

Deciphering Molecular Aspects of Potential α -Glucosidase Inhibitors within *Aspergillus terreus*: A Computational Odyssey

Supporting data

Table S1. Designated chemical library of *Aspergillus terreus*-isolated metabolites

Compound name; Isomeric SMILES	Ligand Code	MW	TPSA
2<i>R</i>-(<i>-</i>)-6-hydroxymellein O=C1C2=C(C=C(O)C=C2O)C[C@@H](C)O1	SK-001	194.19	66.76
(<i>-</i>)-(3<i>R</i>)-6-methoxymellein O=C1C2=C(C=C(OC)C=C2O)C[C@@H](C)O1	SK-002	208.21	55.77
6-(4'-hydroxy-2'-methyl phenoxy)-(<i>-</i>)-(3<i>R</i>)-mellein O=C1C2=C(C=C(OC3=CC=C(O)C=C3C)C=C2O)C[C@@H](C)O1	SK-003	300.31	76.00
(3<i>R</i>,4<i>R</i>)-6,7-dimethoxy-4-hydroxymellein O=C1C2=C(C=C(OC)C(OC)=C2O)[C@@H](O)[C@@H](C)O1	SK-004	254.24	85.23
Asperterrestide B O=C([C@@H]([C@@H](O)C1=CC=CC=C1)N(C)C([C@@H](C(C)C)NC([C@@H](C)N2)=O)=O)NC3=CC=CC=C3C2=O	SK-005	466.54	127.83
Asperterrestide A O=C([C@@H]([C@@H](O)C1=CC=CC=C1)N(C)C([C@@H](C(CC)C)NC([C@@H](C)N2)=O)=O)NC3=CC=CC=C3C2=O	SK-006	480.56	127.83
Arisugasin H CC(O[C@@H]1C[C@H](O)[C@]2(C)[C@@]3(O)CC4=C(C=C(C5=CC=C(OC)C=C5)OC4=O)O[C@]3(C)CC[C@@]2(O)C1(C)C)=O	SK-007	526.60	135.67
Arisugasin D CC(O[C@@H]1CC[C@]2(C)[C@@]3(O)CC4=C(C=C(C5=CC=C(OC)C=C5)OC4=O)O[C@]3(C)CC[C@@]2(O)C1(C)C)=O	SK-008	512.60	115.44
Terretrione B O=C(C(C(C)C)N(C)C(C1CC2=CC=CC=C2)=O)N(C)C1=O	SK-009	302.37	57.69
Terretrione C O=C(C(C(CC)C)N(C)C(C1CC2=CC=CC=C2)=O)N(C)C1=O	SK-010	316.40	57.69
1-methyl emodin O=C1C2=C(C=C(C)C=C2OC)C(C3=CC(O)=CC(O)=C13)=O	SK-011	284.27	83.83
Aspernolide A O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC(CCC(C)(C)O4)=C4C=C3)OC2=O)OC	SK-012	424.45	102.30
Aspernolide F O=C([C@](C(C1=CC=C(O)C=C1)=C2OCC)(CC3=CC=C(O)C(C/C=C(C)\C)=C3)OC2=O) OC	SK-013	452.50	102.30
Aspernolide B CC(C)(CCC1=C(C=CC(=C1)C[C@@]2(C(=C(C(=O)O2)O)C3=CC=C(C=C3)O)C(=O)OC) O)O	SK-014	442.46	133.52
Aspernolide C CC(C)(CCC1=C(C=CC(=C1)C[C@@]2(C(=C(C(=O)O2)O)C3=CC=C(C=C3)O)C(=O)OC) O)OC	SK-015	456.49	122.53
Aspernolide E O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC(C=CC(C)(C)O4)=C4C=C3)OC2=O)OC	SK-016	422.43	102.30
Aspernolide G O=C([C@](C(C1=CC=C(O)C=C1)=C2OCC)(CC3=CC=C(O)C[C@H](O)C(C)(O)C)=C3)OC2=O)OC	SK-017	486.52	142.76
1,8-dihydroxy-3-methoxy-6-methylanthracene-9,10-dione O=C1C2=C(C=C(C)C=C2O)C(C3=CC(OC)=CC(O)=C13)=O	SK-018	284.27	83.83
Methyl, 6-acetyl-4-methoxy-5,8-dihydroxynaphthalene-2-carboxylate O=C(C1=CC(OC)=C2C(O)=C(C(C)=O)C=C(O)C2=C1)OC	SK-019	290.27	93.07
Methyl, 6-acetyl-4- methoxy-5,7,8-trihydroxynaphthalene-2-carboxylate O=C(C1=CC(OC)=C2C(O)=C(C(C)=O)C(O)=C(O)C2=C1)OC	SK-020	306.27	113.29

Stigmasta-4,6,8(14), 22-tetraen-3-one	SK-021	406.65	17.07
<chem>CC[C@@H](C(C)C)/C=C/[C@@H](C)[C@H]1CCC2=C3C=CC4=CC(CC[C@]4(C)[C@@]3([H]))CC[C@]12C=O</chem>			
Stigmast-4-ene-3-one	SK-022	412.70	17.07
<chem>CC[C@@H](C(C)C)CC[C@@H](C)[C@H]1CC[C@@]2([H])[C@]3([H])CCC4=CC(CC[C@]4(C)[C@@]3([H]))CC[C@]12C=O</chem>			
(22E,24R)-stigmasta-5,7,22-trien-3-beta-ol	SK-023	410.69	20.23
<chem>CC[C@H](C(C)C)/C=C/[C@@H](C)[C@H]1CC[C@@]2([H])C3=CC=C4C[C@@H](O)CC[C@]4(C)[C@@]3([H])CC[C@]12C</chem>			
(S)-6, 8-dimethoxy-3-methylisochroman-1-one	SK-024	222.24	44.77
<chem>O=C1O[C@@H](C)CC2=C1C(OC)=CC(OC)=C2</chem>			
Lovastatin	SK-025	404.55	72.84
<chem>CC[C@H](C)C(O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@H](C)[C@@H](O)C3)OC3=O)[C@@]12[H])=O</chem>			
3-hydroxy-5-[[4-hydroxy-3-(3-methyl-2-buten-1-yl)phenyl]methyl]-4-(4-hydroxyphenyl)- 2(5H)-furanone	SK-026	366.41	86.99
<chem>O=C1OC(CC2=CC=C(O)C(C/C=C(C)\C)=C2)C(C3=CC=C(O)C=C3)=C1O</chem>			
Aspergillamide A	SK-027	474.61	94.60
<chem>CC(C)C[C@H](NC(C)=O)C(N([C@@H](CC1=CC=CC=C1)C(N/C=C\C2=CNC3=C2C=CC=C3)=O)C)=O</chem>			
Aspergillamide B	SK-028	474.61	94.30
<chem>CC(C)C[C@H](NC(C)=O)C(N([C@@H](CC1=CC=CC=C1)C(N/C=C/C2=CNC3=C2C=CC=C3)=O)C)=O</chem>			
Aspergillamide C	SK-029	490.60	114.52
<chem>CC[C@H](C)[C@H](NC(C)=O)C(N([C@@H](CC1=CC=C(O)C=C1)C(N/C=C\C2=CNC3=C2C=CC=C3)=O)C)=O</chem>			
Aspergillamide D	SK-030	490.60	114.52
<chem>CC[C@H](C)[C@H](NC(C)=O)C(N([C@@H](CC1=CC=C(O)C=C1)C(N/C=C/C2=CNC3=C2C=CC=C3)=O)C)=O</chem>			
Methyl, 2-(3-formyl-4-hydroxybenzyl)-4-hydroxy-3-(4-hydroxyphenyl)-5-oxo-2,5-dihydrofuran-2-carboxylate	SK-031	384.34	130.37
<chem>O=C1OC(CC2=CC=C(O)C(C=O)=C2)(C(OC)=O)C(C3=CC=C(O)C=C3)=C1O</chem>			
Methyl, 3,4,5-trimethoxy-2-(2- (nicotinamido)benzamido) benzoate	SK-032	465.46	125.09
<chem>O=C(OC)C1=CC(OC)=C(OC)C(OC)=C1NC(C2=CC=CC=C2NC(C3=CN=CC=C3)=O)=O</chem>			
Kigelin	SK-033	238.24	65.00
<chem>O=C1C2=C(C=C(OC)C(OC)=C2O)C[C@@H](C)O1</chem>			
Questin	SK-034	284.27	83.83
<chem>O=C1C2=C(C=C(O)C=C2OC)C(C3=CC(C)=CC(O)=C13)=O</chem>			
5-[(3,4-dihydro-2,2-dimethyl-2H-1-benzopyran-6-yl)- methyl]-3-hydroxy-4-(4-hydroxyphenyl)-2(5H)-furanone	SK-035	366.41	76.00
<chem>O=C1OC(CC2=CC=C3C(CCC(C)(C)O3)=C2)C(C4=CC=C(O)C=C4)=C1O</chem>			
4-(4-hydroxyphenyl)-5- (4-hydroxyphenylmethyl)-2-hydroxyfuran-2-one	SK-036	284.31	69.92
<chem>OC1OC(CC2=CC=C(O)C=C2)C(C3=CC=C(O)C=C3)=C1</chem>			

