](C[C@@H]([C@H]1OC(=O)[C@H](C)[C@H](O)/C=C/[C@H](C)[C@H](O)C[C@H](O)[C@H](C)[C@@H](O)CC[C@H](C)[C@H](O)C[C@@]2(O[C@H](C[C@H](C[C@@H](C[C@H]([C@@H]([C@@H](/C=C/C=C/[C@@H]1C)O)C)O)OC(=O)CC(=O)O)O)C[C@H](OC(=O)CC(=O)O)[C@H]2O)O)C)C)N	754	Yes
1614	Niphimycin E	CN=C(NCCC/C=C/CCC[C@@H](C[C@@H]([C@H]1OC(=O)[C@H](C)[C@H](O)/C=C/[C@H](C)[C@H](O)C[C@H](O)[C@H](C)[C@@H](O)CC[C@H](C)[C@H](OC(=O)CC(=O)O)C[C@@]2(O[C@H](C[C@H](C[C@@H](C[C@H]([C@@H]([C@@H](/C=C/C=C/[C@@H]1C)O)C)O)OC(=O)CC(=O)O)O)C[C@H](O)[C@H]2O)O)C)C)N	755	Yes
1615	Guanidylfungin B	OC(=O)CC(=O)OC1/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(O)OC(CC(CC(CC(C(C(/C(=C/CCC(C(OC(=O)C1C)C(C/C(=C/CCCCCN=C(N)N)/C)C)C)/C)O)C)O)O)O)CC(C2O)O	756	Yes
1616	Methyl guanidylfungin A	CN=C(NCCCCC/C=C(/CC(C1OC(=O)C(C)C(O)/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(C(C(/C(=C/CCC1C)/C)O)C)O)O)OC(=O)CC(=O)O)CC(O)C2O)OC)C)\C)N	757	Yes
1617	Malolactomycin D	OC1CC(OC(=O)CC(=O)O)CC2CC(O)C(C(O2)(O)CC(O)C(C)CCC(O)C(C)C(O)CC(O)C(C)C(O)C/C=C(\C(C(C(=O)OC(C(/C=C\C=C\C(C(C(CC(C1)O)O)C)O)C)C(C/C(=C/CCCCCN=C(N)N)/C)C)C)O)/C)O	758	Yes
1618	Malolactomycin A	CN/C(=N\C)/NCCCCC/C=C(/CC(C1OC(=O)C(C)C(O)/C(=C\CC(O)C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(CC(C(C(/C=C/C=C\C1C)O)C)O)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)/C)C)\C	759	Yes
1619	Amycin B	C/N=C(/NCCC/C=C/CCCC(CC(C1OC(=O)C(C)C(O)/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(C(C(/C=C\C=C\C1C)O)C)O)O)O)CC(O)C2O)O)C)C)\N	760	Yes
1620	Nificin	C/N=C(/NCCC/C=C/CCCC(CC(C1OC(=O)C(C)C(O)/C=C/C(C)C(O)CC(O)C(C)C(O)CCC(C)C(O)CC2(OC(CC(CC(CC(C(C(/C=C/C=C\C1C)O)C)O)O)O)OC(=O)CC(=O)O)CC(O)C2O)O)C)C)\N	761	Yes
1621	Indolactam V	OC[C@H]1NC(=O)[C@H](C(C)C)N(c2c3c(C1)c[nH]c3ccc2)C	762	Yes
1622	Lyngbyatoxin	OCC1NC(=O)C(C(C)C)N(c2c3c(C1)c[nH]c3c(cc2)C(CCC=C(C)C)(C=C)C)C	763	No
1623	Pendolmycin	OC[C@H]1NC(=O)[C@H](C(C)C)N(c2c3c(C1)c[nH]c3c(cc2)C(C=C)(C)C)C	763	No
1624	Teleocidin	OC[C@H]1NC(=O)[C@H](C(C)C)N(c2c3c(C1)c[nH]c3c(cc2)[C@](CCC=C(C)C)(C=C)C)C	763	Yes
1625	Cytoblastin	OCC(C(c1c[nH]c2c1cccc2)c1ccc2c3c1[nH]cc3CC(CO)NC(=O)C(N2C)C(C)C)O	763	No
1626	UNII-T7972EPW8P	COc1c2ccccc2n2c1c1n(C)c3c(c1[C@@]1([C@@]2(O)C(=O)N(C1=O)C)O)cc(cc3)Cl	764	No
1627	CHEBI:84366	COc1c2ccccc2n2c1c1[nH]c3c(c1[C@@]1([C@@]2(O)C(=O)N(C1=O)C)O)cc(cc3)Cl	764	Yes
1628	CHEBI:84367	COc1c2cc(Cl)ccc2n2c1c1[nH]c3c(c1[C@@]1([C@@]2(O)C(=O)N(C1=O)C)O)cc(cc3)Cl	764	No
1629	CHEBI:84368	COc1c2ccccc2n2c1c1[nH]c3c(c1[C@@]1([C@@]2(O)C(=O)N(C1=O)C)O)cccc3	764	No
1630	CHEBI:84370	COc1c2cc(Cl)ccc2n2c1c1[nH]c3c(c1C(=O)[C@@]2(O)C(=O)NC)cc(cc3)Cl	764	No
1631	CHEBI:84369	COc1c2ccccc2n2c1c1[nH]c3c(c1C(=O)[C@@]2(O)C(=O)NC)cc(cc3)Cl	764	No
1632	7-Chloro-11-hydroxy-20-methoxy-N-methyl-12-oxo-3,13-diazapentacyclo[11.7.0.02,10.04,9.014,19]icosa-1(20),2(10),4(9),5,7,14,16,18-octaene-11-carboxamide	COc1c2ccccc2n2c1c1[nH]c3c(c1C(C2=O)(O)C(=O)NC)cc(cc3)Cl	764	No
1633	CHEBI:65639	COc1c2cc(Cl)ccc2n2c1c1[nH]c3c(c1[C@@](C2=O)(O)C(=O)NC)cc(cc3)Cl	764	No
1634	7,17-Dichloro-11-hydroxy-20-methoxy-N-methyl-12-oxo-3,13-diazapentacyclo[11.7.0.02,10.04,9.014,19]icosa-1(20),2(10),4(9),5,7,14(	COc1c2cc(Cl)ccc2n2c1c1[nH]c3c(c1C(C2=O)(O)C(=O)NC)cc(cc3)Cl	764	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	19),15,17-octaene-11-carboxamide			
1635	Rebeccamycin	CO[C@@H]1[C@@H](CO)O[C@H]([C@@H]([C@H]1O)O)n1c2c(Cl)cccc2c2c1c1[nH]c3c(c1c1c2c(=O)[nH]c1=O)cccc3Cl	765	Yes
1636	4'N-Formyl-7-oxoholyrin A	O=CN[C@@H]1C[C@@H](O[C@H]([C@@H]1O)C)n1c2c3[nH]c4c(c3c3c(c2c2c1cccc2)c(=O)[nH]c3=O)cccc4	766	No
1637	7-Oxoholyrin A	O[C@@H]1[C@H](N)C[C@@H](O[C@H]1C)n1c2c3[nH]c4c(c3c3c(c2c2c1cccc2)c(=O)[nH]c3=O)cccc4	766	No
1638	7-Oxostaurosporine	CN[C@H]1CC2O[C@@]([C@@H]1OC)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3c(=O)[nH]c1=O	766	No
1639	7-Oxo-K252d	O[C@H]1[C@H](C)O[C@H]([C@@H]([C@@H]1O)O)n1c2c3[nH]c4c(c3c3c(c2c2c1cccc2)c(=O)[nH]c3=O)cccc4	766	No
1640	7-Oxo-MLR-52	CO[C@@H]1[C@@H](O)[C@@H](O)[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3c(=O)[nH]c1=O	766	No
1641	3'Demethyl-RK-1409	CO[C@@H]1[C@H](N)C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3c(=O)[nH]c1=O	766	No
1642	RK-1409	CN[C@H]1C[C@@H]2O[C@@]([C@@H]1OC)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3c(=O)[nH]c1=O	766	No
1643	7-Oxo-K252b	O=c1[nH]c(=O)c2c1c1c3ccccc3n3c1c1c2c2ccccc2n1[C@@H]1O[C@@]3(C)[C@](C1)(O)C(=O)O	766	No
1644	4'-Demethylamino-4'-oxostaurosporine	CO[C@@H]1C(=O)C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1645	Tan 1030A	O/N=C\1/CC2OC(C1OC)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1646	CHEMBL94678	COC(=O)[C@]1(O)C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1647	K252a-Me	COC(=O)[C@@]1(OC)C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1648	K252a	COC(=O)C1(O)C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1649	Antibiotic K 252a	COC(=O)C1(O)CC2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1650	Streptocarbazole B	COC1=C(C)O[C@@H]2C[C@@]1(OC)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1651	Steptocarbazole A	OCC1=C(OC)C2(CC(O1)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3C(=O)NC1)OC	766	No
1652	CID 72501072	COC1=C(C)OC2CC1(OC)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1653	Staurosporine M2	CC(=O)c1cccn1[C@@H]1C[C@H]2O[C@]([C@@H]1O)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1654	Holyrine A	O[C@@H]1[C@H](N)C[C@@H](O[C@H]1C)n1c2c(c3c1cccc3)c1C(=O)NCc1c1c2[nH]c2c1cccc2	766	No
1655	Holyrine B	O=C1NCc2c1c1c(c3c2c2ccccc2[nH]3)n(c2c1cccc2)[C@H]1C[C@@H](N)[C@H](C(O1)(C)O)O	766	No
1656	3'N-Formylholyrine A	O=CN[C@@H]1C[C@@H](O[C@H]([C@@H]1O)C)n1c2c(c3c1cccc3)c1C(=O)NCc1c1c2[nH]c2c1ccc2	766	No
1657	3'-N-Acetylholyrine A	CC(=O)N[C@@H]1C[C@@H](O[C@H]([C@@H]1O)C)n1c2c(c3c1cccc3)c1C(=O)NCc1c1c2[nH]c2c1cccc2	766	No
1658	RK-1409B	CO[C@H]1[C@@H](O)CC2O[C@@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3C(=O)NC1	766	No
1659	3'-O-Demethyl-4'-N-demethyl-4'-N-acetyl-4'-epi-staurosporine	CC(=O)N[C@H]1CC2O[C@]([C@@H]1O)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1660	K252d	O[C@H]1[C@H](C)OC([C@@H]([C@@H]1O)O)n1c2c(c3c1cccc3)c1C(=O)NCc1c1c2[nH]c2c1cccc2	766	No
1661	Fradcarbazole C	N#CN([C@@H]1C[C@H]2O[C@]([C@@H]1OC)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O)C	766	No
1662	4'-N-Acetyl-staurosporine	CO[C@@H]1[C@@H](C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O)N(C(=O)C)C	766	No
1663	7-Hydroxystaurosporine	CN[C@H]1CC2O[C@@]([C@@H]1OC)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3[C@@H](NC1=O)O	766	No
1664	Staurosporine M1	CC(=O)N[C@@H]1C[C@H]2O[C@]([C@@H]1O)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1665	(R)-L-Digitoxosyl-arcyriaflavin A	O=C1NCc2c1c1c3ccccc3n3c1c1c2c2ccccc2n1[C@]1(O[C@@H]3C[C@H]([C@H]1O)O)C	766	No
