

Supplementary Material

An Effective Search of Triterpenes with Anti-HSV-1 Activity Using Classification Model by Logistic Regression

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S1. The canonical SMILES of collected triterpene with information of anti-HSV-1 activity and their references.

S2. The result of cytotoxicity assay

S3. References

S. 1. The canonical SMILES of collected triterpene with information of anti-HSV-1 activity and their references.

<chem>CC[C@@H](C(C)C)/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC=C2[C@]1(C)C[C@@H](C2)O)C</chem>	(Wachsman et al. 2004)
<chem>CC[C@@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C[C@@H](O)[C@H](C2)O)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)OC(=O)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)OC(=O)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)Br)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)Br)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)O)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)O)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)O)C)O)O)C(C)C</chem>	
<chem>CC[C@H](C(C)C)/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)O)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2COC(=O)[C@@H]2[C@]1(C)C[C@@H](O)[C@H](C2)O)C)O)O)C(C)C</chem>	
<chem>CC[C@@H](C(C)C)/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC=CC2)F)C</chem>	
<chem>CC[C@@H](C(C)C)/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)F)Cl)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)OF)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)OF)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)F)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)F)O)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)F)O)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)F)O)C)O)O)C(C)C</chem>	
<chem>CC[C@@H](C(C)C)/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@H]([C@@H]2[C@]1(C)CC[C@@H](C2)Br)Cl)O)C</chem>	
<chem>CC[C@@H](C(C)C)/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CCC2=CC(=O)CC[C@]12C)C</chem>	
<chem>CC[C@@H](C(C)C)/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@@H]([C@@H]2[C@]1(C)C[C@@H](O)[C@H](C2)O)F)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)O)C)O)O)C(C)C</chem>	
<chem>CC([C@@H]([C@H]1OC(O[C@@H]1[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C[C@@H]1OC(O[C@H]1C2)(C)C)(C)C)C)C</chem>	
<chem>CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C[C@@H](O)[C@H](C2)O)F)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)O)C)O)O)C(C)C</chem>	
<chem>CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CCC2=CC(=O)CC[C@]12C)C)O)O)C(C)C</chem>	

CC[C@H]([C@@H])([C@H])([C@H])([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CCC2=CC(=O)CC[C@]12C(C)O)O)C(C)C	
OCC1O[C@@H](OC2[C@@H](OC[C@H]([C@H]2O)C)O[C@H]2CC[C@]3([C@H]([C@]2(C)CO)CC[C@@]2([C@@H]3CC[C@]34[C@@]2(C)C[C@H]([C@@]2([C@H]4CC(C)(C)CC2)CO3)O)C)C([C@@H]([C@@H]1O[C@@H]1OC[C@@H]([C@H]([C1O)O)O)O[C@@H]1OC(CO)[C@H]([C@H]([C1O)O)O)C	(Amoros et al. 1987)
OC[C@H]1O[C@@H](OC(=O)[C@@]23CC[C@H]([C@@]([C@H]3C3=CC[C@H]4[C@@]([C@@]3(C2)C)(C)CC[C@H]2[C@]4(C)C[C@H]([C@@H](C2(C)C)O)O)(C)O)C)[C@@H]([C@H]([C@@H]1O)O)O	(Simões et al. 1999)
OCC1O[C@H](O[C@H]2[C@H](O)C[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3[C@](C)O)[C@H](C)CC2)C(=O)O)C)C([C@@H]([C@@H]1O)O)O	
CC(=O)[C@H]1CC[C@]2([C@H]1CCC3[C@@]([C@]1(C)CC2)(C)CCC1[C@]3(C)CC[C@H]([C@@]1(C)C(=O)O)O)C(=O)O	(Li et al. 2007)
CO[C@@H]1CC[C@]2(C([C@]1(C)S(=O)(=O)O)CC[C@@]1(C2CC[C@H]2[C@@]1(C)CC[C@@]1([C@@H]2[C@@H](CC1)C(=C)C)C(=O)O)C	
CC(=O)O[C@H]1CC[C@]2(C(C1(C)C)CC[C@@]1(C2CC[C@H]2[C@@]1(C)CC[C@@]1([C@@H]2[C@@H](CC1)C(=C)C)C(=O)O)C	
COC(=O)[C@@]12CC[C@H]([C@@H]2[C@@H]2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CC[C@@H](C3(C)C)O)C(=C)C	
COC(=O)[C@@]12CC[C@H]([C@@H]2[C@@H]2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CC[C@@H](C3(C)C)OC(=O)C)C(=C)C	
C[C@@H]1CC[C@]2([C@H]([C@H]1C)C1=CCC3[C@@]([C@@]1(CC2)C)(C)CCC1[C@]3(C)C[C@@H](O)[C@H](C1(C)C)O)C(=O)O	
CC(=O)O[C@@H]1C[C@@]2(C)C(C([C@@H]1OC(=C)C)(C)C)CC[C@@]1(C2CC=C2[C@@]1(C)CC[C@@]1([C@@H]2[C@@H](C)[C@H](C)CC1)C(=O)O)C	
COC(=O)[C@@]12CC[C@H]([C@@H]([C@@H]2C2=CCC3[C@@]([C@@]2(CC1)C)(C)CCC1[C@]3(C)C[C@H]([C@H](C1(C)C)O)O)C	(Ryu et al. 1992)
COC(=O)[C@@]12CC[C@H]([C@@H]([C@@H]2C2=CCC3[C@@]([C@@]2(CC1)C)(C)CCC1[C@]3(C)C[C@H]([C@H](C1(C)C)OC(=O)C)OC(=O)C)C	
C[C@@H]1CC[C@]2([C@H]([C@H]1C)C1=CCC3[C@@]([C@@]1(CC2)C)(C)CCC1[C@]3(C)CC[C@@H](C1(C)C)O)C(=O)O	
CC(=O)O[C@H]1CC[C@]2(C(C1(C)C)CC[C@@]1(C2CC=C2[C@@]1(C)CC[C@@]1([C@@H]2[C@@H](C)[C@H](C)CC1)C(=O)O)C	
COC(=O)[C@@]12CC[C@H]([C@@H]([C@@H]2C2=CCC3[C@@]([C@@]2(CC1)C)(C)CCC1[C@]3(C)CC[C@@H](C1(C)C)O)C	
O=C1C=C2[C@@H]3[C@@H](C)[C@H](C)CC[C@@]3(CC[C@]2([C@]2([C@H]1[C@@]1(C)CC[C@@H](C([C@@H]1CC2)(C)C)O)C)C(=O)O	
C[C@@H]1CC[C@]2([C@H]([C@H]1C)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CCC1[C@]3(C)C[C@@H](O)[C@H](C1(C)C)O)C(=O)O	
O[C@H]1COC([C@@H]([C@H]1O)O)O[C@@H]1CC[C@]2(C(C1(C)C)CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2[C@](C)O)[C@H](C)CC1)C(=O)O)C	
OC[C@H]1O[C@@H](OC(=O)[C@@]23CC[C@H]([C@@]([C@H]3C3=CC[C@H]4[C@@]([C@@]3(C2)C)(C)CCC2[C@]4(C)CC[C@H](C2(C)C)OC2OC[C@@H]([C@@H]([C@H]2O)O)O)(C)O)C)[C@@H]([C@H]([C@@H]1O)O)O	
C[C@@H]1CC[C@]2([C@@H]([C@]1(C)O)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CCC(=O)C1(C)C)C(=O)O	(Ryu et al. 1993)
O=C1C=C2[C@@H]3[C@@H](C)[C@H](C)CC[C@@]3(CC[C@]2([C@]2([C@H]1[C@@]1(C)CC[C@@H]1CC2)(C)C)C)C(=O)O	
C[C@@H]1CC[C@]2([C@@H]([C@H]1C)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)O)C(=O)O	
O[C@H]1CC[C@]2([C@H]([C@H]1C)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)O)C(=O)O	
O=C1C=C2[C@@H]3[C@@H](C)[C@H](C)CC[C@@]3(CC[C@]2([C@]2([C@H]1[C@@]1(C)CCC(=O)C([C@@H]1CC2)(C)C)C)C(=O)O	
N#CC[C@]1(C)C(CC[C@@]2(C1CCC1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=C)C)C(=O)O)C)C(=O)C	
N#CC[C@@]1(C)C(CC[C@@]2(C1CCC1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=C)C)C(=O)O)C)C(=O)O)C	
CCC(NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC([C@](C1CC2)(C)CC#N)C(=O)(C)C)C(=C)C)CO	(Tolmacheva et al. 2019)
CC[C@@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC([C@](C1CC2)(C)C#N)C(=O)(C)C)C(=C)C)CO	

CC[C@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC([C@](C1CC2)(C)CC#N)C(C=O)(C)C)C(=O)C)CO	
N#CC[C@@]1(C)C(CC[C@@]2(C1CCC1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=O)C)C(=O)NC(CO)CC(C)C	
N#CC[C@@]1(C)C(CC[C@@]2(C1CCC1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=O)C)C(=O)OC)C(C(=O)NC(CO)CC(C)C	
CCC(NC(=O)C(C1CC[C@@]2(C([C@@]1(C)CC#N)CCC1[C@@]2(C)CCC23[C@@H]1[C@@H](OC2)C(CC3)(C)C)C(C)C)CO	
CC(=O)[C@@H]1CC[C@@]2([C@H]1C1CCC3[C@@]([C@]1(C)CC2)(C)CCC1[C@]3(C)CCC(=O)C1(C)C)C(=O)O	
CCC(NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CCC(=O)C3(C)C)C(=O)C)CO	
CC[C@@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)C(CC(=O)C3(C)C)C(=O)C)CO	
CC[C@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CC(C(=O)C3(C)C)C(=O)C)CO	
CCC(NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CC[C@@H](C3(C)C)O)C(=O)C)CO	
CC[C@@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)C[C@@H](C3(C)C)O)C(=O)C)CO	
CC[C@@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CC[C@@H](C3(C)C)O)C(=O)C)CO	
CC[C@@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)C[C@@H](C3(C)C)O)C(=O)C)COC(=O)C	
O/N=C/C(C1CC[C@@]2(C([C@@]1(C)CC#N)CCC1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=O)C)C(=O)NC(C)C)C(C)C	
CC[C@@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)C(CC(=O)C3(C)C)C(=O)C)CO	
CC[C@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CC(C(=O)C3(C)C)C(=O)C)CO	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C[C@H](O)[C@@H](C2)O)C)C	(Pujol et al. 2016)
[Na]OS(=O)(=O)O[C@H]1C[C@]2(C)[C@H]3CC[C@]4([C@H]([C@@H]3CC(=O)[C@H]2C[C@H]1OS(=O)(=O)O[Na])CC[C@@H]4[C@@H](CCCC(C)C)C	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C[C@@H](O)[C@H](C2)O)C)C	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C[C@@H](OS(=O)(=O)[O-])[C@H](C2)OS(=O)(=O)[O-])C)C.[Na+].[Na+]	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C[C@H](O)[C@H](C2)O)C)C	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C[C@H](OS(=O)(=O)[O-])[C@H](C2)OS(=O)(=O)[O-])C)C.[Na+].[Na+]	
O/N=C/1\C[C@H]2[C@@H]3CC[C@H]([C@@]3(C)CC[C@@H]2[C@@]2([C@@H]1C[C@H](OS(=O)(=O)[O-])[C@H](C2)OS(=O)(=O)[O-])C)[C@@H](CCCC(C)C)C.[Na+].[Na+]	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@H]([C@@H]2[C@]1(C)C[C@H](O)[C@H](C2)O)O)C)C	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@H]([C@@H]2[C@]1(C)C[C@H](OS(=O)(=O)[O-])[C@H](C2)OS(=O)(=O)[O-])OS(=O)(=O)[O-])C)C.[Na+].[Na+].[Na+]	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@@H]([C@@H]2[C@]1(C)C[C@H](O)[C@H](C2)O)O)C)C	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@@H]([C@@H]2[C@]1(C)C[C@H](OS(=O)(=O)[O-])[C@H](C2)OS(=O)(=O)[O-])OS(=O)(=O)[O-])C)C.[Na+].[Na+].[Na+]	
CC(CCC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@H]([C@@H]2[C@]1(C)C[C@H](OS(=O)(=O)[O-])[C@H](C2)OS(=O)(=O)[O-])O)C)C.[Na+].[Na+]	
N#CC[C@@]1(C)C(CC[C@@]2(C1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=O)C)C(=O)O)C(C(=O)O)C(C)C	(Tolmacheva et al. 2014)
N#CC[C@@]1(C)C(CC[C@@]2(C1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=O)C)C(=O)O)C(C(=O)O)C(C)C	
OCC(NC(=O)[C@@]12CC[C@H]([C@@H]2[C@@H]2[C@](CC1)(C)[C@]1(C)CC[C@H]([C@](C1CC2)(C)CC#N)C(C=O)(C)C)C(=O)C)CO	