Butyrolactone I O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC=C(O)C(C/C=C(C)\C)=C3)OC2=O)OC	SK-037	424.4	113.29
Butyrolactone II O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC=C(O)C=C3)OC2=O)OC	SK-038	356.33	113.29
Isobutyrolactone II CO[C@]1(C(=C(C(=O)O1)O)C2=CC=C(C=C2)O)CC3=CC=C(C=C3)O	SK-039	328.32	96.22
4-O-Demethylisobutyrolactone II C1=CC(=CC=C1C[C@@]2(C(=C(C(=O)O2)O)C3=CC=C(C=C3)O)O)O	SK-040	314.29	107.22
Butyrolactone III O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC=C(O)C(CC4OC4(C)C)=C3)OC2=O)OC	SK-041	440.45	125.82
Butyrolactone IV CC(C)([C@H]1CC2=C(O1)C=CC(=C2)C[C@@]3(C(=C(C(=O)O3)O)C4=CC=C(C=C4)O)C(=O)OC)O	SK-042	440.45	122.53
Butyrolactone V CC1([C@H](CC2=C(O1)C=CC(=C2)C[C@@]3(C(=C(C(=O)O3)O)C4=CC=C(C=C4)O)C(=O)OC)O)C	SK-043	440.45	122.53
Butyrolactone VI O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC=C(O)C(C[C@H](O)C(C)(O)C)=C3)OC2=O)OC	SK-044	458.46	153.75
Butyrolactone VII CCOC(=O)[C@]1(C(=C(C(=O)O1)O)C2=CC=C(C=C2)O)CC3=CC(=C(C=C3)O)CC=C(C)C	SK-045	438.48	113.29
Butyrolactone VIII CC(=CCC1=C(C=CC(=C1)CC2=C(C(OC2=O)(C(=O)OC)O)C3=CC=C(C=C3)O)O)C	SK-046	424.45	113.29
Emodin O=C1C2=C(C=C(C)C=C2O)C(C3=CC(O)=CC(O)=C13)=O	SK-047	270.24	94.83
Camptothecin O=C1C2=C(C=C(O)C=C2OC)C(C3=CC(C)=CC(O)=C13)=O	SK-048	284.27	83.83
Terremide A O=C(OC)C1=CC=CC(O)=C1NC(C2=CC=CC=C2NC(C3=CC=CN=C3)=O)=O	SK-049	391.38	117.62
Terremide B O=C(OC)C1=CC=CC(O)=C1N2C(C3=CC=CN=C3)=NC4=C(C=CC=C4)C2=O	SK-050	373.37	94.32
Terremide C O=C(OC)C1=CC(OC)=C(OC)C(OC)=C1N2C(C3=CC=CN=C3)=NC4=C(C=CC=C4)C2=O	SK-051	447.45	101.80
Terrelactone A O=C([C@](C(C1=CC=C(OC)C=C1)=C2O)(CC3=CC(C/C=C(C)\C)=C(O)C(OC)=C3)OC2=O)OC	SK-052	468.50	111.53
Aspulvinone B O=C(C(C1=CC(CCC(C)(C)O2)=C2C=C1)=C/3O)OC3=C/C4=CC=C(O)C(C/C=C(C)\C)=C4	SK-053	432.52	79.90
Aspulvinone C CC1(CCC2=CC(=C(C=C2O1)O)/C=C\3/C(=C(C(=O)O3)C4=CC5=C(C=C4)OC(CC5)(C)C)O)C	SK-054	448.51	89.14
Aspulvinone E O=C(C(C1=CC=C(O)C=C1)=C/2O)OC2=C/C3=CC=C(O)C=C3	SK-055	296.28	90.89
Aspulvinone D CC(=CCC1=C(C=CC(=C1)/C=C\2/C(=C(C(=O)O2)C3=C(C=C4C(=C3)CCC(O4)(C)C)O)O)O)C	SK-056	448.51	100.13
Isoaspulvinone E O=C(C(C1=CC=C(O)C=C1)=C/2O)OC2=C\C3=CC=C(O)C=C3	SK-057	296.28	90.89
Aspulvinone F	SK-058	464.51	109.36

<chem>O=C(C(C1=CC(CCC(C)(C)O2)=C2C=C1O)=C/3O)OC3=C/C4=CC5=C(OC(C(C)(O)C)C5)C=C4</chem>			
Aspulvinone G	SK-059	312.28	111.12
<chem>O=C(C(C1=CC=C(O)C=C1O)=C/2O)OC2=C/C3=CC=C(O)C=C3</chem>			
Aspulvinone H	SK-060	432.52	90.89
<chem>O=C(C(C1=CC=C(O)C(C/C=C(C)\C)=C1)=C/2O)OC2=C/C3=CC=C(O)C(C/C=C(C)\C)=C3</chem>			
Rubrolide S	SK-061	348.40	59.67
<chem>O=C(C=C/1C2=CC=C(O)C=C2)OC1=C/C3=CC(CCC(C)(C)O4)=C4C=C3</chem>			
Rubrolide R	SK-062	348.40	70.67
<chem>O=C(C=C/1C2=CC=C(O)C=C2)OC1=C/C3=CC=C(O)C(C/C=C(C)\C)=C3</chem>			
Aspulvinone R	SK-063	466.53	131.35
<chem>O=C(C(C1=CC(CCC(C)(O)C)=C(O)C=C1O)=C/2O)OC2=C/C3=CC=C(O)C(C/C=C(C)\C)=C3</chem>			
Aspulvinone V	SK-064	498.62	79.90
<chem>O=C(C(C1=CC(C=CC(C)(C)O2)=C2C(C/C=C(C)\C)=C1)=C/3O)OC3=C/C4=CC=C(O)C(C/C=C(C)\C)=C4</chem>			
Aspulvinone W	SK-065	448.51	100.13
<chem>O=C(C(C1=CC(C/C=C(C)/C)=C(O)C=C1)=C/2O)OC2=C/C3=CC=C(CC(C(C)(C)O)O4)C4=C3</chem>			
Aspulvinone X	SK-066	448.51	89.14
<chem>O=C(C(C1=CC(CCC(C)(C)O2)=C2C=C1)=C/3O)OC3=C/C4=CC=C(CC(C(C)(C)O)O5)C5=C4</chem>			
Kodaistatin A	SK-067	630.65	202.79
<chem>O=C(C(C1=CC(O)=C(O)C=C1C2=C(CC(/C=C/C(C)=C/C(C)CC)=O)C(C(O)C2(C(C)=O)O)=O)=C/3O)OC3=C/C4=CC=C(O)C=C4</chem>			
Kodaistatin C	SK-068	646.64	223.02
<chem>O=C(C(C1=CC(O)=C(O)C=C1C2=C(CC(/C=C/C(C)=C/C(C)CC)=O)C(C(O)C2(C(C)=O)O)=O)=C/3O)OC3=C/C4=CC=C(O)C(O)=C4</chem>			
Versicolactone G	SK-069	440.49	102.30
<chem>O=C([C@](C(C1=CC=CC=C1)=C2O)(CC3=CC=C(O)C(CCC(C)(OC)C)=C3)OC2=O)OC</chem>			
(+)-Terrein	SK-070	154.16	57.53
<chem>O=C1C=C/C=C/C/[C@H](O)[C@H]1O</chem>			
Butyrolactone I, 2-sulfate	SK-071	504.51	156.67
<chem>O=C([C@](C(C1=CC=C(O)C=C1)=C2OS(=O)(O)=O)(CC3=CC=C(O)C(C/C=C(C)\C)=C3)OC2=O)OC</chem>			
Butyrolactone I, 4``-Sulfated	SK-072	504.51	153.51
<chem>O=C([C@](C(C1=CC=C(O)C=C1)C2=O)(CC3=CC=C(OS(=O)(O)=O)C(C/C=C(C)\C)=C3)OC2=O)OC</chem>			
7``-Hydroxybutyrolactone III	SK- 073	456.44	146.05
<chem>O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC=C(O)C(C(O)C4OC4(C)C)=C3)OC2=O)OC</chem>			
(+)-3',3'-di-(dimethylallyl)-butyrolactone II	SK- 074	492.57	113.29
<chem>CC(=CCC1=C(C=CC(=C1)C[C@@]2(C(=C(C(=O)O2)O)C3=CC(=C(C=C3)O)CC=C(C)C)C(=O)OC)O)C</chem>			
14α-hydroxyergosta-4,7,22-triene-3,6-dione	SK-075	424.62	54.37
<chem>C[C@H](C(C)C)/C=C/[C@@H](C)[C@H]1CC[C@@]2(O)C3=CC(C4=CC(CC[C@]4(C)[C@@]3([H]))CC[C@]12C)=O=O</chem>			
Asterelenin	SK-076	431.49	89.94