1666	MLR-52	CO[C@@H]1[C@@H](O)[C@@H](O)[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1667	Staurosporine	CN[C@@H]1C[C@H]2O[C@]([C@@H]1OC)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1668	N-[(2R,4R,5R,6S)-5-Methoxy-6-methyl-18-oxo-29-oxa-1,7,17-triazaoctacyclo[12.12.2.	CCC(=O)N([C@@H]1C[C@H]2O[C@]([C@@H]1OC)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O)C	766	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	$1^{2,6}.0^{7,28}.0^{8,13}.0^{15,19}.0^{20,27}.0^{21,26}$]nonacosa-8,10,12,14(28),15(19),20(27),21(26),22,24-nonaen-4-yl]-N-methylpropanamide			
1669	3'-N-Demethyl-4'-hydroxystaurosporine	O=C1NCc2c1c1c3ccccc3n3c1c1c2c2ccccc2n1[C@]1(O[C@@H]3C[C@H]([C@H]1O)N)C	766	No
1670	UCN 02	CN[C@H]1CC2O[C@@]([C@@H]1OC)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3[C@H](NC1=O)O	766	No
1671	1-[(2R,4R,5R,6S)-5-Methoxy-6-methyl-18-oxo-29-oxa-1,7,17-triazaoctacyclo[12.12.2.$1^{2,6}.0^{7,28}.0^{8,13}.0^{15,19}.0^{20,27}.0^{21,26}$]nonacosa-8,10,12,14(28),15(19),20(27),21(26),22,24-nonaen-4-yl]-1-methylurea	CO[C@@H]1[C@@H](C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O)N(C(=O)N)C	766	No
1672	(2S,3R,4R,6R)-4-[Hydroxy(methyl)amino]-3-methoxy-2-methyl-29-oxa-1,7,17-triazaoctacyclo[12.12.2.$1^{2,6}.0^{7,28}.0^{8,13}.0^{15,19}.0^{20,27}.0^{21,26}$]nonacosa-8(13),9,11,14(28),15(19),20(27),21,23,25-nonaen-16-one	CO[C@@H]1[C@@H](C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O)N(O)C	766	No
1673	C07349	CN[C@@H]1CC2O[C@]([C@@H]1O)(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	No
1674	Fradcarbazole B	CO[C@@H]1[C@@H](C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O)N(C(=S)N)C	766	No
1675	RK-286C	COC1C(O)CC2OC1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O	766	Yes
1676	Borrelidin N	C[C@@H]1C[C@H](C)C[C@H](C)[C@H](O)/C(=C\C=C\C[C@@H](OC(=O)C[C@H]([C@@H](C1)C)O)C1CCC[C@@H]1C(=O)N)/CNC(=O)C	767	Yes
1677	Borrelidin I	C[C@H]1C[C@@H](C)C[C@H](C)[C@H](O)/C(=C\C=C\C[C@H](OC(=O)C[C@@H]([C@H](C1)C)O)[C@@H]1CCC[C@H]1C(=O)O)/CNC(=O)C	767	No
1678	Borrelidin O	N#C/C/1=C/C=C/C[C@@H](OC(=O)C[C@H]([C@@H](C[C@@](C[C@@H](C[C@@H]([C@@H]1O)C)(C)O)C)O)C)O)C1CCC[C@@H]1C(=O)O	768	No
1679	Borrelidin E	N#C/C/1=C/C=C/C[C@H](OC(=O)C[C@@H]([C@H](C[C@H]([C@@H]([C@H](C[C@@H]([C@H]1O)C)C)O)C)C)O)[C@@H]1CCC[C@H]1C(=O)O	768	No
1680	Borrelidin K	N#CC1=CC=CC[C@H](OC(=O)C[C@@H]([C@H](C[C@H](CC(C[C@@H]([C@H]1O)C)(C)O)C)C)O)[C@@H]1CCC[C@H]1C(=O)O	768	Yes
1681	Borrelidin J	OC[C@@H]1C[C@H](C)C[C@H](C)[C@@H](O)CC(=O)O[C@@H](CC=CC=C([C@@H]([C@H](C1)C)O)C#N)[C@@H]1CCC[C@H]1C(=O)O	768	No
1682	Borrelidin M	N#C/C/1=C/C=C/C[C@@H](OC(=O)C[C@H]([C@@H](C[C@@H](C[C@@H](C[C@@H]([C@H]1O)C)C)C)C)O)C1CCC[C@@H]1C(=O)N	769	No
1683	Borrelidin A	N#C/C/1=C/C=C/C[C@@H](OC(=O)C[C@H]([C@@H](C[C@@H](C[C@@H](C[C@@H]([C@@H]1O)C)C)C)C)O)C1CCC[C@@H]1C(=O)O	769	No
1684	Borrelidin F	N#C/C/1=C/C=C/C[C@H](OC(=O)C[C@@H]([C@H](C[C@H](C[C@H](C[C@@H]([C@@H]1O)C)C)C)C)O)[C@@H]1CCC[C@H]1C(=O)O	769	Yes
1685	Borrelidin	N#C/C/1=C/C=C/C[C@H](OC(=O)C[C@@H]([C@H](C[C@H](C[C@H](C[C@@H]([C@H]1O)C)C)C)C)O)[C@@H]1CCC[C@H]1C(=O)O	769	No
1686	Borrelidin CR1	N#C/C/1=C/C=C/C[C@@H](OC(=O)C[C@H]([C@@H](C[C@@H](C[C@@H](C[C@@H]([C@@H]1O)C)C)C)C)O)C1CCC[C@@H]1C(=O)N	769	No
1687	BC194	N#C/C/1=C/C=C/C[C@H](OC(=O)C[C@@H]([C@H](C[C@H](C[C@H](C[C@@H]([C@H]1O)C)C)C)C)O)[C@@H]1CC[C@H]1C(=O)O	769	No
1688	Borrelidin H	[C-]#[N+]/C/1=C/C=C/C[C@H](OC(=O)C[C@@H]([C@H](C[C@H](C[C@H](C[C@@H]([C@@H]1O)C)C)C)C)O)[C@@H]1CCC[C@H]1C(=O)O	769	No
1689	SF 2415A2	CC1=C(C2=C(C(=[N+]=[N-])C1=O)C(=O)C3(C(C2=O)(O3)CC=C(C)C)C/C=C(\C)/CCC=C(C)C)O	770	Yes
1690	Zincphyrin IV	OC(=O)CCC1=C(C)C2=NC1=Cc1[nH]c(c(c1C)CCC(=O)O)C=c1[nH]c(=CC3=NC(=C2)C(=C3CCC(=O)O)C)c(c1CCC(=O)O)C	771	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1691	Zinc corproporphyrin III	OC(=O)CCC1=C(C)C2=NC1=Cc1[nH]c(c(c1C)CCC(=O)O)C=c1[nH]c(=CC3=NC(=C2)C(=C3C)CCC(=O)O)c(c1CCC(=O)O)C.[Zn+2]	771	No
1692	Coporphyrin III	OC(=O)CCC1=C(C)C2=NC1=Cc1[nH]c(c(c1C)CCC(=O)O)C=c1[nH]c(=CC3=NC(=C2)C(=C3C)CCC(=O)O)c(c1CCC(=O)O)C	771	Yes
1693	Coproporphyrin I	OC(=O)CCC1=C(C)C2=N/C/1=C\c1[nH]c(c(c1C)CCC(=O)O)/C=c/1\[nH]/c(=C\C3=N/C(=C\2)/C(=C3C)CCC(=O)O)/c(c1C)CCC(=O)O	771	No
1694	CHEMBL482339	COc1cc2c(cc1OCCCC#Cc1ccccc1C#Cc1ccccc1)N=C[C@H]1N(C2=O)CCC1	772	Yes
1695	Bahamaolide A	O[C@H]1CC[C@H](C)[C@@H](OC(=O)/C=C/C=C/C=C/C=C/C=C/C=C/C[C@H](C[C@@H](C[C@@H](C[C@@H](C[C@H](C[C@@H](C[C@H](C[C@H](C1)O)O)O)O)O)O)O)O)C(C)C	773	Yes
1696	Butyrolactol B	CC(CC/C=C/C=C/CC/C=C/C=C/CC(C(C(C(C(C(C1OC(=O)C(C1O)O)O)O)O)O)O)C)C	774	Yes
1697	Butyrolactol A	CC(C(C(C(C(C(C1OC(=O)C(C1O)O)O)O)O)O)O)C/C=C/C=C/CC/C=C\C=C\CCC(C)(C)C	774	No
1698	Takanawaene C	CCCC1OC(=O)C(C)C(O)CC(O)CCCC(O)CC(O)CC(C(C(/C=C/C=C/C=C/C=C/C=C/C1C)O)C)O	775	Yes
1699	Takanawaene B	CCC1OC(=O)C(C)C(O)CC(O)CCCC(O)CC(O)CC(C(C(/C=C/C=C/C=C/C=C/C=C/C1C)O)C)O	775	No
1700	15-Glycidylfilipin III	CCCCC[C@H]([C@@H]1[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)[C@H](O)[C@H](OC[C@@H](CO)O)/C(=C/C=C/C=C/C=C/C=C/[C@@H]([C@H](OC1=O)C)O)/C)O	776	Yes
1701	Fungichromin	CCCCC[C@H](C1[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)[C@@H](O)[C@H](O)/C(=C/C=C/C=C/C=C/C=C/[C@@H]([C@H](OC1=O)C)O)/C)O	777	Yes
1702	Fungichromin B	CCCCCCC(C1C(O)CC(O)CC(O)CC(O)CC(O)CC(O)C(O)C(O)/C(=C/C=C/C=C/C=C/C=C/C=C/C(C(OC1=O)C)O)/C)O	777	No
1703	Takanawaene A	OC1CCCC(O)CC(O)C(C)C(=O)OC(C)C(C)/C=C/C=C/C=C/C=C/C=C/C=C/C(CC(CC(C1)O)O)O	778	Yes
1704	16alpha,17alpha-epoxyfilipin V	CCCCC[C@H]([C@@H]1[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)[C@]2([C@H](/C=C/C=C/C=C/C=C/[C@@H]([C@H](OC1=O)C)O)O2)C)O	779	Yes
1705	16beta,17beta-epoxyfilipin V	CCCCC[C@H]([C@@H]1[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@]2([C@@H](/C=C/C=C/C=C/C=C/[C@@H]([C@H](OC1=O)C)O)O2)C)O	779	No
1706	Filipin	CCCCC[C@H]([C@@H]1[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@H](O)/C(=C/C=C/C=C/C=C/C=C/[C@@H]([C@H](OC1=O)C)O)/C)O	780	Yes
1707	Strevertene B	CCC1C(O)CC(O)CC(O)CCCC(O)CC(O)C(C(=O)O)C(O)/C=C/C=C/C=C/C=C/C=C/C(C(OC1=O)C)C	781	Yes
1708	Tetronothiodin	OC1C/C=C/CC(C)C2C(SCC2C(=O)C2=C(C3(C(C/C=C/C=C/C1)C=C(C)C(C3)C)OC2=O)O)C(=O)C(=O)O	782	Yes
1709	TPU-0043	CCCC[C@@H]1[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@H](O)/C(=C/C=C/C=C/C=C/C=C/[C@@H](C(OC1=O)C)O)/C	783	Yes
1710	Strevertene A	OC1CCCC(O)CC(O)C(C(=O)O)C(O)/C=C/C=C/C=C/C=C/C=C/C(C(OC(=O)C(C(CC(C1)O)O)C)C)C	784	Yes
1711	Reedsmycin C	CCC(C1OC(=O)/C=C\C=C/C=C/C=C/C=C/CC(O)CC(CC(CC(CC(CC(CC(CC(/C=C/C1C)O)O)O)O)O)O)O)O)C	785	Yes
1712	Reedsmycin D	CCC(C1OC(=O)/C=C/C=C/C=C/C=C/C=C\CC(O)CC(CC(CC(CC(CC(CC(CC(/C=C/C1C)O)O)O)O)O)O)O)O)C	785	No
1713	Reedsmycin E	CCC(C1OC(=O)/C=C/C=C\C=C\C=C/C=C/CC(O)CC(CC(CC(CC(CC(CC(CC(/C=C/C1C)O)O)O)O)O)O)O)O)C	786	Yes
1714	Reedsmycin A	CCC(C1OC(=O)/C=C/C=C/C=C/C=C/C=C/CC(O)CC(CC(CC(CC(CC(CC(CC(/C=C/C1C)O)O)O)O)O)O)O)O)C	786	No
1715	Flavofungin III	O[C@H]1C[C@H](O)C[C@@H](O)C[C@@H](O)/C=C/[C@H](C)[C@@H](OC(=O)/C=C/C=C/C=C/C=C/[C@H]([C@H](C[C@@H]([C@@H]([C@@H](C[C@@H](C[C@@H](C1)O)O)O)C)O)O)O)C(C)C	787	Yes
1716	Faeriefungin B	CCC(C1OC(=O)/C=C/C=C/C=C/C=C/C=C/CC(O)C(C)C(CC(CC(CC(CC(CC(CC(/C=C/C1C)O)O)O)O)O)O)O)C	788	Yes
1717	Flavofungin II	CC[C@@H]([C@@H]1OC(=O)/C=C/C=C/C=C/C=C/C=C/C[C@H](O)[C@H](C)[C@@H](C[C@@H](C[C@@H](C[C@H](C[C@@H](C[C@H](C[C@H](/C=C/[C@@H]1C)O)O)O)O)O)O)O)C	788	No
