InChikey	Canonical smiles
PFCVZKFJHRCLCC-PGOIBATFSA-N	CC(=C)C1CC[C@]2([C@H]1[C@H]1CC[C
JXSVIVRDWWRQRT-UYDOISQJSA-N	OC[C@]1(C)[C@@H](O)[C@H](O)C[C@]
DTGKSKDOIYIVQL-UHFFFAOYSA-N	OC1CC2C(C1(C)CC2)(C)C
DTGKSKDOIYIVQL-WEDXCCLWSA-N	O[C@H]1C[C@@H]2C([C@@]1(C)CC2)(
DSSYKIVIOFKYAU-GMSGAONNSA-N	O=C1C[C@@H]2C([C@]1(C)CC2)(C)C
INOSMXBKABLUIL-DCKDXSSCSA-N	CC1=CCC(=C)[C@@H]2[C@@H](CC1)C
NPNUFJAVOOONJE-FLFDDASRSA-N	CC1=CCCC(=C)[C@@H]2[C@@H](CC1)
NJICGAVMYWKCMW-GWJXCKMPSA-N	CC(=CCC[C@@]([C@H]1CC[C@@]2([C
UFJPCTSKTPSJTK-SGAOCFLWSA-N	OCC([C@H]1CC[C@@]2([C@@H]1CC[C
OPFTUNCRGUEPRZ-QLFBSQMISA-N	C=C[C@]1(C)CC[C@H](C[C@H]1C(=C)C
PSZDOEIIIJFCFE-OSQDELBUSA-N	OC[C@]12CC[C@@]3(C(C(=CC[C@H]4[C
FAMPSKZZVDUYOS-PGPZXUPKSA-N	CC1=CCC(C)(C)C=CCC(=CCC1)C
DTGKSKDOIYIVQL-OYNCUSHFSA-N	O[C@H]1C[C@H]2C([C@]1(C)CC2)(C)C
DTGKSKDOIYIVQL-MRTMQBJTSA-N	O[C@@H]1C[C@@H]2C([C@@]1(C)CC2
MIJYXULNPSFWEK-GTOFXWBISA-N	O[C@H]1CC[C@]2([C@H](C1(C)C)CC[C
HFPZCAJZSCWRBC-UHFFFAOYSA-N	Cc1ccc(cc1)C(C)C
WEEGYLXZBRQIMU-UHFFFAOYSA-N	CC12CCC(CC1)C(O2)(C)C
CRPUJAZIXJMDBK-UHFFFAOYSA-N	C=C1C2CCC(C1(C)C)C2
UAHWPYUMFXYFJY-UHFFFAOYSA-N	C=CC(=C)CCC=C(C)C
OGLDWXZKYODSOB-UHFFFAOYSA-N	CC1=CCC(C=C1)C(C)C
IHPKGUQCSIINRJ-CSKARUKUSA-N	C=C/C(=C/CC=C(C)C)/C
XMGGYMWWDOXHJM-UHFFFAOYSA-N	CC1=CCC(CC1)C(=C)C
WUOACPNHFRMFPN-UHFFFAOYSA-N	CC1=CCC(CC1)C(O)(C)C
MIJYXULNPSFWEK-UHFFFAOYSA-N	OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1
BQOFWKZOCNGFEC-UHFFFAOYSA-N	CC1=CCC2C(C1)C2(C)C
HAVYZKHVTLAPDZ-PRUKLFJYSA-N	C=C1CCCC(=CCC(C=CC1)(C)C)C
NPNUFJAVOOONJE-WDZFZDKYSA-N	CC1=CCCC(=C)C2C(CC1)C(C2)(C)C
NVEQFIOZRFFVFW-UHFFFAOYSA-N	C=C1CCC2OC2(CCC2C1CC2(C)C)C
OPFTUNCRGUEPRZ-UHFFFAOYSA-N	C=CC1(C)CCC(CC1C(=C)C)C(=C)C
HIGQPQRQIQDZMP-FLIBITNWSA-N	C/C(=C/COC(=O)C)/CCC=C(C)C
DSSYKIVIOFKYAU-UHFFFAOYSA-N	O=C1CC2C(C1(C)CC2)(C)C
XGFDWZLOGKFUGO-UHFFFAOYSA-N	OCC1(C)CC(O)CC2(C1(O)CCC1(C2CC=C
AZBICJOBHDKYGG-LUAWRHEFSA-N	CCOC(=O)c1c(NC(=O)/C=C\c2ccc(c(c2)C
PSZDOEIIIJFCFE-UHFFFAOYSA-N	OCC12CCC3(C(=CCC4C3(C)CCC3C4(C)
LBMAECHMNKURES-UHFFFAOYSA-N	C=C1CC2CCCC3C1(C)CCCC(C23)(C)C
NJICGAVMYWKCMW-UHFFFAOYSA-N	CC(=CCCC(C1CCC2(C1CCC1C2(C)CCC
VHVOLFRBFDOUSH-NSCUHMNNSA-N	C/C=C/c1ccc2c(c1)OCO2
BCKIAEZZQAYKGK-UHFFFAOYSA-N	CC1CC=C(C(C1)C)C
RUJPNZNXGCHGID-UHFFFAOYSA-N	CC(=C)C1CCC(CC1)(C)O
WTARULDDTDQWMU-UHFFFAOYSA-N	C=C1CCC2CC1C2(C)C
KQAZVFVOEIRWHN-UHFFFAOYSA-N	CC1=CCC2(C1C2)C(C)C
CDOSHBSSFJOMGT-UHFFFAOYSA-N	C=CC(CCC=C(C)C)(O)C
PFCVZKFJHRCLCC-UHFFFAOYSA-N	CC(=C)C1CCC2(C1C1CCC3C(C1(C)CC2
UHWIZIJICYWABA-UHFFFAOYSA-N	CC(=CC(=O)OC1c2c(ccc3c2oc(=O)cc3)O
UFJPCTSKTPSJTK-UHFFFAOYSA-N	OCC(C1CCC2(C1CCC1C2(C)CCC2C1(C
AOWMBRPPHGNFDX-UHFFFAOYSA-N	OC(=O)C1CC(C)(C)CC2C1CCC1(C2=CC
KMKFOIBUKYMVRJ-UHFFFAOYSA-N	OCC1OC(OC(=O)C23CCC(CC3C3=CCC4
INOSMXBKABLUIL-YHYXMXQVSA-N	CC1=CCC(=C)C2C(CC1)C(C2)(C)C
YAPXSYXFLHDPCK-HKWUFEEASA-N	C/C/1=C\CC/C(=C\CCC(/C=C\C(CC1)C(C
JXSVIVRDWWRQRT-UHFFFAOYSA-N	OCC1(C)C(O)C(O)CC2(C1CCC1(C2CC=C
PRVKSKWNDSLRBY-UHFFFAOYSA-N	CCCC(=O)c1c(O)c(Cc2c(O)c(CC3=C(O)C
XTGYWZXUYFAABL-WLRTZDKTSA-N	OC/C=C/1\CN2CCC34C2CC1C1=CCC(=C
LSKFUSLVUZISST-UHFFFAOYSA-N	OCC(C(c1ccc(c(c1)OC)O)O)O
BPLQKQKXWHCZSS-UHFFFAOYSA-N	C=CCc1cc(OC)c(c(c1)OC)OC
ZBPQOWMVWIKUHQ-UHFFFAOYSA-N	OCC12CCC3C(=CCC4C3(C)CCC3C4(C)C
PREBVFJICNPEKM-YDWXAUTNSA-N	O=C(CC(=O)/C=C/c1ccc(cc1)O)/C=C/c1c
DSSYKIVIOFKYAU-GMSGAONNSA-N	O=C1C[C@@H]2C([C@]1(C)CC2)(C)C

```
ULDHMXUKGWMISQ-VIFPVBQESA-N      CC(=C)[C@H]1CC=C(C(=O)C1)C
FINHMKGKINIASC-UHFFFAOYSA-N      Cc1nc(C)c(nc1C)C
XISBISVWIJDEQH-CQSZACIVSA-N      CC(=C)CCC[C@H](C1=CCC(=CC1)C)C
ZIUSSTSXXLLKKK-KOBPDPAPSA-N      COc1cc(/C=C/C(=C/C(=O)/C=C/c2ccc(c(c
QRMPRVXWPCLVNI-YYFQZIEXSA-N      CC([C@@H]1C[C@]23O[C@]1(O)CC(=C
KDPFMRXIVDLQKX-WDZFZDKYSA-N      CC1=CCC[C@@H](C)C(=O)C[C@H](C(=
RDFLLVCQYHQOBU-ZOTFFYTFSA-N      OC[C@H]1O[C@@H](Oc2cc(O)cc3c2cc(
JLJLRLWOEMWYQK-OBDJNFEBSA-N      OC(=O)C1[C@H]2[C@]3([C@H]4[C@]51
ZOWHLBOPCIHIHW-KQBHUUJHSA-N      OC(=O)[C@H]1[C@H]2[C@]3([C@H]4[C
WZRRJZYYGOOHRC-UQJCXHNCSA-N      OC(=O)C1[C@H]2[C@]3([C@H]4[C@]51
MHVYWTXXZIFXDT-YGNOGLJPSA-N      OC(=O)[C@H]1[C@H]2[C@]3([C@H]4[C
CQDCLVASIPBLIZ-ZXUMCLPVSA-N      CC1C[C@@]23C[C@H]1CC[C@H]3[C@]
CPGCVOVWHCWVTP-UHFFFAOYSA-N      CCCCCCCCCCCCCCCCCCCC(CCCCCC
YGSDEFSMJLZEOE-UHFFFAOYSA-N      OC(=O)c1ccccc1O
QFVCWQNGOCGQJL-WFYKWJGLSA-N      COc1cc(/C=C/C(=O)C(C(Cc2ccc(cc2)C)O
GSLDEZOOOSBFGP-UHFFFAOYSA-N      C=C1CCOC1=O
SQRUWMQAWMLKPR-DZEUPHNYSA-N      OCCC(=C)C(=O)O[C@@H]1O[C@H](CO
KVRQQFBSAHPTAB-FUYPYFFWSA-N      OC[C@H]1O[C@@H](OC(=O)C(=C)C(CC
FMHJNIRDGYFPEC-CHICSPHLSA-N      OC[C@H](C(=C)C(=O)OC[C@H]1OC(O)[
IZSSLGQVLPHINU-SESNJUDKSA-N      OCCC(=C)C(=O)O[C@@H]1O[C@H](CO
FZPYMZUVXJUAQA-ZDUSSCGKSA-N      CC(=CC(=O)C[C@@H](C1=CCC(=CC1)C
TXIKNNOOLCGADE-DHMWGJHJSA-N      CC(=C1C[C@H]2[C@H]([C@@](CC1=O)
IVSZLXZYQVIEFR-UHFFFAOYSA-N      Cc1cccc(c1)C
IHPKGUQCSIINRJ-NTMALXAHSA-N      C=C/C(=C\CC=C(C)C)/C
WKOLLVMJNQIZCI-UHFFFAOYSA-N      COc1cc(ccc1O)C(=O)O
GYHFUZHODSMOHU-UHFFFAOYSA-N      CCCCCCCCC=O
INNSGICBAVEKCC-UHFFFAOYSA-N      CC(=C)C1CCC2(C(C1)(C)C=C)CCC2C
HFPZCAJZSCWRBC-UHFFFAOYSA-N      Cc1ccc(cc1)C(C)C
XVOHELPNOXGRBQ-LXQMTTSMSA-N      CC1=CC(=O)c2c(CC(=CCC1)C)occ2C
WUOACPNHFRMFPN-UHFFFAOYSA-N      CC1=CCC(CC1)C(O)(C)C
WEEGYLXZBRQIMU-UHFFFAOYSA-N      CC12CCC(CC1)C(O2)(C)C
GRWFGVWFFZKLTI-UHFFFAOYSA-N      CC1=CCC2CC1C2(C)C
WTARULDDTDQWMU-UHFFFAOYSA-N      C=C1CCC2CC1C2(C)C
NDVASEGYNIMXJL-UHFFFAOYSA-N      C=C1CCC2(C1C2)C(C)C
DSSYKIVIOFKYAU-UHFFFAOYSA-N      O=C1CC2C(C1(C)CC2)(C)C
WBYWAXJHAXSJNI-SREVYHEPSA-N      OC(=O)/C=C\c1ccccc1
OYHQOLUKZRVURQ-HZJYTTRNSA-N      CCCCC/C=C\C/C=C\CCCCCCCC(=O)O
TUNFSRHWOTWDNC-UHFFFAOYSA-N      CCCCCCCCCCCCCCC(=O)O
MBIPADCEHSKJDQ-UHFFFAOYSA-N      CC1CCC=C2C1(C)C1C(C1(C)C)CC2
IQSPYJZCWMAJLU-WAYWQWQTSA-N      CC1CC=CC(C)CCC(CC1)C(C)C
BOBTWVZHSPRDFC-UHFFFAOYSA-N      CC1=CC2C(CC1)C(C)(O)CCC2(C)C
VLXDPFLIRFYIME-UHFFFAOYSA-N      CC(C1CCC2(C3C1C2C(=CC3)C)C)C
ICWHTQRTTHCUHW-UHFFFAOYSA-N      CC1CCC=C(C21CCC(C2)C(O)(C)C)C
GIBQERSGRNPMEH-UHFFFAOYSA-N      CC(=C1CCC(C2=C(C1)C(C)CC2)C)C
TWVJWDMOZJXUID-UHFFFAOYSA-N      CC1CCC(CC2=C1CCC2C)C(O)(C)C
SECPZKHBENQXJG-FPLPWBNLSA-N      CCCCCC/C=C\CCCCCCCC(=O)O
DTGKSKDOIYIVQL-UHFFFAOYSA-N      OC1CC2C(C1(C)CC2)(C)C
JMSVCTWVEWCHDZ-UHFFFAOYSA-N      COc1cc(cc(c1O)OC)C(=O)O
CRPUJAZIXJMDBK-UHFFFAOYSA-N      C=C1C2CCC(C1(C)C)C2
NPNUFJAVOOONJE-WDZFZDKYSA-N      CC1=CCCC(=C)C2C(CC1)C(C2)(C)C
KGEKLUUHTZCSIP-UHFFFAOYSA-N      CC(=O)OC1CC2C(C1(C)CC2)(C)C
UAHWPYUMFXYFJY-UHFFFAOYSA-N      C=CC(=C)CCC=C(C)C
CDOSHBSSFJOMGT-UHFFFAOYSA-N      C=CC(CCC=C(C)C)(O)C
OGLDWXZKYODSOB-UHFFFAOYSA-N      CC1=CCC(C=C1)C(C)C
IHPKGUQCSIINRJ-CSKARUKUSA-N      C=C/C(=C/CC=C(C)C)/C
YKFLAYDHMOASIY-UHFFFAOYSA-N      CC1=CCC(=CC1)C(C)C
ITYNGVSTWVVPIC-UHFFFAOYSA-N      CC1CCC2C1C1C(C1(C)C)CCC2=C
PHWISBHSBNDZDX-UHFFFAOYSA-N      CC(C1CCC(=C)C=C1)CCC=C(C)C
```

FMXKKHBXBBAQBC-UHFFFAOYSA-N	CC1=CCCC(C1=C)(C)C
XLPDVYGDNRIQFV-UHFFFAOYSA-N	Cc1ccc(cc1)C(O)(C)C
XPGWKKLDFXNBPJ-UHFFFAOYSA-N	CC1CCC2C1C1C(C1(C)C)CCC12OC1
WPYMKLBDIGXBTP-UHFFFAOYSA-N	OC(=O)c1ccccc1
OWMJDOUOHDOUFG-FNCQTZNRSA-N	O=C(CCc1ccccc1)/C=C/C=C/c1ccccc1
FRMCCTDTYSRUBE-UHFFFAOYSA-N	C=C1CCC2C(C3C1CCC3(C)O)C2(C)C
XMGQYMWWDOXHJM-UHFFFAOYSA-N	CC1=CCC(CC1)C(=C)C
DPRCKWANIKZGTF-NTUHNPAUSA-N	OC(CCc1ccccc1)CC/C=C/c1ccccc1
FAMPSKZZVDUYOS-KXWHQPPKSA-N	CC1=CCC(C)(C)C=CCC(=CCC1)C
LCOSCMLXPAQCLQ-UHFFFAOYSA-N	CC1=CC2C(=C(C)CCCC2(C)C)CC1
FKWGCEDRLNNZOZ-UHFFFAOYSA-N	CC(=CCCC(c1ccc(c(c1)O)C)C)C
CRDAMVZIKSXKFV-YFVJMOTDSA-N	OC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
QMVPMAAFGQKVCJ-UHFFFAOYSA-N	OCCC(CCC=C(C)C)C
BWHPKBOLJFNCPW-HZPYOLDOSA-N	COc1cc(CCC(=O)C=C(/C=C/c2ccc(c(c2)C
OELMAFBLFOKZJD-UHFFFAOYSA-N	COc1cc(CCC(CC(CCc2ccc(c(c2)OC)O)O)O
RRAFCDWBNXTKKO-UHFFFAOYSA-N	C=CCc1ccc(c(c1)OC)O
LFJQCDVYDGGFCH-UHFFFAOYSA-N	CC(C1CCC(=C)C=C1)C
VFLDPWHFBUODDF-KYPMKJFLSA-N	COc1cc(/C=C/C(=O)CC(=O)/C=C\c2ccc(c
RECUKUPTGUEGMW-UHFFFAOYSA-N	CC(c1ccc(c(c1)O)C)C
MOYAFQVGZZPNRA-UHFFFAOYSA-N	CC1=CCC(=C(C)C)CC1
PDSNLYSELAIEBU-UHFFFAOYSA-N	C=C1C2CCC3C1(C)CCCC(C23)(C)C
BQOFWKZOCNGFEC-UHFFFAOYSA-N	CC1=CCC2C(C1)C2(C)C
GNWJYPQYWBLOGD-UHFFFAOYSA-N	CC1CCC(C2(C1CC(CC2)C(C)C)C)O
BOPIMTNSYWYZOC-UHFFFAOYSA-N	C=C1CCCC2(C1CC(CC2)C(O)(C)C)C
GFJIQNADMLPFOW-UHFFFAOYSA-N	C=CC1(C)CCC(CC1C(=C)C)C(O)(C)C
YOVSPTNQHMDJAG-UHFFFAOYSA-N	C=C1CCCC2(C1CC(CC2)C(=C)C)C
JESIHYIJKKUWIS-UHFFFAOYSA-N	Cc1ccc(cc1)C(O)C
USDOQCCMRDNVAH-UHFFFAOYSA-N	CC1=CCC2C(C1)C(CC=C2C)C(C)C
WGTRJVCFDUCKCM-UHFFFAOYSA-N	CC1CCC2=C(C)CCC3C(C12)C3(C)C
NPJICTMALKLTFW-UHFFFAOYSA-N	CCC(C(C)C)CCC(C1CCC2C1(C)CCC1C2
CUUMXRBKJIDIAY-UHFFFAOYSA-N	CC(C1CC=C(c2c1cc(C)cc2)C)C
SPCXZDDGSGTVAW-UHFFFAOYSA-N	CC1CCC2C(C3=C(CCC13)C)C2(C)C
KZJWDPNRJALLNS-UHFFFAOYSA-N	CCC(C(C)C)CCC(C1CCC2C1(C)CCC1C2
NGSWKAQJJWESNS-UTCJRWHESA-N	OC(=O)/C=C\c1ccc(cc1)O
QAIPRVGONGVQAS-RQOWECAXSA-N	OC(=O)/C=C\c1ccc(c(c1)O)O
FFRFJIZJLZXEJX-PORYWJCVSA-N	COc1cc(/C=C\C(=O)CC(=O)/C=C\c2ccc(c
MXDMETWAEGIFOE-UHFFFAOYSA-N	C=CC1(C)CCC(=CC1C(=C)C)C(C)C
RMZHSBMIZBMVMN-UHFFFAOYSA-N	C=C1CCCC2(C1CC(=C(C)C)CC2)C
FARHRLFSUJIINR-UHFFFAOYSA-N	CC(=O)CCC1C2C1(C)CC(=O)C(C2)C(O)(
BCMMNIMNKUKKCI-UHFFFAOYSA-N	O=C1OC2C(=C1C)CC1C(C2)(C)C(O)CC(
MUYJSOCNDLUHPJ-CLTKARDFSA-N	COc1cc(CCC(=O)CC(=O)/C=C\c2ccc(c(c2
PFIXJSCFTAVWBW-UHFFFAOYSA-N	CC1=C2C(=O)c3c(CC2(C(CC1)O)C)occ3
QXEXMTIZXNCRJO-UHFFFAOYSA-N	Cc1coc2c1C(=O)C1C(C2)(C)C(O)CCC1(
FNMDHMSGEIODFP-UHFFFAOYSA-N	CC(C1=CCC(C2C(C1)C(C)(O)CC2)(C)O)
JWUVBGKPYDWLJC-UHFFFAOYSA-N	CC(=O)CCC1=CCC(=C(C)C)C(=O)CC1C
JBUPYYZICGGNGI-UHFFFAOYSA-N	CC(C1CC2(OC1=O)C(C)CCC2C(=C)C)C
KHOTZHZBHNDKOB-UHFFFAOYSA-N	CC(=C1CC2(OC1=O)C(C)CCC2C(=C)C)C
ISFMXVMWEWLJGJ-UHFFFAOYSA-N	CC(=C1CC23OC1(O)C=C(C3CCC2)C)C
LWEBVMKVDYHHRS-UHFFFAOYSA-N	CC(=O)CCC1C2C1(C)CC1C(=C(C)C(=O)
AWUBJLRYWHOLFW-WZUFQYTHSA-N	O=C(CC(=O)/C=C\c1ccc(cc1)O)CCc1ccc(
JZIQIHGNLNKQKF-UHFFFAOYSA-N	CC(=O)CCC1C2C1(C)CC1(C(=C(C)C(=O
QRMPRVXWPCLVNI-UHFFFAOYSA-N	CC(C1CC23OC1(O)CC(=C)C3CCC2)C
JXBMAOPQNNTXPM-UHFFFAOYSA-N	CCC(=O)CC1=CCC(=C(C)C)C(=O)CC1C
YBJIFGYQRRWWFW-UHFFFAOYSA-N	CC1CCc2c(C1=O)c1c(C)coc1cc2C
HICAMHOOTMOHPA-UHFFFAOYSA-N	C=CC1(C)Cc2occ(c2CC1C(=C)C)C
IZLBLUIBVMGMIY-UTCJRWHESA-N	COc1cc(/C=C\C2=CC(=O)CC(O2)c2ccc(c
NEQGOKAKPXXESR-ACCUITESSA-N	OC(CC(=O)CCc1ccccc1)/C=C/c1ccccc1

