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SUPPLEMENTARY MATERIALS

Table 1. SMILES code notation for the cholic acid derivatives.

L.p.	SMILES code
1.	CCCC(=O)OC1CCC2(C)C(CC(O)C3C4CCC(C(C)CCC(O)=O)C4(C)C(O)CC23)C1
2.	CCCC(=O)OC1CC2CC(O)CCC2(C)C3CC(OC(=O)CCC)C4(C)C(CCC4C13)C(C)CCC(O)=O
3.	CCCC(=O)OC1CCC2(C)C(C1)CC(OC(=O)CCC)C3C4CCC(C(C)CCC(O)=O)C4(C)C(CC23)OC(=O)CCC
4.	CCCCCCCCCC(=O)OC1CCC2(C)C(CC(O)C3C4CCC(C(C)CCC(O)=O)C4(C)C(O)CC23)C1
5.	CCCCCCCCCC(=O)OC1CCC2(C)C(C1)CC(OC(=O)CCCCCCCCC)C3C4CCC(C(C)CCC(O)=O)C4(C)C(O)CC23
6.	CCCCCCCCCC(=O)OC1CC2CC(O)CCC2(C)C3CC(OC(=O)CCCCCCCCC)C4(C)C(CCC4C13)C(C)CCC(O)=O
7.	CCCCCCCCCC(=O)OC1CCC2(C)C(C1)CC(OC(=O)CCCCCCCCC)C3C4CCC(C(C)CCC(O)=O)C4(C)C(CC23)OC(=O)CCCCCCCCC
8.	CCCCCCCCCC(=O)OC1CCC2(C)C(CC(O)C3C4CCC(C(C)CCC(=O)OC)C4(C)C(O)CC23)C1
9.	CCCCCCCCCC(=O)OC1CCC2(C)C(C1)CC(OC(=O)CCCCCCCCC)C3C4CCC(C(C)CCC(=O)OC)C4(C)C(O)CC23
10.	CCCCCCCCCC(=O)OC1CC2CC(O)CCC2(C)C3CC(OC(=O)CCCCCCCCC)C4(C)C(CCC4C13)C(C)CCC(=O)OC
11.	CCCCCCCCCC(=O)OC1CCC2(C)C(C1)CC(OC(=O)CCCCCCCCC)C3C4CCC(C(C)CCC(=O)OC)C4(C)C(CC23)OC(=O)CCCCCCCCC
12.	CCCCCCCCCCCCCCCC(=O)OC1CCC2(C)C(CC(O)C3C4CCC(C(C)CCC(O)=O)C4(C)C(O)CC23)C1
13.	CCCCCCCCCCCCCCCC(=O)OC1CC2CC(O)CCC2(C)C3CC(OC(=O)CCCCCCCCCCCCCCC)C4(C)C(CCC4C13)C(C)CCC(O)=O
14.	CCCCCCCCCCCCCCCC(=O)OC1CCC2(C)C(C1)CC(OC(=O)CCCCCCCCCCCCCCC)C3C4CCC(C(C)CCC(O)=O)C4(C)C(CC23)OC(=O)CCCCCCCCCCCCC
15.	CC(CCC(O)=O)C1CCC2C3C(O)CC4CC(CCC4(C)C3CC(O)C12C)OC(=O)CCC(=O)OCCOCCO
16.	CC(CCC(O)=O)C1CCC2C3C(CC4CC(O)CCC4(C)C3CC(OC(=O)CCC(=O)OCCOCCO)C12C)OC(=O)CCC(=O)OCCOCCO
17.	CC(CCC(O)=O)C1CCC2C3C(CC4CC(CCC4(C)C3CC(OC(=O)CCC(=O)OCCOCCO)C12C)OC(=O)CCC(=O)OCCOCCO)OC(=O)CCC(=O)OCCOCCO
18.	CCCCCCCCCC(=O)OCCOCCOC(=O)CCC(=O)OC1CCC2(C)C(CC(O)C3C4CCC(C(C)CCC(O)=O)C4(C)C(O)CC23)C1
19.	CCCCCCCCCC(=O)OCCOCCOC(=O)CCC(=O)OC1CC2CC(O)CCC2(C)C3CC(OC(=O)CCC(=O)OCCOCCOC(=O)CCCCCCCCC)C4(C)C(CCC4C13)C(C)CCC(O)=O
20.	CCCCCCCCCC(=O)OCCOCCOC(=O)CCC(=O)OC1CCC2(C)C(C1)CC(OC(=O)CCC(=O)OCCOCCOC(=O)CCCCCCCCC)C3C4CCC(C(C)CC(O)=O)C4(C)C(CC23)OC(=O)CCC(=O)OCCOCCOC(=O)CCCCCCCCC
21.	CCCCCCCCCC(=O)OCC(COC(=O)CCC(=O)OC1CCC2(C)C(CC(O)C3C4CCC(C(C)CCC(O)=O)C4(C)C(O)CC23)C1)OC(=O)CCCCCCCCC
