

## **Supporting information for**

# **Deep Learning-Assisted Performance Prediction and Rational Design of Sensitizers in Dye-Sensitized Solar Cells**

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**Table S1. SMILES for dyes in the database.**

| No. | SMILES  |
|-----|---|
| 1   | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(c2c1nns2)c1ccc(cc1)/C=C(\[C@@H]1SC(=S)NCC(=O)OC1=O)/[C@H]1SC(=S)NCC(=O)OC1=O</chem>  |
| 2   | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C(C)(C)C)/C(=O)O</chem>                           |
| 3   | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(c2c1nns2)c1ccc(s1)/C=C(/[C@H]1SC(=S)NC1=O)\[C@H]1SC(=S)NCC(=O)OC1=O.C1C(=O)O1</chem> |
| 4   | <chem>N#C/C(=C/c1ccc(s1)c1ccc(cc1)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C(C)(C)C)/C(=O)O</chem>                                    |
| 5   | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2c(c1)n1c3ccc(cc3c3c1c2cc(c3)C(C)(C)C(C)(C)C)/C(=O)O</chem>                         |
| 6   | <chem>CCCCCc1cc(sc1c1sc(c(c1)CCCCC)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)n1c3ccc(cc3c3c1c2cc(c3)C(C)(C)C(C)(C)C</chem>             |
| 7   | <chem>N#C/C(=C\c1ccc(s1)c1ccc2c(c1)c1cccc1n2c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O</chem>                                   |
| 8   | <chem>N#C/C(=C/c1ccc(s1)c1ccc(s1)c1ccc2c(c1)c1cccc1n2c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O</chem>                          |
| 9   | <chem>N#C/C(=C\c1ccc(s1)c1ccc2c(c1)c1cccc1n2c1ccc(cc1)C=C(c1cccc1)c1cccc1)/C(=O)O</chem>                                  |
| 10  | <chem>N#C/C(=C\c1ccc(s1)/C=C\c1ccc(s1)c1ccc2c(c1)c1cccc1n2c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O</chem>                     |
| 11  | <chem>CCCCCCCCOe1ccc2c(c1)n(CC)c1c2cc(cc1)c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)/C=C(\C(=O)O)/C#N</chem>        |
| 12  | <chem>CCCCCCCCOe1ccc2c(c1)n(CC)c1c2cc(cc1)c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)/C=C(\C(=O)O)/C#N</chem>        |
| 13  | <chem>CCCCCc1cc(sc1c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)/C=C(/C(=O)O)\C#N)c1sc(cc1CCCCC)c1ccc2c(c1)c1cccc1n2CC</chem>          |
| 14  | <chem>O=C(O)CN1C(=S)S/C(=C/c2ccc(s2)c2ccc3c(c2)c2cccc2n3c2ccc3-c4c(C(c3c2)(C)C)cccc4)/C1=O</chem>                         |
| 15  | <chem>O=C(O)CN1C(=S)S/C(=C/c2ccc(s2)c2ccc(s2)c2ccc3c(c2)c2cccc2n3c2ccc3-c4c(C(c3c2)(C)C)cccc4)/C1=O</chem>                |
| 16  | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(c2c1nns2)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>   |
| 17  | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(c2c1nns2)c1ccc(cc1)/C=C(\C(=O)O)/C#N</chem>  |
| 18  | <chem>CCCCCc1cc(sc1c1sc(c(c1)CCCCC)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)c1cccc1n2CC</chem>  |
| 19  | <chem>Cc1cc(sc1c1cc(c(s1)/C=C(\C(=O)O)/C#N)C)c1ccc2c(c1)c1cccc1n2c1cccc1</chem>   |
| 20  | <chem>CCCCCc1cc(sc1c1cc(c(s1)/C=C(/C(=O)O)\C#N)CCCCC)c1ccc2c(c1)c1cccc1n2c1cc(cc1)OC</chem>                               |
| 21  | <chem>N#C/C(=C\c1ccc(s1)c1ccc(c2c1nns2)c1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O</chem>  |
| 22  | <chem>N#C/C(=C\c1ccc(s1)c1ccc(c2c1nns2)c1ccc2c(c1)c1cccc1n2c1cccc1)/C(=O)O</chem>   |
| 23  | <chem>CCCC[C@@H](Cn1c2ccc(cc2c2c1cccc2)c1ccc(c2c1nns2)c1ccc(s1)/C=C(\C(=O)O)/C#N)CC</chem>                                |
| 24  | <chem>CCCC[C@@H](COe1ccc(cc1)n1c2ccc(cc2c2c1cccc2)c1ccc(c2c1nns2)c1ccc(s1)/C=C(/</chem>                                   |

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|    | C(=O)O\C#N)CC  |
| 25 | N#C/C(=C/c1ccc(s1)c1ccc(c2c1nsn2)c1ccc2c(c1)n(c1cccc1)c1c2cccc1)/C(=O)O  |
| 26 | CCCC[C@H](COc1ccc(cc1)n1c2cccc2c2c1cc(cc2)c1ccc(c2c1nsn2)c1ccc(s1)/C=C(/C(=O)O)\C#N)CC   |
| 27 | N#C/C(=C\c1ccc(cc1)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C)/C(=O)O   |
| 28 | N#C/C(=C\c1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O  |
| 29 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2c(c1)c1cccc1n2CC)/C(=O)O   |
| 30 | N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)c1ccc(cc1n2CC)c1ccc(s1)/C=C(/C(=O)O)\C#N)/C(=O)O |
| 31 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(c2)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C)c1ccc(s1)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 32 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(c2)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N  |
| 33 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(c2)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 34 | CN1c2ccc(cc2Sc2c1ccc(c2)/C=C(\C(=O)O)/C#N)n1c2ccc(cc2c2c1ccc(c2)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C                            |
| 35 | CCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(\C(=O)O)/C#N)n1c2ccc(cc2c2c1ccc(c2)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C                         |
| 36 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(\C(=O)O)/C#N)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C  |
| 37 | CCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(\C(=O)O)/C#N)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C   |
| 38 | COc1c2c3sc(cc3sc2c2c(c1OC)c1sc(cc1s2)/C=C(\C(=O)O)/C#N)c1ccc(c2=[N]=C(C=[N]=c12)c1csc(c1)C)c1ccc(s1)C)c1ccc2c(c1)c1cccc1n2C  |
| 39 | CCCC[C@H](COc1c2c3sc(cc3sc2c2c(c1OCC(C)C)c1sc(cc1s2)/C=C(\C(=O)O)/C#N)c1ccc(c2c1nsn2)c1ccc2c(c1)c1cccc1n2C[C@H](CCCC)CC  |
| 40 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc2c(c1)c1cccc1n2CC)/C(=O)O   |
| 41 | C[C@H](COc1c2c3sc(cc3sc2c2c(c1OCC(C)C)c1sc(cc1s2)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)n(C)c1c2cc(cc1)c1sc2c(c1)sc1c2c(OCC(C)C)c(OCC(C)C)c2c1sc1c2sc(c1)/C=C(\C(=O)O)/C#N)CC        |
| 42 | CCCCCclcc(sc1c1sc(c1)CCCC)c1sc(c1)CCCC/C=C(/P(=O)(O)O)\C#N)c1sc(cc1CCCC)c1ccc2c(c1)c1cccc1n2CC   |
| 43 | CCCCn1c2ccc(cc2c2c1ccc(c2)/C=C(/C(=O)O)\C#N)/C=C(/C(=O)O)\C#N  |
| 44 | CCCCn1c2ccc(cc2c2c1ccc(c2)N(c1ccc(cc1)OC)c1cccc1)N(c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC  |
| 45 | CCCCn1c2ccc(cc2c2c1ccc(c2)N(c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC)N(c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC  |
| 46 | N#C/C(=C\c1ccc(cc1)C#Cc1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O   |
| 47 | CC(COc1c2c3sc(cc3sc2c2c(c1OCC(C)C)c1sc(cc1s2)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)c1cccc1n2CC(C)C  |