ZYPUZCWWTYIGFV-WDZFZDKYSA-N	CC1=CCCC(C)C(=O)CC(=C(C)C)C(=O)C
BQSLMQNYHVFRDT-UHFFFAOYSA-N	C=CC1(C)CCC(=C(C)C)CC1C(=C)C
PXPIJNMPDAFWSF-XBXARRHUSA-N	OC(CCc1ccc(cc1)O)CC/C=C/c1ccccc1
ZVMJXSJCBLRAPD-UHFFFAOYSA-N	C=CC1(C)Cc2occ(c2C(=O)C1C(=C)C)C
ATJVZXXHKSYELS-FNORWQNLSA-N	CCOC(=O)/C=C/c1ccc(c(c1)OC)O
DHNGCHLFKUPGPX-TWGQIWQCSA-N	CCOC(=O)/C=C\c1ccc(cc1)OC
OELWYQGRQUQQPD-XBXARRHUSA-N	OC(CCc1ccc(c(c1)O)O)CC/C=C/c1ccccc1
VMDXHYHOJPKFEK-ADUATRDFSA-N	CC1=CCc2c(CC(=CCC1)C)occ2C
ZLESWHXADLWJPV-YHYXMXQVSA-N	CC1=CCCC(C)C(=O)Cc2c(C1)occ2C
OYONKNQJEXRUQZ-VLLDNGIUSA-N	OC/C(=C\1/CC=C(C)CCC=C(CC1=O)C)/C
RBXMGYRKSKKXNT-UHFFFAOYSA-N	CC(C1CCC(C)C(=O)CCC2(C(C1)O2)C)C
SLGKCOCDZZQQLY-LXQMTTSMSA-N	CC1=CCCC(=CCC2=C(C(=O)OC2C1)C)C
NKDVMZOMVJQUDC-UTCJRWHESA-N	COc1cc(/C=C\C(=O)CC(=O)CC(c2ccc(c(c
RKQDKXOBRXTSFS-QZFXXANLSA-N	CC1=CCCC2(C)OC2CC(C=CC1)(C)C
GLKQAHXBJLGAFT-UHFFFAOYSA-N	CC1CCC2C1C1C(C1(C)C)CC1C2(C)O1
XXFPSLVWNRANRW-UHFFFAOYSA-N	CC(=O)CCC1CCC(=C(C)C)C(=O)C=C1C
FPRYGNYXOFHMLF-UHFFFAOYSA-N	CC1=C2CCC(C2C2C(CC1)C2(C)C)(C)O
TXIKNNOOLCGADE-UHFFFAOYSA-N	CC(=C1CC2C(C(CC1=O)(C)O)CCC2(C)O
VZWGRQBCURJOMT-UHFFFAOYSA-N	CCCCCCCCCCCCOC(=O)C
STRABSCAWZINIF-UHFFFAOYSA-N	CC(=C1CCC2(C(C1)C(C)(O)CCC2)C)C
OZNHATCGPKOFBH-UHFFFAOYSA-N	CC1CCC23C1C1C(C1(C)C)CCC3(O2)C
IEDKVDCIEARIIU-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCCC(=O)C
YZBOVSFWWNVKRJ-UHFFFAOYSA-N	CCCCOC(=O)c1ccccc1C(=O)O
JWRBAZYQWTVQSD-UHFFFAOYSA-N	CC(=C1CC23OC1(O)CC(=C3CCC2C)C)C
DAUDFKSHOYLOOB-UHFFFAOYSA-N	CC(=C1CC2C(=C(CC1=O)C)CCC2(C)O)C
MQJGAHXKAZGEGI-IUNAMMOKSA-N	COc1cc(/C=C\C(=O)CC(=O)/C=C\c2cc(OC
NMKYCFSNAWAALS-UHFFFAOYSA-N	CC1=CC2(O)OC3(C1CCC3C)CC12OC1(O
TZUNCSSGETYEPM-UHFFFAOYSA-N	Cc1cc(O)c2c(c1)C(Cc1c2cc2C(O)C(C(C)C
CSKINCSXMLCMAR-UHFFFAOYSA-N	CC1CCC2=C1CC1CCC2(C1(C)C)C
XNGKCOFXDHYSGR-UHFFFAOYSA-N	CC(=CCCc1cocc1)C
HSRRCZPSLXXKJL-XEQVNJCQSA-N	COc1cc(/C=C\C(=O)CC(=O)/C=C\c2ccc(c
IYDMICQAKLQHLA-UHFFFAOYSA-N	c1ccc(cc1)c1ccccc2c1cccc2
XLEYFDVVXLMULC-UHFFFAOYSA-N	CC(=O)c1c(O)cc(cc1O)O
AFDXODALSZRGIH-DAXSKMNVSA-N	COc1ccc(cc1)/C=C\C(=O)O
JSWOSPDHAFLJHZ-UHFFFAOYSA-N	CC1=Cc2c(CC1)c(C)cc1c2c(C)co1
YFDIAFVTFRYMNI-UHFFFAOYSA-N	CC(=CC(=O)CC(C1CC(O)C(C2C1O2)(C)O
HJFYFYWETUVIHT-UHFFFAOYSA-N	COc1cc(CCC(=O)CC(=O)CCc2ccc(cc2)O)
OVURIZIJDDTXJS-FNCQTZNRSA-N	OC(CCc1ccccc1)/C=C/C=C/c1ccccc1
ISIMGBQRFXXNON-VHOZIDCHSA-N	COc1cc(/C=C\C(=O)/C=C\c2ccc(c(c2)OC)
CVIVANCKIBYAOP-UITAMQMPSA-N	CC1=CCCC2(C)OC2CC(=O)c2c(C1)occ2C
BQDXDGDOYPUUOD-UHFFFAOYSA-N	O=C1OC2C(=C1C)CC1C(C(C2)(C)O)CCC
HPNXJLIPUVXDNH-UHFFFAOYSA-N	CC1=C2CC3C(C)(O)CCC3(C(C=C2OC1=
ZHVYOZUDBBMXPD-UHFFFAOYSA-N	OC1CCC2C1CC1=C(C)C(=O)OC1CC2(C
ONMRIEOINXLXQN-UHFFFAOYSA-N	CC1=C2CC3C(C)(O)CCC3(C(C=C2OC1=
CKDRPCYJCDMPFO-UHFFFAOYSA-N	C=C1Cc2occ(c2C(=O)C2(C1CCC2)O)C
FYIUFPCMCZWNKH-UHFFFAOYSA-N	O=C1OC2(C(=C1C)CC1C3(C(C2O)(C)O3
JUDCTVXWYFNGQQ-YNYJRQSBSA-N	COc1cc(/C=C\C=C\C(=O)/C=C\c2ccc(c(c2
DXGIJGSOOPTGDC-UHFFFAOYSA-N	O=C1OC2(C(=C1C)CC1C(C(C2)(C)O)CC
GIHNTRQPEMKFKO-HQCVNHCJSA-N	CC1=CCC(C)(C)C=CC(=O)C(=CCC1)C
PALMCMYYFAHUGA-DGSDLINQSA-N	O=C(/C=C\c1ccc(cc1)O)/C=C/C=C\c1ccc(
URJZIVZWAWBZCT-ZSOIEALJSA-N	CC(=O)OC(CCc1ccccc1)CC/C=C\c1ccccc
VNFWNGSEJXPCSW-QPEQYQDCSA-N	O=C(CCc1ccccc1)CC/C=C\c1ccccc1
GTHJHHZMCSHKDZ-UHFFFAOYSA-N	CC(=C1CC2OC2(C)CCC2C(CC1=O)(C)O
ZWEHNKRNPOVVGH-UHFFFAOYSA-N	CCC(=O)C
YGZDWJVKOQPZDX-UHFFFAOYSA-N	CC1CCc2c1cc(cc2C)C(=O)O
PCBKWKNYISJGPJ-BUHFOSPRSA-N	CCCCCCCCCCCC/C=C/CC(=O)O
DLPRXTUOPLIHNV-FOCLMDBBSA-N	CCCCCCCCCCCCCC/C=C/CC(=O)O
RNZJKBXCMRFWKJ-CCKMTBCVSA-N	CC(=O)OCC(C1C=C2OC2(C)CC=CC(CC

InChIKey	SMILES
SVJCSSAWCKGHMZ-HVOHDJRZSA-N	OC/C(=C/1\CC2OC2(C)CCC=C(CC1=O)C
OQZCUYXRSFWCJU-UHFFFAOYSA-N	CC(CCC1C2C1(C)CC(=O)C(=C(C)C)C2)C
FTVWIRXFELQLPI-UHFFFAOYSA-N	Oc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2O)O
LGEKQNSNNQGALI-UHFFFAOYSA-N	CC(=O)CCC1C2C1(C)CCC(=O)C2
SNEAPXILYVCZFK-UHFFFAOYSA-N	Cc1cc(O)c2c(c1)c(ccc2C)C(C)C
ZMIQNSSHYBJKIL-UHFFFAOYSA-N	CC(=CC(=O)CC(C1=CC=C(CC1)C)C)C
QVRYUUYYIWAQHV-AVWDGMTFSA-N	COc1cc(/C=C\C(=O)/C=C\c2ccc(cc2)O)cc
NAAJVHHFAXWBOK-UHFFFAOYSA-N	CC(=CC(=O)CC(c1ccc(cc1)C)C)C
OZQAPQSEYFAMCY-UHFFFAOYSA-N	CC1=CCCC2(C1CC(CC2)C(=C)C)C
XOCANRBEOZQNAQ-UHFFFAOYSA-N	CC(=CC(=O)CC(C1CC=C(C=C1)C)C)C
LRDZCBICVMXPBB-UHFFFAOYSA-N	CC(=CC(=O)CC(=C)C1CCC(=CC1)C)C
ABLPGPHZENVRRH-UHFFFAOYSA-N	C=CC1(C)CC(=O)C(=C(C)C)CC1C(=C)C
QJOWFYQIUZMPRY-UHFFFAOYSA-N	CC(=CC(=O)CC(C1C=CC(C(C1)O)(C)O)C
ZRSXYQBSTGSATR-UHFFFAOYSA-N	O=CC(c1ccc(c2c1cc(C)cc2)C=O)C
UYPPHUAQDGUVKN-UHFFFAOYSA-N	CC1CCC2C3(C1(C)C1C(C1(C)C)CC3)O2
UYEWRTKHKAVRDI-ASVGJQBISA-N	COc1cc(/C=C/C(=O)OCC(=O)/C=C/c2ccc
NVEQFIOZRFFVFW-UHFFFAOYSA-N	C=C1CCC2OC2(CCC2C1CC2(C)C)C
JSNRRGGBADWTMC-NTCAYCPXSA-N	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
WRYLYDPHFGVWKC-UHFFFAOYSA-N	CC1=CCC(CC1)(O)C(C)C
FUCYIEXQVQJBKY-UHFFFAOYSA-N	CC1=CC2C(=C(C)CCC2C(C)C)CC1
ZQPPMHVWECSIRJ-KTKRTIGZSA-N	CCCCCCCC/C=C\CCCCCCCC(=O)O
DOIRQSBPFJWKBE-UHFFFAOYSA-N	CCCCOC(=O)c1ccccc1C(=O)OCCCC
IPCSVZSSVZVIGE-UHFFFAOYSA-N	CCCCCCCCCCCCCCCC(=O)O
GLZPCOQZEFWAFX-YFHOEESVSA-N	OC/C=C(\CCC=C(C)C)/C
NGSWKAQJJWESNS-ZZXKWVIFSA-N	OC(=O)/C=C/c1ccc(cc1)O
IWQURBSTAIRNAE-UHFFFAOYSA-N	CC(C1=CC2C(C(CC1)(C)O)CCC2(C)O)C
QIQXTHQIDYTFRH-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCCC(=O)O
DEBDFZGNZTYPMF-UHFFFAOYSA-N	CC(=C1CC23OC1(O)CC(=C)C3CCC2C)C
VMYXUZSZMNBRCN-UHFFFAOYSA-N	CC(=CCCC(c1ccc(cc1)C)C)C
SSRDTRQCJGXMGT-PXNMLYILSA-N	CC1=CCCC2(C)C3CC(C2C(=O)c2c(C1)oc
KKOXKGNSUHTUBV-UHFFFAOYSA-N	CC(=CCCC(C1CC=C(C=C1)C)C)C
IXQJBPRUTQTCMW-UHFFFAOYSA-N	CC(=C1CC2C(C)(O)CCC2(C(=CC1=O)C)
HUZJLWLCLJEXEL-UHFFFAOYSA-N	CC(=O)CCC1C2C1(C)CC(=O)C(=C(C)C)C
OGJFTQVVQQMGJG-UHFFFAOYSA-N	Cc1cc2oc(=O)c(c2cc2c1CCC2C)C
OPFTUNCRGUEPRZ-UHFFFAOYSA-N	C=CC1(C)CCC(CC1C(=C)C)C(=C)C
CAULGCQHVOVVRN-SVGXSMIJSA-N	CC1=CCC(=C(C)C)C(=O)CC(=CCC1)C
YHQGMYUVUMAZJR-UHFFFAOYSA-N	CC1=CC=C(CC1)C(C)C
LMVGRKPOXLBIFQ-UHFFFAOYSA-N	Cc1cc2occ(c2cc2c1ccc2C)C
GXEGJTGWYVZSNR-OMQMMEOVSA-N	CC1=CCCC(=CCC(=C(C)C)CC1)C
NUQDPKOFUKFKFD-UHFFFAOYSA-N	CC1CCC2C(C3=C1CCC3C)C2(C)C
WMOPMQRJLLIEJV-UHFFFAOYSA-N	CC1=C2CC(CCC2(CCC1)C)C(O)(C)C
PREBVFJICNPEKM-JTAXDKCCSA-N	O=C(CC(=O)/C=C/c1ccc(cc1)O)/C=C\c1cc
HJTVQHVGMGKONQ-LUZURFALSA-N	COc1cc(/C=C/C(=O)CC(=O)/C=C/c2ccc(c
ITIGZFMSPAFZAE-UHFFFAOYSA-N	C=C1CC(=O)C(=C(C)C)CC2C1CCC2(C)C
OSIFVLKZUWRNBN-UHFFFAOYSA-N	CC(=CC(=O)CC(c1ccc(c(c1)O)C)C)C
MBUWIGIPGMJVMN-UHFFFAOYSA-N	CC1=CC(=O)C(=C(C)C)CC2(C1CCC2(C)C
RHBOHEXDGUVIIY-UHFFFAOYSA-N	CC1=CC(=O)C(=C(C)C)CC2C1CCC2(C)C
NRBFEAZFHRHFFQ-UHFFFAOYSA-N	CC(=CC(CC(c1ccc(cc1)C)C)O)C
WYIJOOQDLOBLCP-UHFFFAOYSA-N	CC(=CC(=O)CC(c1ccc(cc1O)C)C)C
XZRVRYFILCSYSP-UHFFFAOYSA-N	CC(=CCCC(=C)C1CCC(=CC1)C)C
JIJQKFPGBBEJNF-UHFFFAOYSA-N	CC(C1CCC(=C)C=C1)CC(=O)C=C(C)C
WTWBUQJHJGUZCY-UHFFFAOYSA-N	O=Cc1ccc(cc1)C(C)C
KJPRLNWUNMBNBZ-QPJJXVBHSA-N	O=C/C=C/c1ccccc1
PUSAAHYGRLPDMQ-UHFFFAOYSA-N	O=C(OCC1OC(OC(=O)CC[N+](=O)[O-])C
YXAKCQIIROBKOP-HSSGTREWSA-N	O/C(=C\C(=O)/C=C/c1ccc(cc1)O)/C=C/c1
SNVNUOWZKGGIRP-HCKUEKJXSA-N	OC/C(=C/CC/C(=C\Cc1cc(O)ccc1O)/C)/CC
SGAYOTORECIFCJ-UHFFFAOYSA-N	CC(=CCCC1(C)C2CCC1(C)C(C2)O)C
OIRFZVJHADZVMD-UHFFFAOYSA-N	CC(=CCCC1=CCCC(C1)C(=C)CCC=C(C)