1718	Faeriefungin A	OC1CC(O)CC(O)CC(O)/C=C/C(C)C(OC(=O)/C=C/C=C/C=C/C=C/C=C/CC(C(CC(CC(C1)O)O)O)C)O)C(C)C	789	Yes
1719	Flavofungin VIII	O[C@@H]1C[C@@H](O)C[C@@H](O)C[C@@H](O)C[C@@H]2C[C@H]([C@H](O2)/C=C/C=C/C=C/C=C/C(=O)O[C@H]([C@H](/C=C/[C@@H](C[C@@H](C[C@H](C1)O)O)O)C)C)C)O	789	No
1720	Flavofungin I	O[C@H]1C[C@H](O)C[C@@H](O)C[C@@H](O)/C=C/[C@H](C)[C@@H](OC(=O)/C=C/C=C/C=C/C=C/C=C/C[C@@H]([C@@H]([C@@H](C[C@@H](C[C@@H](C1)O)O)O)C)O)C(C)C	790	Yes
1721	14-Demethylmycoticin A	CCC1OC(=O)/C=C/C=C/C=C/C=C\C=C\CC(O)C(C)C(CC(CC(CC(CC(CC(CC(/C=C\C1C)O)O)O)O)O)O)O	791	Yes
1722	Reedsmycin B	CCC(C1OC(=O)/C=C/C=C/C=C\C=C/C=C/CC(O)CC(CC(CC(CC(CC(CC(CC(/C=C/C1C)O)O)O)O)O)O)O)O)C	792	Yes
1723	Flavofungin VI	O[C@H]1C[C@H](O)C[C@@H](O)C[C@@H](O)/C=C/[C@H](C)[C@@H](OC(=O)/C=C/C=C/C=C/C=C/[C@@H]2O[C@H]([C@@H]([C@@H](C[C@@H](C[C@@H](C1)O)O)O)C)C[C@@H]2O)C(C)C	793	Yes
1724	Flavofungin VII	O[C@H]1C[C@H](O)C[C@@H](O)C[C@@H](O)/C=C/[C@H](C)[C@@H](OC(=O)/C=C/C=C/C=C/C=C/[C@@H]2O[C@H]([C@@H]([C@@H](C[C@@H](C[C@@H](C1)O)O)O)C)C[C@H]2O)C(C)C	793	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1725	Flavofungin IX	O[C@@H]1C[C@@H](O)C[C@@H](O)/C=C/[C@H](C)[C@@H](OC(=O)/C=C/C=C/C=C/C=C/[C@@H]2O[C@H](C[C@@H](C[C@@H](C[C@H](C1)O)O)O)[C@H](C)[C@@H](O)C[C@H]2O)C(C)C	794	Yes
1726	Flavofungin V	CC[C@@H]([C@@H]1OC(=O)/C=C/C=C/C=C/C=C/[C@H]2O[C@H](C[C@H]2O)[C@H](C)[C@@H](C[C@@H](C[C@@H](C[C@H](C[C@@H](C[C@H](C[C@H](/C=C/[C@@H]1C)O)O)O)O)O)O)O)C	795	Yes
1727	Flavofungin IV	O[C@H]1C[C@H](O)C[C@@H](O)C[C@@H](O)/C=C/[C@H](C)[C@@H](OC(=O)/C=C/C=C/C=C/C=C/[C@H]2O[C@@H]([C@@H]([C@@H](C[C@@H](C[C@@H](C1)O)O)O)C)C[C@H]2O)C(C)C	796	Yes
1728	32,33-Didehydroroflamycoin	OC1CC(O)CC(O)CC(O)CC2(O)CC(O)CC(O2)CC=CC=CC=CC=C(C(=O)OC(C(C=CC(CC(CC(C1)O)O)O)C)C(C)C)C	797	Yes
1729	DDHR	OC1CC(O)CC(O)CC(O)CC2(O)CC(O)CC(O2)C/C=C/C=C/C=C/C=C/C=C(/C(=O)OC(C(/C=C/C(CC(CC(C1)O)O)O)C)C(C)C)\C	798	Yes
1730	PN00053	CCC(C1OC(=O)/C(=C/C=C/C=C/C=C/C=C/CC2CC(O)CC(O2)(O)CC(CC(CC(CC(CC(CC(CC(/C=C/C1C)O)O)O)O)O)O)O)/C)C	799	Yes
1731	1alpha,25-Dihydroxyvitamin D3	OC1CC(O)C(=C)/C(=C\C=C\2/CCCC3(C2(C)CCC3C(CCCC(O)(C)C)C)C)/C1	800	Yes
1732	Roseosporol A	OC[C@@H]1C[C@H](O)[C@](C[C@]1(C)/C=C/C=C(C)C)(C)O	801	Yes
1733	Chaxamycin A	O=C1/C=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](O)[C@@H]([C@H]([C@H](/C=C(/C(=O)c2c3C(=O)C(=C(N1)C(=O)c3c(O)c(c2O)C)C)\C)C)O)C	802	Yes
1734	CHEBI:69810	O=C1/C=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](O)[C@@H]([C@H]([C@H](/C=C(/C(=O)c2c3C(=O)C(=C(N1)C(=O)c3cc(c2O)C)C)\C)C)O)C	803	Yes
1735	Chaxamycin C	OC[C@H]1/C=C(\C)/C(=O)c2c3C(=O)C(=C(C(=O)c3c(c(c2O)C)O)NC(=O)/C=C\C=C\[C@@H]([C@@H]([C@H]([C@H]([C@H]([C@@H]([C@@H]([C@H]1O)C)O)C)O)C)O)C)C	803	No
1736	Chebi:69812	CC(=O)O[C@@H]1[C@H](C)[C@@H](O)/C=C/O[C@]2(C)Oc3c([C@@H]2O)c2C(=O)C(=C(C(=O)c2c(c3C)O)NC(=O)/C=C\C=C\[C@@H]([C@@H]([C@H]([C@H]([C@H]1C)O)C)O)C)C	804	Yes
1737	Tolypromycin Y	COC1/C=C/OC2(C)Oc3c(C2=O)c2C(=C/C(=N/C(=O)/C(=C\C(=O)C4C(C(C(C(C(C(C1C)OC(=O)C)C)O)C)O)C4)/C)/C(=O)c2c(c3C)O)NC1CCC(OC1C)O	805	Yes
1738	Rifabutin	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C2=O)c2C4=NC5(NC4=C(C(=O)c2c(c3C)O)NC(=O)/C(=C\C=C\[C@@H]([C@@H]([C@H]([C@H]([C@H]([C@@H]([C@@H]1C)OC(=O)C)C)O)C)O)C)/C)CCN(CC5)CC(C)C	806	Yes
1739	Rifamycin O	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C2=O)c2c(c(c3C)O)C(=O)C(=CC32OCC(=O)O3)NC(=O)/C(=C\C=C\[C@@H]([C@@H]([C@H]([C@H]([C@H]([C@@H]([C@@H]1C)OC(=O)C)C)O)C)O)C)/C	807	Yes
1740	Carbazomycin D	COc1ccc2c(c1)c1c(OC)c(OC)c(c(c1[nH]2)C)C	808	Yes
1741	Carbazomycin A	COc1c(OC)c(C)c(c2c1c1ccccc1[nH]2)C	808	No
1742	Carbazomycin C	COc1ccc2c(c1)c1c(O)c(OC)c(c(c1[nH]2)C)C	809	No
1743	Carbazomycin F	COc1ccc2c(c1)c1c(O)c(OC)c(c(c1[nH]2)C=O)C	809	No
1744	Carbazomycin B	COc1c(C)c(C)c2c(c1O)c1ccccc1[nH]2	809	No
1745	Carbazomycin E	O=Cc1c(C)c(OC)c(c2c1[nH]c1c2cccc1)O	809	Yes
1746	Terferol	COc1cc(c2ccccc2)c(c(c1c1ccccc1)O)O	810	Yes
1747	Murrayanine	COc1cc(C=O)cc2c1[nH]c1c2cccc1	811	Yes
1748	Aminoansamycin D	O=C1Nc2cc(O)cc(c2O)[C@@H](C/C=C/C=C/[C@H]([C@@H]1C)O)Cc1ccccc1C(=O)O	812	Yes
1749	Aminoansamycin E	O=C1Nc2cc(O)cc(c2O)[C@@H](C/C=C/C=C/[C@H]([C@@H]1C)O)Nc1cc(O)ccc1C(=O)O	813	Yes
1750	Aminoansamycin C	CO[C@@H]1C/C=C/C=C/[C@H]([C@@H](C(=O)Nc2c(c1cc(O)c2)O)C)O	814	Yes
1751	Aminoansamycin B	Oc1cc2NC(=O)[C@@H](C)[C@H](O)/C=C/C=C/C[C@H](c(c1)c2O)O	814	No
1752	Youssoufene A1	C/C=C/C=C\C=C\C=C/[C@H]1C[C@@H](C=C/C/1=C\CC(=O)O)[C@@H](c1ccccc1/C=C\C=C\C=C/C=C/C)CC(=O)O	815	Yes
1753	Aminoansamycin A	CC(=O)O[C@@H]1C[C@H]2/C=C/C[C@H]([C@@H](C(=O)Nc3c(c1cc(O)c3)O2)C)O	816	Yes
1754	Bisindolylmaleimide IV	O=C1NC(=O)C(=C1c1c[nH]c2c1cccc2)c1c[nH]c2c1cccc2	817	Yes
1755	3'-epi-5'-Methoxy-K252d	CO[C@@H]1[C@H](O)[C@H](O)[C@@H](O[C@H]1n1c2c(c(c1C)C=C)c1C(=O)NCc1c1c2[nH]c2c1ccc2)C	818	Yes
1756	9-Hydroxy-3'-N-acetylholyrine A	CC(=O)N[C@@H]1C[C@@H](O[C@H]([C@@H]1O)C)n1c2c(c3c1cccc3)c1C(=O)NCc1c1c2[nH]c2c1cc(cc2)O	819	No
1757	3-Hydroxy-3'-N-acetylholyrine A	CC(=O)N[C@@H]1C[C@@H](O[C@H]([C@@H]1O)C)n1c2c(c3c1ccc(c3)O)c1C(=O)NCc1c1c2[nH]c2c1cccc2	819	Yes
1758	3-Hydroxyholyrine A	Oc1ccc2c(c1)c1c3C(=O)NCc3c3c(c1n2[C@H]1C[C@@H](N)[C@H]([C@@H](O1)C)O)[nH]c1c3cccc1	819	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1759	9-Hydroxyl-3'-N-acetyl-4'-Hydroxylstaurosporine	CC(=O)N[C@@H]1C[C@H]2O[C@](C[C@@H]1O)(C)n1c3ccc(cc3c3c1c1n2c2ccccc2c1c1c3CNC1=O)O	819	No
1760	Fradcarbazole A	CO[C@@H]1[C@@H](C[C@H]2O[C@]1(C)n1c3ccccc3c3c1c1n2c2ccccc2c1c1c3CNC1=O)N(c1ncc(s1)c1c[nH]c2c1cccc2)C	820	Yes
1761	Juglorubin	OC(=O)/C=C/C1C2[C-](C3C1C(=O)c1c(O)cccc1C(=O)O[C@@H](C3)CC(=O)O)C(=O)c1c(C2=O)cccc1O	821	Yes
1762	Herboxidiene	CO[C@H]([C@H](C1O[C@]1(C)C[C@@H](/C=C/C=C(/[C@H]1O[C@H](CC[C@@H]1C)CC(=O)O)\C)C)[C@H](O)C	822	No
1763	18-Deoxy-25-demethylherboxidiene	CC[C@@H]([C@H]([C@H]1O[C@]1(C)C[C@@H](/C=C/C=C(/[C@H]1O[C@H](CC[C@@H]1C)CC(=O)O)\C)C)C)O	822	No
1764	25-Demethyl-herboxidiene	OC(=O)C[C@H]1CC[C@@H]([C@H](O1)/C(=C/C=C/[C@H](C[C@@]1(C)O[C@@H]1[C@@H]([C@H]([C@H](O)C)O)C)C)/C)C	822	Yes
1765	18-Deoxyherboxidiene	CC[C@@H]([C@H]([C@H]1O[C@]1(C)C[C@@H](/C=C/C=C(/[C@H]1O[C@H](CC[C@@H]1C)CC(=O)O)\C)C)C)OC	822	No
1766	25-Demethyl-herboxidiene C	OC(=O)C[C@H]1CC[C@@H]([C@H](O1)C1(C)OC1/C=C/[C@H](C[C@H]1O[C@@H]1[C@@H]([C@H]([C@H](O)C)O)C)C)C	822	No
1767	Herboxidiene A1	CO[C@H]1[C@@H](C)OC([C@@H]1C)C(C[C@@H](/C=C/C=C(/[C@H]1O[C@H](CC[C@H]1C)CC(=O)O)\C)C)(C)C	823	Yes
1768	Herboxidiene B1	CO[C@H]1[C@@H](C)O[C@@]([C@@H]([C@@H]1C)O)(C)C[C@@H](/C=C/C=C(/[C@H]1O[C@H](CC[C@@H]1C)CC(=O)O)\C)C	823	No
1769	5,6-Dihydroxy-25-demethyl-herboxidiene A1	OC(=O)C[C@H]1C[C@@H](O)[C@@]([C@H](O1)/C(=C/C=C/[C@H](CC(C1O[C@@H]([C@@H]([C@H]1C)O)C)(C)C)C)/C)(C)O	824	Yes
1770	5-Hydroxy-25-demethyl-herboxidiene A1	OC(=O)C[C@H]1C[C@@H](O)[C@@H]([C@H](O1)/C(=C/C=C/[C@H](CC(C1O[C@@H]([C@@H]([C@H]1C)O)C)(C)C)C)/C)C	824	No
1771	5,6-Dihydroxy-herboxidiene A1	CO[C@H]1[C@@H](C)OC([C@@H]1C)C(C[C@@H](/C=C/C=C(/[C@H]1O[C@@H](CC(=O)O)C[C@H]([C@@]1(C)O)O)\C)C)(C)C	824	No