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| 48 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)c1ccc(cc1n2CC)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)/C(=O)O</chem> |
| 49 | <chem>N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1ccc2c(c1)c1cccc1n2CC)/C(=O)O</chem>   |
| 50 | <chem>CCCCCCCCCCCCn1c2ccc(cc2c2c1ccc(e2)c1ccc(s1)/C=C(/C(=O)O)\C#N)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C</chem>  |
| 51 | <chem>CCCCCCCCCCCCn1c2ccc(cc2c2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 52 | <chem>CCCCCCCCCCCCn1c2ccc(cc2c2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)c1ccc(s1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 53 | <chem>CCCCCCCCCCCCn1c2ccc(cc2c2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)c1ccc(s1)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N</chem>   |
| 54 | <chem>N#C/C(=C/c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)c1ccc(cc1)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)/C(=O)O</chem>   |
| 55 | <chem>CCCCCclcc(se1c1ccc(s1)c1ccc2c(c1)c1cccc1n2CC)c1sc(c(c1)CCCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 56 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)n1c2cccc2c2c1cccc2)c1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O</chem>   |
| 57 | <chem>N#C/C(=C/c1ccc(s1)/C=C/c1ccc(cc1)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)/C(=O)O</chem>  |
| 58 | <chem>CCCN1c2cc(ccc2c2c1cc(cc2)N(c1ccc2-c3c(C(c2c1)(CCC)CCC)cccc3)c1cccc1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 59 | <chem>CCCN1c2cc(ccc2c2c1cc(cc2)N(c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 60 | <chem>CCCN1c2cc(ccc2c2c1cc(cc2)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)N(c1ccc2-c3c(C(c2c1)(CCC)CCC)cccc3)c1cccc1</chem>   |
| 61 | <chem>CCCN1c2cc(ccc2c2c1cc(cc2)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)N(c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1ccc2-c3c(C(c2c1)(CC)CC)cccc3</chem>  |
| 62 | <chem>CCCCCclcc(se1c1se(c(c1)CCCCC)/C=C(/C(=O)O)\C#N)c1sc(cc1CCCCC)c1ccc2c(c1)c1cccc1n2CC</chem>   |
| 63 | <chem>COCCCClcc(se1c1se(c(c1)CCCCOC)c1se(c(c1)CCCCOC)/C=C(/C(=O)O)\C#N)c1sc(cc1CCCCOC)c1ccc2c(c1)c1cccc1n2CC</chem>  |
| 64 | <chem>CCCCCclcc(se1c1se(c(c1)CCCCC)/C=C(/C(=O)O)\C#N)c1sc(cc1CCCCOC)c1sc(cc1CCCCOC)c1ccc2c(c1)c1cccc1n2CC</chem>   |
| 65 | <chem>CCCN1c2cc(ccc2c2c1cc(cc2)N(c1cccc1)c1cccc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 66 | <chem>N#C/C(=C/c1ccc(s1)C#Cc1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O</chem>   |
| 67 | <chem>CCCN1c2cc(ccc2c2c1cc(cc2)N(c1cccc1)c1cccc1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 68 | <chem>N#C/C(=C\c1ccc2c(c1)c1cccc1n2CC)/C(=O)O</chem>   |
| 69 | <chem>CCCCCN1c2ccc(cc2c2c1cccc2)n1cc(c2c1cccc2)/C=C(/C(=O)O)\C#N</chem>  |
| 70 | <chem>CCCCCclcc(se1c1ccc(s1)c1ccc(s1)c1sc(cc1CCCCC)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)c1cccc1n2CC</chem>   |

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| 71 | CCCCC1c1cc(sc1c1cc(c(s1)c1sc2c(c1)cc(c1c2n(CC)c2c1cccc2)c1cccc1)CCCCC)c1sc(cc1CCCCC)/C=C(/C(=O)O)\C#N                                 |
| 72 | N#C/C(=C/c1ccc(s1)c1ccc(s1)c1ccc(s1)c1sc2c(c1)ccc1c2n(c2c1cccc2)c1cc(c(cc1C(C)(C)C)OC)C(C)(C)C)/C(=O)O                                |
| 73 | N#C/C(=C/c1ccc(s1)c1ccc(s1)c1ccc(s1)c1cc2c(s1)c1[nH]c3c(c1cc2)cccc3)/C(=O)O   |
| 74 | CCCCCCCn1c2ccc(cc2c2c1cc1c3cccc3n(c1c2)CCCCCCC)c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)/C=C(/C(=O)O)\C#N                      |
| 75 | CCCCCCCn1c2ccc(cc2c2c1cc1c3cccc3n(c1c2)CCCCCCC)c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)[CH][C](C(=O)O)C#N                                     |
| 76 | CCCC[C@@H](Cn1c2ccc(cc2c2c1ccc(c2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)c1=[N]=c3cccc3=[N]=c1n2C[C@@H](CCCC)CC)CC                     |
| 77 | CCCC[C@H](Cn1c2ccc(cc2c2c1ccc(c2)c1ccc(o1)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)c1=[N]=c3cccc3=[N]=c1n2C[C@@H](CCCC)CC)CC                      |
| 78 | CCCCCn1c2ccc(cc2c2c1ccc(c2)/C=C/1\SC(=S)N(C1=O)CC(=O)O)/C=C/1\SC(=S)N(C1=O)CC(=O)O  |
| 79 | CCCCn1c2cc(ccc2c2c1cc(cc2)c1ccc(s1)[C]1c2ccc(n2[B](n2c1ccc2c1ccc(s1)C1=CC=[N]=C[CH]1)(F)F)c1ccc(s1)C1=CC=[N]=C[CH]1)N(c1cccc1)c1cccc1 |
| 80 | CCCCC1c1cc(sc1/C=C(\C(=O)O)/C#N)c1sc2c(c1)c1nn(nc1c1c2sc(c1)c1ccc2c(c1)n(C[C@@H](CCCC)CC)c1c2cccc1)C[C@@H](CCCC)CC                    |
| 81 | CC(Cn1nc2c(n1)c1cc(sc1c1c2cc(s1)c1ccc2c(c1)n(CC(C)C)c1c2cccc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)C  |
| 82 | N#C/C(=C/c1ccc(cc1)/C=C/c1ccc2c(c1)c1cccc1n2c1ccc(cc1)C)/C(=O)O   |
| 83 | CCCCOC1c1cc(sc1c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)/C=C(/C(=O)O)\C#N)c1sc(cc1COCCCC)c1ccc2c(c1)c1cccc1n2CC                                |
| 84 | CCCCn1c2cc(ccc2c2c1cc(cc2)/C=C(/C(=O)O)\C#N)n1c2cccc2c2c1cccc2  |
| 85 | CCCCn1c2cc(ccc2c2c1cc(cc2)n1c2cccc2c2c1cccc2)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 86 | Cn1c2cc(ccc2c2c1cc(cc2)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 87 | CCCCn1c2cc(ccc2c2c1cc(cc2)n1c2cccc2c2c1cccc2)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 88 | CCCCn1c2cc(ccc2c2c1cc(cc2)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N                                 |
| 89 | CCCCC1c1cc(sc1c1sc(c(c1)CCCCC)/C=C(/C(=O)O)\C#N)c1sc(cc1CCCCC)c1ccc2c(c1)c1cccc1n2CC  |
| 90 | CCCCC1c1cc(sc1c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1sc(cc1CCCCC)c1ccc2c(c1)c1cccc1n2CC  |
| 91 | CCCCC1c1cc(sc1c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)/C=C(/C(=O)O)\C#N)c1sc(cc1CCCCC)c1sc(cc1CCCCC)c1ccc2c(c1)c1cccc1n2CC    |
| 92 | CCCCC1c1cc(sc1c1sc(c(c1)CCCCC)c1ccc2c(c1)c1cccc1n2CC)c1sc(cc1CCCCC)c1sc(cc1CCCCC)/C=C(\C(=O)O)/C#N                                    |
| 93 | N#C/C(=C/c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc2c(c1)c1cccc1n2CC)/C(=O)O  |
| 94 | CCCCC1c1cc(sc1c1sc(c(c1)CCCCC)c1ccc2c(c1)c1cccc1n2CC)c1sc(cc1CCCCC)/C=C(\C(=O)O)/C#N  |