BQLZQPGWNVTIHR-UHFFFAOYSA-N	OCC1OC(Oc2cc3oc(c4ccc(cc4)O)c(c(=O)
MPYYVGIJHREDBO-UHFFFAOYSA-N	CC(CC(=O)OC1CC2C(C1(C)CC2)(C)C)C
MLOIFQIPYKRTPY-KZZDLZNXSA-N	COc1cc(/C=C/C(=O)CC(=O)/C=C/c2ccc(c
IQTVWGJWEJIBHJ-UHFFFAOYSA-N	N#Cc1ccc(cc1)Nc1cc(Oc2c(C)cc(cc2C)C)
NKSUFXDOOSPKIX-UHFFFAOYSA-N	Cc1ccc(cc1)C1(C)CCCC(O1)(C)C
FZPYMZUVXJUAQA-UHFFFAOYSA-N	CC(=CC(=O)CC(C1=CCC(=CC1)C)C)C
XISBISVWIJDEQH-UHFFFAOYSA-N	CC(=C)CCCC(C1=CCC(=CC1)C)C
ULDHMXUKGWMISQ-UHFFFAOYSA-N	CC(=C)C1CC=C(C(=O)C1)C
KWVISVAMQJWJSZ-UHFFFAOYSA-N	CC1CCC2(NC1)OC1C(C2C)C2(C(C1)C1C
CXTATJFJDMJMIY-UHFFFAOYSA-N	CCCCCCCC(=O)OC(C[N+](C)(C)C)CC(=O
BSBFFVUBOUMCCS-UHFFFAOYSA-N	COc1cc2CCN(C3c2cc1Oc1ccc(cc1O)CC1
VFLDPWHFBUODDF-FCXRPNKRSA-N	COc1cc(/C=C/C(=O)CC(=O)/C=C/c2ccc(c
WWZKQHOCKIZLMA-UHFFFAOYSA-N	CCCCCCCC(=O)O
PAYRUJLWNCNPSJ-UHFFFAOYSA-N	Nc1ccccc1
NGZXDRGWBULKFA-UHFFFAOYSA-N	COc1cc2CCN(C3c2cc1Oc1cc(ccc1O)CC1
SNVNUOWZKGGIRP-SCNFBCNRSA-N	OC/C(=C/CC/C(=C/Cc1cc(O)ccc1O)/C)/C
UEPVWRDHSPMIAZ-IZTHOABVSA-N	COc1cc(/C=C/C(=C/C(=O)/C=C/c2ccc(cc2
TZDMGBLPGZXHJI-UHFFFAOYSA-N	C=C1C(=O)CC2CC1C2(C)C
QMAYBMKBYCGXDH-UHFFFAOYSA-N	CC1=CC2C(CC1)C(=CCC2C(C)C)C
LCYXQUJDODZYIJ-UHFFFAOYSA-N	C=C1C(O)CC2CC1C2(C)C
KEMQGTRYUADPNZ-UHFFFAOYSA-N	CCCCCCCCCCCCCCCC(=O)O
VKOBVWXKNCXXDE-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCCCC(=O)O
RGZSQWQPBWRIAQ-UHFFFAOYSA-N	CC(=CCCC(C1CCC(=CC1)C)(O)C)C
QTGAEXCCAPTGLB-QZFXXANLSA-N	CC1=CCC(C)(C)C=CCC2C(C(CC1)O2)C
IGODOXYLBBXFDW-UHFFFAOYSA-N	CC(=O)OC(C1CCC(=CC1)C)(C)C
QZZGJDVWLFXDLK-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCCCCCCC(=O
KXSDPILWMGFJMM-UHFFFAOYSA-N	CC(C12CCC(C2C1)(C)O)C
GEHPRJRWZDWFBJ-FOCLMDBBSA-N	CCCCCCCCCCCCC/C=C/C(=O)O
BKATZVAUANSCKN-UHFFFAOYSA-N	CC(=O)OCC1=CCC2CC1C2(C)C
WQEPLUUGTLDZJY-UHFFFAOYSA-N	CCCCCCCCCCCCCCC(=O)O
HIGQPQRQIQDZMP-DHZHZOJOSA-N	C/C(=C\COC(=O)C)/CCC=C(C)C
KQAZVFVOEIRWHN-UHFFFAOYSA-N	CC1=CCC2(C1C2)C(C)C
SEKHAGCBKYMSBO-UHFFFAOYSA-N	CC(CCC=C(C)C)CCCC(=O)O
YYWZKGZIIKPPJZ-UHFFFAOYSA-N	CC1(O)CCC2CC1C2(C)C
DCSCXTJOXBUFGB-UHFFFAOYSA-N	CC1=CC(=O)C2CC1C2(C)C
XBGUIVFBMBVUEG-PFONDFGASA-N	CC(=CCC/C(=C/1\CCC(=CC1)C)/C)C
QPTHNVGZXBEQOJ-UHFFFAOYSA-N	CC(=O)CC(c1ccc(cc1)C)C
SECPZKHBENQXJG-BQYQJAHWSA-N	CCCCCC/C=C/CCCCCCCC(=O)O
ZQPPMHVWECSIRJ-MDZDMXLPSA-N	CCCCCCCC/C=C/CCCCCCCC(=O)O
XBWACJDEQIZTPR-UHFFFAOYSA-N	CC(C1CCC2(C3C1C1C(C21C)C3)C)C
OYHQOLUKZRVURQ-AVQMFFATSA-N	CCCCC/C=C/C/C=C/CCCCCCCC(=O)O
DTOSIQBPPRVQHS-IUQGRGSQSA-N	CC/C=C/C/C=C/C/C=C/CCCCCCCC(=O)C
CXENHBSYCFFKJS-VDQVFBMKSA-N	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
FQTLCLSUCSAZDY-SDNWHVSQSA-N	C=CC(CC/C=C(/CCC=C(C)C)\C)(O)C
VKUJZPYJXUSOEW-AATRIKPKSA-N	CC(/C=C/CC(c1ccc(cc1)C)C)C
GAIBLDCXCZKKJE-BZXLUOIMSA-N	CC1=CCCC(=C)C=CC(CC1)C(C)C
WONIGEXYPVIKFS-UHFFFAOYSA-N	CC1=CC(O)C2CC1C2(C)C
KMRMUZKLFIEVAO-UHFFFAOYSA-N	O=CC1=CCC2CC1C2(C)C
GLZPCOQZEFWAFX-JXMROGBWSA-N	OC/C=C(/CCC=C(C)C)\C
WTEVQBCEXWBHNA-JXMROGBWSA-N	O=C/C=C(/CCC=C(C)C)\C
JXZQZARENYGJMK-UHFFFAOYSA-N	CC(=CCCC(C1=CCC(=CC1)C)C)C
YMBFCQPIMVLNIU-UHFFFAOYSA-N	CC(=CCCC1(C)C2CC=C(C1C2)C)C
WRHGORWNJGOVQY-UHFFFAOYSA-N	CC1=CC2C(CC1)C(=C)CCC2C(C)C
FIKTURVKRGQNQD-VHEBQXMUSA-N	CCCCCCCCCCCCCCCC/C=C/C(=O)O
NEHNMFOYXAPHSD-UHFFFAOYSA-N	O=CCC(CCC=C(C)C)C
RRBYUSWBLVXTQN-UHFFFAOYSA-N	CC12C3C1CC(C2(C)C)C3
UKMSUNONTOPOIO-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCCCCCCCCC(=O)O
UPVZPMJSRSWJHQ-UHFFFAOYSA-N	CC(C1CCC2(C3C1C2C(=C)CC3)C)C

```
OGCGGWYLHSJRFY-UHFFFAOYSA-N      O=CCC1CC=C(C1(C)C)C
ZRALSGWEFCBTJO-UHFFFAOYSA-N      NC(=N)N
CGJJPOYORMGCGE-UHFFFAOYSA-N      O=CC(CC(=O)O)N
ULEBESPCVWBNIF-UHFFFAOYSA-N      NC(=NCCCC(C(=O)N)N)N
FULLTSYFDLSFSF-UHFFFAOYSA-N      OCCCCN=C(N)N
QNAYBMKLOCPYGJ-UHFFFAOYSA-N      CC(C(=O)O)N
DJNCIOAUQVURTQ-UHFFFAOYSA-N      CC(CCCC(C1CCC2=C3C(CCC12C)C1(C)
CKLJMWTZIZZHCS-UHFFFAOYSA-N      OC(=O)CC(C(=O)O)N
HVYWMOMLDIMFJA-UHFFFAOYSA-N      CC(CCCC(C1CCC2C1(C)CCC1C2CC=C2
ODKSFYDXXFIFQN-UHFFFAOYSA-N      OC(=O)C(CCCN=C(N)N)N
ZRALSGWEFCBTJO-UHFFFAOYSA-N      NC(=N)N
BPYKTIZUTYGOLE-BMNRKXRESA-N      C=CC1=C(C)/C(=C\c2[nH]c(c(c2C)CCC(=
GWZYPXHJIZCRAJ-UDMDDCJJSA-N      C=CC1=C(C)/C(=C\c2[nH]c(c(c2C)CCC(=
RUDATBOHQWOJDD-CGAHXEJXSA-N      O[C@@H]1CC[C@]2([C@@H](C1)C[C@
BHQCQFFYRZLCQQ-OELDTZBJSA-N      O[C@@H]1CC[C@]2([C@@H](C1)CC([C
KXGVEGMKQFWNSR-LLQZFEROSA-N      O[C@@H]1CC[C@]2([C@@H](C1)CC[C
DNVPQKQSNYMLRS-CLTUJMCISA-N      OC1CC[C@]2(C(=CC=C3[C@H]2CC[C@
SMEROWZSTRWXGI-HVATVPOCSA-N      O[C@@H]1CC[C@]2([C@@H](C1)CC[C
XOAAWQZATWQOTB-UHFFFAOYSA-N      NCCS(=O)(=O)O
MIJYXULNPSFWEK-UHFFFAOYSA-N      OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1
DNVPQKQSNYMLRS-BQYQJAHWSA-N      OC1CCC2(C(=CC=C3C2CCC2(C3CCC2(
WCGUUGGRBIKTOS-UHFFFAOYSA-N      CC1CCC2(C(C1C)C1=CCC3C(C1(CC2)C
GWZYPXHJIZCRAJ-NAUAOTQLSA-N      C=CC1=C(C)/C(=C/c2[nH]c(c(c2C)CCC(=
BPYKTIZUTYGOLE-VVCLLGATSA-N      C=CC1=C(C)/C(=C/c2[nH]c(c(c2C)CCC(=
WVULKSPCQVQLCU-UHFFFAOYSA-N      OC1CCC2(C(C1)CCC1C2CC(O)C2(C1CC
JUFYZLWTPPZFMH-UHFFFAOYSA-N      O=C(OC(C(=O)O)Cc1ccc(c(c1)O)O)CCc1
DLYVTEULDNMQAR-UHFFFAOYSA-N      COC(=O)CCC(C1CCC2C1(C)C(O)CC1C2
ZHUOOEGSSFNTNP-UHFFFAOYSA-N      COC(=O)CCC(C1CCC2C1(C)C(O)CC1C2
AWDRATDZQPNJFN-UHFFFAOYSA-N      OC1CCC2(C(C1)CCC1C2CC(O)C2(C1CC
WBWWGRHZICKQGZ-UHFFFAOYSA-N      OC1CCC2(C(C1)CC(C1C2CC(O)C2(C1C
RUDATBOHQWOJDD-UHFFFAOYSA-N      OC1CCC2(C(C1)CC(C1C2CCC2(C1CCC
OJLLODMRNXRZIT-UHFFFAOYSA-N      COc1c(O)c(OC)cc2c1c(=O)n(cc2)C
GRQROVWZGGDYSW-UHFFFAOYSA-N      COC(=O)CCC(C1CCC2C1(C)CCC1C2C(
KXGVEGMKQFWNSR-UHFFFAOYSA-N      OC1CCC2(C(C1)CCC1C2CC(O)C2(C1CC
ZESRJSPZRDMNHY-UHFFFAOYSA-N      OCC(=O)C1CCC2C1(C)CCC1C2CCC2=C
XCGSFFUVFURLIX-UHFFFAOYSA-N      O=C(C1CN(C)C2C(=C1)c1cccc3c1c(C2)c
RFDAIACWWDREDC-UHFFFAOYSA-N      OC1CCC2(C(C1)CC(C1C2CC(O)C2(C1C
HVYWMOMLDIMFJA-UHFFFAOYSA-N      CC(CCCC(C1CCC2C1(C)CCC1C2CC=C2
OEYIOHPDSNJKLS-UHFFFAOYSA-N      OCC[N+](C)(C)C
SNKFFCBZYFGCQN-BJMVGYQFSA-N      O=C(OC(C(=O)O)Cc1ccc(c(c1)O)O)/C=C/
HPYDSVWYXXKHRD-UHFFFAOYSA-N      OC(=O)CNC(=O)C(Cc1ccc(cc1)O)N
DJNCIOAUQVURTQ-UHFFFAOYSA-N      CC(CCCC(C1CCC2=C3C(CCC12C)C1(C)
BHQCQFFYRZLCQQ-UHFFFAOYSA-N      OC1CCC2(C(C1)CC(C1C2CC(O)C2(C1C
SMEROWZSTRWXGI-UHFFFAOYSA-N      OC1CCC2(C(C1)CCC1C2CCC2(C1CCC2
RCNSAJSGRJSBKK-YKSNQIBWSA-N      C=CC1=C(C)C(=NC1=O)/C=c\1/[nH]/c(=C
KRAPUBRHQOHVHM-IFADSCNNSA-N      C=CC1=C(C)/C(=C/C2=C(C)C(C(=N2)CC
DAIDKOMWNKGKSP-UHFFFAOYSA-N      CCCNC(=O)CCCC1CCC2(C1(C)C(O)CC1
BPYKTIZUTYGOLE-IFADSCNNSA-N      C=CC1=C(C)/C(=C/c2[nH]c(c(c2C)CCC(=
POJWUDADGALRAB-PVQJCKRUSA-N      NC(=O)N[C@@H]1NC(=O)NC1=O
CBMYJHIOYJEBSB-ULTMTAQRSA-N      O[C@@H]1CC[C@]2([C@@H](C1)CC[C
CBMYJHIOYJEBSB-GCXXXECGSA-N      O[C@@H]1CC[C@]2([C@@H](C1)CC[C
RAJWOBJTTGJROA-WZNAKSSCSA-N      O=C1CC[C@]2([C@H](C1)CC[C@@H]1[
RAJWOBJTTGJROA-QJISAEMRSA-N      O=C1CC[C@]2([C@@H](C1)CC[C@@H]
CBMYJHIOYJEBSB-YISWTCPOSA-N      O[C@H]1CC[C@]2([C@@H](C1)CC[C@
YEWSFUFGMDJFFG-QAGGRKNESA-N      O=C1CC[C@]2(C(=C1)C=C[C@@H]1[C@
AEMFNILZOJDQLW-QAGGRKNESA-N      O=C1CC[C@]2(C(=C1)CC[C@@H]1[C@
QGXBDMJGAMFCBF-HLUDHZFRSA-N      O[C@@H]1CC[C@]2([C@H](C1)CC[C@
OFNSUWBAQRCHAV-OYQUVCAXSA-N      C/C(=C\C=C\C=C(\C=C\C=C(\C=C\[C@]1
```

MDFFNDBAEOHIDY-UHFFFAOYSA-N	COc1c2OCOc2c2c3c1ccnc3C(=O)c1c2cc
MUNWAHDYFVYIKH-WDSKDSINSA-N	O[C@H]1C[C@H]([N+](C1)(C)C)C(=O)[O-
DTGKSKDOIYIVQL-UHFFFAOYSA-N	OC1CC2C(C1)(C)CC2)(C)C
DTGKSKDOIYIVQL-QXFUBDJGSA-N	O[C@@H]1C[C@H]2C([C@]1(C)CC2)(C)
RECUKUPTGUEGMW-UHFFFAOYSA-N	CC(c1ccc(c(c1)O)C)C
GXGJIOMUZAGVEH-UHFFFAOYSA-N	CCc1ccc(c2c(c1)c(C)cc2)C
NYOXRYYXRWJDKP-SHLKSLFASA-N	CC(CCC[C@@H]([C@H]1CC[C@H]2[C@
HVYWMOMLDIMFJA-DPAQBDIFSA-N	CC(CCC[C@H]([C@H]1CC[C@H]2[C@]1
VQMSRUREDGBWKT-UHFFFAOYSA-N	OC(=O)c1ccnc2c1cccc2
VKOSQMWSWLZQPA-UHFFFAOYSA-N	COc1cc2oc(cc(=O)c2c(c1OC)O)c1ccc(c(c
RSLTVQQROJUNCD-ALCCZGGFSA-N	O=C1CCCCCCCC/C=C\CCC1
FUGDHQXYVPQGLJ-UHFFFAOYSA-N	O=C1CCCCCCCCCCCC1
XOEMDGMZEQVNDD-XQRVVYSFSA-N	O=C1CCCCCCC/C=C\CCC1
YZPIVPVXEUAVNR-UHFFFAOYSA-N	C1CCCCCCCc2nc(CC1)ccc2
MPLDCQODSRHTBW-UHFFFAOYSA-N	Oc1ccc2c(c1)nc(oc2=O)c1ccccc1
SVZLTRRSGWXPBL-UHFFFAOYSA-N	Oc1ccc(c(c1)Nc1cc(O)ccc1C(=O)O)C(=O)
QFZHDMKCXNVVKG-PVYCLFTASA-N	O=C1OC[C@H]2O[C@@H](Oc3cc4c(O[C
MDSZBCFPVUABGB-PVYCLFTASA-N	[O-]c1ccc(cc1)c1[o+]c2cc(O)cc3c2cc1O[C
VOXZDWNPVJITMN-SFFUCWETSA-N	Oc1ccc2c(c1)CC[C@@H]1[C@@H]2CC[
VOXZDWNPVJITMN-ZBRFXRBCSA-N	Oc1ccc2c(c1)CC[C@@H]1[C@@H]2CC[
VADSVXSGIFBZLI-IBEHDNSVSA-N	C=CCc1ccc(c(c1)OC)O[C@@H]1O[C@H
GCLHKQZTLUKUTE-UHFFFAOYSA-N	CC(=O)c1c(C)cc2c(c1O)c(O)c(cc2)c1ccc2
OZIPFYKAIOOVEJ-ODWUMMNUSA-N	CC/C=C\CCO[C@@H]1O[C@H](CO)[C@
QGXBDMJGAMFCBF-BNSUEQOYSA-N	O[C@@H]1CC[C@]2([C@@H](C1)CC[C
QGXBDMJGAMFCBF-LUJOEAJASA-N	O[C@H]1CC[C@]2([C@H](C1)CC[C@@H
VMYTXBKVYDESSJ-HKQXQEGQSA-N	O[C@@H]1CC[C@]2(C(=C1)CC[C@@H]
FMGSKLZLMKYGDP-USOAJAOKSA-N	O[C@H]1CC[C@]2(C(=CC[C@@H]3[C@
GQQXMGOLSQFKPZ-ODWDTFMPSA-N	OC[C@H]1O[C@@H](OCC/C=C\CC2=C(
RZGFUGXQKMEMOO-BSANDHCLSA-N	OCC/C=C\C[C@@H]1[C@H](CCC1=O)C
JFDNMLUPLXZXGV-RKAGECJXSA-N	OC[C@H]1O[C@@H](OCC/C=C\C[C@@
FPDSMLMTMDHJQT-UHFFFAOYSA-N	CC1CCCCCCC(c2nc(C1)ccc2)O
XEKNCTZVXNUNGM-UHFFFAOYSA-N	OC1C(C)CCCCCCCc2nc1ccc2
DOUMFZQKYFQNTF-WUTVXBCWSA-N	O=C(O[C@@H](C(=O)O)Cc1ccc(c(c1)O)O
UWKAYLJWKGQEPM-LBPRGKRZSA-N	C=C[C@](OC(=O)C)(CCC=C(C)C)C
YVBJWBLZYPRBNN-LWUSAIQQSA-N	OC[C@H]1O[C@@H](O[C@]2(C)CC=C(C
JGXUYPSOOTZEGY-LWUSAIQQSA-N	CC(=O)OC[C@H]1O[C@H](O[C@]2(C)CC
MDDBLJFAZVVHGO-YXIOUMEFSA-N	OC[C@H]1O[C@H](O[C@]2(C)CC=C(C[C
HDVPJYNBUXNSEW-YXIOUMEFSA-N	OC[C@H]1O[C@H](O[C@]2(C)CCC(=C[C
CVMWCRDXSQGRSJ-UHFFFAOYSA-N	CC1CCCCCCCCCC(=O)C1
XCZTYYQNVNLGKI-LVUHIJSRSA-N	OCC/C=C\C[C@@H]1[C@H](CCC1=O)C
AJWIFVNLXHFTFD-AHXFZLPISA-N	OC[C@H]1O[C@@H](OCC/C=C\C[C@@
IEVYLQISZQFFGA-JXMROGBWSA-N	OC/C(=C/CCC(=C)C=C)/C
YGUUXLXMTKARJN-DHZHZOJOSA-N	C=CC(=C)CC/C=C(/COC(=O)C)\C
RPESHUOYYLJEQJ-HTQZYQBOSA-N	C[C@H](CC[C@H](C(C)C)OS(=O)(=O)O)
GVPGXFIINYYZAR-UHFFFAOYSA-N	CC1CCCCCCCCCCCC(C1)O
ALHUZKCOMYUFRB-UHFFFAOYSA-N	CC1CCCCCCCCCCCC(=O)C1
IMNKABOILQOFDL-UHFFFAOYSA-N	CC1CCCCCCCc2nc(C1)ccc2
QBGSZFGDIXJTOI-UHFFFAOYSA-N	C1CCCCCc2nc(CC1)ccc2
OSOIQJGOYGSIMF-UHFFFAOYSA-N	O=C1CCCCCCCCCCCCCC1
YQKQOLPNKNHLBO-DVAIZSLESA-N	OC[C@H]1O[C@@H](O[C@@H](COC(=
HHNPREGNVCFCOP-MHSMMQCRSA-N	OC[C@H](O[C@@H]1O[C@H](CO)[C@H
BTRIXFBTQFTXAB-SGKFEUNSSA-N	OC[C@H]1O[C@@H](O[C@@H](COC(=
FCDLCPWAQCPTKC-UHFFFAOYSA-N	Oc1cc(cc2c1C(=O)c1c(C2=O)cccc1O)C(=
WRYLYDPHFGVWKC-JTQLQIEISA-N	CC1=CC[C@@](CC1)(O)C(C)C
QKYDQSUAFNWVTI-UDNSVAPOSA-N	O=C1CC[C@]2(C(=C1)CC[C@@]1(C2CC
KXSDPILWMGFJMM-AEJSXWLSSA-N	CC([C@]12CC[C@@]([C@@H]2C1)(C)O
MGSRCZKZVOBKFT-UHFFFAOYSA-N	Cc1ccc(c(c1)O)C(C)C
BAIRXMVFPKLWSE-UHFFFAOYSA-N	COc1cc(ccc1O)c1cc(=O)c2c(o1)c(OC)c(c(c