1772	5-Hydroxy-herboxidiene B1	CO[C@H]1[C@@H](C)O[C@@]([C@@H]([C@@H]1C)O)(C)C[C@@H](/C=C/C=C(/[C@H]1O[C@@H](CC(=O)O)C[C@H]([C@@H]1C)O)\C)C	824	No
1773	5,6-Dihydroxyherboxidiene B1	CO[C@H]1[C@@H](C)O[C@@]([C@@H]([C@@H]1C)O)(C)C[C@@H](/C=C/C=C(/[C@H]1O[C@@H](CC(=O)O)C[C@H]([C@@]1(C)O)O)\C)C	824	No
1774	5-Hydroxyherboxidiene A1	CO[C@H]1[C@@H](C)OC([C@@H]1C)C(C[C@@H](/C=C/C=C(/[C@H]1O[C@@H](CC(=O)O)C[C@H]([C@@H]1C)O)\C)C)(C)C	824	No
1775	5- Hydroxy-25-demethyl-herboxidiene B1	OC(=O)C[C@H]1C[C@@H](O)[C@@H]([C@H](O1)/C(=C/C=C/[C@H](C[C@]1(C)O[C@H](C)[C@@H]([C@H]([C@H]1O)C)O)C)/C)C	824	No
1776	5,6-Dihydroxy-25-demethylherboxidiene B1	OC(=O)C[C@H]1C[C@@H](O)[C@@]([C@H](O1)/C(=C/C=C/[C@H](C[C@]1(C)O[C@H](C)[C@@H]([C@H]([C@H]1O)C)O)C)/C)(C)O	824	No
1777	Herboxidiene C	CC[C@H]([C@H]([C@H]1O[C@H]1C[C@@H](/C=C/C1OC1(C)[C@H]1O[C@H](CC[C@H]1C)CC(=O)O)C)C)[C@H](O)C	825	Yes
1778	Kandenol E	O=C1C=C(C)[C@@]23[C@@](C1)(C)C[C@H]([C@H](C2)C(O3)(C)C)O	826	Yes
1779	3-Methyl-antibiotic G-15F	CC1=CC2=C(C(O1)C)C(=O)c1c(C2=O)ccc(c1O)[C@@H]1O[C@H](C)[C@H]([C@@H](C1)N(C)C)O	827	Yes
1780	Jadomycin furan 4	OCc1cc(C)cc2c1c1c(o2)C(=O)c2c(C1=O)cccc2O[C@H]1C[C@H](O)[C@H](C(O1)C)O	828	Yes
1781	Jadomycin furan 3	O=Cc1cc(C)cc2c1c1c(o2)C(=O)c2c(C1=O)cccc2O[C@H]1C[C@H](O)[C@H](C(O1)C)O	828	No
1782	CHEMBL1922539	CC/C=C/1\C[C@@H]2N(C1)C(=O)c1c(NC2)cccc1	829	Yes
1783	CHEMBL1922537	CC/C=C/1\C[C@@H]2N(C1)C(=O)c1c(NC2)c(OC)ccc1	829	No
1784	(5E,8R,9E)-3-(Carbamoylmethyl)-8,10-dimethyl-7-oxododeca-5,9,11-trienoic acid	C=C/C(=C/[C@H](C(=O)/C=C/CC(CC(=O)O)CC(=O)N)C)/C	830	Yes
1785	Methyl (5E,8R,9E)-3-(carbamoylmethyl)-8,10- dimethyl-7-oxododeca-5,9,11-trienoate	COC(=O)CC(CC(=O)N)C/C=C/C(=O)[C@@H](/C=C(/C=C)\C)C	830	No
1786	CHEBI:66788	CC/C=C/C=C(/C(C(CC(/C=C/C=C/C1OC(=O)C=CC1OC)OC)C)O)\OC	831	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1787	Sultriecin	CCCCC/C=C/C=C/C=C/C(C(C(OS(=O)(=O)O)C/C=C/C1OC(=O)C=CC1O)C)O	832	Yes
1788	CHEBI:69413	CC/C=C/[C@H]1C/C=C/C=C\[C@H](OC)[C@@H](O)[C@@H](O)[C@@H](C)/C=C/C[C@H](/C=C/C=C(/C=C/C(=O)O1)\C)C	833	Yes
1789	CHEBI:69411	CC/C=C/[C@H]1C/C=C/C=C\[C@H](O)C[C@@H](O)[C@@H](C)/C=C/C[C@H](/C=C/C=C(/C=C/C(=O)O1)\C)C	833	No
1790	Atacamycin A	CC/C=C\1/C/C=C/C=C\C(OC)C(O)C(O)C(C)/C=C/C(C(/C=C/C=C(/C=C/C(=O)O1)\C)C)OC	834	Yes
1791	Atacamycin B	CC/C=C\1/C/C=C/C=C\C(OC)C(O)C(O)C(C)/C=C/CC(/C=C/C=C(/C=C/C(=O)O1)\C)C	835	Yes
1792	Atacamycin C	CC/C=C\1/C/C=C/C=C\C(OC)CC(O)C(C)/C=C/CC(/C=C/C=C(/C=C/C(=O)O1)\C)C	835	No
1793	CHEBI:69412	CC/C=C/[C@H]1C/C=C/C=C\[C@H](O)[C@@H](O)[C@@H](O)[C@@H](C)/C=C/C[C@H](/C=C/C=C(/C=C/C(=O)O1)\C)C	836	Yes
1794	Emycin D	CC1CC(=O)c2c(C1)ccc1c2C2OC(O1)c1c2cccc1O	837	Yes
1795	(R)-3-Hydroxy-7-((1S,3R)-3-hydroxy-7-methoxy-2,3-dihydro-1H-inden-1-yl)-3-methyl-3,4-dihydronaphthalen-1(2H)-one	COc1cccc2c1[C@@H](C[C@H]2O)c1ccc2c(c1)C(=O)C[C@](C2)(C)O	838	No
1796	(R)-3-Hydroxy-7-((1S,3S)-3-hydroxy-7-methoxy-2,3-dihydro-1H-inden-1-yl)-3-methyl-3,4-dihydronaphthalen-1(2H)-one	COc1cccc2c1[C@@H](C[C@@H]2O)c1ccc2c(c1)C(=O)C[C@](C2)(C)O	838	No
1797	(R)-7-((1S,3R)-3-Ethoxy-7-methoxy-2,3-dihydro-1H-inden-1-yl)-3-hydroxy-3-methyl-3,4-dihydronaphthalen-1(2H)-one	CCO[C@@H]1C[C@H](c2c1cccc2OC)c1ccc2c(c1)C(=O)C[C@](C2)(C)O	838	No
1798	(R)-7-((1S,3S)-3-Ethoxy-7-methoxy-2,3-dihydro-1H-inden-1-yl)-3-hydroxy-3-methyl-3,4-dihydronaphthalen-1(2H)-one	CCO[C@H]1C[C@H](c2c1cccc2OC)c1ccc2c(c1)C(=O)C[C@](C2)(C)O	838	No
1799	(R)-7-((1S,3R)-3,7-Dimethoxy-1,3-dihydroisobenzofuran-1-yl)-3-hydroxy-3-methyl-3,4-dihydronaphthalen-1(2H)-one	COc1cccc2c1[C@@H](O[C@H]2OC)c1ccc2c(c1)C(=O)C[C@](C2)(C)O	838	No
1800	1,4-Dimethoxy-3-(3'-hydroxy-3'-methyl-1'-tetralone)-1(3H)-isobenzofuran	COc1cccc2c1[C@H](O[C@H]2OC)c1ccc2c(c1)C(=O)C[C@](C2)(C)O	838	Yes
1801	(R)-7-((1R,3S)-3,7-Dimethoxy-1,3-dihydroisobenzofuran-1-yl)-3-hydroxy-3-methyl-3,4-dihydronaphthalen-1(2H)-one	COc1cccc2c1[C@H](O[C@@H]2OC)c1ccc2c(c1)C(=O)C[C@](C2)(C)O	838	No
1802	(3R,8S,13S)-3-Hydroxy-9-methoxy-3-methyl-3,4,8,13-tetrahydro-8,13-epoxybenzo[e]naphtho[2,1-b]oxepin-1(2H)-one	COc1cccc2c1[C@@H]1Oc3c([C@H]2O1)c1C(=O)C[C@](Cc1cc3)(C)O	839	Yes
1803	(3R,8R,13R)-3-Hydroxy-9-methoxy-3-	COc1cccc2c1[C@H]1Oc3c([C@@H]2O1)c1C(=O)C[C@](Cc1cc3)(C)O	839	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
	methyl-3,4,8,13-tetrahydro-8, 13-epoxybenzo[e]naphtho[2,1-b]oxepin-1(2H)-one			
1804	Versipelostatin A	OC[C@@H]1C[C@@H](C)[C@H](O[C@H]2C[C@H](O)[C@@H]([C@H](O2)C)O[C@H]2C[C@H](OC)[C@H]([C@@H](O2)C)O[C@H]2C[C@H](O)[C@@H]([C@H](O2)C)O)[C@H](C)CCC(C)[C@H]2[C@]3(C(=C(C(=O)[C@@]4([C@H](/C(=C/1)/CC)C(=C[C@H]1[C@H]4[C@@H](C)C(=O)C[C@@H]1C)C)CC)C(=O)C3)O)C[C@H](C(=C2)C)C	840	Yes
1805	Lobophorin F	COC(=O)N[C@H]1[C@@H](C)O[C@H](C[C@]1(C)[N+](=O)[O-])O[C@H]1C/C=C(\C)/[C@@H]2C=C[C@H]3[C@H]([C@]2(C)C(=C2C(=O)[C@]4([C@H](/C=C/1\C)C=C(C)[C@@H](C4)C)OC2=O)O)[C@@H](C)C[C@@H]([C@@H]3O[C@@H]1O[C@@H](C)[C@@H]([C@@H](C1)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O)O)C	841	Yes
1806	Lobophorin	OCC1CCC23C(C1)/C=C(\C)/[C@H](C/C=C(/[C@H]1[C@](C(=O)C([C@H]3O)C(=O)O2)(C)[C@@H]2[C@@H](C)C[C@@H]([C@@H]([C@H]2C=C1)O[C@H]1OC(C)[C@H]([C@@H](C1)O[C@@H]1C[C@@H](O)[C@@H](C(O1)C)OC1C[C@@H](O)C(C(O1)C)OC)O)C)\C)O[C@@H]1OC(C)C(C(C1)(C)N(=O)=O)NC(=O)OC	842	Yes
1807	Lobophorin E	COC(=O)N[C@H]1[C@@H](C)O[C@H](C[C@]1(C)[N+](=O)[O-])O[C@H]1C/C=C(\C)/[C@@H]2C=C[C@H]3[C@H]([C@]2(C)C(=C2C(=O)[C@]4([C@H](/C=C/1\C)C=C(C)[C@@H](C4)C)OC2=O)O)[C@@H](C)C[C@@H]([C@@H]3O[C@@H]1O[C@@H](C)[C@@H]([C@@H](C1)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O[C@@H]1C[C@@H](O)[C@H]([C@@H](O1)C)OC)O)C	843	Yes
1808	Lobophorin B	COC(=O)N[C@H]1[C@@H](C)O[C@H](C[C@]1(C)[N+](=O)[O-])O[C@H]1C/C=C(/C)\[C@@H]2C=C[C@H]3[C@H]([C@]2(C)C(=C2C(=O)[C@]4([C@H](/C=C\1/C)C=C(CO)[C@@H](C4)C)OC2=O)O)[C@@H](C)C[C@@H]([C@@H]3O[C@@H]1O[C@@H](C)[C@@H]([C@@H](C1)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O[C@@H]1C[C@@H](O)[C@H]([C@@H](O1)C)OC)O)C	844	Yes
1809	Lobophorin C	COC(=O)N[C@@H]1[C@H](C)O[C@H](C[C@@]1(C)N)OC1C/C=C(\C)/[C@H]2C=C[C@@H]3[C@@H]([C@@]2(C)C(=O)C2=C(C4([C@H](/C=C\1/C)C=C(CO)[C@H](C4)C)OC2=O)O)[C@H](C)C[C@H]([C@H]3O[C@H]1O[C@@H](C)[C@@H]([C@@H](C1)O[C@@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O[C@@H]1C[C@@H](O)[C@H]([C@@H](O1)C)OC)O)C	845	Yes
1810	Kijanimicin	COC(=O)N[C@H]1[C@@H](C)O[C@H](C[C@]1(C)[N+](=O)[O-])O[C@H]1C/C=C(\C)/[C@@H]2C=C[C@H]3[C@H]([C@]2(C)/C(=C\2/C(=O)[C@]4([C@H](/C=C/1\C)C=C(CO)[C@@H](C4)C)OC2=O)/O)[C@@H](C)C[C@@H]([C@@H]3O[C@@H]1O[C@@H](C)[C@@H]([C@@H](C1)O[C@@H]1O[C@@H](C)C(C(C1)O[C@H]1C[C@H](O)[C@H]([C@@H](O1)C)O)O[C@@H]1C[C@@H](O)[C@H]([C@@H](O1)C)OC)O)C	846	Yes
1811	Lobophorin K	COC(=O)N[C@H]1[C@@H](C)O[C@H](C[C@]1(C)NO)O[C@H]1CC=C(C)[C@@H]2C=C[C@H]3[C@H]([C@]2(C)C(=C2C(=O)[C@]4([C@H](C=C1C)C=C(CO)[C@@H](C4)C)OC2=O)O)[C@@H](C)C[C@@H]([C@@H]3O[C@@H]1O[C@@H](C)[C@@H]([C@@H](C1)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O[C@@H]1C[C@@H](O)[C@H]([C@@H](O1)C)OC)O)C	847	Yes