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|     | cc(s1)/C=C(\C(=O)O)/C#N  |
| 120 | CCCCC[C]1c2c(c(c(n2[B](n2c1c(C)c(c2C)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(c1)n(c1ccc(cc1)OC)c1c2cccc1)C                          |
| 121 | CCCCC[C]1c2c(c(c(n2[B](n2c1c(C)c(c2C)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(c1)n(CCCCCC)c1c2cccc1)C                                |
| 122 | CCCCC[C]1c2c(c(c(n2[B](n2c1c(C)c(c2C)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(c1)c1cccc1n2c1ccc(cc1)OC)C                             |
| 123 | CCCCC[C]1c2c(c(c(n2[B](n2c1c(C)c(c2C)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(c1)c1cccc1n2CCCCCCCC)C                                 |
| 124 | N#C/C(=C\c1ccc(s1)c1ccc2c(c1)c1ccc(cc1n2CC)c1ccc(cc1)C=C(c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C)/C(=O)O                             |
| 125 | N#C/C(=C/c1ccc2c(c1)c1ccc(cc1n2CC)c1ccc(s1)c1ccc(s1)c1ccc(cc1)C=C(c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C)/C(=O)O                    |
| 126 | N#C/C(=C/c1ccc2c(c1)c1ccc(cc1n2CC)c1ccc(s1)c1ccc(cc1)C=C(c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C)/C(=O)O                             |
| 127 | CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)/C=C/1\SC(=S)N(C1=O)CC(=O)O  |
| 128 | CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)/C=C(\C(=O)O)/C#N  |
| 129 | CCCCCn1c2ccc(cc2c2c1cccc2)/C=C(\c1ccc(s1)C=C1C(=O)NC(=O)NC1=O)/C#N   |
| 130 | CCCCCn1c2ccc(cc2c2c1cccc2)/C=C(\c1ccc(s1)/C=C\1\SC(=S)NCC(=O)OC1=O)/C#N  |
| 131 | CCCCCn1c2ccc(cc2c2c1cccc2)/C=C(\c1ccc(s1)/C=C(/C(=O)O)\C#N)/C#N  |
| 132 | CCCCC[C@H](C)c1ccc(se1c1se2-c3c(C4=NON[C]4e2e1)cc(s3)c1se(cc1C[C@H])(CCCC)CCCC)c1ccc2c(c1)c1cccc1n2CC)/C=C(/C(=O)O)\C#N)CCCC |
| 133 | CCCCOe1ccc(cc1)N(c1ccc2c(c1)n(CCCC)c1c2ccc(c1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCC                            |
| 134 | CCCCn1c2ccc(cc2c2c1cc(cc2)c1ccc(s1)/C=C(/C(=O)O)\C#N)N(c1ccc(cc1)OCCCC)c1ccc(cc1)OCCCC                                       |
| 135 | CN1/C(=C[CH]e2ccc3c(c2)c2cccc2n3C)/C(c2c1ccc(c2)C(=O)O)(C)C.[I]  |
| 136 | CCCCCCCCOe1ccc(cc1)c1c2c3cccc3n(e2c(e2c1n(CCCCCC)c1c2cc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCCCCCC)CCCCCCCC          |
| 137 | CCCCCCCCn1c2ccc(cc2c2c1c(c1ccc(cc1)OCC)c1c(c2c2ccc(cc2)OCC)n(c2c1cccc2)CCCCCCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N                   |
| 138 | CCCCCCCCn1c2ccc(cc2c2c1c(c1ccc(cc1)N(CC)CC)c1c(c2c2ccc(cc2)N(CC)CC)n(c2c1cccc2)CCCCCCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N           |
| 139 | CCCCCCCCn1c2ccc(cc2c2c1c(c1ccc(cc1)CC)c1c(c2c2ccc(cc2)CC)n(c2c1cccc2)CCCCCCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N                     |
| 140 | CCCCCCCCc1ccc(se1c1ccc(s1)c1se(cc1CCCCCCCC)/C=C(\C(=O)O)/C#N)c1cc2c(c3c1cccc3)n(c1e2cc(OC)cc1)[C@@H](CCCC)CC                 |
| 141 | CCCC[C@H](n1c2ccc(cc2c2c1c1cccc1c(c2)c1ccc(o1)/C=C(/C(=O)O)\C#N)OC)CC  |
| 142 | CCCC[C@@H](n1c2ccc(cc2c2c1c1cccc1c(c2)c1ccc(s1)/C=C(\C(=O)O)/C#N)OC)CC   |
| 143 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)c1cc2c3c(c1)c1cccc1n3c1c2cccc1)/C(=O)O   |
| 144 | N#C/C(=C\c1ccc(cc1)c1ccc(cc1)c1cc2c3c(c1)c1cccc1n3c1c2cccc1)/C(=O)O  |