<chem>O=C(NC1=CC=CC=C21)[C@@]3(O)C[C@@]4(C(C=C)(C)C)C5=CC=CC=C5N(C(C)=O)[C@@]4([H])N3C2=O</chem>			
(3E,7E)-4,8-dimethylundeca-3,7-diene-1,11-diol <chem>OCC/C=C(C)/CC/C=C(C)/CCCO</chem>	SK-077	212.33	40.46
Monacolin L <chem>O=C1O[C@H](CC[C@H]2[C@@H](C)C=CC3=C[C@H](C)CC[C@]23[H])C[C@@H](O)C1</chem>	SK-078	304.43	46.53
Pulvinic acid <chem>C1=CC=C(C=C1)C2=C/C(=C/C3=CC=CC=C3)\C(=O)O/OC2=O)O</chem>	SK-079	308.28	87.74
Terrephenol A <chem>CC(=CCC1=C(C(=CC(=C1)C[C@@]2(C(=C(C(=O)O2)O)C3=CC=C(C=C3)O)C(=O)OC)OC)O)C</chem>	SK-080	454.48	122.53
Terrephenol B <chem>CC(=CCC1=C(C(=CC(=C1O)C[C@@]2(C(=C(C(=O)O2)O)C3=CC=C(C=C3)O)C(=O)OC)OC)C</chem>	SK-081	454.48	122.53
Terrephenol C <chem>O=C([C@](C(C1=CC=C(OC)C=C1)=C2O)(CC3=CC(C/C=C(C)/C)=C(O)C(OC)=C3)OC2=O)OC</chem>	SK-082	468.50	111.53
Terrenolide S <chem>CCOC1=C([C@](OC1=O)(CC2=CC=C(C=C2)O)C(=O)OC)C3=CC=C(C=C3)O</chem>	SK-083	384.38	102.30
Xenofuranone A <chem>COC1=C(C(OC1=O)CC2=CC=CC=C2)C3=CC=CC=C3</chem>	SK-084	280.32	35.54
Xenofuranone B <chem>C1=CC=C(C=C1)CC2C(=C(C(=O)O2)O)C3=CC=CC=C3</chem>	SK-085	266.30	46.53
Luteoride E <chem>O=C(OC)/C(CC1=CNC2=C1C=CC=C2C/C=C(C)\C)=N/O</chem>	SK-086	300.36	74.69
3-hydroxy-5-(4-hydroxybenzyl)-4-(4-hydroxyphenyl)furan-2(5H)-one <chem>O=C1C(O)=C(C2=CC=C(O)C=C2)C(CC3=CC=C(O)C=C3)O1</chem>	SK-087	298.29	86.99
5-[(3,4-Dihydro-2,2-dimethyl-2H-1-benzopyran-6-yl)-methyl]-3-hydroxy-4-(4-hydroxyphenyl)-2(5H)-furanone <chem>O=C1OC(CC2=CC=C3C(CCC(C)(C)O3)=C2)C(C4=CC=C(O)C=C4)=C1O</chem>	SK-088	366.41	76.00
Arisugasin A <chem>O=C1[C@]2(C)[C@@]3(O)CC4=C(C=C(C5=CC=C(OC)C(OC)=C5)OC4=O)O[C@]3(C)CC[C@@]2(O)C(C)(C)C=C1</chem>	SK-089	496.56	115.44
Terreulactone A <chem>C[C@@]12CC[C@]34[C@@]([C@]1(CC5=C(O2)C=C(OC5=O)C6=CC=C(C=C6)OC)O)(C(=O)[C@](C3(C)C)(C(=O)O4)OC)C</chem>	SK-090	510.54	121.52
Terreulactone B <chem>C[C@@]12CC[C@]3([C@@]([C@]1(CC4=C(O2)C=C(OC4=O)C5=CC=C(C=C5)OC)O)(C=CC(=O)C3(C)C)C)O</chem>	SK-091	466.53	106.21
Terreulactone C <chem>C[C@]12CCC(=O)C([C@@]1(CC[C@@]3([C@@]2(CC4=C(O3)C=C(OC4=O)C5=CC=C(C=C5)OC)O)C)O)(C)C</chem>	SK-092	468.55	103.21
Terreulactone D <chem>C[C@@]12CC[C@]3([C@@]([C@]1(CC4=C(O2)C=C(OC4=O)C5=CC(=C(C(=C5)OC)OC)OC)O)(C(=O)C=C(C3(C)C)OC)C)O</chem>	SK-093	556.61	133.91