CSCBRJMLQJUDBK-HHYIAMCXSA-N	OC[C@H]1O[C@H]2O[C@]3(C)CC=C(C[
WFMIUXMJJBBOGJ-UHFFFAOYSA-N	CC(=O)Oc1cc(C)ccc1C(C)C
SMYFGRWZEIQLPY-XSNSHTBXSA-N	NC(=O)N[C@@H]1CC[C@]2(C(=C1)CCC
RQUJDLYPEZVGRT-JSGNRIOWSA-N	NC(=O)N[C@@H]1CC[C@]2(C(=C1)CCC
OCDWKDASQKOTIQ-ZSAROZDLSA-N	OC[C@H]1O[C@@H](O[C@@H]2C[C@(
MFAONEQLPARJAO-UHFFFAOYSA-N	NC(=O)NC1=NC(=O)NC1=O
UYEMGAFJOZZIFP-UHFFFAOYSA-M	[O-]c1cc(O)cc(c1)C(=O)O
YXOLAZRVSSWPPT-UHFFFAOYSA-N	Oc1ccc(c(c1)O)c1oc2cc(O)cc(c2c(=O)c1O
RPESHUOYYLJEQJ-UHFFFAOYSA-N	CC(CCC(C(C)C)OS(=O)(=O)O)O
DJNCIOAUQVURTQ-UHFFFAOYSA-N	CC(CCCC(C1CCC2=C3C(CCC12C)C1(C)
CPBQNAKTSMCPNH-GZTJUZNOSA-N	COc1cc(/C=C/C(=O)OC2CCC3(C(=CCC4
GMNAPBAUIVITMI-UHFFFAOYSA-N	CNC(C1C(O)CC2(C1(C)CCC13C2CCC2C
PNHDWCKYXTWGLA-UHFFFAOYSA-N	CC(COC1OCC(C(C1OC(=O)C)OC(=O)C)
ZMEIKTTXONUYNX-UHFFFAOYSA-N	OCC1OC(OC2C(O)COC(C2O)OC2C(OC
PCSWXVJAIHCTMO-UHFFFAOYSA-P	Nc1cc(C)[n+](c2c1cccc2)CCCCCCCCCC[
VJDBDVUFFPRHSF-UHFFFAOYSA-N	OCC1OC(Oc2cc(O)cc3c2c(O)c(c(c3)C)C)C(
RAJWOBJTTGJROA-UHFFFAOYSA-N	O=C1CCC2(C(C1)CCC1C2CCC2(C1CCC
QGXBDMJGAMFCBF-UHFFFAOYSA-N	OC1CCC2(C(C1)CCC1C2CCC2(C1CCC2
CBMYJHIOYJEBSB-UHFFFAOYSA-N	OC1CCC2(C(C1)CCC1C2CCC2(C1CCC2
YEWSFUFGMDJFFG-UHFFFAOYSA-N	O=C1CCC2(C(=C1)C=CC1C2CCC2(C1C
FMGSKLZLMKYGDP-UHFFFAOYSA-N	OC1CCC2(C(=CCC3C2CCC2(C3CCC2=(
VOXZDWNPVJITMN-UHFFFAOYSA-N	Oc1ccc2c(c1)CCC1C2CCC2(C1CCC2O)(
MUMGGOZAMZWBJJ-UHFFFAOYSA-N	O=C1CCC2(C(=C1)CCC1C2CCC2(C1CC
VPQWBNWSLZYYFH-UHFFFAOYSA-N	CC1CCCCCCCCCC(=O)C1
BKIMMITUMNQMOS-UHFFFAOYSA-N	CCCCCCCCC
QQKAHDMMPBQDAC-UHFFFAOYSA-N	COc1cc2CCNC3c2c(c1OC)c1ccccc1C3
ZFMSMUAANRJZFM-UHFFFAOYSA-N	COc1ccc(cc1)CC=C
AEMFNILZOJDQLW-UHFFFAOYSA-N	O=C1CCC2(C(=C1)CCC1C2CCC2(C1CC
POJWUDADGALRAB-UHFFFAOYSA-N	NC(=O)NC1NC(=O)NC1=O
OVSKIKFHRZPJSS-UHFFFAOYSA-N	OC(=O)COc1ccc(cc1Cl)Cl
MMOXZBCLCQITDF-UHFFFAOYSA-N	CCN(C(=O)c1cccc(c1)C)CC
HVYWMOMLDIMFJA-UHFFFAOYSA-N	CC(CCCC(C1CCC2C1(C)CCC1C2CC=C2
UYEMGAFJOZZIFP-UHFFFAOYSA-N	Oc1cc(O)cc(c1)C(=O)O
LQGNCUXDDPRDJH-XICIJMSXSA-N	CC(CC[C@H]([C@@]([C@H]1CC[C@@]:
BJRNKVDFDLYUGJ-RMPHRYRLSA-N	OC[C@H]1O[C@@H](Oc2ccc(cc2)O)[C@
CTNHZEZBBGIUJB-HRQAAHFGSA-N	OC[C@@]12[C@@H](O)CC(C[C@H]2C2
SPCSEMLFKVZFJN-CUCCWGAISA-N	OC[C@@]12[C@@H](O)CC(C[C@H]2C2
PADNECYMNLPKRN-JAGYOTNFSA-N	OC[C@]12[C@H](O)C[C@@]3(C(=CC[C(
PADNECYMNLPKRN-HAIONMGCSA-N	OC[C@]12[C@H](O)C[C@@]3(C(=CC[C(
CJGRGYBLAHPYOM-LNVOCJLCSA-N	OC[C@H]1O[C@@H](OC(=O)/C=C\c2cc
CJGRGYBLAHPYOM-HOLMNUNMSA-N	OC[C@H]1O[C@@H](OC(=O)/C=C/c2cc
UTIATVZKLZDAQF-FFHNCUASSA-N	O=C(/C=C/c1ccccc1)OC[C@H]1O[C@@H
NAKQJOAAYRWURE-QKZSZZOLSA-N	OCCC(=C)C(=O)OC[C@H]1O[C@@H](O
NAKQJOAAYRWURE-OAXOJBTLSA-N	OCCC(=C)C(=O)OC[C@H]1O[C@@H](O
CQLRUIIRRZYHHS-LFXZADKFSA-N	OC[C@H]1O[C@@H](Oc2c(oc3c(c2=O)c
POQICXMTUPVZMX-UXYNSRGZSA-N	OC[C@@H]1O[C@H]([C@@H]([C@H]1C
RWBQKECPTANRKY-SIUDIOLQSA-N	CC(CCC(=O)[C@@]([C@H]1CC[C@@]2(
IILSBUXFTVZCJS-JTGVHUCZSA-N	O[C@H]1C[C@@]2(C)C(C[C@H]1O)C(=(
YHGVYECWZWIVJC-TVZJSHMMSA-N	OC[C@@]12CCC(C[C@H]2C2=CC[C@H
PZZRDJXEMZMZFD-BWYUNELBSA-N	Oc1cc(O)c2c(c1)oc(c(c2=O)O[C@@H]1O
DJSISFGPUUYILV-ZFORQUDYSA-N	OC(=O)[C@H]1O[C@@H](Oc2cc3oc(cc(=
SKKXALUAXPQBOM-FUCRAMRQSA-N	O[C@H]1[C@@H](O[C@H]([C@@H]([C@
PWSLQEGYLXOJNB-UOXIVHGRSA-N	O[C@H]1[C@@H](O[C@H]([C@@H]([C@
JPUKWEQWGBDDQB-DTGCRPNFSA-N	OC[C@H]1O[C@@H](Oc2c(oc3c(c2=O)c
AZDRQVAHHNSJOQ-UHFFFAOYSA-N	[AlH3]
RYGMFSIKBFXOCR-UHFFFAOYSA-N	[Cu]
CWYNVVGOOAEACU-UHFFFAOYSA-N	[Fe+2]
WAEMQWOKJMHJLA-UHFFFAOYSA-N	[Mn+2]

BLRPTPMANUNPDV-UHFFFAOYSA-N	[SiH4]
PWYYWQHXAPXYMF-UHFFFAOYSA-N	[Sr+2]
PTFCDOFLOPIGGS-UHFFFAOYSA-N	[Zn+2]
IIDJRNMFWXDHID-UHFFFAOYSA-N	OP(=O)(C(P(=O)(O)O)(Cc1cccnc1)O)O
ONCBFIXZBSEBNG-YQCHCMBFSA-N	COC(=O)C1=C(O)c2c3=C1C1=[NH+]/C(=
JLVVSXFLKOJNIY-UHFFFAOYSA-N	[Mg+2]
BVKZGUZCCUSVTD-UHFFFAOYSA-N	OC(=O)O
XEEYBQQBJWHFJM-UHFFFAOYSA-N	[Fe]
PWHULOQIROXLJO-UHFFFAOYSA-N	[Mn]
HCHKCACWOHOZIP-UHFFFAOYSA-N	[Zn]
REDXJYDRNCIFBQ-UHFFFAOYSA-N	[AlH3+3]
DFYRUELUNQRZTB-UHFFFAOYSA-N	COc1cc(ccc1O)C(=O)C
IYGYMKDQCDOMRE-ROUUACIJSA-N	CN1CCc2c([C@H]1[C@H]1OC(=O)c3c1c
QUOZWMJFTQUXON-UXXRCYHCSA-N	OC[C@H]1O[C@@H](Oc2ccc(cc2OC)C(=
KSENPDOZJGRJHR-GPWVBDSWSA-N	OC[C@H]1O[C@@H](O[C@H]2C[C@H]3
GOWXUGYRPHOTEQ-QYNXQQORSA-N	OC[C@H]1O[C@@H](O[C@H]2C[C@@H
RJWJHRPNHPHBRN-FKVJWERZSA-N	OCC1=C[C@H]([C@H]2[C@H]1[C@@H]
VFCGRXCCUHLLIP-UHFFFAOYSA-N	COc1c(OC)ccc2c1c[n+]1CC(O)c3c(c1c2)c
YBHILYKTIRIUTE-UHFFFAOYSA-N	COc1c(OC)ccc2c1c[n+]1CCc3c(c1c2)cc1c
CBTFERBMQQAROP-BZNQNGANSA-N	OC[C@H]1O[C@@H](Oc2ccc(c(c2)C(=O)
LHDWRKICQLTVDL-PZYDOOQISA-N	OC[C@H]1O[C@@H](OC2OC=C[C@@H
YYFOFDHQVIODOQ-UHFFFAOYSA-O	COc1cc2CC[n+]3c(c2cc1O)cc1c(c3)c(OC)
XYHOBCMEDLZUMP-UHFFFAOYSA-N	C1Oc2c(O1)cc1c(c2)CC[n+]2c1cc1ccc3c(
FELOSQQXIHRUSH-UHFFFAOYSA-N	COc1cc2CCN(Cc2cc1O)C
BMCZTYDZHNTKPR-INIZCTEOSA-N	COc1c(OC)ccc2c1CN1CCc3c([C@@H]1C
XPOJSWHIKCNLEQ-UHFFFAOYSA-N	COc1cc2C(=O)Cc3ccc4c(c3CN(CCc2cc1O
NJJDSCKXYWRUOY-HUYWQKACSA-N	COC(=O)[C@H]1O[C@@H](O[C@H]2CC
PVOOFKAEZIVTOE-HWVFMACMSA-N	OC[C@H]1O[C@@H](OCC23CCC(CC3O
FNUPUYFWZXZMIE-LSDHHAIUSA-N	Oc1ccc2c(c1)O[C@@H]([C@H](C2=O)O)
FNUPUYFWZXZMIE-CABCVRRESA-N	Oc1ccc2c(c1)O[C@H]([C@@H](C2=O)O)
CXQWRCVTCMQVQX-LSDHHAIUSA-N	Oc1cc2O[C@H](c3ccc(c(c3)O)O)[C@H](O
YQUVCSBJEUQKSH-UHFFFAOYSA-N	OC(=O)c1ccc(c(c1)O)O
PQQITYGQJLPDFC-RKQHYHRCSA-N	OC[C@H]1O[C@@H](OCCc2ccc(c(c2)O)
FPJQGFLUORYYPE-UHFFFAOYSA-N	COc1cc2c(cc1OC)CC[n+]1c2cc2ccc3c(c2
KSEBMYQBYZTDHS-HWKANZROSA-N	COc1cc(/C=C/C(=O)O)ccc1O
LVNFIOGAAUPIPC-BJGSYIFTSA-N	COc1cc(/C=C/C(=O)OC[C@H]2O[C@@H
XHEFDIBZLJXQHF-UHFFFAOYSA-N	Oc1ccc2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O
VKUXVDUAEAQCSK-MJLPRLLOSA-N	OC[C@H]1O[C@@H](OCCc2ccc(c(c2)O)
FUZMQNZACIFDBL-KYJUHHDHSA-N	COc1ccc2cc1Oc1ccc(cc1)C[C@@H]1N(C
OSSHOTLYZGBYFR-IVMMKFTPSA-N	CC(=O)OC[C@H]1O[C@@H](OC2OC=C
KWVNDXWEYANTFF-AAOUOOLPSA-N	COc1cc(ccc1OC(=O)C)C(=O)O[C@H]1[C
NHKDEMRRYWOJOF-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCCCCCCCCCCC
OCPXLBDSVHVVEA-QSKFOJEASA-N	OC[C@H]1O[C@@H](OCCc2ccc(c(c2)O)
MXTLAHSTUOXGQF-UHFFFAOYSA-O	COc1cc2c(cc1O)CC[n+]1c2cc2ccc(c(c2c1
JANLDILJJLTVDB-YHZAWZKLSA-N	OC[C@H]1O[C@@H](OC2OC=C[C@@H
GAYKAIAESJROGN-SAOYRWCPSA-N	OC[C@H]1[C@H](CO[C@@H]1c1ccc(c(c
KBDSLGBFQAGHBE-FGPVBJILSA-N	O=C1OC[C@]23[C@H](C1)OC([C@@H]2
FBPFZTCFMRRESA-UHFFFAOYSA-N	OCC(C(C(C(CO)O)O)O)O
LRHHPZILMPIMIY-GGKKSNITSA-N	OC[C@H]1O[C@@H](OC2OC=C[C@@H
QQKAHDMMPBQDAC-CQSZACIVSA-N	COc1cc2CCN[C@H]3c2c(c1OC)c1ccccc1
KBDSLGBFQAGHBE-ICSMZNQQSA-N	O=C1OC[C@]23[C@H](C1)OC(C2CC(=C
IAFYZOROUCWFHK-RZWNPTOTSA-N	COc1cc2c(cc1OC)CCN([C@H]2Cc1ccc(c
QUCQEUCGKKTEBI-UHFFFAOYSA-N	COc1cc2CC[n+]3c(c2cc1OC)cc1c(c3)c(OC
RTZZUFGHDIARKI-HWLNPCHJSA-N	O=C(OC[C@H]1O[C@@H](OC2OC=C[C
PPTUZELFQUKUGJ-NQLBIMQHSA-N	O[C@H]1C[C@H]2C(=CCC3[C@@]2(C)C
GOZCEKPKECLKNO-RKQHYHRCSA-N	OC[C@H]1O[C@@H](Oc2ccc(cc2)C(=O)
SCIGYBYAZUFDLA-KRQBOUTOSA-N	OC[C@H]1O[C@@H](OC2OC=C[C@@H
AKNILCMFRRDTEY-NUGKWEEESA-N	OC[C@H]1O[C@@H](OC2OC=C[C@@H

RMSKZOXJAHOIER-GGKKSNITSA-N	OC[C@H]1O[C@@H](OC2OC=C[C@@H
HGXBRUKMWQGOIE-AFHBHXEDSA-N	COc1cc(ccc1O)[C@H]1O[C@H]2[C@@
RMJMFPNPBUGUMP-NGESMGFYSA-N	OCC[C@H]1c2cocc2[C@@H]([C@@H]1(
DTHUVZQMVMVXNB-LVSIQRNOSA-N	OC(=O)C[C@H]1c2cocc2[C@@H]([C@@
IKRQGQZHSMYUJJ-DWFIKQFRSA-N	COC(=O)C[C@@H]1[C@@H](O)[C@H](c
CBZYUWGJNYOKHT-ZKDZFUIGSA-N	OC[C@H]1O[C@@H](O[C@H]2[C@H](O
MTKGYCQUEWGDQW-CRVIUCGDSA-N	OC[C@H]1O[C@@H](O[C@H]2[C@H](O
LHUSSIYFBNCANU-HSVUOORVSA-N	COC(=O)[C@@]1(O)C=C(C2=CC(=O)C3
INVGWHRKADIJHF-UHFFFAOYSA-N	C[n+]1cc2c3OCOc3ccc2c2c1c1cc3OCOc
WAABIQNSMBCVLC-FSORARIGSA-N	OC[C@H]1O[C@@H](O[C@H]2[C@H](O
FKUWQWJFTAWUKB-KOIGGHRSSA-N	OC[C@H]1O[C@@H](OCCc2ccc(c(c2)O)
YWNUNVSMOKMJMG-LJAQVGFWSA-N	COc1ccc2cc1Oc1ccc(cc1)CC1=NCCc3c1
XEZKWYLHAOYOCL-AWEZNQCLSA-N	COc1cc2c(cc1OC)C[C@H]1c3c2c2OCOc
GOQUMRHFJDDYAU-UHFFFAOYSA-N	COc1cc2c(cc1OC)C(=O)c1c3c2c2OCOc2
KMLPLPOAFAPFFE-HNNXBMFYSA-N	COc1cc2c(cc1OC)C[C@H]1c3c2c(OC)c(c
JUQBPFGIFICIIN-UHFFFAOYSA-N	COc1c(O)ccc2c1CN(C)CCc1c(C(=O)C2)c
JTZZGWPIBBTYNE-MPBGBICISA-N	COc1cc2c(cc1OC)CCN1[C@@H]2[C@H]
UYNHKOIUEXICNQ-VMPREFPWSA-N	COc1c(OC)c2Oc3cc4c(cc3OC)CCN([C@H
JFOOZQIJNIJCOW-UHFFFAOYSA-N	COc1ccc2cc1Oc1ccc(cc1)CC1NCCc3c1c
FLBHMRBWGPQQKJ-UHFFFAOYSA-N	OC(=O)CCc1ccc(c(c1O)O)O
VZJHQCZRCSACOX-KVBCGVIQSA-N	OC[C@@]12O[C@H]2[C@H]([C@H]2[C@
GOHHRVCULPSXEU-OCHMABMRSA-N	OC[C@H]1O[C@@H](O[C@H]2OC=CC3
DKHAWRPWAKXFNA-MGSHXDRLSA-N	OC/C=C/c1cc2c(c(c1)OC)O[C@H]([C@@
XKNZOUHAGXCOCD-MWICNAQESA-N	OC[C@H]1O[C@@H](OC/C=C/c2cc(O)c3
GPDFNJMVWGKNEM-DPRYFANMSA-N	OC[C@H]1O[C@@H](OC/C=C/c2cc(OC(
NODYDDIWONUPOD-CTOQLXJKSA-N	OCCC(=C)C(=O)OC[C@H]1O[C@@H](O
NKHJLZUONNNHMW-OWLKOJIMSA-N	OCCC(=C)C(=O)OC[C@H]1O[C@@H](O
BCLYFWVPMVZSTR-DYDLCFMWSA-N	OCCC(=C)C(=O)OC[C@H]1O[C@@H](O
JVTZFYYHCGSXJV-UHFFFAOYSA-N	O=Cc1ccc(c(c1)O)OC
CWVRJTMFETXNAD-DUXPYHPUSA-N	O=C(OC1CC(O)(CC(C1O)O)C(=O)O)/C=C
WHUAIEAFPHHTPO-UHFFFAOYSA-N	COC(=O)C12OCC34C2C(OC(=O)C)C(=O
GUIYORVNNIUEBH-VQHVLOKHSA-N	OC(=O)/C=C/C1(C)C(CC(=O)C2(C1CCC1
XGEAUXVPBXUBKN-UHFFFAOYSA-N	COc1cc2CCN(C3c2cc1Oc1c2c(CCN(C2C
KFBCTNNQFGONHB-UHFFFAOYSA-N	COc1cccc2c1nc1occc1c2OC
KFXPBEAXNBSFIQ-UHFFFAOYSA-N	COC(=O)C12OC2(CC=C(C)C)C(=O)c2c(O
YLRXAIKMLINXQY-UHFFFAOYSA-O	COc1ccc2c(c1O)c1c(O)c(OC)cc3c1C(C2)
MAYJEFRPIKEYBL-UHFFFAOYSA-N	O=C1C=CC2(C(C(C(O1)(C)C)CC(=O)C1(C2
KNFSIJCTWSWAOV-UHFFFAOYSA-N	OC1CCC2(C(C1)CC(C1C2CC(O)C2(C1C
GLYPKDKODVRYGP-UHFFFAOYSA-O	COc1ccc2c(c1O)c[n+]1c(c2)c2cc3OCOc3
NKMJZJDVLMDPGO-UHFFFAOYSA-N	Oc1ccc(c2c1oc(CCc1ccccc1)cc2=O)O
MQKFSXLBPPCAGR-UHFFFAOYSA-N	COc1cc2C(=O)NCCc2cc1OC
PGIOBGCIEGZHJH-UHFFFAOYSA-O	COc1cc2c(cc1O)CC[n+]1c2cc2ccc3c(c2c1
KBDSLGBFQAGHBE-UHFFFAOYSA-N	O=C1OCC23C(C1)OC(C2CC(=O)C1(C3C
VSOJKDUWYQCWFM-UHFFFAOYSA-N	O=C1NCCc2c1cc1OCOc1c2
RBBVPNQTBKHOEQ-UHFFFAOYSA-O	COc1cc2C[N+]3(C)CCc4c(C3Cc2cc1O)cc
WDKYDMULARNCIS-GQCTYLIASA-N	CCOC(=O)/C=C/c1ccc(c(c1)O)O
VZTUIEROBZXUFA-UHFFFAOYSA-N	COc1c(OC)ccc2c1CN1CCc3c(C1C2)cc1c
ZHYQCBCBTQWPLC-UHFFFAOYSA-N	COc1c(OC)ccc2c1c(=O)n1c(c2)c2cc3OCO
JRIBPWOXWIRQOQ-WZUFQYTHSA-N	C/C=C(\C(=O)OC(C1Oc2c(C1)c1oc(=O)cc
QBILRDAMJUPXCX-UHFFFAOYSA-N	O=CC12CCC(CC2(O)CCC2C1CCC1(C2((
ODJLBQGVINUMMR-UHFFFAOYSA-N	O=CC12CCC(CC2(O)CCC2C1CCC1(C2((
VHFXPBHLQOPQHJ-UHFFFAOYSA-N	O=C1OC2C(C1=C)CCC(C1C2C(C)(O)CC
DJTVMANCSQLMCX-UHFFFAOYSA-N	OCc1cc(O)c2c(c1)C(c1c(C2=O)c(O)ccc1)(
LOCASNZLOPRAJY-GQCTYLIASA-N	OCC1OC(OC2OC=CC3C2C(C)(O)CC3OC
UPUXGPPBEIXAGT-GQCTYLIASA-N	COc1cc(/C=C/C(=O)OC2CC(C3C2C=CO
PQQITYGQJLPDFC-UHFFFAOYSA-N	OCC1OC(OCCc2ccc(c(c2)O)O)C(C(C1O)
CBTFERBMQQAROP-UHFFFAOYSA-N	OCC1OC(Oc2ccc(c(c2)C(=O)O)O)C(C(C1
JRIBPWOXWIRQOQ-VZUCSPMQSA-N	C/C=C(/C(=O)OC(C1Oc2c(C1)c1oc(=O)cc