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| 145 | <chem>N#C/C(=C\c1ccc(s1)c1cc2c3c(c1)c1cccc1n3c1c2cccc1)/C(=O)O</chem>  |
| 146 | <chem>N#C/C(=C\c1ccc(cc1)c1cc2c3c(c1)c1cccc1n3c1c2cccc1)/C(=O)O</chem>   |
| 147 | <chem>N#C/C(=C/c1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O</chem>   |
| 148 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)n1c2ccc(cc2c2c1ccc(c2)n1c2cccc2c2c1cccc2)n1c2cccc2c2c1cccc2)/C(=O)O</chem>                                   |
| 149 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)n1c2cccc2c2c1cccc2)/C(=O)O</chem>  |
| 150 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)n1c2cccc2c2c1cccc2)/C(=O)O</chem>   |
| 151 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O</chem>  |
| 152 | <chem>N#C/C(=C\c1ccc(cc1)N(c1cccc1)c1ccc(cc1)/C=N/c1ccc2c(c1)c1cccc1n2CC)/C(=O)O</chem>  |
| 153 | <chem>CCCCCn1c2ccc(cc2c2c1ccc(c2)/C=C(/C(=O)O)\C#N)/C=N/c1ccc2c(c1)c1cccc1n2CC</chem>  |
| 154 | <chem>CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=S)NC1=O</chem>  |
| 155 | <chem>CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>  |
| 156 | <chem>CCCC[CH]n1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>   |
| 157 | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(s1)c1ccc2c(c1)c1c(n2c2ccc3-c4c(C(c3c2)(CCCC)CC)cccc4)cc(s1)/C=C(/C(=O)O)\C#N</chem>                               |
| 158 | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>   |
| 159 | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>   |
| 160 | <chem>OC(=O)CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>  |
| 161 | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>   |
| 162 | <chem>OC(=O)CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>  |
| 163 | <chem>OC(=O)CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>  |
| 164 | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>   |
| 165 | <chem>c1ccc(cc1)N(c1ccc2c(c1)[nH]c1c2ccc(c1)c1ccc(s1)C1=CC=[N]=C[CH]1)c1cccc1</chem>   |
| 166 | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>   |
| 167 | <chem>c1ccc(cc1)N(c1ccc2c(c1)[nH]c1c2ccc(c1)c1ccc(s1)C1=CC=[N]=C[CH]1)c1cccc1</chem>   |
| 168 | <chem>CCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>   |
| 169 | <chem>OC(=O)c1ccc(cc1)c1ccc2c(c1)[nH]c1c2ccc(c1)N(c1cccc1)c1cccc1</chem>   |
| 170 | <chem>CCCCC[C]1c2c(c(c(n2[B](n2c1c(C)c(c2C)/C=C(/C(=O)O)\C#N)(F)F)c1ccc(cc1)N(c1cccc1)c1cccc1)C</chem>   |
| 171 | <chem>CCCCC[C]1c2c(c(c(n2[B](n2c1c(C)c(c2C)/C=C(/C(=O)O)\C#N)(F)F)c1ccc(cc1)N(c1cccc1)c1cccc1)C</chem>   |
| 172 | <chem>CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)C=C1C(=O)NC(=O)NC1=O</chem>  |
| 173 | <chem>CCCCCCCC[C@@H](Cn1c2cc(C#Cc3ccc(c4c3nsn4)c3ccc(cc3)C(=O)O)c3c4c2c2c1cc(c1ccc5c(c1)c1cccc1n5C[C@@H](CCCCCCCC)CCCCC)c1c2c(c4ccc3)ccc1)CCCCC</chem> |
| 174 | <chem>CCCCCCCC[C@@H](Cn1c2cc(C#Cc3ccc(c4c3nsn4)c3ccc(cc3)C(=O)O)c3c4c2c2c1cc(c1</chem>   |



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|     | <chem>ccc5c(-c6cccc6[C@]5(C[C@@H](CCCCCCC[CH])CCC[CH2])C[C@H](CCCCCCCC)CCCCC)c1c1c2c(c4ccc3)ccc1)CCCCC.[CH2]C.[H].[H]</chem>   |
| 175 | <chem>CCCCCCCC[C@H](Cn1c2ccc3c4c2c1cc(C#Cc1ccc(c5c1n5)c1ccc(cc1)C(=O)O)c1c2c(c4ccc3)ccc1)CCCCC</chem>  |
| 176 | <chem>CCCCCc1cc(sc1c1cc(c(s1)/C=C(/C(=O)Nc1ccc(cc1)[Si](OC)(OC)OC)\C#N)CCC[CH2])c1sc(cc1CC[CH])c1sc(cc1CCCCC)c1ccc2c(c1)c1cccc1n2CC.[CH2]C.[CH2]C[CH2].[H].[H]</chem>                        |
| 177 | <chem>CCCCCc1cc(sc1c1sc(c(c1)CCCCC)/C=C(/C(=O)Nc1ccc(cc1)C(=O)O)\C#N)c1sc(cc1CCCCC)c1sc(cc1CCCCC)c1ccc2c(c1)c1cccc1n2CC</chem>   |
| 178 | <chem>CCCCn1c2ccc(cc2c2c1ccc(e2)c1ccc2c(c1)c1cc(ccc1n2CCCC)c1sc(e2c1OCCO2)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)c1cc(ccc1n2CCCC)c1ccc2c(c1)c1cccc1n2CCCC</chem>                                       |
| 179 | <chem>CCCCn1c2ccc(cc2c2c1ccc(e2)c1ccc2c(c1)c1cccc1n2CCCC)c1ccc2c(c1)c1cc(ccc1n2CCC)c1sc(e2c1OCCO2)/C=C(/C(=O)O)\C#N</chem>   |
| 180 | <chem>CCCCn1c2ccc(cc2c2c1ccc(e2)c1sc(e2c1OCCO2)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)c1cccc1n2CCCC</chem>   |
| 181 | <chem>N#C/C(=C/C1=[N]=C2[C](C=C1)C=C(C=C2)n1c2ccc(cc2c2c1ccc(e2)OC)OC)/C(=O)O</chem>   |
| 182 | <chem>CCCCCCCCCCCCn1c2cccc2c2c1ccc(e2)C1=[N]=c2ccc(cc2=[N]=C1c1ccc2c(c1)c1ccccc1n2CCCCCCCCCCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 183 | <chem>CCCCCn1c2cccc2c2c1ccc(e2)C1=[N]=c2ccc(cc2=[N]=C1c1ccc2c(c1)c1cccc1n2CCCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 184 | <chem>CCCCn1c2ccc(cc2c2c1cccc2)C1=[N]=c2cc(ccc2=[N]=C1c1ccc2c(c1)c1cccc1n2CCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 185 | <chem>N#C/C(=C/c1ccc(s1)c1ccc2=[N]=C(C(=[N]=c2c1)c1ccc2c(c1)c1cccc1n2CC)c1ccc2c(c1)c1cccc1n2CC)/C(=O)O</chem>  |
| 186 | <chem>CCCCCCCCn1c2cccc2c2c1ccc1c2c2c3cc(ccc3n(c2cc1)CCCCCCC)/C=C(/C(=O)O)\C#N</chem>   |
| 187 | <chem>N#C/C(=C\c1sc2-c3c(C(c2c1)(C)C)cc(s3)c1ccc(s1)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)/C(=O)O</chem>   |
| 188 | <chem>N#C/C(=C\c1sc2-c3c(C(c2c1)(C)C)cc(s3)c1ccc(s1)c1ccc(s1)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)/C(=O)O</chem>  |
| 189 | <chem>CCCCCCCCc1cc(sc1c1sc2-c3c(C(c2c1)(C)C)cc(s3)/C=C(/C(=O)O)\C#N)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C</chem>   |
| 190 | <chem>CCCCCn1c2ccc(cc2c2c1cccc2)c1c(/C=C(/C(=O)O)\C#N)sc(c1c1ccc2c(c1)c1cccc1n2CCCCC)/C=C(/C(=O)O)\C#N</chem>  |
| 191 | <chem>CCCCn1c2cc(ccc2c2c1cc(cc2)c1ccc(s1)c1ccc2n1[B](F)(F)n1c(ccc1[C]2c1ccc(s1)/C=[C]\C#N)c1ccc(s1)c1ccc2c(c1)n(CCCC)c1c2ccc(c1)N(c1cccc1)c1cccc1N(c1cccc1)c1cccc1.[C][CH]/C=N\CH[CH]</chem> |
| 192 | <chem>N#C/C(=C/c1ccc(cc1)C#Cc1ccc2c(c1)n(c1ccc(cc1)C(F)(F)F)c1c2ccc(c1)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)/C(=O)O</chem>  |
| 193 | <chem>N#C/C(=C/c1ccc(cc1)C#Cc1ccc2c(c1)n(c1ccc(cc1)C(F)(F)F)c1c2ccc(c1)C#Cc1ccc(cc1)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)/C(=O)O</chem>   |
| 194 | <chem>N#C/C(=C\c1ccc(cc1)C#Cc1ccc(s1)c1ccc(s1)C#Cc1ccc(cc1)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(C)(C)C)/C(=O)O</chem>  |
| 195 | <chem>N#C/C(=C\c1ccc2c(c1)c1c(n2C)ccc2c1c1c3cccc3n(c1cc2)C)/C(=O)O</chem>  |