OC[C@@H](CNC(=O)[C@@]12CC[C@H]([C@@H]2[C@@H]2[C@](CC1)(C)[C@]1(C)CC[C@H]([C@] [C@H]1CC2)(C)CC#N)C(C=O)(C)C)C(=C)C)O	
OC[C@H](C(C)C)NC(=O)[C@@]12CC[C@H]([C@@H]2[C@@H]2[C@](CC1)(C)[C@]1(C)CC[C@H]([C@] [C@H]1CC2)(C)CC#N)C(C=O)(C)C)C(=C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@ H](CC2)C(=C)C)C(=O)NC(CO)(C)C)C(C=O)(C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@ H](CC2)C(=C)C)C(=O)OC)C(C(=O)NC(CO)CO)(C)C	
OC[C@@H](CNC(=O)C([C@@H]1CC[C@@]2([C@@H]([C@@]1(C)CC#N)CC[C@H]1[C@@]2(C)CC[C@] [C@@]2([C@@H]1[C@@H](CC2)C(=C)C)C(=O)OC)C)(C)C)O	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@ H](CC2)C(=C)C)C(=O)OC)C(C(=O)N[C@H](C(C)C)CO)(C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@ H](CC2)C(=C)C)C(=O)OC)C(C(=O)NC(CO)(C)C)(C)C	
OCC(NC(=O)C([C@@H]1CC[C@@]2([C@@H]([C@@]1(C)CC#N)CC[C@H]1[C@@]2(C)CC[C@@]23 [C@H]1[C@@H](OC2)C(CC3)(C)C)C)(C)C)CO	
OCC(CNC(=O)C([C@@H]1CC[C@@]2([C@@H]([C@@]1(C)CC#N)CC[C@H]1[C@@]2(C)CC[C@@] 23[C@H]1[C@@H](OC2)C(CC3)(C)C)C)(C)C)O	
OCC(C(C)C)CNC(=O)C([C@@H]1CC[C@@]2([C@@H]([C@@]1(C)CC#N)CC[C@H]1[C@@]2(C)CC[C@] [C@@]23[C@H]1[C@@H](OC2)C(CC3)(C)C)C)(C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]23[C@H]1[C@@H] [C@@H](OC2)C(C)C(CC3)C)C(C(=O)NC(CO)(C)C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@ H](CC2)C(=C)C)C(=O)NC(CO)CO)C(C(=O)NC(CO)CO)(C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@ H](CC2)C(=C)C)C(=O)NC[C@@H](CO)O)C(C(=O)N[C@H](C(C)C)CO)(C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@ H](CC2)C(=C)C)C(=O)NCC(C(C)C)CO)C(C(=O)N[C@H](C(C)C)CO)(C)C	
N#CCC1[C@@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2) C(=C)C)C(=O)OC)C(COC(=O)C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]23[C@H]1[C@@H] [C@@H](OC2)C(C)C(CC3)C)C(COC(=O)C)C	
N#CCC1[C@@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2) C(=C)C)C(=O)OC)C(COC(=O)CCC(=O)O)C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]23[C@H]1[C@@H] [C@@H](OC2)C(C)C(CC3)C)C(COC(=O)CCC(=O)O)C)C	
N#CCC1[C@@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2) C(=C)C)C(=O)OC)C(COC(=O)CC(C(=O)O)C)C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]23[C@H]1[C@@H] [C@@H](OC2)C(C)C(CC3)C)C(COC(=O)CCC(C(=O)O)C)C)C	
N#CCC1[C@@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2) C(=C)C)C(=O)OC)C(COC(=O)CC(C(=O)O)C)C)C	
N#CC[C@@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]23[C@H]1[C@@H] [C@@H](OC2)C(C)C(CC3)C)C(COC(=O)CCC(C(=O)O)C)C)C	
N#CCC1[C@@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2) C(=C)C)C(=O)OC)C(COC(=O)CC(C(=O)O)C)C)C	
COC(=O)[C@@]12CC[C@H](C2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)C(=CC3(C)C)C(=O) O)C(=C)C	(Konysheva et al. 2017)
OC(=O)C1=CC(C2[C@@]1(C)C1CCC3[C@@]([C@@]1(CC2)C)(C)CC[C@@]12C3[C@@H](OC1)C(C) (C)CC2)(C)C	
COC(=O)[C@@]12CC[C@H](C2C2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)C(=C(C3(C)C)C)C(=O) O)C(=C)C	
OC(=O)C1=C(C)C(C2[C@@]1(C)C1CCC3[C@@]([C@@]1(CC2)C)(C)CC[C@@]12C3[C@@H](OC1)C (C)C)CC2)(C)C	
NCC1=CC(C2[C@@]1(C)C1CCC3[C@@]([C@@]1(CC2)C)(C)CC[C@@]12C3[C@@H](OC1)C(C)(C)C C2)(C)C	(Baltina, L. A., Jr. et al. 2017)
Oc1ccc(cc1)CC(C(=O)O)NC(=O)C1O[C@H](O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H] 3C(=O)C=C3[C@@]2(C)CC[C@@]2([C@H]3C[C@](C)(CC2)C(=O)NC(C(=O)O)Cc2ccc(cc2)O)C)C)C ([C@@H]([C@@H]1O)O)O[C@H]1OC(C(=O)NC(C(=O)O)Cc2ccc(cc2)O)[C@H]([C@H](C1O)O)O	

O[C@H]1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(C)(C)CC1)C)C	(Kuo et al. 2011)
C=C(C(C)C)CC[C@H]([C@H]1CC[C@@]2([C@]1(C)CC[C@@]13[C@H]2CC[C@@H]2[C@]3(C1)CC[C@@H]([C@H]2C)O)C)C	
OC[C@@]12[C@H](O)C[C@@H](C[C@@]2(O)CC[C@@H]2[C@H]1[C@H](O)C[C@]1([C@]2(O)C[C@H]1C1=CC(=O)OC1)C)O[C@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1O)O)O.O.O.O.O.O.O.O.O	(Su et al. 2008)
OC[C@@]12[C@H](O)C[C@@H](C[C@@]2(O)CC[C@@H]2[C@H]1[C@H](O)C[C@]1([C@]2(O)C[C@H]1C1=CC(=O)OC1)C)O[C@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1O)O)O	
O[C@H]1CC[C@]2([C@H](C1)CC[C@@H]1[C@@H]2CC[C@]2([C@]1(O)C[C@@H]([C@@H]2C1=CC(=O)OC1)O)C)C	
OC[C@]12CC[C@@H](C[C@@]2(O)CC[C@@H]2[C@H]1CC[C@]1([C@]2(O)CC[C@@H]1C1=C(C(=O)OC1)C)O	
O=C1OCC(=C1)[C@H]1CC[C@]2([C@]1(C)CC[C@H]1[C@H]2CC[C@H]2[C@]1(C)CC[C@@H](C2)O[C@H]1C[C@H](O)[C@@H]([C@H](O1)C)O)O	(Bertol et al. 2011)
O=C1OCC(=C1)[C@H]1CC[C@]2([C@]1(C)CCC1C2CC[C@H]2[C@]1(C)CC[C@@H](C2)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)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](O)C[C@@H](O[C@H]2C)O[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C)[C@@H]([C@H]([C@@H]1O)O)O	
CC(=O)OC1C(O)CC(OC1C)OC1C(O)CC(OC1C)OC1C(O)CC(OC1C)OC1CCC2(C(C1)CCC1C2CCC2(C1(O)CCC2C1=CC(=O)OC1)C)C	
OC[C@H]1O[C@@H](O[C@@H]2[C@@H](C)O[C@H](C[C@@H]2OC(=O)C)O[C@H]2[C@@H](O)C[C@@H](O[C@@H]2C)O[C@H]2[C@@H](O)C[C@@H](O[C@@H]2C)O[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C)[C@@H]([C@H]([C@@H]1O)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](O)C[C@@H](O[C@H]2C)O[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)C[C@@H]([C@@H]3C2=CC(=O)OC2)O)C)C)[C@@H]([C@H]([C@@H]1O)O)O	
O=C1OCC(=C1)[C@H]1CC[C@]2([C@]1(C)[C@H](O)C[C@H]1[C@H]2CC[C@H]2[C@]1(C)CC[C@@H](C2)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)O)O	
OC[C@H]1C[C@@H](O[C@H]2[C@@H](O)C[C@@H](O[C@H]2C)O[C@H]2[C@@H](O)C[C@@H](O[C@@H]2C)O[C@H]2[C@@H](O)C[C@@H](O[C@@H]2C)O[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3C[C@@H](O)[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C)[C@@H]([C@H]([C@@H]1O)O)O	
CO[C@H]1C[C@H](O[C@H]2CC[C@]3([C@](C2)(O)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CCC3C2=CC(=O)OC2)C)C=O)O[C@@H]([C@H]1O[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	
CO[C@H]1C[C@H](O[C@H]2[C@@H](O)C[C@@H](O[C@@H]2C)O[C@H]2[C@@H](O)C[C@@H](O[C@@H]2C)O[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C)O[C@@H]([C@H]1O)C	
CO[C@H]1[C@@H](O)C[C@@H](O[C@@H]1C)O[C@H]1[C@@H](O)C[C@@H](O[C@@H]1C)O[C@@H]1[C@@H](O)C[C@@H](O[C@@H]1C)O[C@H]1CC[C@]2([C@@H](C1)CC[C@@H]1[C@@H]2C[C@]2([C@]1(O)CC[C@@H]2C1=CC(=O)OC1)C)C	
O=C[C@@]12CC[C@@H](C[C@@]2(O)CC[C@@H]2[C@H]1CC[C@]1([C@]2(O)CC[C@@H]1C1=CC(=O)OC1)C)O[C@@H]1O[C@@H](O)[C@@H]([C@H]([C@H]1O)O)O	
O=C[C@@]12CC[C@@H](C[C@@]2(O)CC[C@@H]2[C@H]1CC[C@]1([C@]2(O)CC[C@@H]1C1=CC(=O)OC1)C)O[C@H]1C[C@H](O)[C@@H]([C@H](O1)C)O	
CO[C@H]1C[C@H](O[C@H]2CC[C@]3([C@](C2)(O)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C=O)O[C@@H]([C@H]1O)C	
O[C@H]1CC[C@]2([C@H](C1)CC[C@@H]1[C@@H]2C[C@@H](O)[C@]2([C@]1(O)CC[C@@H]2C1=CC(=O)OC1)C)C	
O=C1OCC(=C1)[C@H]1CC[C@]2([C@]1(C)[C@H](O)C[C@H]1[C@H]2CC[C@H]2[C@]1(C)CC[C@@H](C2)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)O)O	
O=C1OCC(=C1)[C@H]1CC[C@]2([C@]1(C)CC[C@H]1[C@H]2CC[C@H]2[C@]1(C)CC[C@@H](C2)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)O)O	
O[C@H]1CC[C@]2(C=CC[C@@H]3[C@@H]2CC[C@]2([C@H]3CC[C@@H]2C(=O)C)C1)C	(Davola et al. 2015)
CC(=O)O[C@H]1CC[C@]2(C=CCC3C2CC[C@]2(C3C[C@H]([C@@H]2C(=O)C)C(=O)O)C1)C	

