

| smile | dili | |
|--------------------------|------|---|
| CNCC[C@@H] | | 1 |
| CN1CCC[C@H]1 | | 0 |
| CN(C)CCCN1C | | 1 |
| CN1CCN(CC1) | | 1 |
| NC(=O)C([C@H]) | | 0 |
| CNCC[C@H](C) | | 1 |
| CNC1(CCCCC1)C | | 0 |
| CC(N)COc1c(C)cc(C)cc1 | | 1 |
| CCN(CC)CC#C | | 0 |
| CN(C)C(=O)C | | 0 |
| Nc1nc2ccc(O)cc2n1 | | 1 |
| CC[C@H]1OC(=O)C1 | | 1 |
| CN(C)CCOC(=O)C | | 0 |
| Oc1ccc2C[C@H](O)C2 | | 0 |
| CNCCC=C1c2ccc(C)cc21 | | 1 |
| C[C@H](Cc1ccc(C)cc1)C | | 0 |
| NC(=O)N1c2ccc(C)cc2N1 | | 1 |
| CCN(CC)CC(=O)C | | 0 |
| CN(C)C(=O)C | | 0 |
| CC(C)[C@H](O)C | | 1 |
| CC(=O)OCC(N)C | | 0 |
| CCCCNc1ccc(C)cc1 | | 0 |
| OC(=O)Cc1ccc(C)cc1 | | 1 |
| CNC(C)C(O)c1ccc(C)cc1 | | 0 |
| OCC(NC(=O)C)C | | 0 |
| CC(C)NCC(O)C | | 0 |
| Cc1ccnc2N(C)CC2c1 | | 1 |
| Nc1ccc(cc1)S(=O)(=O)1 | | 1 |
| CCOC(=O)c1ccc(C)cc1 | | 0 |
| Cn1cnc2n(C)ccc2n1 | | 0 |
| CS(=O)(=O)N | | 1 |
| CC(C)NNC(=O)C | | 1 |
| CN1CCCCC1C | | 0 |
| COc1ccc(Cc2ccc(C)cc2)cc1 | | 1 |
| O=c1[nH]cnc1 | | 1 |
| CCCCc1oc2cc(C)cc2c1 | | 1 |
| OC(CCN1CCC1)C | | 0 |
| OC(=O)c1cn(C)ccc1 | | 1 |
| Cn1cc[nH]c1C | | 1 |
| OC(=O)Cc1ccc(C)cc1 | | 1 |
| CCC1(C(=O)N)CC1 | | 0 |
| OCC(O)C(O)C | | 0 |

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|--------------|---|
| O=C(CCNNC(| 1 |
| CC(=O)Nc1cc | 1 |
| Cc1cc(no1)C(| 1 |
| Fc1c[nH]c(=C | 0 |
| NC(=O)NO | 1 |
| CCN(CC)C(=S | 1 |
| Cc1nnc(NS(= | 0 |
| CN(C)CCOC(c | 0 |
| Nc1ncn(C2O(| 1 |
| Cc1ncc2CN=(| 0 |
| NNC(=O)c1cc | 1 |
| OCCN(C(=O)(| 0 |
| CCc1oc2cccc | 1 |
| Cc1oncc1C(= | 1 |
| CC(C)(C(=O)c | 0 |
| Cc1ncc(CO)c(| 0 |
| OC(=O)c1ccc | 1 |
| COc1cc(NC(C | 0 |
| CN1C(c2cccc(| 1 |
| C[N+]1(C)CC(| 0 |
| CNC1(C)C2CC | 0 |
| COc1ccc(OC) | 0 |
| CC(C)NCC(O) | 0 |
| CN1CC(c2ccc | 1 |
| OC(=O)COC(= | 0 |
| CC(=O)N(O)C | 0 |
| CC[N+](CC)(C | 0 |
| NCCc1ccc(O) | 0 |
| Cc1ccc(cc1)N | 0 |
| CC[N+](C)(C) | 0 |
| CNCCCC1c2cc | 0 |
| CC(C)[N+](C) | 0 |
| CN1C2CC(CC: | 0 |
| NC(=N)NCCN | 0 |
| CCN(CC)CCO(| 0 |
| C[N+]1(C)CC(| 0 |
| COc1cccc1C | 0 |
| CN1C(=O)OC | 1 |
| CN1CCN(CC1 | 0 |
| CN(C)CCOC(c | 0 |
| CC(C)(C)NCC(| 0 |
| Clc1ccc(OCC(| 1 |
| CCCSc1ccc2n | 1 |