NMVUNDOHFYILSF-UHFFFAOYSA-N	CC1CC(O)(CC(C1O)O)C(=O)O
UHPMCKVQTMMPCG-UHFFFAOYSA-N	COC1=CC(=O)c2c(C1=O)c(O)c(c(c2O)C)(
LCXREBMNASQAOC-UHFFFAOYSA-N	Cc1c2cc3OCOc3cc2c[n+]2c1c1cc3OCOc
BEAROWPOUPFNRD-UHFFFAOYSA-N	O=C1OCC23C(C1)OC(C2CC(=O)C1(C3C
VTMFDSJJVNQXLT-HWKANZROSA-N	COc1cc(/C=C/C(=O)OC2C(O)CC(CC2O)(
PGIOBGCIEGZHJH-UHFFFAOYSA-O	COC1=CC2=C3C=c4ccc5c(c4=C[NH+]3C
CPYDMLXRLHYXSV-GQCTYLIASA-N	COC(=O)C1(O)CC(OC(=O)/C=C/c2ccc(c(
QBUIDYLGKMWNEA-UHFFFAOYSA-O	COc1cc2CC[n+]3c(c2cc1OC)cc1c(c3)c(O)
USDOQCCMRDNVAH-UHFFFAOYSA-N	CC1=CCC2C(C1)C(CC=C2C)C(C)C
WWRCMNKATXZARA-UHFFFAOYSA-N	CC(c1ccccc1C)C
DUNCVNHORHNONW-UHFFFAOYSA-N	C=CC(=C)CCCC(O)(C)C
DJCOYPJXFKNBCF-UHFFFAOYSA-N	COc1c(OC)ccc2c1C(=O)N1C2(O)C(=O)c2
OHDQLTAYHMLRBA-UHFFFAOYSA-N	COc1ccc2c(c1O)c1c(OC)c(OC)cc3c1C(C2
HFDVRLIODXPAHB-UHFFFAOYSA-N	CCCCCCCCCCCCC=C
YESPQCLKTIRGLU-UHFFFAOYSA-N	Cc1c2[n+](CCc3c2cc2OCOc2c3)cc2c1cc
SMERZMDSMLIVHC-UHFFFAOYSA-N	COc1c(OC)ccc2c1c[n+]1CCc3c(c1c2C)cc
HYWIKTJORZAXSP-UHFFFAOYSA-O	COc1cc2CC[N+]3(C(c2c(c1OC)O)Cc1c(C
OGFXBIXJCWAUCH-UHFFFAOYSA-N	OCC1Cc2cc(OC)c(cc2C(C1CO)c1ccc(c(c1
XQINTCORIZHGFD-UHFFFAOYSA-O	COc1ccc2c(c1O)c1c(OC)c(OC)cc3c1C(C2
BDRRAMWDUCXAKG-UHFFFAOYSA-N	COc1cc(ccc1O)C(O)C
JZUTXVTYJDCMDU-UHFFFAOYSA-N	COc1c(OC)ccc2c1C(=O)OC2C1N(C)CCc2
IZTUINVRJSCOIR-UHFFFAOYSA-N	c1ccc(cc1)Cc1nccc2c1cccc2
MHXCIKYXNYCMHY-UHFFFAOYSA-N	OCC1C(COC1c1ccc(c(c1)OC)O)Cc1ccc(c
WPQJUYMGQNBENF-UHFFFAOYSA-N	COc1c(OC)ccc2c1c[n+]1CCc3c(c1c2[O-])
OEYIOHPDSNJKLS-UHFFFAOYSA-N	OCC[N+](C)(C)C
OEGWOBMNQDATKP-UHFFFAOYSA-O	COc1c(O)ccc2c1c[n+]1CCc3c(c1c2)cc1c(
UAHWPYUMFXYFJY-UHFFFAOYSA-N	C=CC(=C)CCC=C(C)C
RRAFCDWBNXTKKO-UHFFFAOYSA-N	C=CCc1ccc(c(c1)OC)O
VJOBNGRIBLNUKN-UHFFFAOYSA-N	COc1cc(ccc1O)C1OCC2C1COC2c1cc(OC
HVTCKKMWZDDWOY-UHFFFAOYSA-O	COc1c(OC)ccc2c1c[n+]1CCc3c(c1c2)cc(c
VNGXAACSTLPKAN-UHFFFAOYSA-N	COc1cc2cc(n3c2c(c1)c1cc2OCOc2cc1c3=
WUOACPNHFRMFPN-UHFFFAOYSA-N	CC1=CCC(CC1)C(O)(C)C
BNXZOIDSAUKXGW-UHFFFAOYSA-O	COc1cc2CC[n+]3c(c2cc1O)cc1c(c3)c2OC
ALZAZMCIBRHMFF-UHFFFAOYSA-N	COc1c(OC)ccc2c1CN(C)c1c2ccc2c1cc1O
YOVSPTNQHMDJAG-UHFFFAOYSA-N	C=C1CCCC2(C1CC(CC2)C(=C)C)C
UCAFJBSQKXVPDX-UHFFFAOYSA-N	O=c1c2c(ccc3c2OCO3)cc2n1CCc1c2cc2c
JGUZGNYPMHHYRK-UHFFFAOYSA-N	COc1cc(O)c2c(c1)oc(c(c2=O)O)c1ccc(c(c
XLTFNNCXVBYBSX-UHFFFAOYSA-N	COc1c(O)cc(c2c1oc(cc2=O)c1ccccc1)O
CWKBTNZNPCPAPB-UHFFFAOYSA-N	COc1ccc2c(c1O)c(=O)n1c(c2)c2cc3OCOc
AEQDJSLRWYMAQI-UHFFFAOYSA-N	COc1cc2CCN3C(c2cc1OC)Cc1c(C3)c(OC
OZQAPQSEYFAMCY-UHFFFAOYSA-N	CC1=CCCC2(C1CC(CC2)C(=C)C)C
FRMCCTDTYSRUBE-UHFFFAOYSA-N	C=C1CCC2C(C3C1CCC3(C)O)C2(C)C
KZJWDPNRJALLNS-UHFFFAOYSA-N	CCC(C(C)C)CCC(C1CCC2C1(C)CCC1C2
CLFBXHKECKSQM-UHFFFAOYSA-N	COc1cc2CC[n+]3c(c2cc1OC)cc1c(c3)cc(c
QYVZEPLDLPYECM-XUTLUUPISA-N	CCCCCCCCCCCCCCCCCOC(=O)/C=C
HGXBRUKMWQGOIE-UHFFFAOYSA-N	COc1cc(ccc1O)C1OCC2C1COC2c1ccc(c
HFPZCAJZSCWRBC-UHFFFAOYSA-N	Cc1ccc(cc1)C(C)C
FLIACVVOZYBSBS-UHFFFAOYSA-N	CCCCCCCCCCCCCCCC(=O)OC
WKOLLVMJNQIZCI-UHFFFAOYSA-N	COc1cc(ccc1O)C(=O)O
RAGZUCNPTLULOL-HWKANZROSA-N	COc1cc(/C=C/C(=O)OC2CC(O)(CC(C2O)
WGSMVBQMRKGVJX-UHFFFAOYSA-O	COc1cc2CC[n+]3c(c2cc1O)c(C)c1c(c3)c2
NZZNHGSHLAHPCG-VYUBKLCTSA-N	OC[C@H]1O[C@H]([C@@H]([C@H]([C@
ZGVGUTOTMNVHSX-VYUBKLCTSA-N	OC[C@H]1O[C@H]([C@@H]([C@H]([C@
FXNFHKRTJBSTCS-UHFFFAOYSA-N	Oc1cc2oc(cc(=O)c2c(c1O)O)c1ccccc1
IPQKDIRUZHOIOM-IAAKTDFRSA-N	OC[C@H]1O[C@@H](Oc2cc3oc(cc(=O)c
IKIIZLYTISPENI-ZFORQUDYSA-N	OC(=O)[C@H]1O[C@@H](Oc2cc3oc(cc(=
SGNBVLSWZMBQTH-ZRUUVFCLSA-N	O[C@H]1CC[C@]2(C(=CC[C@@H]3[C@@
RTIXKCRFFJGDFG-UHFFFAOYSA-N	Oc1cc(O)c2c(c1)oc(cc2=O)c1ccccc1

```
QUAPPCXFYKSDSV-LBPRGKRZSA-N      COc1c(O)cc2c(c1O)C(=O)C[C@H](O2)c1
RXSYNUMMIWXLLC-UHFFFAOYSA-N      COc1c(O)c2oc(cc(=O)c2c(c1OC)O)c1ccc
ZQSIKQQCMJOPGE-PUIBNRJISA-N      OC[C@H]1O[C@@H](Oc2cc(O)c3c(c2OC
RYJWOWHMBGOYAT-ZQUMRXHJSA-N      COc1cc(O[C@@H]2O[C@H](C(=O)O)[C@
DSNICWRJCXGVEE-UHFFFAOYSA-N      COc1c(OC)cccc1c1cc(=O)c2c(o1)c(OC)c(
QCKBVAGWPBRRQJ-UHFFFAOYSA-N      COc1c(OC)c(OC)c(c2c1oc(cc2=O)c1cccc
SBHXYTNGIZCORC-ZDUSSCGKSA-N      Oc1cc2O[C@@H](CC(=O)c2c(c1)O)c1ccc
BEIRZEADQYKQFA-NRFANRHFSA-N      Oc1cc(O)c2c(c1)oc(cc2=O)c1c(O)ccc(c1c
IPCSVZSSVZVIGE-UHFFFAOYSA-N      CCCCCCCCCCCCCCCC(=O)O
IHFBPDAQLQOCBX-UHFFFAOYSA-N      COc1c(O)cc2c(c1O)c(=O)cc(o2)c1ccc(cc1
IHLSBQVBFDTNTC-UHFFFAOYSA-N      COc1c(OC)cc(c2c1oc(cc2=O)c1ccccc1)O
NZOUUYOSKJFMKB-UHFFFAOYSA-N      COc1c(O)cc(c2c1oc(cc2=O)c1ccccc1)OC
VDWSYBFEQXWINA-GFKCUEKNSA-N      OC[C@H]1O[C@@H](OCCc2ccc(c(c2)O)
OEZZJTAJYYSQKM-UHFFFAOYSA-N      COc1c(O)cc(c2c1oc(cc2=O)c1ccc(cc1)O)(
OVMFOVNOXASTPA-VYUBKLCTSA-N      OC[C@H]1O[C@H]([C@@H]([C@H]([C@
NXHQVROAKYDSNW-UHFFFAOYSA-N      Oc1ccc(cc1)c1cc(=O)c2c(o1)c(O)c(cc2O)(
ZTHLHHDJRXJGRX-UHFFFAOYSA-N      COc1cc2oc(cc(=O)c2c(c1O)O)c1ccccc1
DGLBFMRIIDZOJI-QKYBYQKWSA-N      OC[C@H]1O[C@@H](Oc2ccc(c3c2c(=O)
ZFKKRRMUPBBYRS-UHFFFAOYSA-N      Oc1cc(O)c2c(c1O)oc(cc2=O)c1ccccc1
XXKJOVIWINPZSF-NRFANRHFSA-N      Oc1ccc(c(c1)[C@@H]1CC(=O)c2c(O1)cc
LKOJGSWUMISDOF-UHFFFAOYSA-N      COc1c(O)cc2c(c1O)c(=O)cc(o2)c1ccccc1
QXIPXNZUEQYPLZ-QSUZLTIMSA-N      COc1cc(O[C@@H]2O[C@H](C(=O)O)[C@
NBQYBZYBTNQEQG-LSDHHAIUSA-N      Oc1cc2O[C@H](c3c(O)cccc3O)[C@H](C(
NULZZCUABWZIRV-UHFFFAOYSA-N      Oc1cc(O)c2c(c1)oc(c(c2=O)O)c1c(O)cccc
CVBUKMMMRLOKQR-UHFFFAOYSA-N      O=C(c1ccccc1)CC(=O)C
BWHOZHOGCMHOBV-BQYQJAHWSA-N      CC(=O)/C=C/c1ccccc1
SAJHRQBGZMZGMA-UHFFFAOYSA-N      COc1cc2OC(CC(=O)c2c(c1)O)c1c(O)cccc
KOBUGDLTCAJTND-DOARKGTESA-N      OC[C@H]1O[C@@H](Oc2cccc(c2[C@@H
DJSISFGPUUYILV-ZFORQUDYSA-N      OC(=O)[C@H]1O[C@@H](Oc2cc3oc(cc(=
XCBMYKIKEHGYAR-UHFFFAOYSA-N      COc1c(O)cc(c2c1oc(cc2=O)c1ccccc1O)O
KZJWDPNRJALLNS-VJSFXXLFSA-N      CC[C@@H](C(C)C)CC[C@H]([C@H]1CC
CZRGNFVQUYWGKP-UHFFFAOYSA-N      COc1cc(O)c2c(c1OC)oc(cc2=O)c1ccccc1
GMQFOKBGMKVUQZ-UHFFFAOYSA-N      COc1cccc(c1c1cc(=O)c2c(o1)c(OC)c(c(c2
HCXVJBMSMIARIN-WACSKALWSA-N      CC[C@H](C(C)C)/C=C/C([C@H]1CCC2[C
CZMRCDWAGMRECN-UGDNZRGBSA-N      OC[C@H]1O[C@@]([C@H]([C@@H]1O)
CPFJPTACQDZPLS-UHFFFAOYSA-N      COc1c(O)ccc(c1c1cc(=O)c2c(o1)c(OC)c(c
BJNCWLSOQIVKIX-LSDHHAIUSA-N      Oc1cc2O[C@H](c3ccccc3O)[C@H](C(=O
XVXXIRQXOYAJAF-ZDUSSCGKSA-N      Oc1ccc(c(c1)[C@@H]1CC(=O)c2c(O1)cc
YQTWPPLBGYVRIV-SFTVRKLSSA-N      OC[C@H]1O[C@@H](Oc2cc3O[C@@H](
ODNWHTWVHZTXPB-CGXGPNJMSA-N      OC(=O)[C@H]1O[C@@H](Oc2cc3O[C@H
STAGATUVRDVEAT-UHFFFAOYSA-N      Oc1cc(O)c2c(c1)oc(cc2=O)c1cccc(c1O)O
WJXXUIYFPVIHDH-UHFFFAOYSA-N      Oc1cc(O)c2c(c1)oc(cc2=O)c1c(O)cccc1O
LHEFNLQSEVZHOI-ZFORQUDYSA-N      OC(=O)[C@H]1O[C@@H](Oc2cc(O)c3c(c
XFUBPGKNMBCAHX-AATRIKPKSA-N      COc1cc(O)cc(c1C(=O)/C=C/c1c(O)cccc1C
JWTCUCPQIJFEBS-YXJFMNLASA-N      COc1c(OC)c(OC)c2c(c1O[C@@H]1O[C@
GWRFNPJGKCUUSJ-UHFFFAOYSA-N      COc1cc(O)c2c(c1OC)oc(cc2=O)c1c(O)ccc
OBPTWCJIAIXDRP-UHFFFAOYSA-N      COc1cccc(c1c1cc(=O)c2c(o1)c(OC)c(cc2C
BYGRZBWUKYXRHL-UHFFFAOYSA-N      COc1c(O)c2oc(cc(=O)c2c(c1OC)O)c1ccc
OFYPDAKTVZXXPC-UHFFFAOYSA-N      Oc1cc(O)c2c(c1)oc(cc2=O)c1ccccc1O
AZRVQJNRDWOJQR-QNDFHXLGSA-N      OC[C@H]1O[C@@H](Oc2ccccc2c2cc(=C
MMDUKUSNQNWVET-VYUBKLCTSA-N      OC[C@H]1O[C@H]([C@@H]([C@H]([C@
HVULMIKUBSLJMI-BQYQJAHWSA-N      COc1cc(O)ccc1C(=O)/C=C/c1c(O)cccc1O
FCXRFTLSXMRXTM-LBPRGKRZSA-N      COc1c(O)cc2c(c1O)C(=O)C[C@H](O2)c1
LUSOAMBDAXTEBX-AWEZNQCLSA-N      COc1cc(O)cc2c1C(=O)C[C@H](O2)c1c(C
VHNWVABJHPRFGC-UHFFFAOYSA-N      COc1c(O)cc2c(c1O)c(=O)cc(o2)c1ccccc1(
NKSITEVSJGHWCO-UHFFFAOYSA-N      COc1cc(O)c2c(c1O)oc(cc2=O)c1ccccc1O
OHRJVTNFYFYUPW-DRASZATQSA-N      OC[C@H]1O[C@@H](Oc2ccccc2c2cc(=C
ZREMOZUHVILNPD-DRASZATQSA-N      OC[C@H]1O[C@@H](Oc2cc(O)c3c(c2OC
```