1812	Lobophorin A	COC(=O)N[C@H]1[C@@H](C)O[C@H](C[C@]1(C)N)O[C@H]1C/C=C(/C)\[C@@H]2C=C[C@H]3[C@H]([C@]2(C)C(=C2C(=O)[C@]4([C@H](/C=C\1/C)C=C(CO)[C@@H](C4)C)OC2=O)O)[C@@H](C)C[C@@H]([C@@H]3O[C@@H]1O[C@@H](C)[C@@H]([C@@H](C1)O[C@H]1C[C@@H](O)[C@H]([C@@H](O1)C)O[C@@H]1C[C@@H](O)[C@H]([C@@H](O1)C)OC)O)C	848	Yes
1813	Lobophorin CR4	CO[C@@H]1[C@@H](O)C[C@H](O[C@@H]1C)O[C@@H]1[C@@H](O)CC(O[C@@H]1C)O[C@H]1C[C@@H](O[C@@H]([C@@H]1O)C)O[C@H]1[C@@H](C)C[C@@H]([C@@H]2[C@@H]1C=C[C@@H]1[C@@]2(C)C(=O)C2=C(O)[C@]3(OC2=O)C[C@@H](C)C(=C[C@H]3/C=C(/[C@H](C/C=C/1\C)O)\C)C)C	849	Yes
1814	Abamectin	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)/C=C/C=C/3\CO[C@H]4[C@]3(O)[C@@H](C=C([C@H]4O)C)C(=O)O[C@H]3C[C@@H](C/C=C/2\C)O[C@]2(C3)C=C[C@@H]([C@H](O2)C(CC)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C.CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1[C@@H](C)/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)C=C[C@@H]([C@H](O1)C(C)C)C	850	No
1815	Avermectin A1b	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1[C@@H](C)/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3OC)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)C=C[C@@H]([C@H](O1)C(C)C)C	850	No
1816	Ivermectin B1b	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1[C@@H](C)/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)CC[C@@H]([C@H](O1)C(C)C)C	850	No
1817	Tenvermectin B	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1[C@@H](C)/C=C\C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)CC[C@@H]([C@H](O1)CC)C	850	No
1818	CTK8E8557	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)C=CC=C3CO[C@H]4[C@]3(O)[C@@H](C=C([C@H]4O)C)C(=O)O[C@H]3C[C@@H](CC=C2C)O[C@]2(C3)C=C[C@@H]([C@H](O2)[C@H](CC)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1819	Avermectin A1a	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)/C=C/C=C/3\CO[C@H]4[C@]3(O)[C@@H](C=C([C@H]4OC)C)C(=O)O[C@H]3C[C@@H](C/C=C/2\C)O[C@]2(C3)C=C[C@@H]([C@H](O2)C(CC)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	No
1820	Tenvermectin C	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)/C=C/C=C/3\CO[C@H]4[C@]3(O)[C@@H](C=C([C@@H]4O)CC)C(=O)O[C@H]3C[C@@H](C/C=C/2\C)O[C@]2(C3)CC[C@@H]([C@H](O2)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	No
1821	Tenvermectin A	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1[C@@H](C)/C=C\C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)CC[C@@H]([C@H](O1)C)C	850	No
1822	Delta2,3-tenvermectin A	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1[C@@H](C)/C=C/C=C/2\CO[C@]3([C@]2(O)C(=C[C@@H]([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)CC[C@@H]([C@H](O1)C)C)C	850	No
1823	Ivermectin	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)/C=C/C=C/3\CO[C@H]4[C@]3(O)[C@@H](C=C([C@H]4O)C)C(=O)O[C@H]3C[C@@H](C/C=C/2\C)O[C@]2(C3)CC[C@@H]([C@H](O2)[C@H](CC)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	No
1824	Avermectin A2a	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)/C=C/C=C/3\CO[C@H]4[C@]3(O)[C@@H](C=C([C@H]4OC)C)C(=O)O[C@H]3C[C@@H](C/C=C/2\C)O[C@]2(C3)C[C@H](O)[C@@H]([C@H](O2)C(CC)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	No
1825	CHC-B2	CO[C@H]1C[C@H](O[C@@H]2/C(=C/C[C@@H]3C[C@H](OC(=O)[C@H]4[C@@]5(/C(=C/C=C/[C@@H]2C)/CO[C@@H]5[C@H](O)C(=C4)C)O)C[C@@]2(O3)C[C@H](O)[C@@H](C(O2)C2CCCCC2)C)/C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	No
1826	Tenvermectin D	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1[C@@H](CC)/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)CC[C@@H]([C@H](O1)C)C	850	No
1827	Doramectin	CO[C@H]1C[C@@H](O[C@H](C1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)OC1[C@@H](C)/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)C=C[C@@H]([C@H](O1)C1CCCCC1)C	850	No
1828	Avermectin A1	COC1CC(O[C@H]2[C@@H](C)/C=C/C=C/3\CO[C@H]4[C@]3(O)[C@@H](C=C([C@H]4OC)C)C(=O)O[C@H]3C[C@@H](C/C=C/2\C)O[C@]2(C3)C=C[C@@H]([C@H](O2)[C@H](CC)C)C)OC(C1OC1CC(OC)C(C(O1)C)O)C	850	No
1829	Avermectin B1b	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1[C@@H](C)/C=C/C=C/2\COC3[C@]2(O)C(C=C([C@H]3O)C)C(=O)OC2CC(C/C=C/1\C)O[C@]1(C2)C=C[C@@H]([C@H](O1)C(C)C)C	850	No
1830	(3S,4'S,5R,5'S,6'R,7R,9E,11S,12S,13E,15E,16aS,18S,20aR)-3,3',4,4',5',6',7,8,11,12,16a,17,18,20a-Tetradecahydro-4',16a,18-trihydroxy-5',10,12,16,19-pentamethyl-1-oxo-6'-(propan-2-yl)-1H-Spiro[3,7-methano[2,6]benzodioxacyclooctadecine-5,2'-pyran]-11-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl-alpha-L-arabino-hexopyranosyl)-3-O-methyl-alpha-L-arabino-hexopyranoside	COC1CC(OCC1OC1CC(OC)C(C(O1)C)O)O[C@H]1[C@@H](C)/C=C/C=C(\C)/[C@]2(O)C[C@H](O)C(=C[C@H]2C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)C[C@H](O)[C@@H]([C@H](O1)C(C)C)C)C	850	No
1831	Avermectin	CO[C@H]1CC(O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1C(C)/C=C\C=C/2\COC3[C@]2(O)C(C=C([C@H]3O)C)C(=O)OC2CC(C/C=C\1/C)OC1(C2)CC[C@@H](CO1)C	850	No
1832	Avermectin A2b	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C)O[C@H]1[C@@H](C)/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3OC)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)C[C@H](O)[C@@H]([C@H](O1)C(C)C)C	850	No
1833	Avermectin B2b	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)/C=C/C=C/3\CO[C@H]4[C@]3(O)[C@@H](C=C([C@H]4O)C)C(=O)O[C@H]3C[C@@H](C/C=C/2\C)O[C@]2(C3)C[C@H](O)[C@@H]([C@H](O2)C(C)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	No
1834	Avermectin B2a	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)/C=C/C=C/3\COC4[C@]3(O)C(C=C([C@H]4O)C)C(=O)OC3CC(C/C=C/2\C)O[C@]2(C3)C[C@H](O)[C@@H]([C@H](O2)C(CC)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1835	Avermectin B(1)A	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)/C=C/C=C/3\COC4[C@]3(O)C(C=C([C@H]4O)C)C(=O)OC3CC(C/C=C/2\C)O[C@]2(C3)C=C[C@@H](C(O2)[C@H](CC)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	Yes
1836	13-Epi-Avm B(sub 2)	CO[C@H]1C[C@H](O[C@H]2[C@@H](C)/C=C/C=C/3\CO[C@H]4[C@]3(O)[C@@H](C=C([C@H]4O)C)C(=O)O[C@H]3C[C@@H](C/C=C/2\C)O[C@]2(C3)C[C@H](O)[C@@H]([C@H](O2)[C@H](CC)C)C)O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O)C	850	No
1837	Okilactomycin	CC1CCCC2C=C(C(=O)O)C(CC32C2OC(C(C1)C)C(=C)C(=O)C2(C(=O)O3)C)C	851	Yes
1838	Avermectin B1a 4"-beta-L-fucoside	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O[C@@H]1O[C@H](CO)[C@@H]([C@@H]([C@H]1O)O)O)C)O[C@H]1[C@@H](C)/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)C=C[C@@H]([C@H](O1)[C@H](CC)C)C	852	Yes
1839	Avermectin B1a 4"-beta-D-galactoside	CC[C@@H]([C@H]1O[C@@]2(C=C[C@@H]1C)O[C@@H]1C/C=C(\C)/[C@@H](O[C@H]3C[C@H](OC)[C@H]([C@@H](O3)C)O[C@H]3C[C@H](OC)[C@H]([C@@H](O3)C)O[C@H]3C[C@@H](O)[C@@H]([C@H](O3)CO)O)[C@@H](C)/C=C/C=C\3/[C@]4([C@H](C(=O)O[C@H](C2)C1)C=C(C)[C@H]([C@H]4OC3)O)O)C	853	Yes
1840	Avermectin B1a 4"-beta-2-deoxy-D-glucoside	CO[C@H]1C[C@@H](O[C@H]([C@@H]1O[C@H]1C[C@H](OC)[C@H]([C@@H](O1)C)O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@H]1O)O)O)C)O[C@H]1[C@@H](C)/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C/1\C)O[C@]1(C2)C=C[C@@H]([C@H](O1)[C@H](CC)C)C	854	Yes