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|--------------|---|
| COc1cc2nc(n | 0 |
| COc1ccc2CC3 | 0 |
| COc1ccccc1C | 0 |
| C[N+](C)(C)C | 0 |
| C[N+]1(C)C2(| 0 |
| CN(C)CCOC(C | 0 |
| CC(C)NCC(O) | 0 |
| CCCCCCCCNC | 1 |
| OC1=NC(=O) | 1 |
| CC(COc1cccc | 0 |
| CC(N)C(=O)C | 1 |
| CCc1oc2cccc | 1 |
| NC[C@H](O) | 0 |
| CC#C[C@]1(C | 0 |
| CCN1CC(CCN | 0 |
| CC(C)CCC[C@ | 0 |
| CNC(=O)c1cc | 1 |
| CC(=O)O[C@ | 0 |
| NCC[C@H](C | 0 |
| OC(=O)COc1 | 1 |
| ONC(=O)CCC | 0 |
| OC(Cn1cncn1 | 1 |
| CC1(C)NC(=O | 1 |
| C[C@](O)(CS | 1 |
| NC[C@H]1O | 0 |
| CC(C)(C)NC(= | 0 |
| C[C@]12CC(C | 1 |
| CCOC(=O)C1(| 0 |
| NCCc1ccc(O) | 0 |
| CC(=O)Oc1cc | 0 |
| Clc1ccc2nsc | 1 |
| C[C@H](N)C | 0 |
| COc1cc(ccc1 | 1 |
| CC(C)C(=O)N | 1 |
| OC[C@H]1O(| 0 |
| CNC(=O)Oc1 | 0 |
| CN1CCCN=C1 | 0 |
| CN[C@@H](i | 0 |
| CCN(CC)C(=O | 1 |
| CC[C@@H](C | 0 |
| C[C@]12CC(C | 1 |
| Oc1ccc2c(Oc | 0 |
| CN(C)CC[C@ | 0 |

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|--------------------|---|
| OCCN1C[C@H]1 | 0 |
| CN(C)CCc1c1 | 0 |
| C[C@@H](c1 | 1 |
| COc1cc2CC[N] | 0 |
| FC(F)(F)[C@H]1 | 1 |
| NC(=O)[C@@H]1 | 0 |
| CCC(C)CCCC | 0 |
| CO[C@@H]1 | 0 |
| COc1ccc(C[C@H]1 | 0 |
| CC(N)C12CC3 | 0 |
| COCCOc1cc2i | 1 |
| CN1CCC(CC1) | 1 |
| CC(=O)N1CC1 | 1 |
| CN1CCCC(CN1) | 1 |
| OCC(O)COC(=O) | 1 |
| C[N+](C)(C)C | 0 |
| C(C(C(C(C(CO | 0 |
| NCCCCC(O)= | 0 |
| CC(=O)Nc1nr | 1 |
| CC(C)C1NC(=O) | 1 |
| NCCCC(O)(P(=O)(O)C | 0 |
| CC(=O)Nc1c1 | 0 |
| NCCCNCCSP(=O)(O)C | 0 |
| Cn1c2nc[nH]1 | 0 |
| Cn1cnc(c1Sc1)C | 1 |
| C1=CC=C(C=C1)C | 1 |
| CC(C[N+](C)(C)C | 0 |
| C1CCN(CC1)C | 0 |
| CC(=O)Oc1cc1 | 0 |
| CS(=O)(=O)C | 1 |
| CCCC(C)(COC(=O)C | 0 |
| CN(C)CCC(C1 | 0 |
| Oc1nc2cc(Cl)cc2 | 1 |
| CC(=O)Oc1cc1 | 1 |
| C1C(=O)NC(=O)C1 | 1 |
| OC(=O)c1cc1 | 1 |
| C(C(CS)S)O | 0 |
| CCCC(CCC)C(=O)C | 1 |
| Fc1ccc(cc1)C | 0 |
| Cn1c2ncn(CC2)C | 0 |
| Clc1ccc-2c(c1)C | 0 |
| CC[C@@H](C)C | 1 |
| CCc1cccc2c3c1 | 1 |