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| 196 | [CH2]CCCN1c2cc(ccc2c2c1cc(cc2)c1ccc(s1)c1ccc2n1[B](F)(F)n1c(ccc1[C]2c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc2c(c1)n(CCCC)c1c2ccc(c1)N(c1cccc1)c1cccc1)N(c1cccc1)c1cccc1.[H] |
| 197 | CCCCCN1c2ccc(cc2c2c1ccc(e2)/C=C(/c1ccc(s1)C=C(C(=O)O)C(=O)O)\C#N)/C=C(/c1ccc(s1)C=C(C(=O)O)C(=O)O)\C#N   |
| 198 | CCCN1c2ccc(cc2c2c1ccc(c2)c1ccc(s1)c1ccc(cc1)C(=O)O)c1ccc(s1)c1ccc(cc1)C(=O)O   |
| 199 | CCCN1c2ccc(cc2c2c1ccc(e2)c1ccc(s1)C1=CC=[N]=C[CH]1)c1ccc(s1)C1=CC=[N]=C[CH]1   |
| 200 | CCCN1c2ccc(cc2c2c1ccc(c2)c1ccc(s1)c1ccc(c(c1)O)O)c1ccc(s1)c1ccc(c(c1)O)O   |
| 201 | CCCN1c2ccc(cc2c2c1ccc(e2)c1ccc(s1)C1=CC=[N]=C[CH]1)c1ccc(s1)c1ccc(cc1)C(=O)O   |
| 202 | CCCN1c2ccc(cc2c2c1ccc(c2)c1ccc(s1)C1=CC=[N]=C[CH]1)c1ccc(s1)c1ccc(c(c1)O)O   |
| 203 | CCCN1c2ccc(cc2c2c1ccc(e2)N(c1cccc1)c1cccc1)c1ccc(c(c1)O)O  |
| 204 | CCCN1c2ccc(cc2c2c1ccc(c2)N(c1cccc1)c1cccc1)c1ccc(s1)C1=CC=[N]=C[CH]1   |
| 205 | Cn1c2ccc(cc2c2c1ccc(e2)c1ccc(s1)C1=CC=[N]=C[CH]1)c1ccc(s1)C1=CC=[N]=C[CH]1   |
| 206 | c12cc(ccc1c1c(C=[N]=C[CH]1)s2)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OCC)c1ccc(cc1)OCC   |
| 207 | CCCCCCCCC1=[N]=C(S[C]1c1ccc2c(c1)n(CCCC)c1c2cccc1)C1=[N]=C([C](S1)c1ccc(s1)/C=C(/C(=O)O)\C#N)CCCCCCCC  |
| 208 | CCCCCOc1ccc(cc1)N(c1cc2c3cc(ccc3n(c2cc1OCCCCC)CCCCC)c1cc2c(s1)c1c(n2c2cccc(e2)OCCCCC)cc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCCC  |
| 209 | COc1cccc(c1)n1c2ccsc2c2c1cc(s2)c1ccc(cc1)N(c1cc2c(cc1OC)n(c1c2cc(cc1)c1sc2c(c1)n(c1c2sc(c1)/C=C(\C(=O)O)/C#N)c1cccc(c1)OC)C)c1ccc(cc1)c1sc2c(c1)n(c1c2sc1)c1cccc(c1)OC       |
| 210 | CCCCCOc1ccc(cc1)N(c1cc2c3cccc3n(c2cc1OCCCCC)CCCCC)c1ccc(cc1)c1cc2c(s1)c1c(n2c2cccc2OCCCCC)cc(s1)/C=C(/C(=O)O)\C#N  |
| 211 | CCOc1cc2n(C)c3c(c2cc1N(c1ccc(cc1)c1cc2c(s1)c1c(n2c2cccc2OC)cc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1cc2c(s1)c1c(n2c2cccc2OC)cc(s1)cccc3   |
| 212 | CCCCCN1c2ccc(cc2c2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 213 | CCCCCN1c2ccc(cc2c2c1ccc(e2)/C=C/c1ccc(cc1)N(c1ccc(cc1)/C=C/c1ccc2c(c1)c1cc(ccc1n2CCCCC)/C=C(/C(=O)O)\C#N)c1cccc1)/C=C(\C(=O)O)/C#N   |
| 214 | Cn1c2ccc(cc2c2c1ccc(e2)/C=C/c1ccc(cc1)N(c1ccc(cc1)/C=C/c1ccc2c(c1)c1cc(ccc1n2C)/C=C(\C(=O)O)/C#N)c1ccc(cc1)/C=C/c1ccc2c(c1)c1cc(ccc1n2C)/C=C(/C(=O)O)\C#N)/C=C(\C(=O)O)/C#N  |
| 215 | N#C/C(=C\c1ccc(s1)c1ccc2c(c1)c1cccc1n2c1ccc(cc1)N(c1ccc(cc1)n1c2cccc2c2c1ccc2)c1ccc(cc1)n1c2cccc2c2c1ccc2)/C(=O)O  |
| 216 | O1C(=O)CNC(=S)S/C=C\c2ccc(s2)c2ccc3c(e2)c2cccc2n3c2ccc(cc2)N(c2ccc(cc2)n2c3cccc3e3c2cccc3)c2ccc(cc2)n2c3cccc3e3c2cccc3)/C1=O   |
| 217 | CCCCCN1c2cc(/C=C/c3ccc(cc3)N(c3cccc3)c3cccc3)ccc2c2c1ccc(e2)/C=C(/C(=O)O)\C#N  |
| 218 | CCCCCN1c2ccc(cc2c2c1cc(/C=C/c1ccc(cc1)N(c1ccc(cc1)/C=C\c1ccc3c(c1)n(CCCC   |