CC(=O)O[C@H]1CC[C@]2(C(=CCC3C2CC[C@]2(C3C[C@H]([C@@H]2C(=O)C)C(=O)Nc2ccccc2)C)C1)C	
CC(=O)O[C@H]1CC[C@]2(C(=CCC3C2CC[C@]2(C3C[C@H]([C@@H]2C(=O)C)C(=O)N(Cc2ccccc2)C(=O)NC(C)(C)C)C)C1)C	
CC(=O)O[C@H]1CC[C@]2(C(=CCC3C2CC[C@]2(C3C[C@H]([C@@H]2C(=O)C)C(=O)N(c2ccccc2)CC(=O)NC(C)(C)C)C)C1)C	
CC(=O)O[C@H]1CC[C@]2(C(=CCC3C2CC[C@]2(C3C[C@H]([C@@H]2C(=O)C)C(=O)N(c2ccc(cc2)Cl)CC(=O)NC(C)(C)C)C)C1)C	
CC(=O)O[C@H]1CC[C@]2(C(=CCC3C2CC[C@]2(C3C[C@H]([C@@H]2C(=O)C)C(=O)N(c2ccc(cc2)F)CC(=O)NC(C)(C)C)C)C1)C	
O=C(NC(C)(C)C)CN(C(=O)[C@@H]1CC2[C@]([C@H]1C(=O)C)(C)CCC1C2CC=C2[C@]1(C)CC[C@@H](C2)O)C1cccc1	
O=C(NC(C)(C)C)CN(C(=O)[C@@H]1CC2[C@]([C@H]1C(=O)C)(C)CCC1C2CC=C2[C@]1(C)CC[C@@H](C2)O)c1ccc(cc1)Cl	
O=C(NC(C)(C)C)CN(C(=O)[C@@H]1CC2[C@]([C@H]1C(=O)C)(C)CCC1C2CC=C2[C@]1(C)CC[C@@H](C2)O)c1ccc(cc1)F	
CC(=O)O[C@H]1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@@H]2C(=O)C=C2[C@@]1(C)CC[C@@]1([C@H]2C[C@](C)(CC1)C(=O)O)C)C	(Zigolo et al. 2018)
OCCNC(=O)[C@@]1(C)CC[C@]2([C@@H](C1)C1=CC(=O)[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)OC(=O)C)C	
OCCCCNC(=O)[C@@]1(C)CC[C@]2([C@@H](C1)C1=CC(=O)[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)OC(=O)C)C	
OCC(NC(=O)[C@@]1(C)CC[C@]2([C@@H](C1)C1=CC(=O)[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)OC(=O)C)C	
CC(CNC(=O)[C@@]1(C)CC[C@]2([C@@H](C1)C1=CC(=O)[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)OC(=O)C)O	(Visalli et al. 2015)
CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C@@]1(C)C(=O)O)C(=O)O	
CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)OS(=O)(=O)C(=O)O	
CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)O)C(=O)O	
CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)CC[C@@H]1[C@]3(C)CCC(=O)C1(C)C)C(=O)O	
OC[C@@]12CC[C@H]([C@@H]2[C@@H]2[C@](CC1)(C)[C@]1(C)CC[C@@H]3[C@]([C@H]1CC2)(C)CC[C@@H](C3(C)C)O)C(=C)C	
CC(=O)OCC1O[C@@H](Oc2nnn(c2)[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C([C@@H]([C@@H]1OC(=O)C)OC(=O)C)OC(=O)C	(Boff et al. 2019)
CC(=O)OCC1O[C@@H](Oc2nnn(c2)[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C([C@@H]([C@@H]1OC(=O)C)OC(=O)C)OC(=O)C	
CC(=O)OCC1O[C@@H](Oc2nnn(c2)[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C([C@@H]([C@@H]1OC(=O)C)OC(=O)C)OC(=O)C	
OCC1O[C@@H](Oc2nnn(c2)[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C([C@@H]([C@@H]1O)O)O	
OCC1O[C@@H](Oc2nnn(c2)[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C([C@@H]([C@@H]1O)O)O	
OCC1O[C@@H](Oc2nnn(c2)[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C([C@@H]([C@@H]1O)O)O	
OCC1O[C@@H](Oc2nnn(c2)[C@H]2CC[C@]3([C@@H](C2)CC[C@@H]2[C@@H]3CC[C@]3([C@]2(O)CC[C@@H]3C2=CC(=O)OC2)C)C([C@@H]([C@@H]1O[C@@H]1OC(CO)[C@H]([C@H](C1O)O)O)O)O	
ClCC(=O)N[C@H]1CC[C@]2([C@@H](C1)CC[C@@H]1[C@@H]2CC[C@]2([C@]1(O)CC[C@@H]2C1=CC(=O)OC1)C)C	
OCCNCC(=O)N[C@H]1CC[C@]2([C@@H](C1)CC[C@@H]1[C@@H]2CC[C@]2([C@]1(O)CC[C@@H]2C1=CC(=O)OC1)C)C	
OCC(=O)N[C@H]1CC[C@]2([C@@H](C1)CC[C@@H]1[C@@H]2CC[C@]2([C@]1(O)CC[C@@H]2C1=CC(=O)OC1)C)C	
N#Cc1ccc(cc1)NCC(=O)N[C@H]1CC[C@]2([C@@H](C1)CC[C@@H]1[C@@H]2CC[C@]2([C@]1(O)CC[C@@H]2C1=CC(=O)OC1)C)C	
O=C(N[C@H]1CC[C@]2([C@@H](C1)CC[C@@H]1[C@@H]2CC[C@]2([C@]1(O)CC[C@@H]2C1=CC(=O)OC1)C)C)CN1CCC(CC1)c1cccc1	