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|---------------|---|
| NC(=O)OCC(| 1 |
| Oc1ccc(cc1)C | 0 |
| CC(C(O)=O)c: | 1 |
| CC(C)(C1=CC= | 0 |
| Cc1c(oc2c(cc | 0 |
| CCOC(=O)c1r | 0 |
| Cc1ccc(C)c(O | 1 |
| C1CN(CCN1C | 0 |
| COc1ccc2n(C | 1 |
| CC(CCc1cccc | 1 |
| Nc1nnc(c(N)i | 1 |
| CCOC(=O)N1 | 0 |
| CC1=CC(=CC= | 0 |
| Cc1cccc(Nc2c | 1 |
| CCOC(=O)C1(| 0 |
| CCCC(C)(COC | 0 |
| CN(C)C(=N)N | 0 |
| Cc1ncc(n1CC | 0 |
| Nc1cc(nc(=N | 0 |
| C1=CC=C(C(= | 0 |
| CC(C)c1cc(O | 1 |
| CCC1=NN(C(= | 1 |
| C1C(C(C(C1 | 0 |
| C(C(CO[N+])(= | 0 |
| CC12CCC3C(C | 1 |
| Nc1nc(O)c(o | 1 |
| CC(C)(CC1=C | 0 |
| CC1=C(C(=O) | 0 |
| C1CCC(CC1)C | 0 |
| C1C(=S)N(C2 | 0 |
| Oc1ccc(cc1)- | 0 |
| CN1CCN(Cc2c | 1 |
| CC1=C(C2=C(| 1 |
| CC(C)(C)C#CC | 1 |
| c1nc(cs1)-c2i | 1 |
| C1CN(CC2=C: | 1 |
| NCC1CCC(CC: | 0 |
| CC(\C=C\C1= | 1 |
| Cc1c(C)c2OC | 1 |
| C1CC[N+](C | 0 |
| CCN(C(C)=O) | 0 |
| CC(=O)OCC(= | 0 |
| [H][C@]12CN | 0 |

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|--------------|---|
| C[C@]12C[C@] | 0 |
| COC1C(CC2C) | 0 |
| CNCC(C1=CC) | 0 |
| CC12CCC3C(C | 1 |
| N[C@@H](C) | 0 |
| CN1CCc2cccc | 0 |
| CC12CCC3C(C | 1 |
| Nc1nc2ncc(C | 0 |
| Nc1ccn([C@] | 1 |
| CC1(O)CCC2C | 1 |
| CC1(CC(=O)N | 0 |
| CN1C2CCC1C | 0 |
| CC1(C)S[C@] | 0 |
| [O-][N+](=O) | 0 |
| CCN(CC)C(C) | 0 |
| OC(=O)c1cc(i | 1 |
| CCC(CO)NC(= | 0 |
| [H][C@@]1(i | 1 |
| CC1(C(=O)N2 | 0 |
| C[N+](C)(C)C | 0 |
| Nc1ccc(cc1)S | 1 |
| OC[C@H]1O | 0 |
| CC(=O)N[C@ | 0 |
| CCC1C(C(C(C | 1 |
| [H][C@@]12 | 0 |
| CC[C@]1(O)(| 0 |
| Fc1ccc(cc1)C | 0 |
| CC12CCC3C(C | 1 |
| Cc1cn([C@@ | 1 |
| CC1(C(=[N+](| 0 |
| CN[C@H]1[C | 0 |
| CN(C)CCCC1C | 1 |
| CC(=O)OC1C | 0 |
| C[C@]12CC[C | 1 |
| CC(=O)N1C2= | 1 |
| CC1C(C(CC(O | 0 |
| COc1cccc2C(| 0 |
| C1=NC2=C(N | 0 |
| [H]OC([H])([| 0 |
| CC1=C(C2=C(| 1 |
| C1CC2=CC=C | 1 |
| Cc1cn(C2CC(I | 1 |
| CC(C1=CC(=C | 1 |

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|--------------|---|
| CC(CCC1=CC= | 0 |
| CC(C)(C)NCC(| 0 |
| C[C@](N)(Cc | 1 |
| COc1ccc(cc1) | 1 |
| CC(=O)OC1C | 0 |
| CC(C1=CC2=C | 1 |
| C1=CC(=C(C= | 1 |
| C1C(C(OC1N; | 1 |
| CCC12CC(=C) | 1 |
| CCC(=O)N(C1 | 0 |
| C[N+]1(CCC2 | 0 |
| OC[C@@H]1 | 1 |
| CCC(=O)N(C1 | 0 |
| CCCCN1CC(C | 0 |
| CN(CC(=O)O) | 1 |
| CCCC(CCC)C(| 1 |
| C1C(N(C2=C | 0 |
| CCNC(=O)N(| 0 |
| CCCN(CCC)C | 1 |
| CCC(C)N1C(= | 1 |
| CNCC(C(C(C | 0 |
| C1=CC=C(C=C | 1 |
| CC1=C(C2=CC | 0 |
| CC(C)NCC(CC | 0 |
| CC(N(O)C(N) | 1 |
| CC[C@@]1(C | 0 |
| CC(CN1CCN(| 0 |
| C1=CN(C(=O) | 1 |
| CCCCCCCN(C | 0 |
| CC1=CC(=C(C | 0 |
| CC(C)c1c(C= | 1 |
| CCCCCN(C)CC | 0 |
| C1=CC(=CC=C | 0 |
| CCCCS(=O)(= | 0 |
| Nc1ncnc2n(c | 0 |
| CCC(C)C1C(= | 0 |
| C1C2C(C2N)C | 1 |
| CCCC1OC2CC | 0 |
| C(N1CCCNCC | 0 |
| CCCC1(CC(=O | 1 |
| C1CC1NC2=N | 1 |
| CC1=CC(=C(C | 1 |
| CN1C2=C(C3= | 1 |