Psoralenone O=C1C(C2=CC(C[C@H](O)C(C)(C)O3)=C3C=C2)=COC4=C1C=C(OC)C(OC)=C4	SK-094	382.41	78.14
Aspulvinone I CC(=CCC1=C(C=CC(=C1)/C=C\2/C(=C(C(=O)O2)C3=CC=C(C=C3)O)O)O)C	SK-095	364.40	90.89
Blasticidin S CN(CC[C@@H](CC(=O)N[C@H]1C=C[C@@H](O[C@@H]1C(=O)O)N2C=CC(=NC2=O)N)N)C(=N)N	SK-096	422.45	215.69
Terreic acid (5,6-epoxy-3-hydroxy-p-toluquinone) CC1=C(C(=O)[C@H]2[C@@H](C1=O)O2)O	SK-097	154.12	66.90
Novobenzomalvin D O=C(NCC(C1=CC=CC=C1)=O)C2=CC=CC=C2N3C(NC4=C(C=CC=C4)C3=O)=O	SK-098	399.41	101.04
Astalluminoxide CC1=NC(OC)=C(CC2=CNC3=C(C/C=C(C)\C)C=CC=C23)N([O-]) C1=O.CC4=NC(OC)=C(CC5=CNC6=C(C/C=C(C)\C)C=CC=C56)N([O-]) C4=O.CC7=NC(OC)=C(CC8=CNC9=C(C/C=C(C)\C)C=CC=C89)N([O-])C7=O.[Al+3]	SK-099	1083.48	255.12
Astechrome CC1=NC(OC)=C(CC2=CNC3=C(C/C=C(C)\C)C=CC=C23)N(O)C1=[OH+]. CC4=NC(OC)=C(CC5=CNC6=C(C/C=C(C)\C)C=CC=C56)N(O)C4=[OH+]. CC7=NC(OC)=C(CC8=CNC9=C(C/C=C(C)\C)C=CC=C89)N(O)C7=[OH+].[Fe]	SK-100	1119.11	263.02
3-hydroxy-5-(4-hydroxybenzyl)-4-(4-hydroxyphenyl)furan-2(5H)-one O=C1OC(CC2=CC=C(O)C=C2)C(C3=CC=C(O)C=C3)=C1O	SK-101	298.29	86.99
3-(p-hydroxyphenyl)-4-hydroxy-S-(p-hydroxybenzylidene)-2(5H)-furanone O=C(C(C1=CC=C(O)C=C1)=C/2O)OC2=C\C3=CC=C(O)C=C3	SK-102	296.28	90.89
Versicolactone B C/C/1=C/C/[C@@H]([C@H]2C[C@@H](CC[C@@H]1O)C(=O)O2)C(=C)C	SK-103	250.34	46.53
Bisdethiodi(methylthio)acetylaranotin CC(OC(C=COC=C1C[C@@]23SC)C1N3C([C@@]4(SC)CC5=COC=CC(OC(C)=O)C5N4C2=O)=O)=O	SK-104	534.61	111.70
Terrusnolide A CC(=CCC1=C(C=CC(=C1)CC(=O)CC2=CC=C(C=C2)O)O)C	SK-105	310.39	57.53
(+)-Geodin CC1=C(C(=C2C(=C1Cl)O[C@]3(C2=O)C(=CC(=O)C=C3OC)C(=O)OC)O)Cl	SK-106	399.18	99.14
Botryosphaerin B C[C@]12CCC[C@]([C@@H]1C=C[C@]3([C@@H]2CC(=O)O3)CO)(C)C(=O)O	SK-107	294.35	83.83
Botryosphaerin F C[C@]12CCC[C@]3([C@@H]1[C@@H]([C@H]([C@H]4C2=CC(=O)OC4)O)OC3=O)C	SK-108	292.33	72.84
13,14,15,16-tetranorlabd-7-ene-19,6b:12,17-diolide O=C(OCC1=C[C@@]2([H])O3)CC1[C@@]([C@@]24[H])(C)CCC[C@]4(C)C3=O	SK-109	276.33	52.61
LLZ1271b O=C([C@@]1(C)CCC[C@]2(C)[C@@H](CC(O)=O)C(C(O)C[C@@]12[H])=C)O	SK-110	296.36	94.83
Anhydrojavanicin CC1=CC2=C(C(=C3C(=O)C=C(C(=O)C3=C2O1)OC)O)C	SK-111	272.26	76.74
8-O-methylbostrycoidin	SK-112	299.28	85.73

<chem>CC1=CC2=C(C=N1)C(=O)C3=C(C2=O)C(=C(C=C3OC)OC)O</chem>			
3β,5α-dihydroxy-(22E,24R)-ergosta-7,22-dien-6-one <chem>O=C1[C@@]2(O)C[C@@H](O)CC[C@]2(C)[C@@]3(C)CC[C@]4(C)[C@@H]([C@@H](/C=C/[C@H](C)C(C)C)C)CC[C@@]4([H])C3=C1</chem>	SK-113	442.68	57.53
3β,5α,14α-trihydroxy-(22E,24R)-ergosta-7,22-dien-6-one <chem>O=C1[C@@]2(O)C[C@@H](O)CC[C@]2(C)[C@@]3(C)CC[C@]4(C)[C@@H]([C@@H](/C=C/[C@H](C)C(C)C)C)CC[C@@]4(O)C3=C1</chem>	SK-114	458.68	77.75
NGA0187 <chem>C[C@H](/C=C/[C@H](C)C(C)C)[C@H]1[C@H](C[C@@H]2[C@@]1(C[C@@H](C3C2[C@H](C(=O)[C@@H]4[C@@]3(CC[C@@H](C4)O)C)O)C)OC(=O)C</chem>	SK-115	504.71	104.06
Beauvericin <chem>CC(C)[C@@H]1C(=O)N([C@H](C(=O)O[C@@H](C(=O)N([C@H](C(=O)O[C@@H](C(=O)N([C@H](C(=O)O1)CC2=CC=CC=C2)C)C(C)C)CC3=CC=CC=C3)C)C(C)C)CC4=CC=CC=C4)C</chem>	SK-116	783.96	139.84
Terrstatin A <chem>C[C@H]1C=CC2=C[C@H](CC[C@@H]2[C@H]1CCC(=O)OC)CO</chem>	SK-117	264.37	46.83
Terrstatin B <chem>C[C@H]1C=CC2=C[C@H](CC[C@@H]2[C@H]1CCC(=O)OC)CO</chem>	SK-118	264.37	46.53
(+)-Asperteretone F <chem>CC(=CCC1=C(C=CC(=C1)C(=O)C2=C(C(=O)O[C@H]2OC)C3=CC=C(C=C3)O)O)C</chem>	SK-119	394.42	93.07
(-)-Asperteretone F <chem>CC(=CCC1=C(C=CC(=C1)C(=O)C2=C(C(=O)O[C@@H]2OC)C3=CC=C(C=C3)O)O)C</chem>	SK-120	394.42	93.07
Sulochrin <chem>CC1=CC(=C(C(=C1)O)C(=O)C2=C(C=C(C=C2OC)O)C(=O)OC)O</chem>	SK-121	332.31	113.29
(2'R)-Westerdijkin A <chem>O=C(OC)CC1=CC=C(OC[C@H](O)C(C)=C)C=C1</chem>	SK-122	250.29	55.77
Methyl, 4-hydroxyphenylacetate <chem>O=C(OC)CC1=CC=C(O)C=C1</chem>	SK-123	166.18	46.53
Ampelopyrone <chem>CC1=C(C=C(OC1=O)CC(C)OC(=O)C)O</chem>	SK-124	226.23	76.74
Sporogen-AO 1 <chem>C[C@H]1[C@@H](CCC2=CC(=O)[C@]3([C@@H]([C@]12C)O3)C(=C)C)O</chem>	SK-125	248.32	49.83
Asperdemin <chem>CC1=CC2=C(C[C@H]3[C@](O2)(C[C@H]([C@@H]4[C@@]3([C@H](CC(=O)OC4(C)C)O)C)O)C(=O)O1</chem>	SK-126	392.45	106.21
(S)-(+)-11-dehydroxydonic acid <chem>CC(=C)CCC[C@@](C)(C1=C(C=C(C=C1)C(=O)O)O)O</chem>	SK-127	264.32	77.75
Asperversin E <chem>CC1=CC2=C(C[C@H]3[C@](O2)(C[C@H]([C@@H]4[C@@]3([C@H](CC(=O)OC4(C)C)O)C)OC(=O)C)C(=O)O1</chem>	SK-128	434.49	112.28
Asperversin G <chem>CC1=CC2=C(C[C@H]3[C@](O2)(C[C@H]([C@@H]4[C@@]3(C=CC(=O)C4(C)C)C)OC(=O)C)C(=O)O1</chem>	SK-129	40.47	82.82