O=C(N[C@H]1CC[C@]2([C@@H](C1)CC[C@H]1[C@H]2CC[C@]2([C@]1(O)CC[C@H]2C1=C C(=O)OC1)C)C)CNc1ccc(cc1)Cl	
O=C1OCC(=C1)[C@H]1CC[C@]2([C@]1(C)CC[C@H]1[C@H]2CC[C@H]2[C@]1(C)CC[C@@H](C2)N CCC(C(C(O)C)O)O)O	
O[C@H]1CC[C@]2([C@@H](C1)CC[C@H]1[C@H]2CC[C@]2([C@]1(O)CC[C@H]2C1=CC(=O) OC1)C)C	
CC(=C)[C@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)CC[C@@H]1[C@]3(C)CC[C@H](C1(C)C)O)C	(Heidary Navid et al. 2014)
C[C@H]1CC[C@]2([C@@H]([C@H]1C)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@H]1[C@ @]3(C)CC[C@H]([C@]1(C)C(=O)O)O)C	(Goswami et al. 2018)
C/C=C/1\C(=O)C[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC[C@@H]2[C@]1(C)C[C@H](O)[C@@H](C 2)O	
O[C@@H]([C@@H](C(O)(C)C)O)C[C@H]([C@H]1CC[C@@]2([C@]1(C)CC[C@@]13[C@H]2CC[C@ @H]2[C@]3(C1)CCC(=O)C2(C)C)C)C	(Joycharat et al. 2008)
C/C=C/1\C(=O)C[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC[C@@H]2[C@]1(C)C[C@H](O)[C@@H](C 2)O	
COC(=O)CC[C@@]12C[C@@]32CC[C@]2([C@@]([C@@H]3CC[C@H]1C(O)(C)C)(C)C[C@H]1[C@ @H]2[C@H](C)C[C@]2(O1)OC(=O)C(=C2)C)C	
CC1=C[C@@]2(OC1=O)O[C@H]1C[C@@]3([C@]([C@H]1[C@@H](C2)C)(C)CC[C@@]12[C@H]3CC [C@H]3[C@]2(C1)CCC(=O)C3(C)C)C	
COC(=O)CC[C@@]12C[C@@]32CC[C@]2([C@@]([C@@H]3CC[C@H]1C(O)(C)C)(C)C[C@H]1[C@ @H]2[C@H](C)C[C@]2(O1)OC(=O)[C@H](C2)C)C	
O=C(C[C@@H](C(=O)O)C)C[C@H]([C@H]1CC[C@@]2([C@]1(C)CC[C@@]13[C@H]2CC[C@@H]2[C@] @]3(C1)CCC(=O)C2(C)C)C)C	
COC(=O)CC[C@@]12C[C@@]32CC[C@]2([C@@]([C@@H]3CC[C@H]1C(O)(C)C)(C)CC[C@@H]2[C@ @H](CC(=O)C[C@@H](C(=O)O)C)C)C	
COC(=O)CC[C@@]12C[C@@]32CC[C@]2([C@@]([C@@H]3CC[C@H]1C(O)(C)C)(C)C[C@H]1[C@ @H]2[C@H](C)C[C@]2(O1)OC(=O)[C@H](C2)C)C	
O=C(C/C=C/(C(=O)O)C)C[C@H]([C@H]1CC[C@@]2([C@]1(C)CC[C@@]13[C@H]2CC[C@@H]2[C@] 3(C1)CCC(=O)C2(C)C)C)C	
O=C1C=C2O[C@@]3(C=C2[C@H](C(O1)(C)C)CCC[C@]1([C@@](CCC3)(C)[C@@H]2[C@@H](C1)O [C@]1[C[C@H]2C)C[C@H](C(=O)O1)C)C)O	
O=C1C=C2O[C@@H]3C=C2[C@H](C(O1)(C)C)CCC[C@]1([C@@](CCC3)(C)[C@@H]2[C@@H](C1) O[C@]1[C[C@H]2C)C[C@H](C(=O)O1)C)C	
CC[C@H]([C@H]([C@@H]([C@H](C1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@]2([C@ 1(C)CC[C@@H](C2)Br)O)C)O)C)C	
CC[C@H]([C@H]([C@@H]([C@H](C1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@]2([C@ 1(C)CC[C@@H](C2)O)F)C)O)C)C	
CC[C@H]([C@H]([C@@H]([C@H](C1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@]2([C@ 1(C)CC[C@@H](C2)O)O)C)O)C)C	
OC[C@H]1O[C@@H](OC[C@H]2O[C@H](OC[C@H]3O[C@@H](O[C@H]4[C@@H](O)C[C@]5([C@ @H](C4(CO)CO)CC[C@@]4([C@@H]5CC=C5[C@@]4(C)C[C@H]([C@@]4([C@H]5CC(C)(C)CC4)C =O)O[C@@H]4OC[C@@H]([C@@H]([C@H]4O[C@@H]4O[C@@H](C)[C@@H]([C@H]([C@H]4O)O O)O[C@@H]4OC[C@H]([C@@H]([C@H]4O)O)O)O)C)C)[C@@H]([C@H]([C@@H]3O)O)O)[C@ @H]([C@H]([C@@H]2O)O)O)[C@@H]([C@H]([C@@H]1O)O)O	
OC[C@H]1O[C@@H](OC[C@H]2O[C@H](OC[C@H]3O[C@@H](O[C@H]4[C@@H](O)C[C@]5([C@ @H](C4(CO)CO)CC[C@@]4([C@@H]5CC=C5[C@@]4(C)C[C@H]([C@@]4([C@H]5CC(C)(C)CC4)C =O)O[C@@H]4OC[C@@H]([C@@H]([C@H]4O[C@@H]4O[C@@H](C)[C@@H]([C@H]([C@H]4O)O O)O)O)O)C)C)[C@@H]([C@H]([C@@H]3O)O)O)[C@@H]([C@H]([C@@H]2O)O)O)[C@@H]([C@H] ([C@@H]1O)O)O	
OC[C@H]1O[C@@H](OC[C@H]2O[C@H](O[C@H]3[C@@H](O)C[C@]4([C@H]([C@]3(C)CO)CC[C@ @]3([C@@H]4CC=C4[C@@]3(C)C[C@H]([C@@]3([C@H]4CC(C)(C)CC3)C(=O)O[C@@H]3OC[C@ @H]([C@@H]([C@H]3O[C@@H]3O[C@@H](C)[C@@H]([C@H]([C@H]3O)O)O[C@@H]3OC[C@ H]([C@@H]([C@H]3O)O[C@@H]3OC[C@]([C@H]3O)(O)CO)O)O)O)C)C)[C@@H]([C@H]([C@@ H]2O)O)O)[C@@H]([C@H]([C@@H]1O)O)O	
OC[C@H]1O[C@@H](OC[C@H]2O[C@H](O[C@H]3[C@@H](O)C[C@]4([C@H]([C@]3(C)CO)CC[C@ @]3([C@@H]4CC=C4[C@@]3(C)C[C@H]([C@@]3([C@H]4CC(C)(C)CC3)C(=O)O[C@@H]3OC[C@ @H]([C@@H]([C@H]3O[C@@H]3O[C@@H](C)[C@@H]([C@H]([C@H]3O)O)O[C@@H]3OC[C@ H]([C@@H]([C@H]3O)O[C@@H]3OC[C@]([C@H]3O)(O)CO)O)O)O)C)C)[C@@H]([C@H]([C@@ H]2O)O)O)[C@@H]([C@H]([C@@H]1O)O)O	
OC[C@H]1O[C@@H](OC[C@H]2O[C@H](O[C@H]3[C@@H](O)C[C@]4([C@H]([C@]3(C)CO)CC[C@ @]3([C@@H]4CC=C4[C@@]3(C)C[C@H]([C@@]3([C@H]4CC(C)(C)CC3)C(=O)O[C@@H]3OC[C@ @H]([C@@H]([C@H]3O[C@@H]3O[C@@H](C)[C@@H]([C@H]([C@H]3O)O)O[C@@H]3OC[C@ H]([C@@H]([C@H]3O)O[C@@H]3OC[C@]([C@H]3O)(O)CO)O)O)O)C)C)[C@@H]([C@H]([C@@ H]2O)O)O)[C@@H]([C@H]([C@@H]1O)O)O	

OC[C@H]1O[C@@H](OC[C@H]2O[C@H](OC[C@H]3O[C@@H](O[C@H]4[C@@H](O)C[C@]5([C@H](C4(CO)CO)CC[C@@]4([C@@H]5CC=C5[C@@]4(C)C[C@H]([C@@]4([C@H]5CC(C)(C)CC4C(=O)O[C@H]4OC[C@H]([C@@H]([C@H]4O[C@@H]4O[C@H](C)[C@@H]([C@H]([C@H]4O)O)O[C@H]4OC[C@H]([C@@H]([C@H]4O)O[C@H]4OC[C@]([C@H]4O)(O)CO)O)O)O)C)[C@H]([C@H]([C@H]3O)O)O)[C@@H]([C@H]([C@H]2O)O)O)[C@@H]([C@H]([C@H]1O)O)O	
N#CC[C@@H](C(C1CCC2C(C1=C)CCC1[C@@]2(C)CC[C@@]23C1[C@@H](OC2)C(CC3)(C)C(C)C)O	(Tolmacheva et al. 2017)
N#C[C@H]([C@@H](C(C1CCC2C(C1=C)CCC1[C@@]2(C)CC[C@@]23C1[C@@H](OC2)C(CC3)(C)C(C)C)Cl)O	
COC(=O)[C@]1(C)CC[C@]2([C@@H](C1)[C@]1(C)CC[C@@]3(C=CC(=C4C3=CC(=O)C(=C4)O)O)[C@]1(CC2)C)C	(Liu et al. 2019)
COC(=O)[C@]1(C)CC[C@]2([C@@H](C1)[C@]1(C)CC[C@@]3(C=CC(=C4C3=CC(=O)C(=C4)O)O)[C@]1(CC2)C)C	
COC(=O)C([C@@H]1CC[C@@]2([C@@H]([C@@]1(C)CC(=O)O)CC=C1[C@@]2(C)CC[C@@]2([C@H]1[C@](C)(O)[C@@H](CC2)CO)C(=O)O)C(C)C	
OCC1=C(C)[C@@H]2[C@](CC1)(CC[C@@]1(C2=CC[C@H]2[C@@]1(C)CC[C@@H]1[C@]2(C)CCC(=O)[C@]1(C)CO)C)C(=O)O	
OC[C@@]1(C)[C@H](O)[C@H](O)C[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@]1(C2=C(C)[C@@H](CC1)C)C(=O)O)C)C	
OC[C@@H]1CC[C@]2([C@@H]([C@H]1C)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)[C@@H](O)C[C@H]1[C@]3(C)CCC(=O)C1(C)C)C(=O)O	
COc1cc(C=C/C(=O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3[C@@H](O)[C@H](C)CC2)C(=O)O)C)C)ccc1O	
CC(=O)[C@@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)[C@@H](O)C[C@@H]1[C@]3(C)CCC(=O)C1(C)C)C(=O)O	
CC(=O)[C@@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)C[C@@H]([C@@H]1[C@]3(C)CCC(=O)C1(C)C)O)C(=O)O	
COc1cc(C=C/C(=O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@H]3[C@@]2(C)CC[C@@]2([C@@H]3[C@@H](CC2)C(O)(C)C)C(=O)O)C)C)ccc1O	
COc1cc(C=C/C(=O)O[C@H]2[C@H](O)C[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3[C@H](C)CC2)C(=O)O)C)C)ccc1O	
OC[C@]1(C)[C@@H](OC(=O)/C=C/c2ccc(c(c2)OC)O)[C@H](O)C[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(CC1)(C)C)C(=O)O)C)C	
COc1cc(C=C/C(=O)O[C@H]2[C@H](O)C[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@H]3[C@@]2(C)CC[C@@]2([C@@H]3[C@@H](CC2)C(=C)C)C(=O)O)C)C)ccc1O	
OC[C@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1(C2=CC(=O)[C@H]2[C@@]1(C)CC[C@@]1([C@H]2[C@@H](C)[C@@H](CC1)C)C)C	
OC[C@@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1(C2=CC(=O)[C@H]2[C@@]1(C)CC[C@@]1([C@H]2[C@@H](C)[C@@H](CC1)C)C)C	
C[C@@H]1CC[C@]2([C@@H]([C@H]1C)[C@H]1C(=O)C=C3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H]([C@]1(C)C(=O)O)O)C	
CCOCC1=C(C)[C@@H]2[C@](CC1)(CC[C@@]1(C2=CC[C@H]2[C@@]1(C)CC[C@@H]1[C@]2(C)C[C@@H](O)[C@H]([C@@]1(C)CO)O)C(=O)O	
CCOCC1=C(C)[C@@H]2[C@](CC1)(CC[C@@]1(C2=CC[C@H]2[C@@]1(C)CC[C@@H]1[C@]2(C)CC[C@@H]([C@]1(C)CO)O)C)C(=O)O	
OC[C@@]1(C)C(=O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2[C@](C)(O)[C@@H](C[C@@H]1O)C)C(=O)O)C	
OC[C@@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2C=CC2=C[C@@](CC[C@@]12C)(CCC(C(=O)C)C(=O)O)C)C	
COc1cc(C=C/C(=O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3[C@@H](O)[C@H](C)CC2)C(=O)O)C)C)ccc1O	
COc1cc(C=C/C(=O)O[C@H]2[C@H](O)C[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC=C3[C@@]2(C)CC[C@@]2([C@@H]3[C@@H](CC2)C(=C)C)C(=O)O)C)C)ccc1O	
OC[C@]1(C)[C@H](O)[C@H](O)C[C@]2([C@H]1CC[C@@]1([C@@H]2[C@@H]2O[C@@H]2[C@]23[C@@]1(C)CC[C@@]1([C@H]3CC(CC1)(C)C)C(=O)O2)C)C	
COc1cc(C=C/C(=O)O[C@H]2[C@H](O)C[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@H]3[C@@]2(C)CC[C@@]2([C@@H]3[C@@H](CC2)C(=C)C)C(=O)O)C)C)ccc1O	
OC[C@]1(C)[C@H](O)[C@H](O)C[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1(C2=C(C)[C@@H](CC1)C)C(=O)O)C	
CC(=O)C(CC[C@@]1(CC[C@@]2(C=C1)C=C[C@H]1[C@@]2(C)CC[C@@H]2[C@]1(C)C[C@H]([C@@H](C2(C)C)O)O)C)C(=O)O	
C[C@@H]1CC[C@]2([C@@H]([C@H]1C)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)C[C@@H](O)[C@@H](C1(C)C)O)C(=O)O	