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|---------------|---|
| C1=CC(=CC=C | 1 |
| CC(C)NC1=N | 1 |
| CN(CCOc1ccc | 0 |
| C(CNCCNCCN | 0 |
| CC1=NC(=CN | 1 |
| Clc1ccc(cc1)[| 1 |
| CNC1CCC2=C | 0 |
| Cc1cc2c(cc1C | 1 |
| CC(C)C[C@@ | 1 |
| COc1cccc1C | 1 |
| CCCCOCC(CN | 1 |
| CC1=C(C(=O) | 0 |
| C1=NC2=C(N | 1 |
| CN(C)CCc1c[r | 0 |
| C1CC2C(=O)N | 0 |
| COc1cc2ncnc | 1 |
| CN(Cc1cnc2n | 1 |
| CCOc1cccc1 | 0 |
| CC(C)COc1cc | 1 |
| CC(CCCC(C)(C | 0 |
| CC[C@@H])([| 1 |
| C[C@H]1COc | 1 |
| Cc1ccc(Nc2c[| 1 |
| CC12CCC3C(C | 0 |
| CC1CCN(C(C1 | 0 |
| C=C1C(CC(C1 | 1 |
| CC(C1=CC=CC | 0 |
| C1CC(CCC1O[| 0 |
| C1C(C(C(C(C1 | 0 |
| CCCCCO1=C | 1 |
| CN1[C@H]2C | 0 |
| CC1=CC(=CC(| 1 |
| CCCCN(CCCC) | 1 |
| CCC(=O)NCC(| 0 |
| CS(=O)(=O)C | 1 |
| [H][C@]1(CC | 1 |
| Cc1cccc1C(= | 1 |
| CCC(C)CCCC | 0 |
| CNC(=O)C1=(| 0 |
| CCC1=C(C2=C | 1 |
| CC[C@H](C)[| 0 |
| CCC(C)C1C(= | 0 |
| COc1cc(OC)c | 1 |

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|--------------|---|
| CC1C(C(CC(O | 0 |
| CC1C(C(C(C(C | 1 |
| CC1C2CC3=C | 0 |
| C[C@](N)(Cc | 0 |
| CC(C)COC(=O | 0 |
| COCCNC(=O) | 0 |
| CCC(C)CC(C)C | 1 |
| CC1=C(C=C(C | 1 |
| CCCCC(C1(CC | 0 |
| CCCc1cc(=O) | 1 |
| C1=NC2=C(N | 1 |
| CC\C(c1cccc | 1 |
| CC(C)c1nnc(C | 1 |
| CN(C)CC1=CC | 1 |
| CCCCCCCCC | 1 |
| CCCCCOC1=C | 1 |
| C=CCN.C1C(C | 0 |
| Cc1ccc(cc1)C | 1 |
| CC(C)C(C)C=C | 0 |
| CN(C)[C@H]: | 1 |
| CCN(CC)C(=O | 0 |
| CC(C)(C)NCC | 1 |
| CN1CCC23C4 | 0 |
| CCCCC(C)(C= | 0 |
| CCCCC(C)(C | 0 |
| CN1CCC23C4 | 0 |
| CN1CCC23C4 | 0 |
| CCN(CC)CCN | 1 |
| CN(C)N=Nc1 | 1 |
| CC=C1C(=O)N | 0 |
| Oc1cn(N=Cc2 | 1 |
| C1=CC=NC(=O | 1 |
| C1CC(C1)CN2 | 0 |
| C1CCC2(C3CC | 0 |
| CC(C)(C)NC(= | 1 |
| CC1C=CC=C(C | 1 |
| CC1=CC2=C(C | 0 |
| CCC1C2(C(C | 1 |
| CC(C)CC(CC(= | 0 |
| CC1CN(CCC1 | 0 |
| C1=CC(=C2N | 1 |
| CC(C)C(CC1= | 0 |
| CC1C=CC=C(C | 1 |