Asperterone B O=C(C(CC1=CC=C(O)C(CCC(C)(O)C)=C1)=C2C3=CC=C(O)C=C3)OC2=O	SK-130	382.41	107.97
Asperterone C O=C(C(CC1=CC=C2C(CCC(C)(C)O2)=C1)=C3C4=CC=C(O)C=C4)OC3=O	SK-131	364.40	76.74
12β,15α,25,28-tetrahydroxyergosta-4,6,8(14),22-tetraen-3-one CC(C)(O)[C@@H](CO)/C=C/[C@@H](C)[C@H]1CC(O)C2=C3C=CC4=CC(CC[C@]4(C)[C@@]3([H])CC(O)[C@]12C)=O	SK-132	456.62	97.98
Terrequinone A CC(=CCC1=C(C(=O)C(=O)C(=C1O)C2=C(NC3=CC=CC=C32)C(C)(C)C=C)C4=CNC5=CC=CC=C54)C	SK-133	490.60	85.95
Oleic acid CCCCCCCC/C=C\CCCCCCCC(=O)O	SK-134	282.5	37.30
Terrefuranone O=C1[C@](C)(/C=C/C=CC)OC(CC(O)C)=C1	SK-135	236.31	46.53
Terremutin hydrate O=C1C(C)=C(O)[C@H](O)[C@@H](O)[C@@H]1O	SK-136	174.15	97.98
Asteric acid O=C(O)C1=C(OC2=C(C(OC)=O)C=C(O)C=C2OC)C=C(C)C=C1O	SK-137	348.31	122.53
Dihydroerdin O=C(O)C1=CC(O)=CC(OC)=C1C(C2=C(O)C(Cl)=C(C)C(Cl)=C2O)=O	SK-138	387.17	124.29
Sulochrin O=C(OC)C1=CC(O)=CC(OC)=C1C(C2=C(O)C=C(C)C=C2O)=O	SK-139	332.31	113.29
Taxol O=C(O[C@@H]([C@]1([H])[C@]2(OC(C)=O)CO[C@]2([H])C[C@H](O)[C@@]31C)[C@](C4(C)C)(O)C[C@H](OC([C@H](O)[C@@H](NC(C5=CC=CC=C5)=O)C6=CC=CC=C6)=O)C(C)=C4[C@@H](OC(C)=O)C3=O)C7=CC=CC=C7	SK-143	853.92	221.31
3,6-dihydroxytoluquinone O=C1C(C)=C(O)C(C=C1O)=O	SK-144	154.12	74.60
Terreusinone O=C(C1=C2C=C([C@H](O)C(C)C)N1)C3=C(NC([C@H](O)C(C)C)=C3)C2=O	SK-145	330.38	106.18
Citreoviridin O=C1C=C(OC)C(C)=C(/C=C/C=C/C=C/C(C)=C/[C@]2(C)O[C@H](C)[C@](C)(O)[C@H]2O)O1	SK-146	402.49	89.14
Asperlide A CC1C(CC2=C(O1)C=CC(=C2)C[C@@]3(C(=C(C(=O)O3)O)C4=CC=CC=C4)C(=O)OC)OC	SK-147	424.45	102.30
Asperlide B O=C([C@](C(C1=CC=CC=C1)=C2O)(CC3=CC4=C(OC(C(C)(O)C)C4)C=C3)OC2=O)OC	SK-148	424.45	102.30
Asperlide C O=C1C(O)=C(C2=CC=C(O)C=C2)[C@@H](CC3=CC4=C(OC(C(C)(O)C)C4)C=C3)O1	SK-149	382.41	96.22
Asperterpene D O=C([C@](OC([C@]1([H])[C@@]2(C)C(C(O)=C3C4(C)C)=O)=O)(C)C([C@]1(C)C([C@]5([H])O[C@]25[C@]3(C)CCC4=O)=C)=O)OC	SK-150	486.52	136.58
Asperterpen E O=C([C@@](C([C@]1(C)C(C[C@]2([H])[C@@]([C@H](O)C([C@@]3([H])C(C)(C)C(CC[C@]32C)=O)=O)(C)[C@]14[H])=C)=O)(C)OC4=O)OC	SK-151	474.55	124.05

Asperterpene F C[C@H]1C([C@@]2(C)[C@@H]([C@]3(C)[C@H]([C@]4(C)CCC(C(C)(C)[C@@H]4C([C@H]3O)=O)=O)CC2=C)C(O1)=O)=O	SK– 152	416.51	97.75
Asperterpene G O=C([C@@](C([C@]1(C)C(C[C@]2([H])[C@@]([C@H](O)C([C@]3([H])C(C)(C)C(CC[C@]32C)=O)=O)(C)[C@@]14[H])=C)=O)(C)OC4=O)OC	SK– 153	474.55	124.05
Asperterpene H O=C([C@@](C([C@]1(C)C(C[C@]2([H])[C@@]([C@H](O)C([C@]3([H])C(C)(C)C(CC[C@]32C)=O)=O)(C)[C@]14[H])=C)=O)(C)OC4=O)OCC	SK– 154	488.58	124.05
Asperterpene I O=C([C@H]1[C@](C)(C([C@](C)(O)C(OC)=O)=O)C(C[C@@]2([H])[C@]3(C)CC[C@@H](O)C(C)(C)[C@@]3([H])C([C@@H](O)[C@]12C)=O)=C)OC	SK– 155	508.61	147.44
Asperterpene J O=C([C@H]1[C@](C)(C([C@](C)(O)C(OC)=O)=O)C(C[C@@]2([H])[C@]3(C)CCC(C(C)(C)[C@]3([H])C([C@@H](O)[C@]12C)=O)=O)=C)OC	SK– 156	506.59	144.28
Asperterpene K O=C([C@H]1[C@](C)(C([C@](C)(O)C(OC)=O)=O)C(C[C@@]2([H])[C@]3(C)CCC(C(C)(C)[C@@]3([H])C(C[C@]12C)=O)=O)=C)OC	SK– 157	490.59	124.05
Asperterpene L O=C([C@H]1[C@](C)(C([C@](C)(O)C(OC)=O)=O)C(C[C@@]2([H])[C@]3(C)CCC(C(C)(C)C3=C(O)C([C@]12C)=O)=O)=C)OC	SK– 158	504.58	144.28
Asperterpene M C[C@H]1C([C@@]2(C(OC)=O)[C@@]3(C)CC([C@H]4[C@](CCC(C4(C)C)=O)(C)[C@@H]3CC([C@@]2(C)C(O1)=O)=C)=O)=O	SK– 159	458.55	103.82
Terretonin A O=C([C@](C([C@@]1(C)C(C[C@@]2([H])[C@](C(C(O)=C3C(C)(C)C(CC[C@@]32C)=O)=O)(C)[C@@]14[H])=C)=O)(C)OC4=O)OC	SK– 160	472.53	124.05
Terretonin B O=C([C@](C([C@@]1(C)C(C[C@@]2(O)[C@](C(C(O)=C3C(C)(C)C(CC[C@@]32C)=O)=O)(C)[C@@]14[H])=C)=O)(C)OC4=O)OC	SK– 161	488.53	144.28
Terretonin D O=C([C@](C([C@@]1(C)C(C[C@@]2([H])[C@]([C@@H](O)C([C@@]3([H])C(C)(C)C(CC[C@@]32C)=O)=O)(C)[C@@]14[H])=C)=O)(C)OC4=O)OC	SK– 162	474.55	124.05
Terretonin G O=C([C@H]1[C@](C)(C([C@](C)(O)C(OC)=O)=O)C(C[C@@]2([H])[C@]3(C)CCC(C(C)(C)[C@@]3([H])C([C@@H](O)[C@]12C)=O)=O)=C)OC	SK– 163	506.59	144.28
Emestrins B O=C([C@@](SC)(CC1=CC=CC=C1)N2)N[C@](SC)(CC3=CC=CC=C3)C2=O	SK– 164	386.54	58.20
Emestrins C O=C([C@](SC)(CC1=CC=CC=C1)N2)N[C@@](SC)(CC3=CC=CC=C3)C2=O	SK– 165	386.54	58.20
Emestrins L CC(O[C@H]([C@@]1([H])N2C([C@](SC)(CC3=CC=CC=C3O)N4)=O)C=COC=C1C[C@@]2(SC)C4=O)=O	SK– 166	476.58	105.17