OC[C@]1(C)C(=O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2[C@@](C)(O)[C@@H](CC1)C)C(=O)O)C)C	
OC[C@]1(C)[C@H](O)[C@H](O)C[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2[C@@](C)(O)[C@@H](CC1)C)C(=O)O)C)C	
O[C@H]1C[C@@]2(C)[C@H](C([C@H]1O)(C)C)CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(C)(C)CC1)C(=O)O)C	
CC(=O)[C@@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)O)C(=O)O	
OC(=O)C[C@@]1(C)[C@@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=O)C)C(=O)O)C)C(=O)O)C)C(=O)O)C)C	
CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)CC[C@@H]1[C@]3(C)C[C@@H](O)[C@@H](C1(C)C)O)C(=O)O	
OC(=O)CC(=O)O[C@@H]1CC[C@]2([C@H](C1(C)C)CCC1=C2C[C@@H](O)[C@]2([C@@]1(C)CC[C@@H]2[C@@H](CC(=O)[C@H](C([C@@H](C(=O)O)C)C)C)C	(Isaka et al. 2017)
OC(=O)CC(=O)O[C@@H]1CC[C@]2([C@H](C1(C)C)CCC1=C2C[C@@H]2O[C@]3(OC(=O)[C@H](C[C@@H]3C)C)[C@H](C[C@@H]3[C@@]2([C@@]1(C)CC3)C)C)C	
OC(=O)CC(=O)O[C@@H]1CC[C@]2([C@H](C1(C)C)CCC1=C2C[C@@H]2O[C@]3(OC(=O)[C@H](C[C@@H]3C)C)[C@H](C[C@@H]3[C@@]2([C@@]1(C)CC3)C)C)C	
OC(=O)CC(=O)O[C@@H]1CC[C@]2([C@H](C1(C)C)CCC1=C2CC[C@]2([C@@]1(C)CCC2[C@@H](C)C(=O)[C@H](C[C@@H](C(=O)O)C)C)C)C	
O/N=C1\CC[C@]2(C(C1(C)C)CC[C@@]1(C2CCC2[C@@]1(C)CC[C@@]1(C2[C@@H](CC1)C(=C)C)C(=O)O)C)C	(Baltina et al. 2003)
COC(=O)[C@@H](C(C)C)NC(=O)NC12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
NNC(=O)[C@@]12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
NNC(=O)[C@@]12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CC/C(=N\O)/C3(C)C)C(=C)C	
CSCC[C@@H](C(=O)OC)NC(=O)[C@@]12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
COC(=O)[C@@H](NC(=O)[C@@]12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
OCCNC(=O)[C@@]12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
O=C=N[C@@]12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
COC(=O)[C@H](NC(=O)NC12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)C)C(=O)C3(C)C)C(=C)C)CC(C)C	
CSCC[C@H](C(=O)OC)NC(=O)NC12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CC/C(=N\O)/C3(C)C)C(=C)C	
CCCCCCCCCCCCCCCCCCCCNC(=O)[C@@]12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
COC(=O)[C@@H](NC(=O)[C@@]12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C)CC(C)C	
COC(=O)[C@H](C(C)C)NC(=O)[C@@]12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
CSCC[C@H](C(=O)OC)NC(=O)NC12CC[C@H](C2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C[C@H]1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
CC(=C)[C@@H]1CC[C@]2(C1C1CC[C@H]3[C@@]([C@@]1(C)CC2)(C)CCC1[C@]3(C)CCC(=O)C1(C)C)C(=O)N	
OC/C(=C/CC[C@H](C[C@H]1CC[C@@]2([C@]1(C)CC=C1C2=CC[C@@H]2[C@]1(C)CC[C@@H](C2(C)C)O)C)C)/C	(Mothana et al. 2003)
OC/C(=C/CC[C@H](C[C@H]1CC[C@@]2([C@]1(C)CCC1=C2C(=O)C[C@@H]2[C@]1(C)CC[C@@H](C2(C)C)O)C)C)/C	
O=C(C[C@](C1=C[C@@H](C[C@@]2([C@]1(C)C(=O)C=C1[C@]32O[C@@H]3C[C@@H]2[C@]1(C)C)CC(=O)C2(C)C)O)(O)C)CC(C(=O)O)C	
CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]1CCC3[C@@]([C@]1(C)CC2)(C)CCC1[C@]3(C)CCC(=O)C1(C)C)C(=O)O	(Baltina et al. 2003)
CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]1CCC3[C@@]([C@]1(C)CC2)(C)CCC1[C@]3(C)CC[C@@H](C1(C)C)O)C(=O)O	

O/N=C/1\CC[C@]2(C(C1(C)C)CC[C@@]1(C2CC[C@H]2[C@@]1(C)CC[C@@]1([C@@H]2[C@@H](C1)C(=C)C)C(=O)O)C)C	
NNC(=O)[C@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
NNC(=O)[C@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CC/C(=N\O)/C3(C)C)C(=C)C	
O=C=N[C@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
COC(=O)[C@@H](C(C)C)NC(=O)N[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
COC(=O)[C@H](NC(=O)N[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1C C2)(C)CCC(=O)C3(C)C)C(=C)C)CC(C)C	
CSCC[C@H](C(=O)OC)NC(=O)N[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
CSCC[C@H](C(=O)OC)NC(=O)N[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CC/C(=NO)/C3(C)C)C(=C)C	
CCCCCCCCCCCCCCCCCNC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
OCCNC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
COC(=O)[C@@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1C C2)(C)CCC(=O)C3(C)C)C(=C)C)C	
COC(=O)[C@H](C(C)C)NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
COC(=O)[C@@H](NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1C C2)(C)CCC(=O)C3(C)C)C(=C)C)CC(C)C	
CSCC[C@@H](C(=O)OC)NC(=O)[C@@]12CC[C@H]([C@@H]2C2[C@@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CCC(=O)C3(C)C)C(=C)C	
CC(=C)[C@@H]1CC[C@]2([C@H]1C1CCC3[C@@]([C@@]1(C)CC2)(C)CCC1[C@]3(C)CCC(=O)C1(C)C)C(=O)N	(Lv et al. 2016)
OC[C@H]1O[C@@H](O[C@@H]2CCC3=C(C2(C)C)CC[C@@H]2[C@@H](C3)CC[C@]3([C@]2(CC[C@H]3[C@@H]3[C@@H](CCC(=O)C(O)(C)C)C(=O)O)C)[C@@H]([C@H]([C@@H]1O)O)O	
C[C@@H]([C@H]1CC[C@@]2([C@]1(C)CC[C@H]1[C@H]2CCC2=C(C1)CC[C@H](C2(C)C)O)C(=O)O)CCC(=O)C(O)(C)C	
C[C@@H]([C@H]1CC[C@@]2([C@]1(C)CC[C@H]1[C@H]2CCC2=C(C1)CC[C@H](C2(C)C)O)C(=O)O)CC[C@H](C(O)(C)C)O	
CC(=O)OCC1O[C@@H](O[C@@H]2CC=C3[C@H](C2(C)C)CC[C@@H]2[C@@H](C3)CC[C@]3([C@]2(CC[C@H]3[C@@H]3[C@@H](CC[C@@H](C(O)(C)C)O[C@H]2OC[C@@H]([C@H](C2O)O)O)C(=O)O)C)C([C@@H]([C@@H]1O)O)O	
C[C@@H]([C@H]1CC[C@@]2([C@]1(C)CCC1=C2CC[C@@H]2[C@]1(C)CCC(C2(C)C)O)C(=O)O)CC[C@@H](C(O)(C)C)O	
C[C@@H]([C@H]1CC[C@@]2([C@]1(C)CCC1=C2CC[C@@H]2[C@]1(C)CCC(C2(C)C)O)C(=O)O)CC[C@@H](C(O)(C)C)O	
CC(=O)OCC1O[C@@H](OC2CC[C@]3([C@H](C2(C)C)CCC2=C3CC[C@]3([C@]2(CC[C@H]3[C@@H]3[C@@H](CC[C@@H](C(O)(C)C)O)C(=O)O)C)C([C@@H]([C@@H]1O)O)O	
OCC1O[C@H](O[C@H](C(O)(C)C)CC[C@H]([C@H]2CC[C@@]3([C@]2(C)CCC2=C3CC[C@@H]3[C@]2(C)CCC(C3(C)C)O)C(=O)O)C)C([C@@H]([C@@H]1O)O)O	
CC([C@@H](O[C@H]1OC[C@H]([C@H](C1O)O)O)CC[C@H]([C@H]1CC[C@@]2([C@]1(C)CCC1=C2CC[C@@H]2[C@]1(C)CCC(C2(C)C)O)C(=O)O)C)C(=O)O)C	
OC[C@]1(C)[C@H](O)[C@H](O)C[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@]13C2=C(C)[C@](CC1)(OO3)C)C)C	(Liu et al. 2018)
OC[C@@]1(C)[C@H](O)[C@H](O)C[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CCC(=C2C(=O)C)CCC(=O)C)C)C	
OC[C@]1(C)[C@H](O)[C@H](O)C[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CCc1c2c(C)c(cc1)C)C)C	
OC[C@@]1(C)[C@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]13C2=C(C)[C@](CC1)(OO3)C)C)C	
OC[C@]1(C)[C@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@]13C2=C(C)[C@](CC1)(OO3)C)C)C	
OC[C@]1(C)[C@H](O)[C@H](O)[C@H]([C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CCc1c2c(C)c(cc1)C)C)C)O	