PVSHCMCDBFRZFY-UHFFFAOYSA-N	COc1c(OC)c(OC)c(c2c1oc(cc2=O)c1cc(O
KBQNEFOZLNJBRZ-RBLJWTLESA-N	COc1c(OC)c(OC)c2c(c1O[C@@H]1O[C@
YGPCNVVYCWOUPL-AJRKLXPLSA-N	COc1cc(O[C@@H]2O[C@H](CO[C@@H
KCQRDVPUUNCDDW-ARSJFUCGSA-N	OC[C@H]1O[C@@H](Oc2ccc(c(c2c2cc(=
DIRSNBJJSCNRKL-DRASZATQSA-N	OC[C@H]1O[C@@H](Oc2cc(O)c(c3c2c(=
LNOHXHDWGCMVCO-NTKSAMNMSA-N	COc1c(O[C@@H]2O[C@H](C(=O)O)[C@
WEEGYLXZBRQIMU-UHFFFAOYSA-N	CC12CCC(CC1)C(O2)(C)C
WRMNZCZEMHIOCP-UHFFFAOYSA-N	OCCc1ccccc1
DANYIYRPLHHOCZ-UHFFFAOYSA-N	COc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)O
XLTFNNCXVBYBSX-UHFFFAOYSA-N	COc1c(O)cc(c2c1oc(cc2=O)c1ccccc1)O
LNOHXHDWGCMVCO-UHFFFAOYSA-N	COc1c(OC2OC(C(=O)O)C(C(C2O)O)O)cc
DTGKSKDOIYIVQL-UHFFFAOYSA-N	OC1CC2C(C1(C)CC2)(C)C
CDOSHBSSFJOMGT-UHFFFAOYSA-N	C=CC(CCC=C(C)C)(O)C
WPYMKLBDIGXBTP-UHFFFAOYSA-N	OC(=O)c1ccccc1
QQQCWVDPMPFUGF-UHFFFAOYSA-N	COc1cc(O)cc2c1C(=O)CC(O2)c1ccccc1
FAMPSKZZVDUYOS-KXWHQPPKSA-N	CC1=CCC(C)(C)C=CCC(=CCC1)C
RRAFCDWBNXTKKO-UHFFFAOYSA-N	C=CCc1ccc(c(c1)OC)O
CSKINCSXMLCMAR-UHFFFAOYSA-N	CC1CCC2=C1CC1CCC2(C1(C)C)C
JVXZRQGOGOXCEC-UHFFFAOYSA-N	Oc1ccc(cc1)c1cc(=O)c2c(o1)cc(c(c2O)O)O
XGJUUNRZFPFMOK-UHFFFAOYSA-N	COc1c(O)ccc(c1c1cc(=O)c2c(o1)c(OC)c(c
XFUBPGKNMBCAHX-WAYWQWQTSA-N	COc1cc(O)cc(c1C(=O)/C=C\c1c(O)cccc1O
UVNUGBQJLDGZKE-UHFFFAOYSA-N	OC(=O)C1OC(Oc2cc3OC(CC(=O)c3c(c2O
GPDJGLOROGNHJD-UHFFFAOYSA-N	O=C1CC(Oc2c1c(O)c(c(c2)O)O)c1ccccc1
SBHXYTNGIZCORC-UHFFFAOYSA-N	Oc1cc2OC(CC(=O)c2c(c1)O)c1ccc(c(c1)O
QCDYOIZVELGOLZ-UHFFFAOYSA-N	COc1ccc(cc1)c1cc(=O)c2c(o1)cc(c(c2O)C
LYWHJXVFIUKXLE-UHFFFAOYSA-N	COc1ccc(c(c1O)OC)c1oc2cc(O)cc(c2c(=O
ADIDQIZBYUABQK-UHFFFAOYSA-N	CC(=C)C1CCC(C2=C(C1)C(C)CC2)C
MMRYSDPTALIPSP-UHFFFAOYSA-N	OCC1OC(OCCc2ccc(c(c2)O)OC)C(C(C1O
PPUFZEKAOXNVLU-UHFFFAOYSA-N	OCCc1ccc(c(c1)O)OC
ZLPXZRZUFKQINJ-UHFFFAOYSA-N	CCOC1OC(CO)C(C(C1(O)c1ccc(c(c1)O)C
XWBJWURSGCGEQR-UHFFFAOYSA-N	CCOC1OC(CO)C(C(C1(O)c1ccc(c(c1)O)C
GSTISHLARMKZOD-UHFFFAOYSA-N	COc1cc(O)c2c(c1O)C(=O)CC(O2)c1cccc
ILRCGYURZSFMEG-UHFFFAOYSA-N	OCC1OC(OCCc2ccc(cc2)O)C(C(C1O)O)C
YCCILVSKPBXVIP-UHFFFAOYSA-N	OCCc1ccc(cc1)O
DJSISFGPUUYILV-UHFFFAOYSA-N	OC(=O)C1OC(Oc2cc3oc(cc(=O)c3c(c2O)
MIWLOORHWQBIHP-UHFFFAOYSA-N	COc1ccc(c(c1)c1cc(=O)c2c(o1)c(OC)c(c(c
DCWXTOWSMXDTNR-UHFFFAOYSA-N	OC1C(Oc2cc3oc(cc(=O)c3c(c2O)O)c2ccc
NPJICTMALKLTFW-UHFFFAOYSA-N	CCC(C(C)C)CCC(C1CCC2C1(C)CCC1C2
KZJWDPNRJALLNS-UHFFFAOYSA-N	CCC(C(C)C)CCC(C1CCC2C1(C)CCC1C2
KOWMJRJXZMEZLD-UHFFFAOYSA-N	COc1cc(cc(c1O)OC)C1OCC2C1COC2c1c
CPTCHGRDJMOIJZ-UHFFFAOYSA-N	CC(C(CCC(C1CCC2C1(C)CCC1C2CCC2
IRAQOCYXUMOFCW-UHFFFAOYSA-N	CC1=CCC23CC1C(C)(C)C2CCC3C
KMOUJOKENFFTPU-UHFFFAOYSA-N	OCC1OC(Oc2cc(O)c3c(c2)oc(cc3=O)c2cc
VSMOENVRRABVKN-UHFFFAOYSA-N	CCCCCC(C=C)O
NFLGAXVYCFJBMK-UHFFFAOYSA-N	CC1CCC(C(=O)C1)C(C)C
KZNIFHPLKGYRTM-UHFFFAOYSA-N	Oc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)O
GAIBLDCXCZKKJE-BZXLUOIMSA-N	CC1=CCCC(=C)C=CC(CC1)C(C)C
CZMRCDWAGMRECN-UHFFFAOYSA-N	OCC1OC(C(C1O)O)(CO)OC1OC(CO)C(C(
ZNWNWEHQFXOPGK-UHFFFAOYSA-N	O=CCCCCCCCCC=O
NBQYBZYBTNQEQG-UHFFFAOYSA-N	Oc1cc2OC(c3c(O)cccc3O)C(C(=O)c2c(c1
PVFGJHYLIHMCQD-UHFFFAOYSA-N	Oc1ccc2c(c1)oc(cc2=O)c1ccc(c(c1)O)O
DPTVRZXQCBYWIK-UHFFFAOYSA-N	OCC1OC(Oc2cc(O)c3c(c2)OC(C(C3=O)C
FBDUYUDFMFZSDJ-UHFFFAOYSA-N	Oc1ccc(cc1)c1cc(=O)c2c(o1)c(OC1OC(C(
ISNRVVKKHPECQN-UHFFFAOYSA-N	OCC1OC(C(C(C1O)O)O)c1c(O)c(C2OC(C
RDGWQFSLTSPRBG-UHFFFAOYSA-N	N#C/C=C(\c1ccccc1)/c1ccccc1
DYDUQRQYDQHKJU-WDZFZDKYSA-N	O=C1/C(=C/c2ccccc2)/Oc2c1c(O)c(c(c2)C
IPQKDIRUZHOIOM-UHFFFAOYSA-N	OCC1OC(Oc2cc3oc(cc(=O)c3c(c2O)O)c2
RTIXKCRFFJGDFG-UHFFFAOYSA-M	Oc1cc([O-])c2c(c1)oc(cc2=O)c1ccccc1

XESIWQIMUSNPRO-UHFFFAOYSA-M	Oc1cc(O)c2c(c1)oc1c(c2=O)cccc1[O-]
WLOAMJAMSFVOOZ-UHFFFAOYSA-N	OCc1ccc(c2c1C(=O)c1cccc(c1C2=O)O)O
OVMFOVNOXASTPA-UHFFFAOYSA-N	OCC1OC(C(C(C1O)O)O)c1c(O)c(C2OCC
NZZNHGSHLAHPCG-UHFFFAOYSA-N	OCC1OC(C(C(C1O)O)O)c1c(O)c(C2OCC
GMYHXOPIKMGWOM-UHFFFAOYSA-N	OCC1CCC(CC1)C(=C)C
QNVPMKAFCVXMFH-UHFFFAOYSA-N	COc1ccc(c(c1)OC1OC(COC2OCC(C2O)(
IDONYWHRKBUDOR-UHFFFAOYSA-N	OCC1OC(Oc2ccc(cc2)CCC(=O)C)C(C(C1
SWIWTAJTJOYCTB-GZTJUZNOSA-N	COc1cc(/C=C/C(=O)OC2CCC3(C(=CCC4
SKWTXGMULLCOGN-SNAWJCMRSA-N	C/C=C/c1ccc(cc1OC)OC
QSEHQWFPCMNMPH-UHFFFAOYSA-N	O=Cc1c(O)c(OC)c(c2c1c(O)c(c(c2)C)c1c(
SGIOAFBVWVUCQP-UHFFFAOYSA-N	Oc1ccc(cc1)c1oc2cc(O)cc(c2c(=O)c1O)O
QZOALWMSYRBZSA-UHFFFAOYSA-N	OCC1OC(OC2CCC3(C(C2)C(=O)CC2C3C(
HGTMGCDIPYGVKA-UHFFFAOYSA-N	CN1CC(C)C2C(C1)C(C)CC2
AOAFVSVYRSUDBN-UHFFFAOYSA-N	CCC(CCCCCCCCCCCC(=O)OC)C
GYDIPQRLDOTECG-MDZDMXLPSA-N	CCC(C(C)C)/C=C/C(C1CCC2C1(C)CCC1
VWDLOXMZIGUBKM-CMDGGOBGSA-N	CCC(C(C)C)/C=C/C(C1CCC2C1(C)CCC1
SVZGCYLXISBVQK-UHFFFAOYSA-N	CCCC(CC(CCc1ccc(c(c1)OC)O)O)O)O
DSTCZBGJCUOFLM-UHFFFAOYSA-N	CCCCCCCCCCCCCCC(=O)OCC1=CC2
PXDASGXIBCEXNH-UHFFFAOYSA-N	OCC1OC(Oc2cc(ccc2O)C(=O)OC)C(C(C1
HNZGKRAKJFZQAY-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(O)CN2C(C3
QWUHUBDKQQPMQG-UHFFFAOYSA-N	COc1cc2oc(cc(=O)c2c(c1O)O)c1ccc(c(c1)
UYOJEKMKWXYOEQ-UHFFFAOYSA-N	COc1cc(c(cc1OC)O)c1coc2c(c1=O)ccc(c2
JRYNOEBZHZTPOT-UHFFFAOYSA-N	COc1cc(ccc1OC)C1=C(O)C(c2c(O1)cc(O
YLOZPZMPWNUOJV-UHFFFAOYSA-N	OCC1OC(Oc2cc(O)c3c(c2OC)oc(cc3=O)c
QXIPXNZUEQYPLZ-UHFFFAOYSA-N	COc1c(OC2OC(C(=O)O)C(C(C2O)O)O)cc
SCZVLDHREVKTSH-UHFFFAOYSA-M	COc1cc(ccc1[O-])c1cc(=O)c2c(o1)cc(cc2O
GLMWHQIFJIURES-UHFFFAOYSA-N	COc1c(O)c(OC)c2c(c1O)c(=O)cc(o2)c1cc
QZAXKZRZMAXPSF-UHFFFAOYSA-N	COc1c(oc2c(c1=O)c(O)c(c(c2)O)O)c1ccc(
DGLBFMRIIDZOJI-UHFFFAOYSA-N	OCC1OC(Oc2ccc(c3c2c(=O)cc(o3)c2cccc
OBVZFHXNNMIIRJ-UHFFFAOYSA-N	O=CC(c1cc(O)c2c(c1OC)oc(cc2=O)c1ccc
LUSOAMBDAXTEBX-UHFFFAOYSA-N	COc1cc(O)cc2c1C(=O)CC(O2)c1c(O)cccc
IDZNVJWQZDSPIX-UHFFFAOYSA-N	COc1cc(O)c2c(c1)oc1c(c2=O)cc(c(c1OC)(
LZERJKGWTQYMBB-UHFFFAOYSA-N	COc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)O(
WMPDAIZRQDCGFH-UHFFFAOYSA-N	COc1cccc(c1)C=O
MOFOLNOWFPVLGZ-UHFFFAOYSA-N	OC(=O)C1OC(Oc2cc(O)c3c(c2O)oc(cc3=O
RBVYFSLWUBLPMG-UHFFFAOYSA-N	COc1c(O)c(OC)c2c(c1O)c(=O)cc(o2)c1cc
CWVRJTMFETXNAD-DUXPYHPUSA-N	O=C(OC1CC(O)(CC(C1O)O)C(=O)O)/C=C
BJNCWLSOQIVKIX-UHFFFAOYSA-N	Oc1cc2OC(c3ccccc3O)C(C(=O)c2c(c1)O)
USQXPEWRYWRRJD-UHFFFAOYSA-N	Oc1cc2OC(CC(=O)c2c(c1)O)c1cc(O)c(c(c
IDRSJGHHZXBATQ-UHFFFAOYSA-N	OC(=O)C1OC(Oc2cc(O)c3c(c2)oc(cc3=O
MMDUKUSNQNWVET-UHFFFAOYSA-N	OCC1OC(C(C(C1O)O)O)c1c(O)c(C2OCC
KSEBMYQBYZTDHS-HWKANZROSA-N	COc1cc(/C=C/C(=O)O)ccc1O
LNQCUTNLHUQZLR-UHFFFAOYSA-N	OCC1OC(Oc2cc3occ(c(=O)c3c(c2OC)O)c
FBSKJMQYURKNSU-QPJJXVBHSA-N	OCC1OC(OCCc2ccc(c(c2)O)O)C(C(C1OC
HKEAFJYKMMKDOR-UHFFFAOYSA-N	OCC1OC(C(C(C1O)O)O)c1c(O)ccc2c1oc
ODDRJEWIOFPAOL-UHFFFAOYSA-N	OCC1OC(C(C1O)O)OOOC1OC(C(C1O)C
CXMXRPHRNRROMY-UHFFFAOYSA-N	OC(=O)CCCCCCCC(=O)O
SGNBVLSWZMBQTH-UHFFFAOYSA-N	OC1CCC2(C(=CCC3C2CCC2(C3CCC2C
SCZVLDHREVKTSH-UHFFFAOYSA-N	COc1cc(ccc1O)c1cc(=O)c2c(o1)cc(cc2O)(
HCXVJBMSMIARIN-CMDGGOBGSA-N	CCC(C(C)C)/C=C/C(C1CCC2C1(C)CCC1
XESIWQIMUSNPRO-UHFFFAOYSA-N	Oc1cc(O)c2c(c1)oc1c(c2=O)cccc1O
UWIBDEQRXHODSE-UHFFFAOYSA-N	COc1c(OC)c(OC)c(c2c1oc(c1cc(O)ccc1O
KJXSIXMJHKAJOD-LSDHHAIUSA-N	Oc1cc2O[C@H](c3cc(O)c(c(c3)O)O)[C@H
BBFQZRXNYIEMAW-UHFFFAOYSA-N	COc1cccc2c1cc([N+](=O)[O-])c1c2c2OCC
LKLWVKCEYSPQHL-HRAATJIYSA-O	COc1cc2CC[N@+]3([C@H](c2cc1O)Cc1c
LKLWVKCEYSPQHL-KKSFZXQISA-O	COc1cc2CC[N@@+]3([C@H](c2cc1O)Cc
XBYDCPLYWSKTAA-UHFFFAOYSA-N	[Hg-][SH2+]
RKJCLPSFLUKWQY-UHFFFAOYSA-N	COC1=C(OC)C(=O)c2c(C1=O)c(O)c1c(c2

Identifier	SMILES
SGUKYTZMQQVPOB-UHFFFAOYSA-N	Nc1ccn(c(=O)n1)C1OC(C(C1)OP(=O)(OC
RWSOTUBLDIXVET-UHFFFAOYSA-N	S
BMOFEAKQXGGUPE-UHFFFAOYSA-N	S[AsH2]
SLXSULZDDPRFBJ-UHFFFAOYSA-N	S[AsH]=S
LOXQKSBAJJTUOX-BZDYRZRUSA-N	OC[C@H]1O[C@@H](O[C@@H]2OC=C(
RIGYMJVFEJNCKD-UHFFFAOYSA-N	COc1ccc(cc1OC)c1oc2cc(OC)c(c(c2c(=O)
IBIPGYWNOBGEMH-DILZHRMZSA-N	OC[C@H]1O[C@@H](O[C@@H]2OC=C3
BEDSGEULUAVXQH-YGCGHWCOSA-N	COc1cc(/C=C/C(=O)O[C@@H]2[C@H](O
QIWWLKDHHMGRQL-SKMDTYRSSA-N	OCC1=CC[C@H]2[C@H]1[C@@H](OC=C
PANKHBYNKQNAHN-MQQNZMFNSA-N	C/C(=C\C=C\C=C(\C=C\C=C(\C(=O)O)/C)
SEBIKDIMAPSUBY-RTJKDTQDSA-N	OC[C@H]1O[C@@H](OC[C@H]2O[C@@
ZVXWFPTVHBWJOU-YYFGDFGFSA-N	OCC1=C[C@@H]([C@H]2[C@H]1[C@@
WSGPLSDARZNMCW-FCVLBCLDSA-N	OCC1=C[C@@H]([C@H]2[C@H]1[C@@
BEKYZOSRHNMGCR-FMZRLEOLSA-N	O=C(O[C@H]1[C@H](OC(=O)/C=C/c2ccc
OOGPWQHGQYUIAW-KDGFOEJISA-N	O=C(O[C@@H]1CC(O)(C[C@H](C1OC(=
UFCLZKMFXSILNL-PSEXTPKNSA-N	O=C(O[C@@H]1[C@H](O)C[C@@](C[C@
AWJLBZCAQJYFDM-UHFFFAOYSA-N	COc1c(c2cc(=O)c3c(o2)cc(cc3O)O)c(OC)
GYHKMDWFVHCCRA-UHFFFAOYSA-N	Oc1ccc(c(c1)O)c1oc2c(c1)ccc(c2)O
WYIDBNAGSMCMET-UHFFFAOYSA-N	Oc1ccc2c(c1)OCc1c2oc2c1ccc(c2)O
ZYVBPTWKKGRSOZ-UHFFFAOYSA-N	COc1cc(c2cc(=O)c3c(o2)cc(cc3O)O)c(c(c
SPCURNZYGRLEBA-OUEWTLASSA-N	OCC1=C[C@H]2[C@H]1[C@@H](OC=C
JJVJSIBMTMIANL-CCVCSVFYSA-N	OC[C@H]1O[C@@H](OC2OC=C([C@@I
RQRMWYOWQUEKAS-IWSPIJDZSA-N	OCC1=CC[C@H]2[C@@H]1COC(=O)[C@
MQBFFYQCZCKSBX-UHFFFAOYSA-N	COc1c(OC)cc(cc1OC)c1cc(=O)c2c(o1)c(O
BMJZOVISEITTRA-AHGLEFSXSA-N	CC(=CC(=O)C[C@H]([C@H]1CC[C@@]2
WXXRZUXRKRIXTA-GARJFASQSA-N	CCO[C@@H]1OC[C@H]2[C@@H]1CC(=
XJMPAUZQVRGFRE-AYDWLWLASA-N	OC[C@H]1O[C@@H](O[C@@H]2OC=C(
JSKCJJNYSGWZDU-BYFUOZQISA-N	OC[C@H]1O[C@@H](OC2OC=C([C@@I
AZKVWQKMDGGDSV-BCMRRPTOSA-N	COC(=O)C1=CO[C@H]([C@H]2[C@@H]
FYZYXYLPBWLLGI-AUOPOVQUSA-N	OCC1=CC[C@H]2[C@@H]1[C@@H](OC
IBFYXTRXDNAPMM-BVTMAQQCSA-N	OC[C@H]1O[C@@H](O[C@@H]2OC=C(
ZJDOESGVOWAULF-OGJQONSISA-N	OC[C@H]1O[C@@H](O[C@@H]2OC=C(
WECGLUPZRHILCT-HZJYTTRNSA-N	CCCCC/C=C\C/C=C\CCCCCCC(=O)OC
PTOZLBJRCJWJKV-VOGKFIJMSA-N	CCCCC/C=C\C/C=C\CCCCCCC(=O)OC
HBOQXIRUPVQLKX-BBWANDEASA-N	CCCCC/C=C\C/C=C\CCCCCCC(=O)OC
IHOXLUDKLLDPHW-UHFFFAOYSA-N	Oc1ccc2c(c1)OCC(=C2)c1ccc(cc1O)O
ZZUBHVMHNVYXRR-UHFFFAOYSA-N	Oc1ccc(cc1)C1=Cc2c(OC1)cc(cc2)O
SHGCFQDGGXDIFG-OWRRKEEJSA-N	OC[C@]1(C)[C@@H](CC[C@]2([C@H]1C
KEOITPILCOILGM-LLJOFIFVSA-N	OC[C@]1(C)[C@@H](CC[C@]2([C@H]1C
ODBRNZZJSYPIDI-VJXVFPJBSA-N	OC[C@H]1O[C@H]([C@@H]([C@H]([C@
RLRGKMMFFVWPHT-NUYPAGBLSA-N	C=C(C(C)C)CCC([C@H]1CC[C@@]2([C@
YXTURDGNXCWFHX-NEPODAOMSA-N	OC[C@]12CC[C@@]3(C(=CC[C@H]4[C@
QGDNIOFJAUCAMW-UHFFFAOYSA-N	COc1cc(O)c2c(c1)oc(cc2=O)c1c(OC)c(OC
QULPQWKDDOBIOC-UHFFFAOYSA-N	COc1c(OC)cc(cc1OC)c1cc(=O)c2c(o1)cc(
UQKOTVMFJYMJEP-UHFFFAOYSA-N	COc1cc(O)c2c(c1)oc(cc2=O)c1cc(OC)c(c(
OVSQVDMCBVZWGM-QSOFNFLRSA-N	OC[C@H]1O[C@@H](Oc2c(oc3c(c2=O)c
PUPKKEQDLNREIM-QNSQPKOQSA-N	Oc1ccc(cc1)c1oc2cc(O[C@@H]3O[C@@
SMMQSMVUPDCNJU-UHFFFAOYSA-N	COc1ccc2c(c1)OCc1c2oc2c1ccc(c2)O
DDKLBJZRUKOEJA-VIZOYTHASA-N	C/C(=C\Cc1c(O)c(O)cc2c1oc1c2COc2c1c
QATWTDFKCQHTAE-UHFFFAOYSA-N	CC(=CCCC1(C)C=Cc2c(O1)c(O)c1c(c2)oc
FLLWZPMYUAPJEA-UHFFFAOYSA-N	COc1ccc2c(c1)OCc1c2oc2c1cc(c(c2)O)O
HEOXCFPTWPWVSG-OVCLIPMQSA-N	COC(=O)c1c(O)c(O)c(c2c1c1COc3c(c1o2
PBLWSVWYIYVLDE-VGOFMYFVSA-N	C/C(=C\Cc1c(O)c(O)cc2c1oc1c2c(=O)oc2
HGQFHBRDQMGDKQ-OVCLIPMQSA-N	C/C(=C\Cc1c(O)c(O)cc2c1oc(c2C)c1ccc(c
HQQKUDSFSYUGTI-UHFFFAOYSA-N	Oc1ccc(c(c1)O)c1oc2c(c1Cc1cc3c(cc1O)c
DMXCZIUMBYRKQW-QPSGOUHRSA-N	C/C(=C\Cc1c(O)c(O)cc2c1oc(c2Cc1cc2c(
WPDUQFCORDILFF-VGOFMYFVSA-N	C/C(=C\Cc1c(O)c(O)cc2c1oc1c2c(=O)oc2c
KPWKGYKPSLJFDC-UHFFFAOYSA-N	COc1cc(c(cc1O)O)C1COc2c(C1=O)ccc(c2