22.	CCCCCCCCCC(=O)OCC(COC(=O)CCC(=O)OC1CC2CC(O)CCC2(C)C3CC(OC(=O)CCC(=O)OCC(COC(=O)CCCCCCCCC)OC(=O)CCCCCCCCC)C4(C)C(CCC4C13)C(C)CCC(O)=O)OC(=O)CCCCCCCCC
23.	CCCCCCCCCC(=O)OCC(COC(=O)CCC(=O)OC1CCC2(C)C(C1)CC(OC(=O)CCC(=O)OCC(COC(=O)CCCCCCCCC)OC(=O)CCCCCCCCC)C3C4CCC(C(C)CCC(O)=O)C4(C)C(CC23)OC(=O)CCC(=O)OCC(COC(=O)CCCCCCCCC)OC(=O)CCCCCCCCC)OC(=O)CCCCCCCCC
24.	CC(C)CCCC(C)CCCC(C)CCCC1(C)CCC2=C(C)C(=C(C)C(=C2O1)C)OC(=O)CCC(=O)OC3CCC4(C)C(CC(O)C5C6CCC(C(C)CCC(O)=O)C6(C)C(O)CC45)C3
25.	CC(C)CCCC(C)CCCC(C)CCCC1(C)CCC2=C(O1)C(=C(C)C(=C2C)OC(=O)CCC(=O)OC3CC4CC(O)CCC4(C)C5CC(OC(=O)CCC(=O)OC6=C(C)C(=C7OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CCC7=C6C)C)C8(C)C(CCC8C35)C(C)CCC(O)=O)C
26.	CC(C)CCCC(C)CCCC(C)CCCC1(C)CCC2=C(C)C(=C(C)C(=C2O1)C)OC(=O)CCC(=O)OC3CCC4(C)C(C3)CC(OC(=O)CCC(=O)OC5=C(C)C6=C(OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC6)C(=C5C)C)C7C8CCC(C(C)CCC(O)=O)C8(C)C(CC47)OC(=O)CCC(=O)OC9=C(C)C(=C%10OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CCC%10=C9C)C
27.	CC(CCC(O)=O)C1CCC2C3C(O)CC4CC(CCC4(C)C3CC(O)C12C)OC(=O)CCC(=O)OCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
28.	CC(CCC(O)=O)C1CCC2C3C(CC4CC(O)CCC4(C)C3CC(OC(=O)CCC(=O)OCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C12C)OC(=O)CCC(=O)OCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
29.	CC(CCC(O)=O)C1CCC2C3C(CC4CC(CCC4(C)C3CC(OC(=O)CCC(=O)OCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C12C)OC(=O)CCC(=O)OCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)OC(=O)CCC(=O)OCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
30.	CC(CCC(O)=O)C1CCC2C3C(O)CC4CC(CCC4(C)C3CC(O)C12C)OC(=O)CCC(=O)OCC[S](=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
31.	CC(CCC(O)=O)C1CCC2C3C(CC4CC(O)CCC4(C)C3CC(OC(=O)CCC(=O)OCC[S](=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C12C)OC(=O)CCC(=O)OCC[S](=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
32.	CC(CCC(O)=O)C1CCC2C3C(CC4CC(CCC4(C)C3CC(OC(=O)CCC(=O)OCC[S](=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C12C)OC(=O)CCC(=O)OCC[S](=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)OC(=O)CCC(=O)OCC[S](=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
33.	CC(CCC(O)=O)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C12C