1841	3"-O-Demethylavermectin A2a	CCC(C1OC2(OC3C/C=C(\C)/C(OC4CC(O)C(C(O4)C)OC4CC(O)C(C(O4)C)O)C(C)/C=C/C=C\4/C5(C(C(=O)OC(C2)C3)C=C(C)C(C5OC4)O)O)CC(C1C)O)C	855	Yes
1842	Fusicomycin B	CCCC(=O)[C@H]([C@H]1O[C@](O)([C@@H](C[C@H]1C)C)[C@@H](C(=O)OC[C@H]([C@H]1CC[C@]2(C1=CC[C@](C)(O)[C@H]1[C@H](C2)[C@H](CO)C[C@H]1O)C)C)C)C	856	Yes
1843	Fusicomycin A	OC[C@@H]1C[C@H]([C@@H]2[C@@H]1C[C@@]1(C)CC[C@@H](C1=CC[C@]2(C)O)[C@@H](COC(=O)[C@H]([C@]1(O)O[C@@H]([C@@H](C[C@H]1C)C)[C@@H](C(=O)CC)C)C)C)O	856	No
1844	Isofusicomycin A	OC[C@@H]1C[C@H]([C@@H]2[C@@H]1C[C@@]1(C)CC[C@@H](C1=CC[C@]2(C)O)[C@@H](COC(=O)[C@@H]([C@]1(O)O[C@@H]([C@@H](C[C@H]1C)C)[C@@H](C(=O)CC)C)C)C)O	856	No
1845	17-Dihydroxycyclooctatin	CCCC(=O)C(C1OC(O)(C(CC1C)C)C(C(=O)OCC([C@H]1CC[C@]2(C1=CC[C@](C)(O)[C@H]1[C@H](C2)[C@H](CO)C[C@H]1O)C)CO)C)C	856	No
1846	17-[16,17-Dihydroxycyclooctatinyl]-hexaketide ester	CCCC(=O)C(C1OC(O)(C(CC1C)C)C(C(=O)OC[C@@H]([C@@H]1CC[C@@]2(C1=CC[C@@](C)(O)[C@H]1[C@@H](C2)[C@@H](CO)C[C@@H]1O)C)CO)C)C	856	No
1847	Cucurbitacin B	CC(=O)OC(/C=C/C(=O)[C@@]([C@H]1[C@H](O)C[C@@]2([C@]1(C)CC(=O)[C@@]1([C@H]2CC=C2[C@H]1C[C@H](O)C(=O)C2(C)C)C)C)(O)C)(C)C	857	Yes
1848	Cucurbitacin B 2-o-beta-D-glucoside	OC[C@H]1O[C@@H](O[C@H]2C[C@H]3[C@]4(C)C(=O)C[C@]5([C@@]([C@@H]4CC=C3C(C2=O)(C)C)(C)C[C@H]([C@@H]5[C@](C(=O)/C=C/C(OC(=O)C)(C)C)(O)C)O)C)[C@@H]([C@H]([C@@H]1O)O)O	858	Yes
1849	13-Deoxytetrodecamycin	C=C1OC(=O)C2=C1O[C@@H]1[C@@H](O)[C@H]3[C@H]([C@](C2=O)([C@@H]1C)C)CCCC3	859	Yes
1850	Milbemycin F	CC1/C=C\C=C/2\COC3C2(O)C(C=C(C3O)COC(=O)c2ccc[nH]2)C(=O)OC2CC(C/C=C(\C1)/C)OC1(C2)CCC(C(O1)C(C)C)C	860	Yes
1851	Milbemycin H	CC1/C=C\C=C(\C)/C2(O)CC(=O)C(=CC2C(=O)OC2CC(C/C=C(\C1)/C)OC1(C2)CCC(C(O1)C(C)C)C)C	861	Yes
1852	AG-F-74879	CCC1OC2(CCC1C)CC1CC(O2)CC=C(C)CC(C)C=CC=C2C3(C(C(=O)O1)C=C(C)C(C3OC2)O)O	862	No
1853	4-Hydroxy-delta-2,3-milbemycin A4	CCC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/C3C(=C[C@@](C)(O)[C@H](C3OC2)O)C(=O)O1	862	Yes
1854	4-Hydroxy-delta-2,3-milbemycin A3	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/C3C(=C[C@@](C)(O)[C@H](C3OC2)O)C(=O)O1	862	No
1855	27-Methoxylmilbemycin alpha 31	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/c3c(C(=O)O1)cc(C)c(c3OC2OC)O	862	No
1856	Milbemycin A4	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/[C@]3([C@H](C(=O)O1)C=C(C)[C@H]([C@H]3OC2)O)O	863	Yes
1857	Milbemycin alpha-2	CO[C@@H]1C(=CC2[C@]3([C@@H]1OC/C/3=C\C=C\[C@H](C)C/C/C(=C/C[C@@H]1C[C@H](OC2=O)C[C@@]2(O1)CC[C@@H]([C@H](O2)C)C)/C)O)C	864	No
1858	C5-O-Methylmilbemycin B2	COC1C(=C[C@@H]2[C@]3(C1OC/C/3=C\C=C\C(C)C/C(=C/C[C@@H]1C[C@H](OC2=O)C[C@@]2(O1)CC[C@@H]([C@H](O2)C)C)/C)O)C	864	No
1859	Milbemycin A3	C[C@H]1/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C(/C1)\C)O[C@]1(C2)CC[C@@H]([C@H](O1)C)C	864	No
1860	VM-44857	C/C=C(/[C@H]1O[C@]2(CC[C@@H]1C)CC1CC(O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/[C@]3(C(C(=O)O1)C=C(C)[C@H](C3OC2)O)O)\C	864	No
1861	Milbemycin B2	CO[C@@H]1C(=C[C@@H]2[C@]3([C@@H]1OC/C/3=C\C=C\[C@H](C)C/C/(=C/C[C@@H]1C[C@H](OC2=O)C[C@@]2(O1)CC[C@@H]([C@](O2)(C)O)C)/C)O)C	864	Yes
1862	Milbemycin beta2	CCC1OC2(CCC1C)CC1CC(O2)C/C=C(/C)\CC(C)/C=C/C=C(\C2(C(C(=O)O1)C=C(C)C(C2)OC)O)/CO	864	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1863	C5-O-Methylmilbemycin B2	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](O2)C/C=C(\C)/CC(C)/C=C/C=C(/[C@]2([C@H](C(=O)O1)C=C(C)[C@H](C2)OC)O)\CO	864	No
1864	Milbemycin J	CC1/C=C\C=C/2\COC3C2(O)C(C=C(C3=O)C)C(=O)OC2CC(C/C=C(\C1)/C)OC1(C2)CCC(C(O1)C)C	865	No
1865	5-Oxomilbemycin A4	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/[C@]3([C@H](C(=O)O1)C=C(C)C(=O)[C@H]3OC2)O	865	Yes
1866	Milbemycin K	CCC1OC2(CCC1C)CC1CC(O2)C/C=C(/C)\CC(C)/C=C\C=C\2/C3(C(C(=O)O1)C=C(C)C(=O)C3OC2)O	865	No
1867	Avermectin A1b aglycone	CO[C@@H]1C(=C[C@@H]2[C@]3([C@@H]1OC/C/3=C\C=C\[C@H](C)[C@H](O)/C(=C/C[C@@H]1C[C@H](OC2=O)C[C@@]2(O1)C=C[C@@H]([C@H](O2)C(C)C)C)/C)O)C	866	Yes
1868	Milbemycin beta1	CO[C@H]1C[C@@]2(O)/C(=C\C=C\[C@H](C)C/C(=C/C[C@H]3C[C@H](OC(=O)[C@@H]2C=C1C)C[C@@]1(O3)CC[C@@H]([C@H](O1)C)C)/C)/CO	867	Yes
1869	C5-O-Methylmilbemycin B1	CO[C@H]1C[C@@]2(O)/C(=C/C=C/C(C)C/C(=C/C[C@@H]3C[C@H](OC(=O)[C@@H]2C=C1C)C[C@@]1(O3)CC[C@@H]([C@H](O1)C)C)/C)/CO	867	No
1870	Milbemycin D	C[C@H]1/C=C/C=C/2\CO[C@H]3[C@]2(O)[C@@H](C=C([C@H]3O)C)C(=O)O[C@H]2C[C@@H](C/C=C(/C1)\C)O[C@]1(C2)CC[C@@H]([C@H](O1)C(C)C)C	868	No
1871	Milbemycin B3	CO[C@@H]1C(=C[C@@H]2[C@]3([C@@H]1OC/C/3=C\C=C\[C@H](C)C/C(=C/C[C@@H]1C[C@H](OC2=O)C[C@@]2(O1)CC[C@@H]([C@@](O2)(O)CC)C)/C)O)C	868	Yes
1872	VM 44866	C/C=C(/[C@H]1O[C@@]2(CC3CC(O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/[C@]4(C(C(=O)O3)C=C(C)[C@H](C4OC2)O)O)[C@@H](C[C@@H]1C)O)\C	868	No
1873	Milbemycin E	COC1CC2(O)/C(=C\C=C/C(C)C/C(=C\CC3CC(OC(=O)C2C=C1C)CC1(O3)CCC(C(O1)C(C)C)C)/C)/CO	869	No
1874	Nemadectin gamma	CO[C@H]1C(=C[C@H]2[C@@]3([C@H]1OC/C/3=C\C=C[C@@H](C)C/C(=C/C[C@H]1C[C@@H](OC2=O)C[C@]2(O1)C[C@@H](O)[C@H]([C@@H](O2)/C(=C/C)/C)C)/C)O)C	869	No
1875	C5-O-Methylmilbemycin B3	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](O2)C/C=C(\C)/CC(C)/C=C/C=C\2/[C@]3([C@H](C(=O)O1)C=C(C)C(C3OC2)OC)O	869	No
1876	Milbemycin G	CO[C@@H]1C(=C[C@@H]2[C@]3(C1OC/C/3=C\C=C\[C@H](C)C/C(=C/C[C@@H]1C[C@H](OC2=O)C[C@@]2(O1)CC[C@@H](C(O2)C(C)C)C)/C)O)C	869	Yes
1877	LL-F 28249lambda	CO[C@@H]1C(=CC2[C@]3(C1OC/C/3=C\C=C\[C@H](C)C/C(=C/CC1CC(OC2=O)CC2(O1)C[C@H](O)[C@@H]([C@H](O2)/C(=C/C(C)C)/C)C)/C)O)C	870	Yes
1878	LL-F 28249gamma	CO[C@@H]1C(=CC2[C@]3(C1OC/C/3=C\C=C\[C@H](C)C/C(=C/CC1CC(OC2=O)CC2(O1)C[C@H](O)[C@@H]([C@H](O2)/C(=C/C)/C)C)/C)O)C	871	Yes
1879	LL-F 28249beta	C/C=C(/[C@H]1OC2(CC3CC(O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/[C@]4(C(C(=O)O3)C=C(C)[C@H](C4OC2)O)O)C[C@@H]([C@@H]1C)O)\C	872	Yes
1880	Nemadectin	CC(/C=C(/[C@H]1OC2(CC3CC(O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/[C@]4(C(C(=O)O3)C=C(C)[C@H](C4OC2)O)O)C[C@@H]([C@@H]1C)O)\C)C	872	No
1881	13alpha-Hydroxy milbemycin beta11	O[C@@H]1/C(=C/C[C@@H]2C[C@H](OC(=O)[C@H]3[C@@](/C(=C/C=C/[C@@H]1C)/C)(O)[C@H](O)[C@H](O)C(=C3)C)C[C@@]1(O2)CC[C@@H]([C@H](O1)C)C)/C	873	Yes
1882	Aplasmomycin	[B-]123O[C@]45O[C@H](C([C@@H](C/C=C/[C@H]6O[C@@H]([C@H](C6)OC(=O)[C@H](O1)[C@]7(O2)O[C@H](C([C@@H](C/C=C/[C@H]8O[C@@H]([C@H](C8)OC(=O)[C@@H]4O3)C)O)(C)C)CC[C@H]7C)C)O)(C)C)CC[C@H]5C.[Na+]	874	Yes
1883	Lucensimycin A	OC(=O)/C=C/C=C/C=C/C1CC2C=CC3C(C2(C(=O)C21C(=O)OC(=C)C2=O)C)CC(C(C3O)C)OC(=O)C	875	Yes
1884	Lucensimycin B	OCC1OC(=O)C2(C1=O)C(/C=C/C=C/C=C/C(=O)O)CC1C(C2=O)(C)C2CC(OC(=O)C)C(C(C2C=C1)O)C	875	No
1885	Soraphen A	CO[C@@H]1/C=C/[C@H](C)C2O[C@](O)([C@H](C)C(=O)O[C@@H](CCCC[C@@H]1OC)c1ccccc1)[C@@H]([C@H]([C@@H]2C)O)OC	876	Yes
1886	3'-O-Decarbamoylirumamycin	CCC(=O)C1(C)OC1C(CC(C1OC(=O)CC2(O)CC=C(C(O2)/C(=C/CCCC(/C=C/C(C(C1C)O)C)OC1CC(O)C(C(O1)C)O)/C)C)C)C	877	Yes
1887	Irumamycin	CCC(=O)C1(C)OC1C(CC(C1OC(=O)CC2(O)CC=C(C(O2)/C(=C/CCCC(/C=C/C(C(C1C)O)C)OC1OC(C)C(C(C1)OC(=O)N)O)/C)C)C)C	877	No
1888	Venturicidin A	CCC(=O)[C@H]([C@H]([C@@H](C[C@H]([C@H]1OC(=O)C[C@@]2(O)CC=C([C@H](O2)/C(=C/CCC[C@H](/C=C/[C@@H](C[C@H]1C)C)O[C@@H]1O[C@H](C)[C@H]([C@@H](C1)OC(=O)N)O)/C)C)C)O)C	878	Yes