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|     | CCC)c1c3cc(cc1)/C=C(/C(=O)O)\C#N)c1cccc1)cc2)/C=C(\C(=O)O)/C#N  |
| 219 | Cn1c2cc(/C=C/c3ccc(cc3)N(c3ccc(cc3)/C=C\c3ccc4c(e3)n(C)c3c4cc(cc3)/C=C(\C(=O)O)/C#N)c3ccc(cc3)/C=C\c3ccc4c(e3)n(C)c3c4cc(cc3)/C=C(\C(=O)O)/C#N)ccc2c2c1ccc(c2)/C=C(\C(=O)O)/C#N |
| 220 | OC(=O)CN1C(=S)S/C(=C\c2ccc(s2)c2ccc(cc2)N(c2ccc(cc2)n2c3ccc(cc3c3e2ccc(e3)C(C)(C)C)C([CH2])(C)C)[C]/(C=C\C(=[CH])n2c3ccc(cc3c3e2ccc(e3)C(C)(C)C)C(C)(C)C)[CH])/C1=O.[H]         |
| 221 | CCCCCN1C(=[N]=C([C]1c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)c1cccc1n2CCC[CH]CC.[H]   |
| 222 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)C1=[N]=C([C](N1CCCC)C)ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N                             |
| 223 | CCCC[C@@H](Cn1c2cc3c(cc2c2c1ccc(c2)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1c(n3C[C@@H](CCCC)CC)ccc(c1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)CC                                      |
| 224 | CCN1/C(=C\C[C]2C(=C(C2=O)c2ccc(s2)n2c3cccc3c3e2cccc3)O)/Cc2c1ccc(c2)C(=O)O  |
| 225 | CCN1/C(=C\C[C]2C(=C(C2=O)c2ccc(s2)n2c3ccc(cc3c3e2ccc(e3)C(C)(C)C)C(C)(C)C)O)/Cc2c1ccc(c2)C(=O)O   |
| 226 | N#C/C(=C/c1ccc(s1)[C]1SC=C(N1)c1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O  |
| 227 | N#C/C(=C/c1ccc(s1)[C]1SC=C(N1)c1ccc(cc1)c1ccc2c(c1)n(c1cccc1)c1c2cccc1)/C(=O)O  |
| 228 | CCCCn1c2cccc2c2c1cc(cc2)c1ccc(cc1)C1=CS[C](N1)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 229 | CCOc1ccc(cc1)c1ccc2c(c1)c1cc(ccc1n2c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC   |
| 230 | CCCCCOc1ccc(cc1)c1ccc2c(c1)c1cc(ccc1n2c1ccc2-c3c(C(c2c1)(C)C)cc(s3)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OCCCCC  |
| 231 | COc1cc(OC)ccc1c1ccc2c(c1)c1cc(ccc1n2c1ccc2-c3c(C(c2c1)(C)C)cc(s3)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1OC)OC  |
| 232 | CCCCCn1c2ccc(cc2c2c1ccc(c2)c1ccc(o1)/C=C(\C(=O)O)/C#N)c1ccc(o1)/C=C(\C(=O)O)/C#N  |
| 233 | CCCCCn1c2ccc(cc2c2c1ccc(c2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 234 | CCCCCn1c2ccc(cc2c2c1ccc(c2)c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)/C=C(\C(=O)O)/C#N  |
| 235 | CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1)/C=C(\C(=O)O)/C#N   |
| 236 | CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(c(c1)F)/C=C(\C(=O)O)/C#N  |
| 237 | CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(cc1F)/C=C(\C(=O)O)/C#N  |
| 238 | CCCCCn1c2ccc(cc2c2c1cccc2)c1ccc(c(c1F)F)/C=C(\C(=O)O)/C#N   |
| 239 | CCCCn1c2ccc(cc2c2c1ccc(c2)/C=C/1\SC(=O)NC1=O)/C=C/1\SC(=O)NC1=O   |
| 240 | CCCCn1c2ccc(cc2c2c1ccc(c2)C=C1C(=O)NC(=O)NC1=O)C=C1C(=O)NC(=O)NC1=O   |
| 241 | CCCCn1c2ccc(cc2c2c1cccc2)C=C1C(=O)NC(=O)NC1=O   |
| 242 | CCCCCn1c2ccc(cc2c2c1cccc2)C=C1C(=O)NC(=O)NC1=O  |
| 243 | CCCCCc1cc(sc1c1ccc(cc1)N(c1ccc2c(c1)c1cccc1n2c1cccc1)c1ccc2c(c1)c1cccc1n2c1cccc1)c1sc(cc1CCCCC)/C=C(\C(=O)O)/C#N  |