OC[C@@]1(C)[C@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CCc1c2c(C)c(cc1)C)C)C	
OC[C@@]1(C)[C@H](O)[C@H](O)C[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CCc1c2c(C)c(cc1)C)C)C	
OC[C@@]1(C)[C@H](O)C[C@H]([C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CCc1c2c(C)c(cc1)C)C)C)O	
CO[C@@H]1[C@@H](O)[C@H](O[C@@H]2[C@@H](O)[C@H](O[C@@H]3[C@@H](C)O[C@H]([C@@H]([C@H]3O)O)O[C@H]3[C@@H](OC[C@H]([C@@H]3O)OS(=O)(=O)[O-])O[C@H]3CC[C@]4([C@H](C3(C)C)CC=C3[C@@H]4CC[C@]45[C@@]3(C)C[C@H]([C@@H]5[C@](OC4=O)(C)CCC=C(C)C)OC(=O)C)O[C@H]([C@H]2O)COS(=O)(=O)[O-])O[C@@H]([C@H]1O)COS(=O)(=O)[O-].[Na+].[Na+].[Na+]	(Maier et al. 2001)
CO[C@@H]1[C@@H](O)[C@H](O[C@@H]2[C@@H](O)[C@H](O[C@@H]3[C@@H](C)O[C@H]([C@@H]([C@H]3O)O)O[C@H]3[C@@H](OC[C@H]([C@@H]3O)OS(=O)(=O)[O-])O[C@H]3CC[C@]4([C@H](C3(C)C)CC=C3[C@@H]4CC[C@]45[C@@]3(C)C[C@H]([C@@H]5[C@](OC4=O)(C)CCCC(C)C)OC(=O)C)O[C@H]([C@H]2O)COS(=O)(=O)[O-])O[C@@H]([C@H]1O)COS(=O)(=O)[O-].[Na+].[Na+].[Na+]	
CO[C@@H]1[C@@H](O)[C@H](O[C@@H]2[C@@H](O)[C@H](O[C@@H]3[C@@H](C)O[C@H]([C@@H]([C@H]3O)O)O[C@H]3[C@@H](OC[C@H]([C@@H]3O)OS(=O)(=O)O)O[C@H]3CC[C@]4([C@H](C3(C)C)CC=C3[C@@H]4CC[C@]45[C@@]3(C)C[C@H]([C@@H]5[C@](OC4=O)(C)CCC=C(C)C)OC(=O)C)O[C@H]([C@H]2O)COS(=O)(=O)O.[NaH]	
CO[C@@H]1[C@@H](O)[C@H](O[C@@H]2[C@@H](O)[C@H](O[C@@H]3[C@@H](C)O[C@H]([C@@H]([C@H]3O)O)O[C@H]3[C@@H](OC[C@H]([C@@H]3O)OS(=O)(=O)O)O[C@H]3CC[C@]4([C@H](C3(C)C)CC=C3[C@@H]4CC[C@]45[C@@]3(C)C[C@H]([C@@H]5[C@](OC4=O)(C)CCCC(C)C)OC(=O)C)O[C@H]([C@H]2O)COS(=O)(=O)O.[NaH]	
CO[C@@H]1CO[C@H]([C@@H]([C@H]1O)O)OCC[C@H](C(C)C)CC[C@H]([C@H]1[C@@H](O)[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(O)C[C@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)OS(=O)(=O)[O-])O)C.[Na+]	(Wang et al. 2002)
OC[C@H]1O[C@H]([C@@H]([C@H]1O)O[C@H]1OC[C@H]([C@@H]([C@H]1OC)O)OC)O[C@H](C(C)C)CC[C@H]([C@H]1C[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(O)C[C@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)O)OS(=O)(=O)[O-])O)C.[Na+]	
OC[C@H]1O[C@H]([C@@H]([C@H]1O)O[C@H]1OC[C@H]([C@@H]([C@H]1OC)O)OC)O[C@H](C(C)C)CC[C@H]([C@H]1C[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(C)[C@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)O)O)C	
CO[C@H]1[C@@H](OC[C@H]([C@@H]1O)O)O[C@H]1[C@H](OCC(C=C)CC[C@H]([C@H]2[C@H]([C@@H]3[C@]2(C)CC[C@H]2[C@@]3(O)C[C@H]([C@@H]3[C@]2(C)CC[C@H]([C@@H]3O)O)O)C)OC[C@H]([C@@H]1OS(=O)(=O)[O-])O.[Na+]	
OC[C@H]1O[C@H]([C@@H]([C@H]1O)O[C@H]1OC[C@H]([C@@H]([C@H]1OC)O)OC)O[C@H](C(C)C)CC[C@H]([C@H]1C[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(C)[C@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)O)O)C	
CO[C@H]1[C@@H](OC[C@H]([C@@H]1O)O)O[C@H]1[C@H](OC[C@H]([C@@H]([C@H]1OC)O)OC)O[C@H]([C@@H]2[C@H]([C@@H]3[C@]2(C)CC[C@H]2[C@@]3(O)C[C@H]([C@@H]3[C@]2(C)CC[C@H]([C@@H]3O)O)O)C)OC[C@H]([C@@H]1OS(=O)(=O)[O-])O.[Na+]	
CO[C@@H]1CO[C@H]([C@@H]([C@H]1O)O)OCC[C@H](C(C)C)CC[C@H]([C@H]1[C@@H](O)[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(C)[C@H]([C@@H]2O)OS(=O)(=O)[O-])O)C.[Na+]	
CO[C@H]1[C@@H](OC[C@H]([C@@H]1O)O)O[C@H]1[C@H](OCC(C=C)CC[C@H]([C@H]2[C@H]([C@@H]3[C@]2(C)CC[C@H]2[C@@]3(O)C[C@H]([C@@H]3[C@]2(C)CC[C@H]([C@@H]3O)O)O)C)OC[C@H]([C@@H]1O)O	
CO[C@H]1[C@@H](OC[C@H]([C@@H]1O)O)O[C@H]1[C@@H](OC[C@H]([C@@H]1OS(=O)(=O)[O-])O)OCC(C=C)CC[C@H]([C@H]1C[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(O)C[C@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)O)O)C.[Na+]	
CO[C@H]1[C@@H](OC[C@H]([C@@H]1O)O)O[C@H]1[C@H](OCC(C=C)CC[C@H]([C@H]2[C@H]([C@@H]3[C@]2(C)CC[C@H]2[C@@]3(O)C[C@H]([C@@H]3[C@]2(C)CC[C@H]([C@@H]3O)O)O)C)OC[C@H]([C@@H]1OS(=O)(=O)O)O.[NaH]	
CO[C@H]1[C@@H](OC[C@H]([C@@H]1O)O)O[C@H]1[C@@H](OC[C@H]([C@@H]1OS(=O)(=O)O)O)OCC(C=C)CC[C@H]([C@H]1C[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(O)C[C@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)O)O)C.[NaH]	
CO[C@H]1[C@@H](OC[C@H]([C@@H]1O)O)O[C@H]1[C@H](OC[C@H]([C@@H]([C@H]1OC)O)OC)O[C@H]([C@@H]2[C@H]([C@@H]3[C@]2(C)CC[C@H]2[C@@]3(O)C[C@H]([C@@H]3[C@]2(C)CC[C@H]([C@@H]3O)O)O)C)OC[C@H]([C@@H]1OS(=O)(=O)O)O.[NaH]	

OC[C@@H]1O[C@H]([C@@H]([C@H]1O)O)[C@@H]1OC[C@H]([C@@H]([C@H]1OC)O)OC)O[C@H](C(C)C)CC[C@H]([C@H]1C[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(O)C[C@@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)O)O)C	
OC[C@H]1O[C@H]([C@@H]([C@H]1O)O)[C@@H]1OC[C@H]([C@@H]([C@H]1OC)O)OC)O[C@H](C(C)C)CC[C@H]([C@H]1C[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(O)C[C@@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)O)OS(=O)(=O)O)O)C.[NaH]	
CO[C@@H]1CO[C@H]([C@@H]([C@H]1O)O)OCC[C@H](C(C)C)CC[C@H]([C@H]1[C@@H](O)[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(O)C[C@@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)O)OS(=O)(=O)O)O)C.[NaH]	
CO[C@@H]1CO[C@H]([C@@H]([C@H]1O)O)OCC[C@H](C(C)C)CC[C@H]([C@H]1[C@@H](O)[C@H]([C@@H]2[C@]1(C)CC[C@H]1[C@@]2(C)[C@@H]([C@@H]2[C@]1(C)CC[C@H]([C@@H]2O)O)OS(=O)(=O)O)O)C.[NaH]	
O=C1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@@H]2CC[C@H]2[C@@]1(C)CCC1[C@]2(C)CC[C@@H]1C(O)(C)C)C	
O[C@H]1C[C@@H]2[C@@]3(C)CCC(=O)C([C@@H]3CC[C@]2([C@@]2([C@@]31OC(=O)[C@]1([C@H]3[C@@H](C)C(C)C)CC1)CC2)C)C(C)C	
CC(=CCC[C@]([C@H]1CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@H]2[C@]1(C)CCC(=O)C2(C)C)C(O)C)C	
CC(=CCC[C@]([C@H]1CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@H]2[C@]1(C)CC[C@@H](C2(C)C)O)C)C	
OC(=O)CC[C@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@H]1[C@]1(C)C[C@@H](O1)C(O)(C)C)C(=C)C	(Poehland et al. 1987)
OC(=O)CC[C@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@H]1[C@]1(C)C[C@@H](O1)C(O)(C)C)C(=C)C	
C[C@@H]1CC[C@]2([C@@H]([C@H]1C)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)C)CC[C@@H]1[C@@]3(C)CCC(=O)C1(C)C)C(=O)O	
CC(=CCCC(=C)[C@H]1CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@H]2[C@]1(C)CC[C@@H](C2(C)C)O)C)C	
OC(=O)CC[C@]1(C)[C@H](CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@@H]1[C@](CCC(=C(C)C)O)C)C(=C)C	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](OC[C@@H]([C@@H]2O)O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O[C@@H]2O[C@@H](C)[C@@H]([C@H]2O)O)O)O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@]34[C@@]2(C)C[C@H]([C@@]2([C@H]4CC(C)(C)CC2)CO3)O)C)[C@@H]([C@H]([C@@H]1O)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](OC[C@@H]([C@@H]2O)O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O[C@@H]2O[C@@H](C)[C@@H]([C@H]2O)O)O)O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@]34[C@@]2(C)C[C@H]([C@@]2([C@H]4C[C@@](C)(C=O)CC2)CO3)O)C)[C@@H]([C@H]([C@@H]1O)O)O	(Bloor and Qi 1994)
OC[C@H]1O[C@@H](O[C@H]2[C@@H](OC[C@@H]([C@@H]2O)O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O[C@@H]2O[C@@H](C)[C@@H]([C@H]2O)O)O)O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@]34[C@@]2(C)C[C@H]([C@@]2([C@H]4CC(C)(C)CC2)CO3)O)C)[C@@H]([C@H]([C@@H]1O)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](OC[C@@H]([C@@H]2O)O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O[C@@H]2O[C@@H](C)[C@@H]([C@H]2O)O)O)O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@]34[C@@]2(C)C[C@H]([C@@]2([C@H]4CC(C)(C)CC2)CO3)O)C)[C@@H]([C@H]([C@@H]1O)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](OC[C@@H]([C@@H]2O)O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O[C@@H]2O[C@@H](C)[C@@H]([C@H]2O)O)O)O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@]34[C@@]2(C)C[C@H]([C@@]2([C@H]4CC(C)(C)CC2)CO3)O)C)[C@@H]([C@H]([C@@H]1O)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](OC[C@@H]([C@@H]2O)O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O[C@@H]2O[C@@H](C)[C@@H]([C@H]2O)O)O)O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@]34[C@@]2(C)C[C@H]([C@@]2([C@H]4CC(C)(C)CC2)CO3)O)C)[C@@H]([C@H]([C@@H]1O)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](OC[C@@H]([C@@H]2O)O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O[C@@H]2O[C@@H](C)[C@@H]([C@H]2O)O)O)O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC[C@]34[C@@]2(C)C[C@H]([C@@]2([C@H]4CC(C)(C)CC2)CO3)O)C)[C@@H]([C@H]([C@@H]1O)O)O	