Emestrins M O=C([C@](SC)(CC1=CC=CC=C1O)N2)N3[C@]4([H])[C@@H](O)C=COC=C4C[C@@]3(SC)C2=O	SK– 167	434.54	99.10
Pseurotin A3 O=C1C(C)=C([C@@H](O)[C@@H](O)/C=C\CC)O[C@]12C(N[C@](OC)(C(C3=CC=CC=C3)=O)[C@@H]2O)=O	SK– 168	431.44	142.39
4-hydroxy-3-(3-methylbut-2-enyl)benzaldehyde O=CC1=CC=C(O)C(C/C=C(C)\C)=C1	SK– 169	190.24	37.30
5-N-acetylardeemin O=C(N1[C@@H]2C)C3=CC=CC=C3N=C1[C@]4([H])C[C@@]5(C(C=C)(C)C)C6=CC=CC=C6N(C(C)=O)[C@@]5([H])N4C2=O	SK– 170	468.56	75.52
Gillusdin O=C(C(C12OC3=C(C(C)=C(Cl)C(O)=C3Cl)C1=O)=CC(C(O)=C2OC)=O)OC	SK– 171	415.18	119.37
Terrelumamide A O=C(OC)C1=CC=CC=C1NC([C@@H](NC(C2=CN=C3N(C)C(NC(C3=N2)=O)=O)=O)[C@H](O)C)=O	SK– 172	456.42	185.38
Terrelumamide B O=C(OC)C1=CC=CC=C1NC([C@@H](NC(C2=CN=C3N(C)C(NC(C3=N2)=O)=O)=O)CO)=O	SK– 173	442.39	185.38
Terreinol O=C1C2(OCCC2)OCC3=C1C=C(O)C(C)=C3O	SK– 174	250.25	76.00
Asterriquinone O=C1C(O)=C(C2=CN(C(C=C)(C)C)C3=C2C=CC=C3)C(C(O)=C1C4=CN(C(C=C)(C)C)C5=C4C=CC=C5)=O	SK– 175	506.60	84.47
Isoasterriquinone O=C1C(O)=C(C2=CN(C3=C2C=CC(C/C=C(C)\C)=C3)C(C(O)=C1C4=CNC5=C4C=CC(C/C=C(C)\C)=C5)=O	SK– 176	506.60	106.18
Terremutin O=C1[C@@]2([H])O[C@@]2([H])[C@H](O)C(O)=C1C	SK– 177	156.14	70.06
Citrinin O=C(C1=C(O)C(C)=C2[C@H](C)[C@@H](C)OC=C2C1=O)O	SK– 178	250.25	83.83
10-phenyl-[12]-cytochalasins Z16 O=C(C/C=C(C)\C([C@@H](C)C/C=C/[C@@]1([H])[C@H](O)C([C@@H](C)[C@@]2([H])[C@H](CC3=CC=CC=C3)N4)=C=O)O[C@]12C4=O	SK– 179	463.57	92.70
Rosellichalasin O=C(C/C=C(C)\C(C(C)C/C=C/C1C2OC2(C)C(C)C3C(CC4=CC=CC=C4)N5)=O)OC13C5=O	SK– 180	463.57	85.00
Cytochalasin E O=C(O/C=C/[C@@](C)(O)C([C@@H](C)C/C=C/[C@@]1([H])[C@]2([H])O[C@]2(C)[C@@H](C)[C@@]3([H])[C@H](CC4=CC=CC=C4)N5)=O)O[C@]13C5=O	SK– 181	495.57	114.46
Cytochalasin Z11 O=C1N[C@@H](CC2=CC=CC=C2)[C@]3([H])[C@H](C)C([C@@H](O)[C@H]/C=C/C[C@H](C)C([C@@H](O)C)=O)[C@]13O)=C	SK– 182	427.54	106.85
Cytochalasin Z13 O=C1N[C@@H](CC2=CC=CC=C2)[C@]3([H])C(C)=C(C)[C@@H](O)[C@H]/C=C/C[C@H](C)C([C@@H](O)C)=O)[C@]13O	SK– 183	427.54	106.85

(+)-isoterrein O=C1C=C(/C=C/C)[C@H](O)[C@@H]1O	SK– 184	154.16	57.53
4-hydroxy-3-(3-methyl-2-buten-1-yl)-benzaldehyde O=CC1=CC=C(O)C(C/C=C(C)\C)=C1	SK– 185	190.24	37.30
Gliotoxin O=C1N2[C@]3([H])[C@@H](O)C=CC=C3C[C@@]42SS[C@@]1(CO)N(C)C4=O	SK– 186	326.40	81.07
Acetylaranotin CC(OC(C=COC=C1CC23SS4)C1N3C(C54CC6=COC=CC(OC(C)=O)C6N5C2=O)=O)=O	SK– 187	504.54	111.70
Terreustoxin C C[C@H]1C([C@@]2(C)[C@@H]([C@]3(C)[C@H]([C@]4(C)CCC(C(C)(C)[C@H]4[C@@H](O)[C@H]3O)=O)CC2=C)C(O1)=O)=O	SK– 188	418.53	100.90
Terretonin N C[C@H]1C([C@@]2(C)[C@@H]([C@@]3(C)C[C@H](O)[C@H]4[C@](CC[C@H](OC(C)=O)C4(C)C)(C)[C@@H]3[C@H](O)C2=C)C(O1)=O)=O	SK– 189	462.58	110.14
Astepyrazinoxide O=C1C(C)=NC(OC)=C(CC2=CNC3=C2C=CC=C3C/C=C(C)\C)N1O	SK– 190	353.42	80.15
Astepyrazinol A O=C1C(C)=NC(OC)=C(CC2=CNC3=C2C=CC=C3C/C=C(C)\C)N1	SK– 191	337.42	70.78
Aspulvinone S O=C(C(C1=CC(C/C=C(C)\C)=C(O)C=C1O)=C/2O)OC2=C/C3=CC(CCC(C)(C)O4)=C4C=C3	SK– 192	448.51	100.13
Astepyrazinol B O=C1NC2=C(C=CC=C2C/C=C(C)\C)[C@@H]1CC(N3)=C(OC)N=C(C)C3=O	SK– 195	353.42	84.09
Asperteretal D O=C1C(CC2=CC=C(O)C(C/C=C(C)\C)=C2)=C(C3=CC=C(O)C=C3)C(OC)O1	SK– 196	380.44	76.00
Asperteretal E O=C1C(CC2=CC(CCC(C)(C)O3)=C3C=C2)=C(C4=CC=C(O)C=C4)C(O)O1	SK– 197	366.41	76.00
Asperteretal F O=C1C(CC2=CC=C(O)C(C/C=C(C)/C)=C2)=C(C3=CC=C(O)C=C3)C(O)O1	SK– 198	366.41	86.99
Asperteretal G1 O=C(O)[C@H](CC1=CC=C(O)C(C/C=C(C)\C)=C1)[C@@H](C2=CC=C(O)C=C2)C(OC)=O	SK– 199	398.45	104.06
Asperteretal G2 O=C(O)[C@@H](CC1=CC=C(O)C(C/C=C(C)\C)=C1)[C@@H](C2=CC=C(O)C=C2)C(OC)=O	SK– 200	398.45	104.06
Asperteretal H O=C(OC)[C@H](O)[C@H](C1=CC=C(O)C=C1)C(CC2=CC=C(O)C(C/C=C(C)\C)=C2)=O	SK– 201	398.45	104.06
Asperteretal I O=C1C(CC2=CC(CC(O)C(C)(C)O3)=C3C=C2)=C(C4=CC=C(O)C=C4)C(O)O1	SK– 202	382.41	96.22
Asperteretone A O=C(O)[C@H](C1=CC=C(O)C=C1)[C@H](CC2=CC=C(C/C=C(C)\C)C(O)=C2)C(OC)=O	SK– 203	398.45	104.06
Asperteretone B O=C1C(C2=CC=C(O)C=C2)=C(CCC3=CC=C(O)C(C/C=C(C)\C)=C3)[C@@H](OC)O1	SK– 204	380.44	76.00
Asperteretone C O=C1C(C2=CC=C(OC)C=C2)=C(CCC3=CC4=C(OC(C(C)(O)C)C4)C=C3)[C@@H](OC)O1	SK– 205	410.47	74.23