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|---------------|---|
| OS(=O)(=O)C | 0 |
| CCCCCCCCC=C | 0 |
| CO[Si](C)(C)C | 0 |
| CCC1C(=O)N(| 1 |
| CC1=CC(=C(C | 1 |
| CNCC(C(C(C(| 0 |
| CC(C(=NO)C) | 0 |
| CCOC(=O)CN | 1 |
| C1CCC(C(C1)I | 1 |
| CC1=C(C=C(C | 1 |
| CC(=O)OC1=C | 0 |
| CC1C=CC=CC | 0 |
| O=N[Fe--](C | 0 |
| CC(C)C(C(=O) | 0 |
| CCC(C)C(C(=C | 0 |
| CCC(C)C(C(=C | 0 |
| CCNC(=NCCC | 0 |
| C1C2CC2N(C: | 0 |
| CCC(C)C1C(= | 0 |
| Nc1ccc(C(O): | 1 |
| CC(=O)Oc1cc | 0 |
| OC(Cn1ccnc1 | 0 |
| CC1=C(C=C(C | 1 |
| CC(CC1=CC=C | 0 |
| CC(C)C1=C(C | 0 |
| C1=CC(=C(C(| 1 |
| C1CCC(CC1)C | 1 |
| CC(C(=O)NC | 1 |
| CC(C)Cc1ccc | 1 |
| CCOC(C(=O)C | 1 |
| CC(=O)Oc1cc | 1 |
| C1CN(CCC1C | 1 |
| CC(COC1=CC= | 1 |
| CN(C)CC=C(C | 1 |
| CC(C1=CC=CC | 1 |
| OC(=O)Cc1cs | 1 |
| CC1=CC2=C(C | 1 |
| C(C(C1C(=C(C | 0 |
| CC(COC1=CC= | 0 |
| CC1=C(SC=[N | 0 |
| CN(C)CCC(C1 | 0 |
| CC(CC1=CC=C | 0 |
| CN1CCC23C4 | 0 |

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|---------------|---|
| CC1C(OCCN1 | 0 |
| N[S+](O-): | 0 |
| CC(O)(P(O)(C | 0 |
| CCC(C1=CC(= | 0 |
| CC(CC1=CC=C | 0 |
| CC(C)CC(C(=C | 0 |
| C(CC(=O)[O-] | 0 |
| CC(C)C(=O)O | 0 |
| CN1CCC23CC | 0 |
| Cc1ccc(cc1)C | 0 |
| C=CC1=CC=C | 0 |
| CC(C(C1CNC2 | 0 |
| Cc1cc2nc3c(r | 0 |
| CC(C)(CO)N.C | 0 |
| C(CC(C(=O)O | 0 |
| CC(C)(CO)C(C | 0 |
| Nc1ccc(cc1)C | 0 |
| CCC(C)C(C(=C | 0 |
| CC(=O)NC1=C | 0 |
| CC(C(=O)[O-] | 0 |
| CSCC[C@H](I | 0 |
| Cl[Cu]Cl | 0 |
| CCC(C)C(C(=C | 0 |
| CCC(C)C1C(=C | 0 |
| CCC(C)C(C(=C | 0 |
| CCC(C)C(C(=C | 0 |
| C[N+]1(CCC2 | 0 |
| CCCC(=O)OC | 0 |
| Cn1c(CCCC(O | 0 |
| C[Si]12OCCN | 0 |
| C1=C(NC=N1 | 0 |
| OC(=O)CN(C | 0 |
| C(C(F)(F)F)(C | 0 |
| CC1=NC2=C(I | 0 |
| CC1(C(NC(S1 | 0 |
| C1=CC=C(C=C | 0 |
| CN(C)C1=CC(| 0 |
| OC(=O)c1c(l) | 0 |
| CSCC[C@H](I | 0 |
| CC(=O)OC1(C | 0 |
| C1CC(N(C1)C | 0 |
| C1C(N(C2=C | 0 |
| CN1C(CNC2= | 0 |

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|--------------------------|---|
| <chem>C1=C(C(=O)N</chem> | 1 |
| <chem>CC1=C2CCC(=</chem> | 1 |
| <chem>CC(=O)NC1C(</chem> | 1 |
| <chem>CCOC1C(CC(=</chem> | 1 |
| <chem>CCCCN1C(=O</chem> | 1 |
| <chem>CON=C(C1=C</chem> | 1 |
| <chem>COc1cccc2O(</chem> | 1 |