O=C1O[C@]23[C@](C1)(O)OC([C@@H]3C[C@@H])([C@@H]1[C@@]3(C2)CC[C@]2([C@]4([C@](O3)(C1=O)O[C@H]1[C@@H])([C@H]4[C@H](C2=O)C)OC(=O)[C@]1(C)O)C)O)(C)C	(Cheng et al. 2010)
O=C1O[C@]23[C@](C1)(O)OC([C@@H]3C[C@@H])([C@@H]1[C@@]3(C2)CC[C@]2([C@]4([C@](O3)(C1=O)O[C@H]1[C@@H])([C@H]4[C@H](C2=O)C)C)O)(C)C	
O=C1C[C@H]([C@H](O1)[C@@H](/C=C\1/C=C(C(=O)O1)C)C)[C@H]1C[C@]2([C@@H]([C@H]1O)C[C@H]1[C@@]3(C2)OC(=O)C[C@@]3(O)OC1(C)C)O	
O=C1O[C@]23[C@](C1)(O)OC([C@@H]3C[C@@H])([C@@H]1[C@@]3(C2)CC[C@]2([C@H]4[C@]([O3)(C1=O)O[C@H]1[C@@H])([C@H]4[C@H](C2=O)C)OC(=O)[C@]1(C)O)C)O)(C)C	
O=C1C[C@@H]2[C@@]3(O1)[C@@H](O)[C@]14CC[C@]5([C@@H]([C@](O1)(C(=O)[C@@H]4CC[C@H]3C(O2)(C)C)O)[C@H]5[C@@H])([C@@H]([C@@H]1C[C@H](C(=O)O1)C)O)C)C	
O=C1O[C@@H](C[C@H]1C)[C@H]([C@H]([C@@H]1[C@H]2[C@]1(C)CC[C@@]13O[C@]2(O)C(=O)[C@@H]1CC[C@H]1[C@@H]1[C@@]2([C@H]3O)OC(=O)[C@@H]([C@H]2OC1(C)C)O)C)O	
O=C1O[C@]23[C@](C1)(O)OC([C@@H]3C[C@@H])([C@@H]1[C@@]3(C2)CC[C@]2([C@H]4[C@]([O3)(C1=O)O[C@H]1[C@@H])(C)C(=O)O[C@@H]1[C@H]4[C@@H](C2=O)C)C)O)(C)C	
O=C1O[C@]23[C@](C1)(O)OC([C@@H]3C[C@@H])([C@@H]1[C@@]3(C2)CC[C@]2([C@H]4[C@]([O3)(C1=O)O[C@H]1[C@@H])(C)C(=O)O[C@@H]1[C@H]4[C@@H](C2=O)C)C)O)(C)C	
CC(=O)O[C@@H]([C@H]([C@@H]1[C@H]2[C@]1(C)CC[C@@]13O[C@]2(O)C(=O)[C@@H]1CC[C@@H]1[C@@]2([C@H]3O)OC(=O)C[C@H]2OC1(C)C)C)[C@@H]1C=C(C(=O)O1)C	
CC(=O)O[C@@H]([C@H]([C@@H]1[C@H]2[C@]1(C)CC[C@@]13O[C@]2(O)C(=O)[C@@H]1CC[C@@H]1[C@@]2([C@H]3O)OC(=O)C[C@H]2OC1(C)C)C)[C@@H]1C[C@H](C(=O)O1)C	
COC(=O)C1(O)OCC23C1C(C)(C(C1C3C(C(C2OC(=O)C=Cc2ccccc2)O)(C)CO1)O)C12OC2(C)C2CC1OC1C2(O)C=CO1	(Liu et al. 2017)
C[C@@H]1CC[C@]2([C@@H]([C@H]1C)[C@]1(C)CC[C@@]3([C@@]([C1=CC2)(C)[C@@H](O)C[C@@]1([C@@H](C3=O)C[C@@H](C1(C)C)O)O)C)C	
C[C@@H]1CC[C@]2([C@@H]([C@H]1C)[C@]1(C)CC[C@@]3([C@@]([C1=CC2=O)(C)[C@@H](O)C[C@@]1([C@@H](C3=O)C[C@@H](C1(C)C)O)O)C)C	
O[C@H]1C[C@]2(C)C[C@@H](O)[C@]3([C@H]([C@@H]2[C@H])([C@@H]1C)C)CC=C1C3=CC=C2[C@]1(C)CCC(=O)C2(C)C	
COC(=O)[C@]12CC[C@H]([C@@H]2[C@@H]2[C@](CC1)(C)[C@]1(C)CC[C@@H]3[C@]([C@H]1CC2)(C)c1c(=O)c2ccccc2[nH]c1C3(C)C)C(=O)C	(Khusnutdinova et al. 2019)
O=c1c2ccccc2[nH]c2c1[C@@]1(C)[C@H](C2(C)C)CC[C@@]2([C@@H]1CC[C@H]1[C@@]2(C)CC[C@]23[C@@H]1[C@@H](OC3=O)C(C)(C)CC2)C	
OC[C@H]1O[C@@H](O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3C[C@@H](O)[C@H]3[C@@]2(C)CC[C@@H]3[C@](CCC=C(C)C)(O)C)C)[C@@H]([C@H]([C@@H]1O)O)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O[C@@H]1OC[C@H]([C@@H]([C@H]1O)O)O)O)O	(Pei et al. 2011)
C[C@@H]1C[C@@H]2[C@@](CC1=O)(C)CC[C@]1([C@@]2(C)CC=C2[C@@]1(C)C=Cc1c2cc(O)c(c1C)O)C	(Sotanaphun et al. 2005)
C[C@@H]1C[C@@H]2[C@@]([C@H](C1=O)O)(C)CC[C@]1([C@@]2(C)CC=C2[C@@]1(C)C=Cc1c2cc(O)c(c1C)O)C	
Oc1cc2c(c(c1O)C)C=C[C@@]1(C2=CC[C@@]2([C@]1(C)CC[C@@]1([C@H]2C[C@](C)(O)C(=O)C1)C)C	
CC1=C2CC[C@@]3([C@]([C@@H]4C2C(C=C1)C(=C(C4=O)O)C)(C)CC[C@@]1([C@H]3C[C@@](C)(O)C(=O)C1)C)C	
CC1=C[C@@H]2[C@@](CC1=O)(C)CC[C@]1([C@@]2(C)CC=C2[C@@]1(C)C=Cc1c2cc(O)c(c1C)O)C	
CC(=O)C[C@H]1C=C2C(=CC[C@@]3([C@]2(C)CC[C@@]2([C@H]3C[C@H](C(=O)C2)C)C)c2c1c(C)c(c(c2)O)O	
CC(=O)C[C@H]1C=C2C(=CC[C@@]3([C@]2(C)CC[C@@]2([C@H]3C[C@H](C(=O)[C@@H]2O)C)C)c2c1c(C)c(c(c2)O)O	
CC(=O)C[C@H]1C=C2C(=CC[C@@]3([C@]2(C)CC[C@@]2([C@H]3C[C@](C(=O)C2)(C)O)C)C)c2c1c(C)c(c(c2)O)O	
CC(=O)/C=c\1/cc2c(=CC[C@@]3([C@]2(C)CC[C@@]2([C@H]3C[C@@H](C(=O)[C@@H]2O)C)C)c2c1c(C)c(O)c(c2)O	
CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]1CC[C@H]3[C@@]([C@]1(C)CC2)(C)CC[C@@H]1[C@]3(C)CCC(=O)C1(C)C)C	(Madureira et al. 2003)
CC(=O)O[C@H]1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@@H]2CC[C@H]2[C@@]1(C)CCC1=CCC[C@H]([C@H]21)C(=C)C)C)C	(Flekhter et al. 2007)
CC(=C)[C@@H]1CCC=C2[C@H]1[C@H]1CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)O	
CC(=O)O[C@H]1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@@H]2CC[C@H]2[C@@]1(C)CC[C@@]13[C@@H]2C2CCC(O1)O[C@]2(O3)C)C)C	

N#CC[C@@]1(C)C(CC[C@@]2(C1CC[C@H]1[C@@]2(C)CC[C@@]2([C@H]1[C@@H](CC2)C(=C)C)C(=O)NCCC(=O)OC)C(C=O)(C)C	(Tolmacheva et al. 2013)
N#CC[C@@]1(C)C(CC[C@@]2(C1CC[C@H]1[C@@]2(C)CC[C@@]2([C@H]1[C@@H](CC2)C(=C)C)C(=O)Nc1ncs1)C(C=O)(C)C	
CCOC(=O)CNC(=O)C(C1CC[C@@]2(C([C@@]1(C)CC#N)CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=C)C)C(=O)OC)C(C)C	
N#CC[C@@]1(C)C(CC[C@@]2(C1CC[C@H]1[C@@]2(C)CC[C@@]2([C@H]1[C@@H](CC2)C(=C)C)C(=O)OC)C(C(=O)Nc1ncs1)(C)C	
CCOC(=O)CCNC(=O)C(C1CC[C@@]2(C([C@@]1(C)CC#N)CC[C@H]1[C@@]2(C)CC[C@@]2([C@@H]1[C@@H](CC2)C(=C)C)C(=O)NCCC(=O)OCC)C(C)C	
OC[C@]12CC[C@H](CC1=CC[C@H]1[C@H]2CC[C@]2([C@H]1CC[C@H]2[C@@H](OC(=O)C)C)OC(=O)C	(Petrera et al. 2003)
O=C[C@]12CC[C@H](CC1=CC[C@H]1[C@H]2CC[C@]2([C@H]1CC[C@H]2[C@@H](OC(=O)C)C)OC(=O)C	
CO/C=C/[C@]12CC[C@H](CC1=CC[C@H]1[C@H]2CC[C@]2([C@H]1CC[C@H]2[C@@H](OC(=O)C)C)O	
CO/C=C/[C@]12CC[C@H](CC1=CC[C@H]1[C@H]2CC[C@]2([C@H]1CC[C@H]2[C@@H](OC(=O)C)C)OC(=O)C	
CC(=O)O[C@H]1CC[C@]23[C@@](C1)(Cl)C(C[C@H]1[C@@H]3CC[C@]3([C@H]1CC[C@H]3[C@@H](OC(=O)C)C)C[C@H]2O	
CC(=O)O[C@H]1CC[C@]23[C@@](C1)(Cl)C(CC2)C[C@H]1[C@@H]3CC[C@]2([C@H]1CC[C@H]2[C@@H](OC(=O)C)C)C	(Yoneda et al. 2018)
O=C1CC[C@]23C(=C1)C(CC2)C[C@H]1[C@@H]3CC[C@]2([C@H]1CC[C@H]2C(=O)C)C	
C/C=C/C(=O)O[C@H]1[C@H](OC(=O)C(=C/C)C(C)C)C[C@H]2[C@@]1(CO)[C@H](O)C[C@@]1(C2=CCC2[C@@]1(C)CCC1[C@]2(C)CC[C@H](C1(C)C)O)C	
C/C=C/C(=O)O[C@H]1[C@H](OC(=O)C(=C/C)C(C)C)C[C@H]2[C@@]1(CO)[C@H](O)[C@H](O)[C@@]1(C2=CCC2[C@@]1(C)CCC1[C@]2(C)CC[C@H](C1(C)C)O)C	
C/C=C/C(=O)O[C@H]1[C@H](O)[C@]2(COC(=O)C)[C@H](O)C[C@@]3(C(=CCC4[C@@]3(C)CCC3[C@]4(C)CC[C@H](C3(C)C)O)[C@H]2CC1(C)C)C	
C/C=C/C(=O)O[C@H]1[C@H](O)[C@]2(CO)[C@H](O)C[C@@]3(C(=CC[C@H]4[C@@]3(C)CC[C@H]3[C@]4(C)CC[C@H](C3(C)C)O)[C@H]2CC1(C)C)C	(Kinjo et al. 2000)
OC[C@]12[C@H](O)C[C@@]3(C(=CCC4[C@@]3(C)CCC3[C@]4(C)CC[C@H](C3(C)C)O)[C@H]2CC[C@@]1(C)C)C	
OC[C@@]1(C)[C@H](CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC[C@H]1O)(C)C)C)O[C@H]1O[C@H](C(=O)O)[C@H]([C@H]([C@H]1O[C@@H]1OC[C@H]([C@H]([C@H]1O[C@@H]1O[C@@H](C)[C@H]([C@H]1O)O)O)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@H]([C@H]([C@H]2O)O)C(=O)O)O[C@H]2CC[C@]3([C@H]([C@@]2(C)CO)CC[C@@]2([C@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3CC(C)C)C[C@H]2O)C)C)[C@@H]([C@H]([C@H]1O)O)O[C@@H]1O[C@@H](C)[C@H]([C@@H]([C@H]1O)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@H]3[C@]4([C@@]5([C@H]2C(C)(C)[C@H](CC5)O[C@@H]2OC[C@H]([C@@H]([C@H]2OC(=O)C)O)O)C4)CC[C@]2([C@@]3(C)C[C@H]([C@@H]2[C@@]2(C)CC[C@H](O2)C(O)(C)C)O)C)[C@@H]([C@H]([C@H]1O)O)O	
OCC1OC(OC2C(OC(C2O)C(=O)O)OC2CCC3(C2(C)C)CCC2(C3CC=C3C2(C)CCC2(C3CC(C)(C)CC2O)C)C(C(C1O)O)OC1OC(C)C(C(C1O)O)O	
O[C@@H]1[C@@H](O[C@H]2OC[C@@H]([C@@H]([C@H]2O[C@@H]2O[C@@H](C)[C@@H]([C@H]([C@H]2O)O)O)O)O)[C@@H](O[C@H]([C@H]1O)C(=O)O)O[C@H]1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(C)(C)C[C@H]1O)C)C	
OC[C@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@H]([C@H]([C@H]2O)O)C(=O)O)O[C@H]2CC[C@]3([C@H]([C@@]2(C)CO)CC[C@@]2([C@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3CC(C)(C)C[C@H]2O)C)C)[C@@H]([C@H]([C@H]1O)O)O	
OC[C@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@H]([C@H]([C@H]2O)O)C(=O)O)O[C@H]2CC[C@]3([C@H]([C@@]2(C)CO)CC[C@@]2([C@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3CC(C)(C)C[C@H]2O)C)C)[C@@H]([C@H]([C@H]1O)O)O	
O[C@@H]1[C@@H](O)[C@@H](O[C@H]([C@H]1O)C(=O)O)O[C@H]1CC[C@]2([C@H](C1(C)C)C[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(C)(C)C[C@H]1O)C)C	
OC[C@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@H]([C@H]([C@H]2O)O)C(=O)O)O[C@H]2CC[C@]3([C@H]([C@@]2(C)CO)CC[C@@]2([C@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3CC(C)(C)C[C@H]2O)C)C)[C@@H]([C@H]([C@H]1O)O)O	