Asperteretone D O=C1C(C2=CC=C(O)C=C2)=C(CC3=CC(CCC(C)(C)O4)=C4C=C3)[C@@H](OC)O1	SK– 206	380.44	65.00
Asperteretone E O=C1C(C2=CC=C(O)C=C2)=C(CC3=CC=C(O)C(C/C=C(C)\C)=C3)C(OC)O1	SK– 207	380.44	76.00
Amauromine B CC(O[C@]1(C[C@@]23[H])C4=CC=CC=C4N[C@@]1([H])N3C([C@]5([H])C[C@@]6(C(C=C)(C)C)C7=CC=CC=C7N[C@@]6([H])N5C2=O)=O)=O	SK– 208	498.58	90.98
Austalide N CC(O[C@@H]1C2=C(C(C)=C3COC(C3=C2OC)=O)O[C@@]4(C)C[C@@H](O)[C@@]5(O6)C(C)(C)O[C@@]6(OC)CC[C@]5(C)[C@@]14[H])=O	SK– 209	532.59	119.01
(R,E)-3-(2,2-dimethylchroman-6-yl)-4-hydroxy-5-((2-(2-hydroxypropan-2-yl)-2,3-dihydrobenzofuran-5-yl)methylene)furan-2(5H)-one O=C(C(C1=CC(CCC(C)(C)O2)=C2C=C1)=C/3O)OC3=C\C4=CC=C(O[C@@H](C(C)(O)C)C5)C5=C4	SK– 210	448.51	89.14
Soyasapogenol B O[C@H]1CC[C@]2(C)[C@@]3([H])CC=C4[C@]5([H])CC(C)(C)C[C@@H](O)[C@]5(C)CC[C@@]4(C)[C@]3(C)CC[C@@]2([H])[C@]1(CO)C	SK– 211	458.73	60.68
Decanoic acid CCCCCCCCCCC(O)=O	SK– 212	172.27	37.30
Dodecanoic acid CCCCCCCCCCCCC(O)=O	SK– 213	200.32	37.30
(9Z,12Z)-N-(2-hydroxyethyl) octadeca-9,12- dienamide CCCCC/C=C\C/C=C\CCCCCCCC(NCCO)=O	SK– 214	323.52	49.33
4β-hydroxy-6,7-dimethoxyisoflavone O=C1C(C2=CC=C(O)C=C2)=COC3=C1C=C(OC)C(OC)=C3	SK– 215	298.29	68.91
Isoterreulactone A O=C1CC[C@]2(C)[C@@]3(O)CC4=C(C=C(C5=CC=C(OC)C=C5)OC4=O)O[C@]3(C)CC[C@@]2(O)C(C)(C)O1	SK– 216	484.55	115.44
12a-dehydroxyisoterreulactone A C[C@]12CCC(=O)OC([C@@]1(CC[C@@]3([C@@H]2CC4=C(O3)C=C(OC4=O)C5=CC=C(OC)C)O)(C)C	SK– 217	468.55	95.21
Blumenol A O=C1C=C(C)[C@@]/C=C/[C@H](O)C(O)C(C)(C)C1	SK– 218	224.30	57.53
Genistein O=C1C(C2=CC=C(O)C=C2)=COC3=C1C(O)=CC(O)=C3	SK– 219	270.24	90.89
Biochanin A O=C1C(C2=CC=C(OC)C=C2)=COC3=C1C(O)=CC(O)=C3	SK– 220	284.27	79.90
Psoralenol O=C1C(C2=CC(CC(O)C(C)(C)O3)=C3C=C2)=COC4=C1C=CC(O)=C4	SK– 221	338.36	79.90
Daidzein O=C1C(C2=CC=C(O)C=C2)=COC3=C1C=CC(O)=C3	SK– 222	254.24	70.67
Fumitremorgin C O=C([C@]1([H])CCCN21)N3[C@@H]/C=C(C)\C)C4=C(C5=C(N4)C=C(OC)C=C5)C[C@@]3([H])C2=O	SK– 223	379.46	65.64

Bisdethiobis(methylthio)gliotoxin O=C1N(C)[C@@](SC)(CO)C(N2[C@@]1(SC)CC3=CC=C[C@H](O)[C@@]23[H])=O	SK– 224	356.47	81.07
Cyclo-(L-Pro-L-Met) O=C(N[C@@H]1CCSC)[C@](CCC2)([H])N2C1=O	SK– 225	228.32	49.41
Cyclo-(L-Pro-L-Tyr) O=C(N[C@H]1CC2=CC=C(O)C=C2)[C@@](CCC3)([H])N3C1=O	SK– 226	260.26	69.64
Cyclo-(L-Pro-L-Phe) O=C([C@H](CCC1)N1C2=O)N[C@H]2CC3=CC=CC=C3	SK– 227	244.29	49.41
Penicitrinone A O=C1C=C2OC3=C4O[C@H](C)[C@@H](C)C4=C(C)C(O)=C3C5=C2C([C@H](C)[C@@H](C)O5)=C1C	SK– 228	380.44	68.91
Penicitrinone B O=C1C=C2OC3=C4OC(C)=C(C)C4=C(C)C(O)=C3C5=C2C([C@H](C)[C@@H](C)O5)=C1C	SK– 229	378.42	72.81
2,3,4-trimethyl-5,7-dihydroxy2,3-dihydrobenzofuran OC1=C(OC(C)C2C)C2=C(C)C(O)=C1	SK– 230	194.23	49.69
Physcion O=C1C2=C(C=C(C)C=C2O)C(C3=CC(OC)=CC(O)=C13)=O	SK– 231	284.27	83.83
Aspergiketal O=C([C@]12OCCC1)C3=C(CO2)C(O)=C(C)C(O)=C3	SK– 232	250.25	76.00
Sinulolide I O=C(OCC)CCCCCCCC[C@@](C(C)=C1C)(O)OC1=O	SK– 233	312.41	72.84
Territrem A O=C1C2(C)C3(O)CC4=C(C=C(C5=CC(OC)=C(OCO6)C6=C5)OC4=O)OC3(C)CCC2(O)C(C)(C)C=C1	SK– 234	510.54	124.67
Territrem B O=C1[C@]2(C)[C@@]3(O)CC4=C(C=C(C5=CC(OC)=C(OC)C(OC)=C5)OC4=O)O[C@]3(C)CC[C@@]2(O)C(C)(C)C=C1	SK– 235	526.58	124.67
Territrem C O=C1[C@]2(C)[C@@]3(O)CC4=C(C=C(C5=CC(OC)=C(O)C(OC)=C5)OC4=O)O[C@]3(C)CC[C@@]2(O)C(C)(C)C=C1	SK– 236	512.55	135.67
Territrem D C[C@@]12CC[C@@]3([C@@]([C@]1(CC4=C(O2)C=C(OC4=O)C5=CC(=C(C(=C5)OC)OC)O)O)(C(=O)C=CC3(C)C)C)O	SK– 237	512.55	135.67
Cowabenzophenone A O=C(C1(C/C=C(C)/CC/C=C(C)\C)C2)[C@@]3(C(C4=CC=CC=C4)=O)C(C)(C)[C@]2([H])C[C@]5([H])C(C)(C)[C@@H](C(C)=C)CC(C3=O)5C1=O	SK– 238	598.80	68.25
Asperteramide O=C(C(CCC1=CC=C(O)C(C/C=C(C)\C)=C1)=C2C3=CC=C(O)C=C3)NC2=O	SK– 239	363.41	90.39
Terreinlactone B O=C1OCCC(/C=C/C)=C1	SK– 240	138.17	26.30
15bβ-hydroxyl-5-N-acetylardeemin O=C1N2C([C@](C[C@]3(C(CC=C)(C)C)C4N(C(C)=O)C5=C3C=CC=C5)(O)N4C([C@H]2C)=O)=NC6=C1C=CC=C6	SK– 241	498.58	95.74
10-phenyl-[12]-cytochalasin Z17	SK– 242	463.57	92.70