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| 244 | CCCCCc1ccc(sc1c1ccc(cc1)N(c1ccc2c(c1)c1ccccc1n2c1ccccc1)c1ccc2c(c1)c1ccccc1n2c1ccccc1)/C=C(\C(=O)O)/C#N                          |
| 245 | N#C/C(=C\c1ccc(cc1)N(c1ccccc1)CCCCCN1c2ccccc2Sc2c1ccc(c2)/C=C(/c1ccc(s1)/C=C(/C(=O)O)\C#N)\C#N)/c1ccc(s1)/C=C(/C(=O)O)\C#N       |
| 246 | N#C/C(=C\c1ccc(cc1)N(c1ccccc1)CCCCCN1c2ccccc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)/C(=O)O   |
| 247 | CCCN1c2ccc(cc2Sc2c1ccccc2)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 248 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccccc2)/C=C(/C(=O)O)\C#N)CC  |
| 249 | N#C/C(=C\c1ccc2c(c1)Oc1c(N2CCCCCN2c3ccccc3Oc3c2ccc(c3)/C=C(/C(=O)O)\C#N)ccccc1)/C(=O)O   |
| 250 | O=C1OC(=O)/C(=C/c2ccc(cc2)N(c2ccc(cc2)N2c3ccccc3Sc3c2ccccc3)c2ccc(cc2)N2c3ccccc3Sc3c2ccccc3)/SC(=S)NC1                           |
| 251 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)OC[C@H](CCCC)CC)c1ccc(s1)[C@@H]1[C@H](O)/C(=C/[C@@H]2N(CCCCCC)c3c(C2(C)C)cc(cc3)C(=O)O)/C1=O         |
| 252 | CCCN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(cc1OCCCC)OCCCC)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 253 | CCCCCN1C(=C2C(=C(N(C2=O)CCCC)C2ccc(cc2)c2ccc(cc2)/C=C(/C(=O)O)\C#N)C1=O)c1ccc(cc1)c1ccc2c(c1)Sc1c(N2CCCC)ccccc1                  |
| 254 | COc1ccc(cc1)N1c2ccc(cc2Sc2c1ccc(c2)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)OC)ccc(c1)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)OC)ccccc1 |
| 255 | COc1ccc(cc1)N1c2ccc(cc2Sc2c1ccccc2)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)OC)ccc(c1)/C=C(/C(=O)O)\C#N                                       |
| 256 | CCCCCOc1ccc(cc1)N1c2ccccc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N  |
| 257 | CN1c2ccc(cc2Sc2c1ccc(c2)c1ccc2c(c1)Sc1c(N2C)ccc(c1)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)Sc1c(N2C)ccccc1                                  |
| 258 | CCCCCN1c2ccc(cc2Sc2c1ccccc2)c1ccc2c(c1)Sc1c(N2CCCC)ccc(c1)/C=C(/C(=O)O)\C#N  |
| 259 | CN1c2ccc(cc2Sc2c1ccc(c2)/C=C\1/SC(=S)NCC(=O)OC1=O)/C=C/1\SC(=S)NCC(=O)OC1=O  |
| 260 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccccc2)/C=C\1/SC(=S)N(C1=O)CC(=O)O)CC  |
| 261 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)/C=C(/C(=O)O)\C#N)CC  |
| 262 | CCCCCCCCCCCC[C@H](CN1c2ccc(cc2Sc2c1ccc(c2)N1CCCC1)/C=C/1\SC(=S)N(C1=O)CC(=O)O)CCCCCCCC   |
| 263 | CC(CN1c2ccc(cc2Sc2c1ccc(c2)n1c2ccccc2c2c1ccccc2)/C=C/1\SC(=S)N(C1=O)CC(=O)O)C  |
| 264 | CC(CN1c2ccc(cc2Sc2c1ccc(c2)N1c2ccccc2Sc2c1ccccc2)/C=C\1/SC(=S)N(C1=O)CC(=O)O)C   |
| 265 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C/1\SC(=S)NCC(=O)OC1=O)c1ccc2c(c1)Sc1c(N2CCCC)ccccc1  |
| 266 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(cc1)C)/C=C/1\SC(=S)N(C1=O)CC(=O)O  |
| 267 | CCCCCCCCCCCC[C@H](CN1c2ccc(cc2Sc2c1ccc(c2)C#N)/C=C/1\SC(=S)NCC(=O)OC1=O)CCCCCCCC   |

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| 268 | CCCCCCCCCCCC[C@H](CN1c2ccc(cc2Sc2c1ccc(e2)/C=C/1\SC(=S)N(C1=O)CC(=O)O)Br)CCCCCCCC  |
| 269 | CCCCCCCCCCCC[C@H](CN1c2ccccc2Sc2c1ccc(e2)/C=C/1\SC(=S)N(C1=O)CC(=O)O)CCCCCCCC  |
| 270 | CCSc1cc2c(cc1/C=C(/C(=O)O)\C#N)Sc1c(N2c2ccc(cc2)OC)cccc1   |
| 271 | CCCN1c2cc(SCC)c(cc2Sc2c1cccc2)/C=C(\C(=O)O)/C#N  |
| 272 | COc1ccc(cc1)N1c2ccc(cc2Sc2c1cccc2)/C=C(/C(=O)O)\C#N  |
| 273 | CCCN1c2ccc(cc2Sc2c1cccc2)/C=C(\C(=O)O)/C#N   |
| 274 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(CCC)CCC)cccc3)c1ccc2-c3c(C(c2c1)(CCC)CCC)cccc3                  |
| 275 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)N(c1ccc(cc1)C(c1cccc1)(C)C)c1ccc(cc1)C(c1cccc1)(C)C  |
| 276 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)c1cccc1n2CCCCC  |
| 277 | CCCCCN1c2ccc(cc2Sc2c1cccc2)/C=C(/C(=O)O)\C#N   |
| 278 | Cc1ccc(cc1)N1c2ccc(cc2Sc2c1ccc(e2)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N                                    |
| 279 | CCCCCc1ccc(cc1)N1c2ccc(cc2Sc2c1ccc(e2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 280 | N#C/C(=C)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N1c2ccccc2Sc2c1cccc2)/C(=O)O   |
| 281 | CCN1c2ccc(cc2Sc2c1cccc2)/C=C/c1sc(e2c1OCCO2)/C=C(/C(=O)O)\C#N  |
| 282 | CCCCCCCN1c2ccc(cc2Sc2c1cccc2)/C=C/c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 283 | CCCCCCCN1c2ccc(cc2Sc2c1cccc2)/C=C/c1sc(cc1/C=C/c1ccc2c(c1)Sc1c(N2CCCCCCC)cccc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N                           |
| 284 | CC1(C)c2cc(ccc2-c2c1cc(cc2)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)N1c2ccccc2Sc2c1ccc(e2)[CH]C1=c2c(=C3[C]1C=CC=C3)cccc2                         |
| 285 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)c1sc(cc1CCCCC)C1=C[CH]N(C=C1)C(=O)O)c1ccc(cc1OCCCCC)OCCCCC   |
| 286 | CCCCCc1cc(se1c1ccc2c(c1)Sc1c(N2CCCCC)cccc1)C1=C[CH]N(C=C1)C(=O)O   |
| 287 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)OC[C@H](CCCC)CC)c1ccc(s1)[C@@H]1[C@H](O)/C(=C/[C@@H]2N(CCCCCC)c3c(C2(C)C)cc(cc3)c2ccc(s2)/C=C(/C(=O)O)\C#N)/C1=O |
| 288 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)OC[C@H](CCCC)CC)c1sc2c(c1)sc(c2)[C@@H]1[C@H](O)/C(=C/[C@@H]2N(CCCCCC)c3c(C2(C)C)cc(cc3)C(=O)O)/C1=O              |
| 289 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)OC[C@H](CCCC)CC)c1ccc(s1)c1ccc(s1)[C@@H]1[C@H](O)/C(=C/[C@@H]2N(CCCCCC)c3c(C2(C)C)cc(cc3)C(=O)O)/C1=O            |
| 290 | N#C/C(=C)c1ccc2c(c1)Sc1c(N2Cc2ccc(cc2)CN2c3ccccc3Sc3c2ccc(e3)/C=C(/C(=O)O)\C#N)cccc1)/C(=O)O   |
| 291 | N#C/C(=C)c1ccc2c(c1)Sc1c(N2CCCN2c3ccccc3Sc3c2ccc(e3)/C=C(/C(=O)O)\C#N)cccc1)/C(=O)O  |
| 292 | CCCCCN1C(=C2C(=C(N(C2=O)CCCCC)c2ccc(cc2)/C=C(/C(=O)O)\C#N)C1=O)c1ccc(cc1)c1ccc2c(c1)Sc1c(N2CCCCC)cccc1                                       |