NYGZYUAVZPIKBZ-UHFFFAOYSA-N	COc1cc2c(cc1O)OC1C2COc2c1ccc(c2)O
IRVDWFYPCQFZTA-PMACEKPBSA-N	CC(=CC[C@@]12COc3c([C@@H]1Oc1c
UCYCRJCXEHJRDP-PMACEKPBSA-N	CC(=CC[C@@]12COc3c([C@@H]1Oc1c
WLDDYRDGRVNYEY-SFTDATJTSA-N	COc1cc2O[C@@H]3[C@@](c2cc1O)(CC
MVDMPADXXDHNOL-JISJETCLSA-N	CC(=CCCCC1(C)Oc2c(O)cc3c(c2CC1O)O[
JEHZELNRHHBZFM-UHFFFAOYSA-N	COc1cc(c(cc1O)O)C1COc2c(C1=O)c(O)c
GLMLQROWOJXFJA-FRKPEAEDSA-N	C/C(=C\Cc1c(O)cc(c2c1occ(c2=O)c1ccc(
JVYKYLOUVXNIMK-VIZOYTHASA-N	C/C(=C\Cc1c(O)c(O)cc(c1O)c1coc2c(c1=O
DJJQWLWXJHJPIH-UHFFFAOYSA-N	Oc1ccc2c(c1)OC=C(C2)c1ccc(cc1O)O
AWVKZYDVQDHNKA-JTQLQIEISA-N	COc1cc([C@@H]2COc3c(C2)ccc(c3)O)c(
NGWYJYHAFLMHNW-UHFFFAOYSA-N	Oc1ccc(c(c1)O)C(=O)C(=O)c1ccc(cc1O)C
ZXALVCPICGWIFY-SNAWJCMRSA-N	CC(=CC(C/C=C/Cc1c(O)cc2c(c1O)C(=O)(
CSZKAJDXUNNJKV-UHFFFAOYSA-N	CC(=CCCC1(C)C=Cc2c(O1)cc1c(c2O)C(=
KRFBMPVGAYGGJE-UHFFFAOYSA-N	COc1ccc(cc1)c1cc(=O)c2c(o1)c(OC)c(c(c:
PTPQTMGOUIHFNR-LGGDGBFUSA-N	OC[C@H]1C=C([C@@H]2[C@H]1C(=CO
KVWWIYGFBYDJQC-GHMZBOCLSA-N	CCCCC[C@@H]1[C@H](CCC1=O)CC(=C
JBBLCGRIZVRWJC-MNIQVYHASA-N	OC[C@H]1O[C@@H](O[C@H]2OC=C(C:
PUCHCUYBORIUSM-UHFFFAOYSA-N	CCCSSC
PTPQTMGOUIHFNR-IYQBLMFUSA-N	OC[C@@H]1C=C([C@@H]2[C@H]1C(=C
IGGUPRCHHJZPBS-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCCCCCCCCCCCCC
YXTKNMNZABXVJX-ZYMWYSJDSA-N	OC[C@H]1O[C@@H](OC[C@H]2O[C@@
PLAPMLGJVGLZOV-VPRICQMDSA-N	OC[C@H]1O[C@H]([C@@H]([C@H]([C@
LBTAFDHXNSPZSZ-QLDIZCGWSA-N	OC[C@H]1O[C@@H](O[C@@H]2CC(=C
IAGSHEHQJJTLLR-FNINEVAMSA-N	OC[C@]1(C)[C@@H](CC[C@]2([C@H]1C
DFBCVZCHRMESFM-IPRKTUQPSA-N	C=C(C(C)C)CC[C@H]([C@H]1CC[C@@]
WSGPLSDARZNMCW-LPGRTNKPSA-N	OCC1=C[C@H]([C@H]2[C@H]1[C@@H]
YSIFYNVXJOGADM-KDYWOABDSA-N	OC[C@H]1O[C@@H](OC2OC=C([C@@
ZZYMHGCHGDEWKR-LBVFNNMGSA-N	CC(=CC(=O)CC([C@H]1CC[C@@]2([C@
JPUKWEQWGBDDQB-DTGCRPNFSA-N	OC[C@H]1O[C@@H](Oc2c(oc3c(c2=O)c
CWVRJTMFETXNAD-DUXPYHPUSA-N	O=C(OC1CC(O)(CC(C1O)O)C(=O)O)/C=O
AZKVWQKMDGGDSV-UHFFFAOYSA-N	COC(=O)C1=COC(C2C1CC=C2CO)O
MIJYXULNPSFWEK-UHFFFAOYSA-N	OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1
OLOOJGVNMBJLLR-UHFFFAOYSA-N	CC(=CCOc1c2occc2cc2c1oc(=O)cc2)C
OVSQVDMCBVZWGM-UHFFFAOYSA-N	OCC1OC(Oc2c(oc3c(c2=O)c(O)cc(c3)O)c
IRVSYXACZHIMTN-UHFFFAOYSA-N	CC(=CCOc1c2C=CCc2cc2c1C=CC(=C)O
QHHVLIUOUPHBGA-UHFFFAOYSA-N	CCOC1OCC2C(C1)CC(=O)CC2(C)C
LLIOFDFSNDWFFZ-UHFFFAOYSA-N	OCC1OC(OC2OCC(C3C2C(=CCC3)CO)(
XLNDUMVWOZNMNJ-UHFFFAOYSA-N	COC(=O)C1COC(C2C1CCC=C2CO)O
SEBIKDIMAPSUBY-CKZAFTHVSA-N	OCC1OC(OCC2OC(OC(=O)/C(=C/C=C/C
IBFYXTRXDNAPMM-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(=CC3)CO)C
IKGXIBQEEMLURG-UHFFFAOYSA-N	Oc1cc(O)c2c(c1)oc(c(c2=O)O)C1OC(COC
YSIFYNVXJOGADM-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(C)(O)CC3O
BWZNVEVIYYLKOG-UHFFFAOYSA-N	OC1CC(C2C1C(=COC2O)C(=O)O)(C)O
ALYNDLNZVKVGQH-QSZPNPOGSA-N	Oc1ccc2c(c1/N=N/c1cccc(c1)/N=N/c1ccc
WCGUUGGRBIKTOS-UHFFFAOYSA-N	CC1CCC2(C(C1C)C1=CCC3C(C1(CC2)C
PGOYMURMZNDHNS-UHFFFAOYSA-N	OCC1(C)C(O)CCC2(C1CCC1(C2CC=C2C
REFJWTPEDVJJIY-UHFFFAOYSA-N	Oc1cc(O)c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)
RWASOQSEFLDYLC-UHFFFAOYSA-N	[BeH2]
JOPOVCBBYLSVDA-UHFFFAOYSA-N	[Cr+6]
RYGMFSIKBFXOCR-UHFFFAOYSA-N	[Cu]
CWYNVVGOOAEACU-UHFFFAOYSA-N	[Fe+2]
WAEMQWOKJMHJLA-UHFFFAOYSA-N	[Mn+2]
PXHVJJICTQNCMI-UHFFFAOYSA-N	[Ni]
XRCKXJLUPOKIPF-UHFFFAOYSA-N	[PbH4]
KXCAEQNNTZANTK-UHFFFAOYSA-N	[SnH4]
PTFCDOFLOPIGGS-UHFFFAOYSA-N	[Zn+2]
FBPFZTCFMRRESA-UHFFFAOYSA-N	OCC(C(C(C(CO)O)O)O)O
OEYIOHPDSNJKLS-UHFFFAOYSA-N	OCC[N+](C)(C)C

JSKCJJNYSGWZDU-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(=C)C(C3)O)
KGDIDCUROGOWDM-UHFFFAOYSA-N	O=CC1=COC(C2C1CC(C2=C)O)OC1OC(
CDAISMWEOUEBRE-UHFFFAOYSA-N	OC1C(O)C(O)C(C(C1O)O)O
ZVXWFPTVHBWJOU-UHFFFAOYSA-N	OCC1=CC(C2C1C(OC=C2C(=O)O)OC1C
WGNYWQMQLMVUIP-DUXPYHPUSA-N	OCC1OC(Oc2coccc2=O)C(C(C1O)OC(=O
REFJWTPEDVJJIY-UHFFFAOYSA-M	Oc1cc(O)c2c(c1)oc(c(c2=O)[O-])c1ccc(c(c
GGNQRNBDZQJCCN-UHFFFAOYSA-N	Oc1ccc(c(c1)O)O
KZNIFHPLKGYRTM-UHFFFAOYSA-M	Oc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2[O-])O
TZBJGXHYKVUXJN-UHFFFAOYSA-M	Oc1ccc(cc1)c1coc2c(c1=O)c([O-])cc(c2)O
ZCOLJUOHXJRHDI-UHFFFAOYSA-N	OCC1OC(Oc2cc(O)c3c(c2)occ(c3=O)c2cc
YCCILVSKPBXVIP-UHFFFAOYSA-N	OCCc1ccc(cc1)O
VMNGEGPLZYRNAA-UHFFFAOYSA-N	ON(Cc1ccc(cc1)O)Cc1ccc(cc1)O
XHCADAYNFIFUHF-UHFFFAOYSA-N	OCC1OC(Oc2cc3ccc(=O)oc3cc2O)C(C(C
SPXYMBLXSLZSEX-UHFFFAOYSA-L	O=C1O[BiH]Oc2c1cccc2
CTOLSFASROFSCG-UHFFFAOYSA-N	OCC1OC(Oc2ccc3c(c2O)oc2c(c3=O)c(O)
JXOHGGNKMLTUBP-UHFFFAOYSA-N	OC1CC(=CC(C1O)O)C(=O)O
KRZBCHWVBQOTNZ-FCXRPNKRSA-N	O=C(OC1CC(O)(CC(C1O)OC(=O)/C=C/c1
UFCLZKMFXSILNL-FCXRPNKRSA-N	O=C(OC1C(O)CC(CC1OC(=O)/C=C/c1cc
IYXQRCXQQWUFQV-FCXRPNKRSA-N	O=C(OC1C(O)CC(CC1O)(OC(=O)/C=C/c1
KXEWLJDTPOIUSH-UHFFFAOYSA-N	OCC1=CCC2C1C(OC=C2C(=O)CO)OC1O
ZJDOESGVOWAULF-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(=CC3)CO)C
SUCGXPHEYBRFIL-UHFFFAOYSA-N	OC1CCNC(C1O)C(=O)O
OXNHRKGZZFWUQZ-QORFUXSJSA-N	COC(=O)/C(=C/C=C/C(=C/C=C/C=C(/C=C
CZSBHMFVVLYIQQ-YWYBPMHCSA-N	OCC1OC(OCC2OC(OC(=O)/C(=C/C=C/C
SEBIKDIMAPSUBY-MVELCSNHSA-N	OCC1OC(OCC2OC(OC(=O)/C(=C/C=C/C
IGWDEVSBEKYORK-UHFFFAOYSA-N	CC(=CCOc1c2ccoc2cc2c1ccc(=O)o2)C
UOURIOWCMYPGGF-UHFFFAOYSA-N	COc1cc(O)c(c(c1C(=O)C)O)C=O
GGGDNPWHMNJRFN-UHFFFAOYSA-N	CC(=O)Nc1c(I)c(N(C(=O)C)C)c(c(c1I)C(=O
GEWMGBJPZDGMSS-UHFFFAOYSA-N	CC(=O)OC(C(=O)O)C1CCC2=C1C(O)OC
DHWBTJZWWBYHEM-UHFFFAOYSA-N	OCC1OC(OC2OC=C3C4C2C(=CC4(C)OC
LOXQKSBAJJTUOX-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(=CC3)COC
DSCVRGCAXJUTEM-UHFFFAOYSA-N	COC(=O)C1C(O)CCCN1C(=O)OC(C)(C)C
OZKNMGZZFOYTHQ-MDZDMXLPSA-N	COC1C2OC(=O)C(C2(O)C(C)C)C2(C1(C)
MGWAVDBGNNKXQV-UHFFFAOYSA-N	CC(COC(=O)c1ccccc1C(=O)OCC(C)C)C
ZTDNKQJEIFATQN-UHFFFAOYSA-N	CNC1CCC2(C(=CCC3C2CCC2(C3CCC2(
TTYDGCKGPQOMOK-UHFFFAOYSA-N	CC(=CC(=O)CC(C1CCC2(C1(C)CCC13C2
OOGPWQHGQYUIAW-KBXRYBNXSA-N	O=C(OC1CC(O)(CC(C1OC(=O)CC(CC(=O
BEKYZOSRHNMGCR-KBXRYBNXSA-N	O=C(OC1C(OC(=O)/C=C/c2ccc(c(c2)O)O
NMVUNDOHFYILSF-UHFFFAOYSA-N	CC1CC(O)(CC(C1O)O)C(=O)O
IQGURDMZNWKPEW-VHYPUYLQSA-N	C/C=C/CCCC/C=C/CC(=O)O
BTTOWNPBHGPOLE-UHFFFAOYSA-N	OCC1=CCC2C1COC(=O)C2(C)CO
KWLOAKAXMOYBRK-XNTDXEJSSA-N	O=C(OC1C(O)CC2(C(C1(C)C)CCC1(C2C
XQUFDDXBHJINGZ-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(C)(O)CC3)C
LBTAFDHXNSPZSZ-UHFFFAOYSA-N	OCC1OC(OC2CC(=C(C(C2)(C)C)C(=O)O
FOONTNRMWNJWCL-UHFFFAOYSA-N	OCC1OC(OCC2C(=CC(=O)CC2(C)C)C)C
ZFRKQXVRDFCRJG-UHFFFAOYSA-N	Cc1c[nH]c2c1cccc2
ZMDOPLQSOGZPJN-UHFFFAOYSA-N	Oc1cc(O)c2c(c1)oc(c(c2=O)OC1OC(COC
RTATXGUCZHCSNG-UHFFFAOYSA-N	Oc1ccc(cc1)c1oc2cc(O)cc(c2c(=O)c1OC1
CRDWYCSWUMQZMG-RSZDNHPTSA-N	OCC1OC(OCC2OC(OC(=O)/C(=C/C=C/C
FZRIRHAXJWMMFP-UHFFFAOYSA-N	CC1CC(C(=O)O)C2C(C1C)C1=CCC3C(C
KIJYSICAJWQCER-UHFFFAOYSA-N	CC(=O)OC1CCC2(C(C1(C)C)CCC1(C2CC
GYDIPQRLDOTECG-MDZDMXLPSA-N	CCC(C(C)C)/C=C/C(C1CCC2C1(C)CCC1
VWDLOXMZIGUBKM-CMDGGOBGSA-N	CCC(C(C)C)/C=C/C(C1CCC2C1(C)CCC1
KZJWDPNRJALLNS-UHFFFAOYSA-N	CCC(C(C)C)CCC(C1CCC2C1(C)CCC1C2
XMLSXPIVAXONDL-SNAWJCMRSA-N	CC/C=C/CC1=C(C)CCC1=O
STCGEEFQLSTNRZ-UHFFFAOYSA-N	CCC1C(CC2C1(C)CCC1C2CC(C2C1(C)C
RMTXUPIIESNLPW-AOSYACOCSA-N	CCC/C=C/C/C=C/CCCCCCCc1cccc(c1O)
WOLHVDCCOJEKFW-UHFFFAOYSA-N	CCCCC1CC(=O)CC1CC(=O)OC

OIPHBJBKSAKTTI-IVZWYUIFSA-N	CCCCCC#C/C=C/C=C/CC/C=C/C(=O)NC
WXGBJURRRZPBDS-UHFFFAOYSA-N	CCCCCCCCCCCCCC(C(CCC(C(CCCCCC
QIQXTHQIDYTFRH-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCCC(=O)O
DAGYDJHSDMRWJX-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCCCCCCCC(CC(
DOIRQSBPFJWKBE-UHFFFAOYSA-N	CCCCOC(=O)c1ccccc1C(=O)OCCCC
UMZZGLBLVAIHPM-UHFFFAOYSA-N	CCOC1(C)OCC2C1CC(=O)CC2(C)C
FAPDDOBMIUGHIN-UHFFFAOYSA-K	Cl[Sb](Cl)Cl
LTUZVVOPXHMYOH-UHFFFAOYSA-N	CN1CCCC21NC(=O)c1c2cccc1
WSGPLSDARZNMCW-UHFFFAOYSA-N	OCC1=CC(C2C1C(OC=C2C(=O)OC)OC1
OVNBCJLEFGLOJC-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(=CC3O)CO
XJMPAUZQVRGFRE-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(O)(CO)C=C
JBBLCGRIZVRWJC-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(CO)(OC)C=
AFFNBNJOIDYUQN-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(=C)C(C3)O)
FYZYXYLPBWLLGI-UHFFFAOYSA-N	OCC1=CCC2C1C(OC=C2C(=O)OC)OC1(
QIWWLKDHHMGRQL-RUDMXATFSA-N	OCC1=CCC2C1C(OC=C2C(=O)OC)OC1(
JJVJSIBMTMIANL-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C2(CO)OC2C
JGHUOJAZXGSFRI-YMOMHROCSA-N	COC(=O)CC1/C(=C/COC(=O)/C=C/c2ccc
ABRULANJVVJLFI-UHFFFAOYSA-N	OCC1OC(C(C(C1O)O)O)c1c(OC)cc2c(c1(
DAUAQNGYDSHRET-UHFFFAOYSA-N	COc1cc(ccc1OC)C(=O)O
YSSFBMRXSHCURK-UHFFFAOYSA-N	COc1cc(ccc1OC)c1cc(=O)c2c(o1)c(OC)c(
RODXRVNMMDRFIK-UHFFFAOYSA-N	COc1cc2ccc(=O)oc2cc1O
GUAFOGOEJLSQBT-UHFFFAOYSA-N	COc1cc2oc(=O)ccc2cc1OC
FCXRFTLSXMRXTM-UHFFFAOYSA-N	COc1c(O)cc2c(c1O)C(=O)CC(O2)c1ccc(c
WKOLLVMJNQIZCI-UHFFFAOYSA-N	COc1cc(ccc1O)C(=O)O
FLCVGMVLNHYJAW-UHFFFAOYSA-N	COc1cc(O)c2c(c1)oc(cc2=O)c1cc(OC)c(c
GIKVSFNAEBQLGB-UHFFFAOYSA-N	COc1cc(OC)c2c(c1)oc(cc2=O)c1cc(OC)c(
JMSVCTWVEWCHDZ-UHFFFAOYSA-N	COc1cc(cc(c1O)OC)C(=O)O
BEDSGEULUAVXQH-NSLJXJERSA-N	COc1cc(/C=C/C(=O)OC2C(O)CC(CC2OC
KCDXJAYRVLXPFO-UHFFFAOYSA-N	COc1cc(C=O)cc(c1O)OC
VJOBNGRIBLNUKN-UHFFFAOYSA-N	COc1cc(ccc1O)C1OCC2C1COC2c1cc(OC
KCFYHBSOLOXZIF-UHFFFAOYSA-N	COc1cc(cc(c1O)OC)C1CC(=O)c2c(O1)cc
LUOAEJWSKPQLJD-UHFFFAOYSA-N	COc1cc(CO)cc(c1O)OC
VTCDZPUMZAZMSB-UHFFFAOYSA-N	COc1c(OC)cc(cc1OC)O
ZRSNZINYAWTAHE-UHFFFAOYSA-N	COc1ccc(cc1)C=O
OOAXTXAQDYRKFM-UHFFFAOYSA-N	COc1ccc(cc1)c1oc2c(OC)c(OC)c(c(c2c(=O
BVEKTSFYGPYCTQ-UHFFFAOYSA-N	COc1ccc(cc1)c1coc2c(c1=O)c(O)cc(c2)O(
WQPZLWXUXYRWDZ-HYQBVQLESA-N	COc1n/c(=C\2/C=CC(=O)C=C2O)/[nH]/c(=
XJZRHAMUBWIJEV-UHFFFAOYSA-N	COC1C=C(C2C1C(=COC2OC1OC(CO)C
PHYYADMVYQURSX-GHXNOFRVSA-N	OCC1OC(S/C(=N\OS(=O)(=O)O)/CCCS(=
NPJICTMALKLTFW-UHFFFAOYSA-N	CCC(C(C)C)CCC(C1CCC2C1(C)CCC1C2
ATQIQIBBBWQWOT-NIBSWVOWSA-N	OCC1OC(OC(=O)/C(=C/C=C/C(=C/C=C/C
DLZFGILSEBIZHZ-UHFFFAOYSA-N	OCC1OC(OCC2OC(OCC3=C(C)C(=O)CC
VULLCGFNYWDRHL-QHUUTLAPSA-N	OCC1OC(OCC2OC(OC(=O)/C(=C/C=C/C
ADIDQIZBYUABQK-UHFFFAOYSA-N	CC(=C)C1CCC(C2=C(C1)C(C)CC2)C
TUNFSRHWOTWDNC-UHFFFAOYSA-N	CCCCCCCCCCCCCC(=O)O
WTUPZYOQFGPHOS-KZZDLZNXSA-N	CCOC(=O)C1(O)CC(OC(=O)/C=C/c2ccc(c
BNXFBCBJALNHOV-UHFFFAOYSA-N	OCC1OC(OCC2=CCC3C2C(OC=C3C(=O
HNVWFUAOTFONLC-XVYDYJIPSA-N	COc1cc(/C=C/C(=O)OC2C(O)CC(CC2OC
QXOKQINPRTYYQK-XVYDYJIPSA-N	COc1cc(/C=C/C(=O)OC2CC(O)(CC(C2O)(
JRYVBZDSFXDJAN-UHFFFAOYSA-N	OCC1OC(OC2OC=C(C3C2C(=CC3)CO)C
DARYRELQFBVEME-NXZHAISVSA-N	COC(=O)C1(O)CC(OC(=O)/C=C/c2ccc(c(
QRWMZZNSGRCHHG-KZZDLZNXSA-N	CCOC(=O)C1(O)CC(OC(=O)/C=C/c2ccc(c(
YCOZIPAWZNQLMR-UHFFFAOYSA-N	CCCCCCCCCCCCCCC
NDJKXXJCMXVBJW-UHFFFAOYSA-N	CCCCCCCCCCCCCCCCC
QNGQIURXCUHNAT-UHFFFAOYSA-N	CC1=CC=CC(CC1=O)(C)C
RJWUMFHQJJBBOD-UHFFFAOYSA-N	CCCCCCCCCCCCCCCC(C)C
LKXMXUPYWQQHNY-UHFFFAOYSA-N	COC(=O)C1=COC(C2C1CC=C2COC(=O)
JZQKTMZYLHNFPL-BLHCBFLLSA-N	CCCCC/C=C/C=C/C=O