1889	Aabomycin A1	CCC(=O)[C@H]([C@H]([C@@H](C[C@H](C1OC(=O)C[C@@]2(O)CC=C(C(O2)/C(=C/CCC[C@H](/C=C/[C@@H](C[C@H]1C)C)O[C@H]1C[C@@H](O)[C@@H]([C@H](O1)C)O)/C)C)C)O)C	879	Yes
1890	2alpha,5alpha,14beta-Triacetoxy-10-hydroxy-10alpha,18-epoxytaxa-4(20),11-diene-9-one	CC(=O)O[C@H]1CC[C@@]2([C@@H](C1=C)[C@H](OC(=O)C)[C@@H]1[C@@H](OC(=O)C)CC3=C([C@](C2=O)(O)OC3)C1(C)C)C	880	No
1891	2alpha,5alpha,14beta-Triacetoxy-9beta-hydroxytaxa-4(20),11-diene-10-one	CC(=O)O[C@H]1CC[C@@]2([C@@H](C1=C)[C@H](OC(=O)C)[C@@H]1[C@@H](OC(=O)C)CC(=C(C(=O)[C@H]2O)C1(C)C)C)C	880	Yes

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1892	2alpha,5alpha,14beta-Triacetoxy-9beta,18-dihydroxytaxa-4(20),11-diene-10-one	OCC1=C2C(=O)[C@@H](O)[C@]3([C@H]([C@@H]([C@H]([C@H](C1)OC(=O)C)C2(C)C)OC(=O)C)C(=C)[C@H](CC3)OC(=O)C)C	880	No
1893	Cochleamycin A	O[C@H]1C[C@@H]2CC(=O)/C(=C\[C@H]3[C@@H](C1)C=C[C@H]1[C@@H]3C[C@@H]([C@@H]1OC(=O)C)C)/C(=O)O2	881	Yes
1894	Cochleamycin A2	O[C@H]1C[C@@H]2CC(=O)/C(=C/[C@H]3[C@@H](C1)C=C[C@H]1[C@@H]3C[C@@H]([C@@H]1OC(=O)C(C)C)C)/C(=O)O2	881	No
1895	Cochleamycin B	CC(=O)O[C@@H]1[C@H](C)C[C@@H]2[C@H]1C=C[C@@H]1[C@H]2C[C@@]23C(C1)C[C@@H](CC2=O)OC3=O	882	Yes
1896	Cochleamycin B2	CC(C(=O)O[C@@H]1[C@H](C)C[C@@H]2[C@H]1C=C[C@@H]1[C@H]2C[C@@]23C(C1)C[C@@H](CC2=O)OC3=O)C	882	No
1897	Cyclostreptin	O[C@@H]1[C@@H](C)[C@@H](C2C1C1C(C(=C2)C)CC2C1C1=C3O[C@]2(C)CCC(OC1=O)[C@H]3C)O	883	Yes
1898	Nargenicin A1	COC1CC2C=CC3C4C2(OC3C(C(C4O)C)OC(=O)c2ccc[nH]2)C(=CC(C(OC1=O)C(O)C)C)C	884	Yes
1899	Pteridic acid G	CC[C@H]1[C@H](O)C[C@]2(O[C@@H]1C)O[C@@H]([C@H](/C=C/C=C/C(=O)OC)C)[C@H]([C@H]([C@@H]2C)O)C	885	Yes
1900	Pteridic acid F	CC[C@H]1[C@H](O)C[C@]2(O[C@@H]1C)O[C@@H]([C@H](/C=C/C=C/C(=O)O)C)[C@H]([C@H]([C@@H]2C)O)C	885	No
1901	Pteridic acid C	CC[C@H]1[C@H](O)C[C@]2(O[C@@H]1C)O[C@@H]([C@H](/C=C/C(=O)O)C)[C@H]([C@H]([C@@H]2C)O)C	885	No
1902	Pteridic acid E	OC(=O)/C=C/C=C/[C@@H]([C@@H]1O[C@@]2(C[C@@H](O)[C@@H]([C@H](O2)C)C)[C@H]([C@@H]([C@@H]1C)O)C)C	886	Yes
1903	Pteridic acid D	OC(=O)/C=C/[C@@H]([C@@H]1O[C@@]2(C[C@@H](O)[C@@H]([C@H](O2)C)C)[C@H]([C@@H]([C@@H]1C)O)C)C	886	No
1904	Hookerolide	O[C@@H]1C[C@@H]2O[C@]3(C=C[C@@H]2C)O[C@H](C/C=C/C=C(/C[C@H](C(=O)O[C@H]([C@H](C(=O)C1)C)C(C)C)C)\C)[C@@H]([C@@H]([C@@H]3C)O)C	887	Yes
1905	Ikarugamycin	CC[C@@H]1[C@H](C)C[C@H]2[C@H]1C=C[C@H]1[C@@H]2C[C@@H]2[C@@H]1C/C=C\C(=O)NCCC[C@H]1C(=O)/C(=C(\C=C\2)/O)/C(=O)N1	888	Yes
1906	Capsimycin	COC([C@@H]1[C@H](C)C[C@H]2[C@H]1[C@H]1O[C@H]1[C@H]1[C@@H]2C[C@@H]2[C@@H]1C/C=C\C(=O)NCCC[C@H]1C(=O)C(=C(/C=C\2)O)C(=O)N1)C	889	Yes
1907	28-N-Methylikarugamycin	CC[C@@H]1[C@H](C)C[C@H]2[C@H]1C=C[C@H]1[C@@H]2C[C@@H]2[C@@H]1C/C=C\C(=O)NCCC[C@H]1C(=O)C(=C(C=C2)O)C(=O)N1C	890	Yes
1908	Aburatubolactam C	CCC1CC2C(C1C)CC1C2C(=O)/C=C/C=C/C(=O)NCCCC2C(=C(C(=O)CC/C=C\1)C(=O)N2C)O	891	Yes
1909	Aburatubolactam B	CCC1CC2C(C1C)CC1C2C(=O)/C=C/C=C/C(=O)NCCC(C2C(=C(C(=O)CC/C=C\1)C(=O)N2C)O)O	892	Yes
1910	Xanthobaccin C	CC[C@H]1C[C@H]2[C@@H]([C@H]1C)[C@H]1[C@H](C2)[C@H]2C/C=C\C(=O)NCCCC3C(=O)C(=C(/C=C/[C@@H]2C[C@@H]1O)O)C(=O)N3	893	No
1911	FI-3	C=C[C@H]1C[C@H]2[C@@H]([C@H]1C)[C@H]1[C@H](C2)[C@H]2C/C=C\C(=O)NCCCC3C(=O)C(=C(/C=C/[C@@H]2C[C@@H]1O)O)C(=O)N3	893	Yes
1912	Dihydromaltophilin	CC[C@H]1C[C@H]2[C@@H]([C@H]1C)[C@H]1[C@H](C2)[C@H]2C/C=C\C(=O)NCCC(C3C(=O)C(=C(/C=C/[C@@H]2C[C@@H]1O)O)C(=O)N3)O	893	No
1913	Heat-stable antifungal factor	CC[C@H]1C[C@H]2[C@@H]([C@H]1C)[C@H]1[C@H](C2)[C@H]2C/C=C/C(=O)NCCC(C3C(=O)C(=C(/C=C/[C@@H]2C[C@@H]1O)O)C(=O)N3)O	893	No
1914	Alteramide A	CC[C@H]1C[C@H]2[C@@H]([C@H]1C)[C@H]1[C@@H](C2)/C=C\C=C/C(=O)NCC[C@@H]([C@H]2C(=O)/C(=C(\C=C/C=C\[C@@H]1O)/O)/C(=O)N2)O	893	No
1915	delta30-Dihydromaltophilin	C=C[C@H]1C[C@H]2[C@@H]([C@H]1C)[C@H]1[C@H](C2)[C@H]2C/C=C\C(=O)NCCC(C3C(=O)C(=C(/C=C/[C@@H]2C[C@@H]1O)O)C(=O)N3)O	893	No
1916	Maltophilin	CCC1CC2C(C1C)C1C(C2)C2C/C=C\C(=O)NCCC(C3C(=O)/C(=C(\C=C\C2CC1=O)/O)/C(=O)N3)O	894	Yes
1917	10-epi-HSAF	CC[C@H]1C[C@@H]2[C@H]([C@@H]1C)[C@@H]1[C@@H](C2)[C@@H]2C/C=C\C(=O)NCC[C@@H]([C@H]3C(=C(C(=O)/C=C/[C@H]2C[C@H]1O)C(=O)N3)O)O	895	Yes
1918	Capsimycin F	CO[C@@H]1[C@@H](O)[C@@H]2[C@H]3C/C=C\C(=O)NCCC[C@@H]4C(=C(C(=O)/C=C\[C@@H]3C[C@@H]2[C@@H]2[C@@H]1[C@H](CC)[C@@H](C2)C)C(=O)N4)O	895	No
1919	10-epi-Maltophilin	CC[C@H]1C[C@@H]2[C@H]([C@@H]1C)[C@@H]1[C@@H](C2)[C@@H]2C/C=C\C(=O)NCC[C@@H]([C@H]3C(=C(C(=O)/C=C/[C@H]2CC1=O)C(=O)N3)O)O	895	No
1920	10-epi-FI-2	CC[C@H]1C[C@@H]2[C@@]([C@@H]1C)(O)[C@@H]1[C@@H](C2)[C@@H]2C/C=C\C(=O)NCCC[C@H]3C(=C(C(=O)/C=C/[C@H]2CC1=O)C(=O)N3)O	895	No
1921	6-epi-Alteramide A	CCC1CC2C([C@H]1C)[C@H]1[C@H](C2)/C=C\C=C/C(=O)NCC[C@@H](C2C(=C(C(=O)/C=C/C=C/[C@@H]1O)C(=O)N2)O)O	895	No
1922	6-epi-Alteramide B	CCC1CC2C([C@H]1C)[C@H]1[C@H](C2)/C=C\C=C/C(=O)NCCCC2C(=C(C(=O)/C=C/C=C/[C@@H]1O)C(=O)N2)O	895	No
1923	Capsimycin G	O=C1NCCC[C@H]2NC(=O)C(=C2O)C(=O)/C=C\[C@H]2[C@H](C/C=C\1)[C@@H]1[C@H](C2)[C@H]2C[C@H]([C@H]([C@@H]2[C@@H]2[C@H]1O2)[C@@H](O)C)C	895	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1924	Capsimycin B	CC[C@@H]1[C@H](C)C[C@H]2[C@H]1[C@H]1O[C@H]1[C@H]1[C@@H]2C[C@@H]2[C@@H]1C/C=C\C(=O)NCCC[C@@H]1C(=C(C(=O)/C=C\2)C(=O)N1)O	895	No
1925	10-epi-deOH-HSAF	CC[C@H]1C[C@@H]2[C@H]([C@@H]1C)[C@@H]1[C@@H](C2)[C@@H]2C/C=C\C(=O)NCCC[C@H]3C(=C(C(=O)/C=C/[C@H]2C[C@H]1O)C(=O)N3)O	896	Yes
1926	10-epi-Hydroxymaltophilin	CC[C@H]1C[C@@H]2[C@@]([C@@H]1C)(O)[C@@H]1[C@@H](C2)[C@@H]2C/C=C\C(=O)NCC[C@@H]([C@H]3C(=C(C(=O)/C=C/[C@H]2CC1=O)C(=O)N3)O)O	897	Yes
1927	Ikarugamycin epoxide	COC(C1C(C)CC2C3C1C1OC1C2C1C(C3)C=CC(=O)C2=C(O)C(NC2=O)CCCNC(=O)C=CC1)C	898	Yes
1928	Capsimycin C	CC[C@@H]1[C@H](C)C[C@H]2[C@H]1[C@H](O)[C@H]([C@H]1[C@@H]2C[C@@H]2[C@@H]1C/C=C\C(=O)NCCC[C@@H]1C(=C(C(=O)/C=C\2)C(=O)N1)O)O	899	Yes
1929	Indotertine B	O=CN1c2ccccc2[C@@]2([C@H]1C=C1CC[C@@H]3[C@]([C@H]1C2)(C)CCCC3(C)C)C[C@@H]1NC(=O)[C@@H](N(C1=O)C)C(C)C	900	Yes
1930	Carmabin A	C#CCCCCC(CC(C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N)Cc1ccc(cc1)OC)C)C)C)C)Cc1ccccc1)C)C)C	901	Yes
1931	Provipeptide A	CC(C[C@@H]1NC(=O)[C@@H]2CCCN2C(=O)[C@@H](NC(=O)[C@@H]2N(C1=O)CCC2)Cc1ccccc1)C	902	Yes
1932	Provipeptide B	CCC(C1NC(=O)C2CCCN2C(=O)C(NC(=O)C2N(C1=O)CCC2)Cc1ccccc1)C	902	No
1933	Aspergilazine A	O=C1N[C@@H](Cc2c[nH]c3c2ccc(c3)n2cc(c3c2cccc3)C[C@@H]2NC(=O)[C@H]3N(C2=O)CCC3)C(=O)N2[C@H]1CCC2	903	Yes
1934	Naseseazine A	O=C1N[C@H](Cc2c[nH]c3c2ccc(c3)[C@@]23C[C@H]4N([C@@H]2Nc2c3cccc2)C(=O)[C@@H]2N(C4=O)CCC2)C(=O)N2[C@@H]1CCC2	903	No
1935	(-)-Lansai B	C=CC(c1ccc2c(c1)[C@]1(C)C[C@@H]3N([C@@H]1N2C)C(=O)[C@H]1N(C3=O)[C@@H]2N(C)c3c([C@@]2(C1)C)cccc3)(C)C	904	Yes
1936	(+)-Nocardioazine B	CC(=CC[C@]12C[C@@H]3N([C@@H]2N(c2c1cccc2)C)C(=O)[C@H]1N(C3=O)[C@H]2Nc3c([C@]2(C1)C)cccc3)C	904	No
1937	Drimentine H	O=CN1c2ccccc2[C@]2([C@@H]1N1C(=O)[C@H](C(C)C)N(C(=O)[C@@H]1C2)C)C[C@H]1C(=C)CC[C@@H]2[C@]1(C)CCCC2(C)C	905	No
1938	Drimentine F	O=C1N(C)[C@@H](C(C)C)C(=O)N2[C@H]1CC1([C@H]2Nc2c1cccc2)C[C@H]1C(=C)CC[C@@H]2[C@]1(C)CCCC2(C)C	905	Yes