<chem>O=C(C/C=C(C)\ C([C@@H](C)C/C=C/[C@H]1[C@H](O)C(C)=C(C)[C@H]2[C@H](CC3=CC=CC=C3)N4)=O)O[C@]12C4=O</chem>			
Neoasterriquinone.	SK–	506.60	106.18
<chem>O=C1C(O)=C(C2=C(C/C=C(C)\ C)NC3=C2C=CC=C3)C(C(O)=C1C4=C(C/C=C(C)\ C)NC5=C4C=CC=C5)=O</chem>	243		
(3R)-6,7,8-trihydroxymellein	SK–	210.19	86.99
<chem>C[C@H]1OC(C2=C(C=C(O)C(O)=C2O)C1)=O</chem>	244		
(3R)-8-methoxy-6-hydroxymellein	SK–	208.21	55.77
<chem>C[C@H]1OC(C2=C(C=C(O)C=C2OC)C1)=O</chem>	245		
4-chloro-3,6-dihydroxytoluquinone	SK–	188.57	74.60
<chem>O=C1C(O)=C(Cl)C(C(C)=C1O)=O</chem>	246		
6-hydroxytoluquinol hydrate	SK–	158.15	77.75
<chem>OC1=C(C)C([C@@H](O)C[C@@H]1O)=O</chem>	247		
Bisdethiobis(methylsulfanyl)acetylaranotin	SK–	534.61	111.70
<chem>CC(O[C@@H](C=COC=C1C[C@@]23SC)[C@@]1([H])N3C([C@]4(SC)CC5=COC=C[C@H](OC(C)=O)[C@@]5([H])N4C2=O)=O)=O</chem>	248		
Bisdethiobis(methylsulfanyl)acetylapoaranotin	SK–	504.63	85.39
<chem>O=C1N2[C@](CC3=COC=C[C@H](OC(C)=O)[C@]32[H])(SC)CN4[C@@]1(SC)CC5=CC=C[C@H](OC(C)=O)[C@@]45[H]</chem>	249		
Bisdethiobis(methylsulfanyl)apoaranotin	SK–	462.59	79.31
<chem>O=C1N2[C@](CC3=COC=C[C@H](OC(C)=O)[C@]32[H])(SC)CN4[C@@]1(SC)CC5=CC=C[C@H](O)[C@@]45[H]</chem>	250		
Asperbutenolide A	SK–	864.90	235.82
<chem>CC(=CCC1=C(C=CC(=C1)C[C@@]2(C(=C(C(=O)O2)OC(C)(C)[C@H](CC3=C(C=CC(=C3)C[C@@]4(C(=C(C(=O)O4)O)C5=CC=C(C=C5)O)C(=O)OC)O)C6=CC=C(C=C6)O)C(=O)OC)O)C</chem>	251		
Asperbutenolide B	SK–	470.47	131.76
<chem>O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC=C(O[C@H](C(C)(O)C)[C@H]4OC)C4=C3) OC2=O)OC</chem>	252		
Asperbutenolide C	SK–	470.47	131.76
<chem>O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC=C(O[C@@H](C(C)(O)C)[C@@H]4OC)C4=C3)OC2=O)OC</chem>	253		
Asperbutenolide D	SK–	384.43	104.06
<chem>O=C(OC)C(CC1=CC=C(O)C(C/C=C(C)\ C)=C1)(O)C(C2=CC=C(O)C=C2)=O</chem>	254		
Asperbutenolide E	SK–	454.48	125.82
<chem>O=C([C@](C(C1=CC=C(O)C=C1)=C2O)(CC3=CC=C(O)C(CC4OC4(C)C)=C3)OC2=O)OCC</chem>	255		
Asperbutenolide F	SK–	354.36	93.07
<chem>O=C(C(C(C1=CC=C(O)C=C1)=C2O)(CC3=CC=CC=C3)OC2=O)OCC</chem>	256		
(S)-Methyl-4-hydroxy-2-[4- hydroxy-3-(3-methyl-but-2-enyl)- benzyl]-3-(4-hydroxy-phenyl)-5- oxo-2,5-dihydro-furan-2- carboxylic acid methyl ester	SK–	424.45	113.29
<chem>O=C(O[C@]1(CC2=CC(C/C=C(C)/C)=C(O)C=C2)C(OC)=O)C(O)=C1C3=CC=C(O)C=C3</chem>	257		
(Z/E)-L-phenylalaninamide	SK–	460.58	94.30
<chem>O=C(C(N(C(C(NC(C)=O)C(C)C)=O)C)CC1=CC=CC=C1)N/C=C/C2=CNC3=CC=CC=C32</chem>	258		
Furanaspermeroterpene A	SK–	558.58	159.59
	259		

<chem>O=C(OC)C[C@@]1([C@](OC2=O)(C(C)=O)O[C@@]3(O)C(C4C5(C)C)=O)[C@@]2(C)C([C@@H](OC(C)=O)C([C@@]13C)[C@]4(C)C=CC5=O)=C</chem>				
Furanaspermeroterpene B	SK–	560.60	159.59	
<chem>O=C(OC)C[C@@]1([C@](OC2=O)(C(C)=O)O[C@@]3(O)C(C4C5(C)C)=O)[C@@]2(C)C([C@@H](OC(C)=O)C([C@@]13C)[C@]4(C)CCC5=O)=C</chem>	260			
Furanaspermeroterpene D	SK–	526.58	122.29	
<chem>O=C(OC)C[C@@]1([C@]2(C)C([C@@]3(C)C4C(C)(C)C(C=C3)=O)[C@H](OC(C)=O)C([C@]15C)=C)C(OC2C4=O)=C(C)OC5=O</chem>	261			
Furanaspermeroterpene E	SK–	574.62	151.75	
<chem>O=C(OC)C[C@@]1([C@]2(C)C([C@@]3(C)C4C(C)(C)C(C[C@H]3OC)=O)[C@H](OC(C)=O)C([C@]15C)=C)C(O[C@@]2(O)C4=O)=C(C)OC5=O</chem>	262			
Furanaspermeroterpene F	SK–	502.56	144.28	
<chem>O=C(OC)C[C@@]1([C@](C(C(O)=C2C(C)(C)C(CC[C@]23C)=O)=O)(C)C3[C@H](O)C([C@]14C)=C)C([C@@H](C)OC4=O)=O</chem>	263			
Furanaspermeroterpene G	SK–	574.62	159.59	
<chem>O=C(OC)C[C@@]1([C@](C(C(O)=C2C(C)(C)C(C[C@@H](OC)[C@]23C)=O)=O)(C)C3[C@H](OC(C)=O)C([C@]14C)=C)C([C@@H](C)OC4=O)=O</chem>	264			
Furanaspermeroterpene H	SK–	588.65	159.59	
<chem>O=C(OC)C[C@@]1([C@](C(C(O)=C2C(C)(C)C(C[C@@H](OCC)[C@]23C)=O)=O)(C)C3[C@H](OC(C)=O)C([C@]14C)=C)C([C@@H](C)OC4=O)=O</chem>	265			