NDFKTBCGKNOHPJ-AATRIKPKSA-N   CCCC/C=C/C=O
YVBAUDVGOFCUSG-UHFFFAOYSA-N   CCCCCc1ccco1
VLCHQFXSBHIBRV-UHFFFAOYSA-N   OCC1OC(OC2OC=C(C3C2C(C)(O)CC3)C
SMUVABOERCFKRW-UHFFFAOYSA-N   O=Cc1cc(C)ccc1C
KKSYAZCUYVRKML-UHFFFAOYSA-N   OCC1OC(OC2OC=C(C3C2C(C)(O)CC3O
LNTHITQWFMADLM-UHFFFAOYSA-N   OC(=O)c1cc(O)c(c(c1)O)O
XLTFNNCXVBYBSX-UHFFFAOYSA-N   COc1c(O)cc(c2c1oc(cc2=O)c1ccccc1)O
JPUKWEQWGBDDQB-UHFFFAOYSA-N   OCC1OC(Oc2c(oc3c(c2=O)c(O)cc(c3)O)c
YQUVCSBJEUQKSH-UHFFFAOYSA-N   OC(=O)c1ccc(c(c1)O)O
SGAWOGXMMPSZPB-UHFFFAOYSA-N   O=CC1=C(C)C=CCC1(C)C
CDOSHBSSFJOMGT-UHFFFAOYSA-N   C=CC(CCC=C(C)C)(O)C
HTPQPMPFXUWUOT-PUNVMFJJSA-N   O=C1C=Cc2c(/C/1=N/Nc1ccc(cc1)/N=N/c
QAIPRVGONGVQAS-DUXPYHPUSA-N   OC(=O)/C=C/c1ccc(c(c1)O)O
ZPVOLGVTNLDBFI-UHFFFAOYSA-N   CC1CCCC(C1=O)(C)C
LFAZJMJJLQUOPK-UHFFFAOYSA-N   OCC1OC(OCC2OC(OC(=O)C3=C(C)C=C
URTXXFGOVQACIC-UHFFFAOYSA-N   OCC1OC(OCC2OC(OC(=O)C3=C(C)CCC
AOMOJMFQSLZWRN-UHFFFAOYSA-N   OCC1(O)COC(C1O)OCC1OC(OCC2C(=C
PFTAWBLQPZVEMU-UHFFFAOYSA-N   Oc1cc2OC(c3ccc(c(c3)O)O)C(Cc2c(c1)O)
FUZZWVXGSFPDMH-UHFFFAOYSA-N   CCCCCC(=O)O
GYFFKZTYYAFCTR-DUXPYHPUSA-N   O=C(OC1C(O)CC(CC1O)(O)C(=O)O)/C=C
IPCSVZSSVZVIGE-UHFFFAOYSA-N   CCCCCCCCCCCCCCCC(=O)O
OPFTUNCRGUEPRZ-UHFFFAOYSA-N   C=CC1(C)CCC(CC1C(=C)C)C(=C)C
IBIPGYWNOBGEMH-UHFFFAOYSA-N   OCC1OC(OC2OC=C3C4C2C(=CC4OC3=
KVWWIYGFBYDJQC-UHFFFAOYSA-N   CCCCCC1C(CCC1=O)CC(=O)OC
TZBJGXHYKVUXJN-UHFFFAOYSA-N   Oc1ccc(cc1)c1coc2c(c1=O)c(O)cc(c2)O
PZNPHSFXILSZTM-UHFFFAOYSA-N   CC1CCC2(OC1)OC1C(C2C)C2(C(C1)C1(
OXNHRKGZZFWUQZ-WTIHNSHESA-N   COC(=O)/C(=C/C=C/C(=C/C=C/C=C(\C=C

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(=

2([C@H]1CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2[C@@H](C)[C@@H

@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(C)(C)CC1)C(=O)O)C)C

;(C(=O)C(=C3O)C(=O)C)(C)C)c(c(c2O)C(=O)CCC)O)c(c(c1O)CC1=C(O)C(C(=O)C(=C1O)C(=

O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@@H]2O)O)O)c([o+]3)c2ccc(c(c2)O)[O-])[C@H](

H]([C@@H]1[C@H]2CC[C@]2([C@@H]1CC[C@@H]2[C@H](CCC(=O)O)C)C)O)C

2O[C@]2(C)C[C@H](CC1(C)C)O)/C)/C)/C=C/C=C(/C=C/C1=C(C)C[C@H](CC1(C)C)O)\C

C@@H]5O[C@H](COC(=O)C(C1)O)[C@@H](O)[C@@H]([C@H]5O)O)cc(cc4[o+]c3c1ccc(c(c

@@H]1O[C@H](COC(=O)CC(C(=O)OC[C@H]2O[C@@H](O3)[C@H](O)[C@H]([C@@H]2O

C(C2O)O)OC2C(OCC(C2O)O)OC2CCC3(C(C2(C)C)CCC2(C3CC=C3C2(C)CC(C2(C3CC(C)(O

2([C@]1(C)C[C@@H](O)C1C2=CC(=O)[C@H]2[C@]1(C)C[C@H](O)[C@@H](C2)O)O)(O)C)(

2=CC[C@H]3[C@@]([C@@]2(C[C@H]1O)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)C
2=CC[C@H]3[C@@]([C@@]2(C[C@H]1O)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H]([C@@]1(
@H]4[C@@]3(C)CC[C@@H]3[C@]4(C)CC[C@@H]([C@]3(C)C=O)O)[C@@H]2CC([C@H]([
@H]4[C@@]3(C)CC[C@@H]3[C@]4(C)CC[C@@H]([C@@]3(C)C=O)O)[C@@H]2CC([C@H]

([C@]1(C)C[C@@H](O)C1C2=CC(=O)[C@H]2[C@]1(C)C[C@H](O)[C@@H](C2)O)O)(O)C)C

]3[C@@]([C@@]2(C[C@H]1O)C)(C)CC[C@@H]1[C@]3(C)CC[C@@H](C1(C)C)O)(C)C

@H]1O)O[C@@H]1OC[C@H]([C@@H]([C@H]1O)O)O)C)Oc1cc2oc(cc(=O)c2c(c1O)O)c1ccc(

C\C4=N/C(=C\c5[nH]c(/C=c(/c2C)\[n-]3)c(CC)c5C=O)/C(=C4C)C=C)/C(C1CCC(=O)OC/C=C(/C

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@]

H]3C(=CC[C@@H]4[C@@]3(C)C(=O)C[C@]3([C@@]4(C)C[C@H]([C@@H]3[C@](C(=O)/C=

[C@]3(C(C2(C)C)CC[C@@]2(C3CCC34[C@@]2(C)C[C@H](C2(C4C[C@](C)(CO)CC2)CO3)

3=CCC4[C@@]([C@@]3(C[C@H]2O)C)(C)CCC2[C@]4(C)CC[C@@H](C2(C)C)O[C@@H]2O

OC)[C@@H]([C@H]([C@@H]1OC(=O)/C=C/c1ccc(c(c1)OC)O)O[C@@H]1O[C@H](CO)[C@

[C@@H]3[C@H]2[C@@]2(COC(=O)C)O[C@H]2[C@H]3OC(=O)C)[C@@H]([C@H]([C@@H

@@H]2C=COC([C@@H]2[C@@]2([C@H]1O2)COC(=O)C)O[C@@H]1O[C@H](COC(=O)C)[

OC)[C@H]([C@H]([C@@H]1O)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)O

H]3[C@H]2[C@@]2(COC(=O)c4ccc(c(c4)OC)O)OC2[C@H]3O)[C@@H]([C@H]([C@@H]1O)(

c1)OC)O)Cc1ccc(c(c1)OC)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O

2CC(=O)[C@@]1([C@@H]3CC[C@@]2(C31O[C@@H]3C(=O)O[C@H]2c1cocc1)C)C)(C)C

H]3[C@H]2[C@@]2(CO)O[C@H]2[C@H]3OC(=O)/C=C/c2ccc(c(c2)O)OC)[C@@H]([C@H]([C

)[C@@]1([C@@H]3CC[C@@]2([C@]31O[C@@H]3C(=O)O[C@H]2c1cocc1)C)C)(C)C

@@H]3[C@H]2[C@@]2(COC(=O)C)O[C@H]2[C@H]3OC(=O)C)[C@@H]([C@H]([C@@H]1C

CC[C@]2([C@@]3(C)C[C@H](C2[C@](C(=O)CCC(O)(C)C)(O)C)O)C)C([C@H]1O)(C)C

H]3[C@H]2[C@@]2(COC(=O)/C=C\c4ccccc4)O[C@H]2[C@H]3O)[C@@H]([C@H]([C@@H]1C

H]3[C@H]2[C@@]2(CO)O[C@H]2[C@H]3OC(=O)c2ccc(c(c2)OC)O)[C@@H]([C@H]([C@@H

H]3[C@H]2[C@@]2(CO)O[C@H]2[C@H]3OC(=O)/C=C/c2ccc(c(c2)OC)O)[C@@H]([C@H]([C

)[C@@H](COC(=O)/C=C/c3ccc(c(c3)O)O)O[C@H]([C@@H]2O)OCCc2ccc(c(c2)O)O)[C@@H
)[C@@H](COC(=O)/C=C/c3ccc(c(c3)OC)O)O[C@H]([C@@H]2O)OCCc2ccc(c(c2)O)OC)[C@

)[C@@H](COC(=O)/C=C/c3ccc(c(c3)OC)O)O[C@H]([C@@H]2O)OCCc2ccc(c(c2)O)O)[C@@
O)[C@H]([C@H]([C@@H]1O)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@H]1O)O)O)O

@@H]1C(OC=C2)O[C@@H]1O[C@H](COC(=O)c2ccc(c(c2)OC)O)[C@H]([C@@H]([C@H]1O
C2[C@@]2(CO)O[C@H]2[C@H]3OC(=O)c2ccccc2)[C@@H]([C@H]([C@@H]1O)O)O

3c(c2)[C@@H](CO)[C@@H](O3)c2cc(OC)c(c(c2)OC)OC)[C@@H]([C@H]([C@@H]1O)O)O
=O)C)c3c(c2)[C@@H](CO)[C@@H](O3)c2cc(OC)c(c(c2)OC)OC)[C@@H]([C@H]([C@@H]1O
C/C=C/c2cc(OC)c3c(c2)[C@@H](CO)[C@@H](O3)c2cc(OC)c(c(c2)OC)OC)[C@@H]([C@H](
C/C=C/c2cc(OC)c3c(c2)[C@@H](COC(=O)C)[C@@H](O3)c2cc(OC)c(c(c2)OC)OC)[C@@H](
C/C=C/c2cc(OC)c3c(c2)[C@@H](CO)[C@@H](O3)c2ccc(c(c2)OC)O)[C@@H]([C@H]([C@@

@H]1O)O)O)c1c(O)c([C@@H]2OC[C@@H]([C@@H]([C@H]2O)O)O)c(c2c1oc(cc2=O)c1cc

@H]1O)O)O)c1c(O)c([C@@H]2OC[C@@H]([C@@H]([C@H]2O)O)O)c2c(c1O)c(=O)cc(o2)c

OC)[C@@H]([C@H]([C@@H]1OC(=O)/C=C/c1ccc(c(c1)O)OC)O[C@@H]1O[C@H](C)[C@H]

@H]1O)O)O)c1c(O)c([C@@H]2OC[C@@H]([C@@H]([C@H]2O)O)O)c(c2c1oc(cc2=O)c1cc

H](CO[C@@H]3OC[C@H]([C@@H]([C@H]3O)O)O)[C@H]([C@@H]([C@H]1O)O)O)c(=O)c

@H]1O)O)O)c1c(O)c([C@@H]2OC[C@@H]([C@@H]([C@H]2O)O)O)c2c(c1O)c(=O)cc(o2)c

2H](CO[C@@H]3OC[C@H]([C@@H]([C@H]3O)O)O)[C@H]([C@@H]([C@H]1O)O)O)c(=O)c

]3OC[C@H]([C@@H]([C@H]3O)O)O)[C@H]([C@@H]([C@H]2O)O)O)c2c(c1OC)oc1c(c2=O)c

CCC3(C2CCC3C(C2CCC(C(O2)OC2OC(C)C(C(C2O)O)O)C)C)C)C)C(C(C1O)O)OC1OC(C)C(

C1OC(CC1OP(=O)(OCC1OC(CC1OP(=O)(OCC1OC(CC1OP(=O)(OCC1OC(CC1OP(=O)(OC

[C@@H]3[C@@H]2C(=CC3)COC(=O)C)C(=O)OC)[C@@H]([C@H]([C@@H]1O)O)O

3[C@@H]4[C@H]2C(=C[C@@H]4OC3=O)COC(=O)C)[C@@H]([C@H]([C@@H]1O)O)O

C2C(=O)OC)O[C@@H]1O[C@H](CO[C@@H]2O[C@H](COC(=O)/C=C\c3ccc(cc3)O)[C@H]([

@H](OC(=O)/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C(=O)O[C@@H]3O[C@H](CO[C@@H]4O

:(c(c2)O)O)C[C@](C[C@H]1OC(=O)CC(CC(=O)O)(O)C)(O)C(=O)O)/C=C/c1ccc(c(c1)O)O
=O)CC(CC(=O)O)(O)C)OC(=O)/C=C/c1ccc(c(c1)O)O)C(=O)O)/C=C/c1ccc(c(c1)O)O

H]3[C@H]2[C@@]2(CO)O[C@H]2C3)C(=O)OC)[C@@H]([C@H]([C@@H]1O)O)O

2([C@]1(C)CC[C@@]13[C@H]2CC[C@@H]2[C@]3(C1)CC[C@@H]([C@@]2(C)C(=O)O)O)C

[C@@H]3[C@H]2[C@](O)(CO)C=C3)C(=O)OC)[C@@H]([C@H]([C@@H]1O)O)O

>=C2C(=O)OC)O[C@@H]1O[C@H](CO[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@@H]2O)

:(COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)COC(=O)CCCCCCC/C=C\C/C=C\CCCCC

CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(CC1)(C)C)C(=O)O)C)C)O[C
CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(CC1)(C)C)C(=O)O)C)C)O[C

2]1(C)CC[C@@]13[C@H]2CC[C@@H]2[C@]3(C1)CC[C@@H]([C@@]2(C)C(=O)O)O)C)C
@@]3(C)CC[C@@H]3[C@]4(C)CC[C@@H](C3(C)C)O)[C@@H]2CC(C[C@@H]1O)(C)C)C

,H](C)[C@@H]([C@H]([C@@H]3O)O)O)cc(c2c(=O)c1O[C@@H]1O[C@@H](C)[C@@H]([C@

@H](OC(=O)[C@@]34CCC(=C)CC4C4=CCC5[C@@]([C@@]4(CC3)C)(C)CCC3[C@]5(C)C[C

CC[C@@]1([C@@H]2CC=C2[C@@]1(C)CC[C@@]1([C@H]2CC(CC1)(C)C)C(=O)O)C)C)O[C
2([C@]1(C)CC[C@@]13[C@H]2CC[C@@H]2[C@]3(C1)C(=O)C[C@@H]([C@@]2(C)C(=O)C

]1(C)CC[C@@]13[C@@H]2CC[C@@H]2[C@]3(C1)[C@@H](O)C[C@@H](C2(C)C)O)C)C)C

(=C/C=C/C=C(/C=C/C=C(/C(=O)OC3OC(COC4OC(CO)C(C(C4O)O)O)C(C(C3O)O)O)\C)\C)/C

(=C/C=C/C=C(/C=C/C=C(/C(=O)OC3OC(CO)C(C(C3O)O)O)\C)\C)/C)/C)C(C(C2O)O)O)C(C(C
(=C/C=C/C=C(\C=C\C=C(/C(=O)OC3OC(COC4OC(CO)C(C(C4O)O)O)C(C(C3O)O)O)\C)/C)/C

O)C)C)[C@@H]([C@H]([C@@H]1O)O)O)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@@H]1(

O[C@H](C(=O)O)[C@H]([C@@H]([C@H]2O[C@@H]2O[C@H](CO)[C@H]([C@@H]([C@@H

H]([C@H]([C@@H]1O)O)O[C@@H]1O[C@H](CO)[C@H]([C@@H]([C@@H]1O)O)O

C1OC(CC1OP(=O)(OCC1OC(CC1OP(=O)(OCC1OC(CC1OP(=O)(OCC1OC(CC1O)n1cnc2c1

O[C@H](CO)[C@H]([C@@H]([C@H]4O)O)O)[C@H]([C@@H]([C@H]3O)O)O)\C)\C)/C)/C)[C@

@@H]1OC[C@@H]([C@@H]([C@H]1O)O[C@@H]1OC[C@H]([C@@H]([C@H]1O)O)O)O
@@H]1OC[C@@H]([C@@H]([C@H]1O[C@@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1O)

@H]([C@@H]([C@@]3(C)CO)O)O)[C@@H]([C@H]([C@@H]2O)O)O)[C@@H]([C@H]([C@(

@@H]1OC[C@@H]([C@@H]([C@H]1O[C@@H]1O[C@@H](C)[C@@H]([C@H]([C@H]1O)

ncnc2N)O)n1ccc(nc1=O)N)O)n1ccc(nc1=O)N)O)n1ccc(nc1=O)N)O)n1cnc2c1ncnc2N)O)n1cn

c2c1ncnc2N)O)n1ccc(nc1=O)N)O)n1cnc2c1ncnc2N)O)COP(=O)(OC1CC(OC1COP(=O)(OC1(

CC(OC1COP(=O)(OC1CC(OC1COP(=O)(OC1CC(OC1COP(=O)(OC1CC(OC1COP(=O)(OC1C

CC(OC1COP(=O)(OC1CC(OC1COP(=O)(OC1CC(OC1COP(=O)(O)O)n1ccc(nc1=O)N)O)n1cn

c2c1nc(N)[nH]c2=O)O)n1cnc2c1nc(N)[nH]c2=O)O)n1ccc(nc1=O)N)O)n1cc(C)c(=O)[nH]c1=O)

O)n1ccc(nc1=O)N)O)n1cnc2c1ncnc2N)O)n1cc(C)c(=O)[nH]c1=O)O