1939	Drimentine C	O=C1N2CCC[C@H]2C(=O)N2[C@H]1C[C@@]1([C@H]2Nc2c1cccc2)C[C@H]1C(=C)CC[C@@H]2[C@]1(C)CCCC2(C)C	905	No
1940	Drimentine G	CC([C@@H]1NC(=O)[C@H]2N(C1=O)[C@@H]1Nc3c(C1(C2)C[C@H]1C(=C)CC[C@@H]2[C@]1(C)CCCC2(C)C)cccc3)C	905	No
1941	Drimentine I	CC([C@@H]1N(C)C(=O)[C@H]2N(C1=O)[C@@H]1N3c4c([C@@]1(C2)C[C@H]1[C@@]3(C)CC[C@@H]2[C@]1(C)CCCC2(C)C)cccc4)C	905	No
1942	C12177	CO[C@@H]1/C=C/C=C(\C)/Cc2cc(NC(=O)C[C@@H](/C(=C/[C@@H]([C@H](CC1=O)O)C)/C)O)cc(c2)O	906	Yes
1943	Ansatrienol J	CO[C@H]1CC(=O)Nc2cc(CC/C=C(\[C@H]([C@H](C(=O)/C=C\C=C/C=C\[C@@H]1O)C)O)/C)cc(c2)O	907	Yes
1944	17-Demethoxy-reblastatin	C[C@@H]1Cc2cc(cc(c2)O)NC(=O)/C(=C/CC[C@@H]([C@H](/C(=C/[C@@H]([C@H]([C@H](C1)O)O)C)/C)O)C)/C	908	Yes
1945	17-Demethoxy-15-hydroxylreblastatin	Oc1cc2NC(=O)/C(=C/CC[C@H](C)[C@H](/C(=C/[C@@H]([C@H]([C@H](C[C@@H]([C@H](c(c1)c2)O)C)O)O)O)C)/C)O)/C	909	Yes
1946	Ansatrienol I	CO[C@@H]1/C=C\C=C/C(O)C(O)C[C@@H](O)[C@H](C)[C@@H](/C(=C\CCc2cc(NC(=O)C1)cc(c2)O)/C)O	910	Yes
1947	Mycotrienol II	CO[C@H]1/C=C\C=C/C=C\C[C@H](O)[C@H](C)[C@H](/C(=C\CCc2c(c(NC(=O)C1)cc(O)c2)O)/C)O	911	Yes
1948	3-O-Demethyltrienomycinol	O[C@@H]1/C=C\C=C/C=C\C[C@@H](O)[C@H](C)[C@@H](/C(=C\CCc2cc(NC(=O)C1)cc(c2)O)/C)O	912	Yes
1949	Trienomycinol	COC1/C=C\C=C/C=C\CC(O)C(C)C(/C(=C\CCc2cc(NC(=O)C1)cc(c2)O)/C)O	912	No
1950	Ansatrienol K	O[C@H]1/C=C/C=C/C[C@H](O)[C@H](C)[C@@H](O)/C(=C\CCc2cc(NC(=O)C1)cc(c2)O)/C	913	Yes
1951	Acyl-desferrioxamine	NCCCCCN(C(=O)CCC(=O)NCCCCCN(C(=O)CCC(=O)NCCCCCN(C(=O)CCCC[C@H](CC)C)O)O)O	914	Yes
1952	3-Chloro-6, 8-dihydroxy-8-alpha-lapachone	Oc1cc(O)c2c(c1)C(=O)[C@@]1(C(C2=O)C[C@H](C(O1)(C)C)O)C[C@@H]1[C@@](C)(O)CC[C@@H](C1(C)C)Cl	915	Yes
1953	MDN-0170	Oc1cc(O)c2c(c1)C(=O)[C@]1(C(=C[C@@H](C(O1)(C)C)O)C2=O)C[C@@H]1[C@@](C)(O)CC[C@@H](C1(C)C)Cl	915	No
1954	27-Oxomilbemycin alpha 31	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](O2)C/C=C(\C)/C[C@@H](C)/C=C/C=C\2/c3c(C(=O)O1)cc(C)c(c3OC2=O)O	916	Yes
1955	13alpha-O-alpha-L-Oleandrosyl-25-ethyl milbemycin beta3	CO[C@H]1CC(O)[C@H](OC1C[C@H]1/C(=C/C[C@H]2CC(OC(=O)c3c(/C(=C/C=C/[C@H]1C)/C)cc(O)c(c3)C)C[C@]1(O2)CC[C@H]([C@@H](O1)CC)C)/C)C	917	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1956	13alpha-O-alpha-L-Oleandrosyl milbemycin beta3	CO[C@H]1CC(O)[C@H](OC1C[C@@H]1[C@H](C)/C=C/C=C(\C)/c2cc(O)c(cc2C(=O)OC2C[C@H](C/C=C/1\C)O[C@@]1(C2)CC[C@H]([C@@H](O1)C)C)C)C	917	Yes
1957	13alpha-O-alpha-L-Oleandrosyl-25-isopropyl milbemycin beta3	CO[C@H]1CC(O)[C@H](OC1C[C@H]1/C(=C/C[C@H]2CC(OC(=O)c3c(/C(=C/C=C/[C@H]1C)/C)cc(O)c(c3)C)C[C@]1(O2)CC[C@H]([C@@H](O1)C(C)C)C)/C)C	917	No
1958	13-alpha-Hydroxy milbemycin beta-3	O[C@@H]1/C(=C/C[C@@H]2C[C@H](OC(=O)c3c(/C(=C/C=C/[C@@H]1C)/C)cc(O)c(c3)C)C[C@@]1(O2)CC[C@@H]([C@H](O1)C)C)/C	918	No
1959	13-alpha-Hydroxy-25-ethy1 milbemycin beta-3	CC[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@H](O2)C/C=C(\C)/[C@@H](O)[C@@H](C)/C=C/C=C(/c2c(C(=O)O1)cc(C)c(c2)O)\C	918	Yes
1960	13-alpha-Hydroxy-4-ethy1 milbemycin beta-3	CCc1cc2C(=O)O[C@H]3C[C@@H](C/C=C(/[C@H]([C@H](/C=C/C=C(/c2cc1O)\C)C)O)\C)O[C@]1(C3)CC[C@@H]([C@H](O1)C)C	918	No
1961	Complestatin B	Oc1ccc(cc1)C(C(=O)O)NC(=O)C1Cc2ccc(cc2)Oc2cc3C(C(=O)NC(C(=O)N1C)c1cc(Cl)c(c(c1)Cl)O)NC(=O)C(NC(=O)C(NC(=O)C(=O)c1cc(Cl)c(c(c1)Cl)O)CC1(c4ccc(c(c2O)c3)cc4NC1=O)O)c1cc(Cl)c(c(c1)Cl)O	919	Yes
1962	Complestatin A	Oc1ccc(cc1)C(C(=O)O)NC(=O)C1Cc2ccc(cc2)Oc2cc3C(C(=O)NC(C(=O)N1C)c1cc(Cl)c(c(c1)Cl)O)NC(=O)C(NC(=O)C(CC1c4ccc(c(c2O)c3)cc4NC1=O)NC(=O)C(=O)c1cc(Cl)c(c(c1)Cl)O)c1cc(Cl)c(c(c1)Cl)O	920	Yes
1963	Complestatin M55	Oc1ccc(cc1)[C@H](C(=O)O)NC(=O)[C@@H]1Cc2ccc(cc2)Oc2cc([C@H](C(=O)N[C@@H](C(=O)N1C)c1cc(Cl)c(c(c1)Cl)O)NC(=O)[C@H](c1cc(Cl)c(c(c1)Cl)O)NC(=O)[C@H](Cc1c[nH]c3c1cccc3)NC(=O)C(=O)c1cc(Cl)c(c(c1)Cl)O)ccc2O	921	Yes
1964	Complestatin S56	Oc1ccc(cc1)[C@H](C(=O)N[C@@H](C(=O)N([C@H](C(=O)N[C@H](c1ccc(cc1)O)C(=O)O)Cc1ccc(cc1)O)C)c1cc(Cl)c(c(c1)Cl)O)NC(=O)[C@H](c1cc(Cl)c(c(c1)Cl)O)NC(=O)[C@H](Cc1c[nH]c2c1cccc2)NC(=O)C(=O)c1cc(Cl)c(c(c1)Cl)O	922	Yes
1965	Isocomplestatin	Oc1ccc(cc1)[C@H](C(=O)O)NC(=O)[C@@H]1Cc2ccc(cc2)Oc2cc3[C@H](C(=O)N[C@@H](C(=O)N1C)c1cc(Cl)c(c(c1)Cl)O)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C(=O)c1cc(Cl)c(c(c1)Cl)O)Cc1c4ccc(c(c2O)c3)cc4[nH]c1)c1cc(Cl)c(c(c1)Cl)O	923	Yes
1966	Complestatin	Oc1ccc(cc1)[C@H](C(=O)O)NC(=O)[C@@H]1Cc2ccc(cc2)Oc2cc3[C@H](C(=O)N[C@@H](C(=O)N1C)c1cc(Cl)c(c(c1)Cl)O)NC(=O)[C@H](NC(=O)[C@H](NC(=O)C(=O)c1cc(Cl)c(c(c1)Cl)O)Cc1c4ccc(c(c2O)c3)cc4[nH]c1)c1cc(Cl)c(c(c1)Cl)O	924	Yes
1967	Chloropeptin I	Oc1ccc(cc1)C(C(=O)O)NC(=O)C1Cc2ccc(cc2)Oc2cc3C(C(=O)NC(C(=O)N1C)c1cc(Cl)c(c(c1)Cl)O)NC(=O)C(NC(=O)C(NC(=O)C(=O)c1cc(Cl)c(c(c1)Cl)O)Cc1c4c(c(c(c2O)c3)ccc4)[nH]c1)c1cc(Cl)c(c(c1)Cl)O	925	Yes
1968	Geralcin C	CCCCCC[N+](=NC(CO)C(=O)N(/C=C\\CCCC)NC(=O)C)[O-]	926	Yes
1969	FL-120A	CC(C)C(=O)O[C@]1([C@@H]([C@H](C2=C([C@H]1OC(=O)C)C(=[N+]=[N-])C3=C2C(=O)C4=C(C3=O)C(=CC=C4)O)O)OC(=O)C)C	927	Yes
1970	L-Rhodinose-L-rhodinose-2-deoxy-L-fucose -beta-rhodomycinone	CC[C@@]1(O)CC(OC2CC(O)C(C(O2)C)OC2CCC(C(O2)C)OC2CCCC(O2)C)C2=C(O)C3C(C(=C2C1)O)C(=O)c1c(C3=O)c(O)ccc1	928	No
1971	L-Rhodinose-L-rhodinose-L-rhodinose-L-rhodinose-beta-rhodomycinone	CC[C@@]1(O)CC(OC2CC(O)C(C(O2)C)OC2CCC(C(O2)C)OC2CCC(C(O2)C)OC2CCC(C(O2)C)O)C2=C(O)C3C(C(=C2C1O)O)C(=O)c1c(C3=O)c(O)ccc1	928	No
1972	L-Rhodinose-2-deoxy-L-fucose-L-rhodinose-epsilon-rhodomycinone	COC(=O)C1C2=C(O)C3C(C(=C2C(C[C@]1(O)CC)OC1CCC(C(O1)C)OC1CC(O)C(C(O1)C)OC1CCC(C(O1)C)O)O)C(=O)c1c(C3=O)cccc1O	928	No
1973	L-Rhodinose-2-deoxy-L-fucose-L-rhodinose-beta-rhodomycinone	OCC1C2=C(O)C3C(C(=C2C(C[C@]1(O)CC)OC1CCC(C(O1)C)OC1CC(O)C(C(O1)C)OC1CCC(C(O1)C)O)O)C(=O)c1c(C3=O)cccc1O	928	No
1974	L-Cinerulose-2-deoxy-L-fucose- L-rhodinose-beta-rhodomycinone	CC[C@@]1(O)CC(OC2CCC(C(O2)C)OC2CC(O)C(C(O2)C)OC2CCC(=O)C(O2)C)C2=C(O)C3C(C(=C2C1O)O)C(=O)c1c(C3=O)c(O)ccc1	928	Yes
1975	Deoxycosmomycin C	CC[C@@]1(O)C[C@H](OC2OC(C)C(C(C2)N(C)C)OC2CCC(C(O2)C)OC2CCC(C(O2)C)O)C2=C(O)C3C(C(=C2[C@H]1OC1OC(C)C(C(C1)N(C)C)OC1CCC(C(O1)C)OC1CCC(C(O1)C)O)O)C(=O)c1c(C3=O)c(O)ccc1	929	Yes
1976	A-83094A	CC/C(=C\C=C\[C@H]1C=C[C@H]2[C@H]([C@@H]1C(=O)c1ccc[nH]1)CCC2)/[C@@H]1O[C@H](CC[C@@H]1C)[C@H](C(=O)O)C	930	Yes
1977	16-Deethylindanomycin methyl ester	CC/C(=C\C=C\C1C=C[C@@H]2[C@@H]([C@H]1C(=O)c1ccc[nH]1)CCC2)/C1O[C@@H](CC[C@H]1C)[C@H](C(=O)OC)C	930	No
1978	16-Deethylindanomycin	CC/C(=C\C=C\[C@H]1C=CC2C([C@@H]1C(=O)c1ccc[nH]1)CCC2)/[C@@H]1OC(CC[C@@H]1C)[C@H](C(=O)O)C	930	No

Comp No[a]	Name	SMILES[b]	Cluster No[c]	Rep[d]
1979	Antibiotic X 14547	CC/C(=C\C=C\[C@H]1C=CC2C([C@@H]1C(=O)c1[nH]ccc1)CC[C@@H]2CC)/[C@@H]1OC(CC[C@@H]1C)[C@H](C(=O)O)C	930	No
1980	66513-28-8	CC/C(=C\C=C/[C@@H]1C=C[C@H]2[C@H]([C@@H]1C(=O)c1[nH]ccc1)CC[C@@H]2CC)/[C@@H]1O[C@H](CC[C@@H]1C)[C@H](C(=O)O)C	930	No
1981	Auroramycin aglycon	CC(C/C/1=C/C(=C/C=C/C=C/[C@@](C)(O)[C@@H](O)/C=C\C=C\C(=C\C=C\C(=C\C[C@@H](NC1=O)C)\C)\C)/C)C	931	Yes

[a]Compound names; [b]The simplified molecular-input line-entry system (SMILES); [c]Cluster number according to *Flexophore* descriptor; [d]Representative compound within each cluster.