O=C(CN1C(=O)CC(C1=O)NC(=O)OCc1cccc1)NCC(=O)Oc1ccc(cc1)[N+](=O)[O-]	
OC[C@@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@@H]2CC(C[C@H]1O)(C)C)C)C	
O[C@H]1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(C)C)[C@H]1O)C)C	
OC[C@@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@@H]2CC(C1=O)(C)C)C)C	
COC(=O)[C@@]1(C)CC[C@]2([C@H](C1)C1=CC(=O)[C@H]3[C@@]([C@@]1(CC2)C)(C)CCC1[C@]3(C)CC[C@@H](C1(C)C)O)C	
OC[C@@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@@H]2CC([C@H]([C@H]1O)O)(C)C)C)C	
OC[C@@]1(C)C[C@H]2C3=CC[C@H]4[C@@]([C@]3(C)CC[C@]2([C@@H]([C@@H]1O)O)(C)CC[C@@H]1[C@]4(C)CC[C@@H]([C@]1(C)CO)O	
OC[C@@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@@H]2C[C@]([C@H]([C@H]1O)O)(C)C(=O)O)C)C	
COC(=O)[C@@]1(C)C[C@H]2C3=CC[C@H]4[C@@]([C@]3(C)CC[C@]2([C@@H]([C@@H]1O)O)(C)CC[C@@H]1[C@]4(C)CC[C@@H]([C@]1(C)CO)O	
OC[C@@]1(C)C[C@H]2C3=CC[C@H]4[C@@]([C@]3(C)CC[C@]2([C@@H]([C@@H]1O)O)(C)CC[C@@H]1[C@]4(C)CC[C@@H]([C@]1(C)CO)O	
OC[C@@]1(C)C[C@@H](O)[C@]2([C@@H](C1)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H]([C@@]1(C)CO)O)C	
OC[C@]1(C)C[C@@H](O)[C@]2([C@@H](C1)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H]([C@]1(C)CO)O)C	
OC[C@@]1(C)C[C@@H](O)[C@]2([C@@H](C1)C1=CC[C@H]3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H]([C@]1(C)CO)O)C	
OC[C@@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@@H]2CC([C@H](C1)O)(C)C)C)C	
OC[C@@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@@H]2CC(C=C1)(C)C)C)C	
OC[C@]1(C)[C@@H](O)CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@@H]2CC(CC1)(C)C(=O)O)C)C	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](O[C@@H]([C@H]([C@@H]2O)O)C(=O)O)O[C@H]2CC[C@]3([C@H]([C@@]2(C)CO)CC[C@@]2([C@@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3CC(C)(C)C[C@H]2O)C)C)[C@@H]([C@H]([C@H]1O)O)O[C@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1O)O)O	
O[C@H]1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(C)C)CC1)C(=O)O)C	
O[C@@H]1[C@@H](O[C@H]2O[C@H](C(=O)O)[C@H]([C@@H]([C@H]2O)O)O)[C@H](O[C@@H]([C@H]1O)C(=O)O)O[C@H]1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@@H]2C(=O)C=C2[C@@]1(C)CC[C@@]1([C@H]2C[C@]([C@]([C@]1O)O)(C)CC1)C(=O)O)C)C	
O=C1C=C2[C@@H]3C[C@]([C@]3(C)CC[C@]2([C@]2([C@H]1[C@@]1(C)CC[C@@H](C([C@@H]1CC2)(C)C)O)C)C(=O)O	
OC[C@@]1(C)[C@@H](CC[C@]2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(C[C@H]1O)(C)C)C)O[C@H]1O[C@H](C(=O)O)[C@H]([C@@H]([C@H]1O)O)O	
COc1cc(C=CC(=O)OC2CC[C@]3(C(C2(C)C)CC[C@@]2(C3C=C[C@]34[C@@]2(C)CC[C@@]2(C4C(C)C)C)CC2)C(=O)O3)C)C)ccc1O	
C[C@@H]1CC[C@]23[C@@H]([C@H]1C)[C@]1(CC[C@H]4[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]4(C)CC[C@@H](C1(C)C)O)OC3=O	
C[C@@H]1CC[C@]2([C@@H]([C@H]1C)C1=CC=C3[C@@]([C@@]1(CC2)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)O)C(=O)O	
O[C@H]1C[C@@H]2[C@@]3(C)CC[C@@H](C([C@@H]3CC[C@]2([C@]2([C@@]31OC(=O)[C@]1([C@H]3CC(C)C)CC1)CC2)C)C)C)O	
O=C1CC[C@]2([C@H](C1(C)C)CC[C@@]1([C@@H]2CC[C@H]2[C@@]1(C)CC[C@@H]1[C@]2(C)C[C@H]1C(O)(C)C)C	
OC[C@H]1O[C@@H](O[C@H]2[C@@H](O[C@@H]([C@H]([C@@H]2O)O)C(=O)O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3CC(C)(C)C[C@H]2O)C)C)[C@@H]([C@H]([C@@H]1O)O)O[C@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1O)O)O	
OC[C@H]1O[C@@H](O[C@H]2O[C@@H](O[C@@H]([C@H]([C@@H]2O)O)C(=O)O)O[C@H]2CC[C@]3([C@H](C2(C)C)CC[C@@]2([C@@H]3CC=C3[C@@]2(C)CC[C@@]2([C@H]3CC(C)(C)C[C@H]2O)C)C)C(C1O)O)O	
CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C[C@@H](O)[C@H](C2)O)O)O)C)C	

(Ikeda et al. 2005)

(Brezáni et al. 2018)

(Poehland et al. 1987)

(Chapman & Hall Chemical Dictionaries)

(Wachsman et al. 2000)

CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@]2([C@]1(C)C)[C@H](O)[C@H](C2)O)C)O)O)C(C)C	
CC(C[C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@H]2[C@]1(C)CC[C@H](C2)OC(=O)C)O)O)C	
CC(C[C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)OC(=O)C)O)O)C	
CC(C[C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)Br)C)O)O)C	
CC(C[C@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)CC[C@@H](C2)Br)C)O)O)C	
CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@]2([C@]1(C)C)[C@H](O)[C@H](C2)O)C)O)O)C(C)C	
CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@]2([C@]1(C)CC[C@@H](C2)Br)O)C)O)O)C(C)C	
CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@]2([C@]1(C)CC[C@@H](C2)OC(=O)C)O)O)O)C(C)C	
CC[C@H]([C@@H]([C@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@H]2[C@]1(C)C)[C@H](O)[C@H](C2)O)C)O)O)C(C)C	
CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@]2([C@]1(C)CC[C@@H](C2)Br)O)C)O)O)C(C)C	
CC[C@H]([C@H]([C@@H]([C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC(=O)[C@@]2([C@]1(C)CC[C@@H](C2)OC(=O)C)O)O)O)C(C)C	
C[C@@H]([C@H]1CC[C@@]2([C@]1(C)CC[C@@]13[C@H]2CC[C@@H]2[C@]3(C1)CC[C@@H](C2(C)C)O)C)CC=CC(O)(C)C	(Shamsabadipour et al. 2013)
OC(=O)[C@]12CC[C@@]3([C@@H](C2=CC(CC1)(C)C)CC[C@H]1[C@@]3(C)CC[C@@H]2[C@]1(C)CCC(=O)C2(C)C)C	(Kurokawa et al. 1999)
COC(=O)[C@@]12CC[C@H]([C@@H]2[C@@H]2[C@](CC1)(C)[C@]1(C)CCC3[C@](C1CC2)(C)CC/C(=N\O)/C3(C)C)C(=C)C	(Flekhter et al. 2004)
O/N=C/1\CC[C@]2(C(C1(C)C)CC[C@@]1(C2CC[C@H]2[C@@]1(C)CC[C@]13[C@@H]2[C@@H](OC3=O)C(C)(C)CC1)C)C	

S. 2. The result of cytotoxicity assay at 25 μM .

compound	Cell viability (%)
1	116.99 ± 5.20
2	116.90 ± 6.99
3	111.94 ± 6.85
4	108.48 ± 4.17
5	121.80 ± 5.60
6	122.43 ± 6.84
7	114.68 ± 3.95
8	122.27 ± 4.78
9	105.53 ± 3.86
10	$14.64 \pm 2.88^{***}$
10 (50 μM)	$1.47 \pm 0.54^{**}$
11	111.53 ± 4.45
11 (50 μM)	113.17 ± 6.08
12	111.81 ± 6.79
12 (50 μM)	111.17 ± 9.73
13	104.16 ± 7.71
14	112.58 ± 18.62
15	114.73 ± 3.93
16	129.88 ± 6.83
16 (50 μM)	$2.96 \pm 1.77^{**}$
17	$16.84 \pm 9.50^{**}$
18	113.47 ± 4.93
19	101.34 ± 4.72
ACV (10 μM)	102.92 ± 13.78

S. 3. References

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