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| 293 | CCCCCN1C(=C2C(=C(N(C2=O)CCCCC)c2ccc3c(c2)Sc2c(N3CCCCC)cccc2)C1=O)c1ccc(cc1)c1ccc(cc1)/C=C(/C(=O)O)\C#N                      |
| 294 | c1cc2c(cc1)Sc1c(cc(cc1)c1cc3c(cc1)c1c(c(c3C3OCCO3)C3OCCO3)cc(cc1)c1ccc(s1)/C=C(\C#N)/C(=O)O)N2C                             |
| 295 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)[CH]C1=C(N/C(=C(\C(=O)O)/C#N)/S1)c1cccc1)c1ccc(cc1OCCCCC)OCCCCC                                 |
| 296 | N#C/C(=C/c1ccc(cc1)N(c1ccc(cc1)N1c2cccc2Sc2c1cccc2)c1ccc(cc1)N1c2cccc2Sc2c1cccc2)/C(=O)O                                    |
| 297 | CN1c2ccc(cc2Sc2c1ccc(c2)/C=C/C1=C[CH]N(C=C1)CC(=O)O)c1ccc(cc1OC)OC.[H]  |
| 298 | CCCCCOc1cc(OCCCCC)ccc1c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(\C(=O)O)/C#N  |
| 299 | COc1cc(OC)ccc1c1ccc2c(c1)Sc1c(N2C)ccc(c1)[CH]/C=C(/N(C)c2c(C1(C)C)cc(cc2)C(=O)O)  |
| 300 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(s1)c1cc(c(s1)/C=C(/C(=O)O)\C#N)CCCCC)c1ccc(s1)c1cc(c(s1)/C=C(\C(=O)O)/C#N)CCCCC)CC |
| 301 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccc(c2)c1cc(c(s1)/C=C(/C(=O)O)\C#N)CCCCC)c1cc(c(s1)/C=C(\C(=O)O)/C#N)CCCCC)CC                   |
| 302 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)/C=C(\C(=O)O)/C#N)CC                                 |
| 303 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1cccc2)c1ccc(s1)/C=C(\C(=O)O)/C#N)CC   |
| 304 | CCCCCCCCOc1ccc(cc1)c1ccc2c(c1)Sc1c(N2CC)ccc(c1)/C=C(/C(=O)O)\C#N  |
| 305 | CCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)O  |
| 306 | CCCCCCCCOc1ccc(cc1)N1c2ccc(cc2Sc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1cc(c(s1)/C=C(/C(=O)O)\C#N                            |
| 307 | CCCCCCCCOc1ccc(cc1)N1c2ccc(cc2Sc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1cccs1  |
| 308 | CCCCCCCCOc1ccc(cc1)N1c2cccc2Sc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 309 | N#C/C(=C/c1ccc2c(c1)c1cccc1n2CCCCCc1ccc(c(c1)Nc1cccc1)/C=C(/C(=O)O)\C#N)/C(=O)O   |
| 310 | CCCCN1c2ccc(cc2Sc2c1cc(SC)cc2)/C=C(/C(=O)O)\C#N   |
| 311 | CCCCN1c2ccc(cc2Sc2c1cc(SC)cc2)/C=C/c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 312 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC                             |
| 313 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1                                       |
| 314 | CN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C=C(c1cccc1)c1cccc1  |
| 315 | N#C/C(=C/c1ccc2c(c1)Sc1c(N2C)ccc(c1)c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O  |
| 316 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1  |
| 317 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1                                   |

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| 318 | CCCCCN1e2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1   |
| 319 | N#C/C(=C\c1ccc2c(c1)Sc1c(N2c2ccc(cc2)C(e2ccc(cc2)C)c2ccc(cc2)C)ccc(c1)c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O                                |
| 320 | N#C/C(=C\c1ccc(s1)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)N(e2ccc(cc2)C)e2ccc(cc2)C)ccc(c1)c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O                       |
| 321 | N#C/C(=C\c1ccc2c(c1)Sc1c(N2c2ccc(cc2)N(e2ccc(cc2)C)e2ccc(cc2)C)ccc(c1)c1ccc(s1)c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O                       |
| 322 | CCCCCN1e2ccc(cc2Sc2c1cccc2)/C=C(/C(=O)O)\C#N  |
| 323 | CCCCCOc1ccc(cc1)c1ccc2c(c1)Sc1c(N2CC)ccc(c1)/C=C(/C(=O)O)\C#N   |
| 324 | CCCCCOc1ccc(cc1)c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(/C(=O)O)\C#N  |
| 325 | CCCCCCCCN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCCC   |
| 326 | CCCCCCCCN1[C@H]2CC=C(C=C2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)c1ccc2-c3c(C(c2c1)(CCCCC)CCCC)cc(cc3)c1ccc2c(c1)N(CCCCCC)c1c(S2)cc(cc1)/C=C(/C(=O)O)\C#N |
| 327 | CN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OC  |
| 328 | CCCCCN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)c1cccc1n2CCCCC   |
| 329 | CCCCCN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc2c(-c3cccc3C2(CCCCC)CCCC)c1  |
| 330 | CCCCCN1e2cccc2c2c1cc(cc2)N1c2cccc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N   |
| 331 | CCCCCC1(CCCCC)c2cc(ccc2-c2c1cccc2)N1c2cccc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N  |
| 332 | CCCCCN1e2ccc(cc2Sc2c1cccc2)/C=C(\C(=O)O)/C#N  |
| 333 | CN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C=C(c1ccc(cc1)N1c2cccc2Sc2c1cccc2)c1ccc(cc1)N1c2cccc2Sc2c1cccc2                             |
| 334 | CN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C=C(c1ccc(cc1)n1c2cccc2c2c1ccc2)c1ccc(cc1)n1c2cccc2c2c1ccc2                                 |
| 335 | Cn1c2ccc(cc2c2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)/C=C(\C1=CC=C(C=[C]1)N1c2cccc2Sc2c1cccc2)/c1ccc(cc1)N1c2cccc2Sc2c1cccc2                      |
| 336 | CCCCCN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C(=C(c1cccc1)c1cccc1)c1cccc1  |
| 337 | CCCCCN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C=C(c1cccc1)c1cccc1   |
| 338 | CCCCCN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)/C=C/c1cccc1  |
| 339 | CCCCCN1e2ccc(cc2Oc2c1cccc2)/C=C(/C(=O)O)\C#N  |
| 340 | CN1e2ccc(cc2Sc2c1ccc(e2)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C=C/c1ccc2c(c1)Sc1c(N2C)ccc(c1)/C=C(/C(=O)O)\C#N                                      |
| 341 | CCCCCN1e2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 342 | CN1e2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc2-c3c(C(c2c1)(C)C)cc(cc3)c1ccc(s1)c1ccc2c(c1)N(C)c1c(S2)cc(cc1)/C=C(\C(=O)O)/C#N        |
| 343 | CCCCCCCCN1e2ccc(cc2Sc2c1ccc(e2)/C=C\1/SC(=S)N(C1=O)CC(=O)O)C#Cc1ccc2c3  |

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|     | c1ccc1c3c(cc2)ccc1  |
| 344 | CCCCC1sc(e2c1OCCO2)c1sc(e2c1OCCO2)c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(/C(=O)O)\C#N  |
| 345 | CCCCC1sc(e2c1OCCO2)c1ccc(s1)c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(/C(=O)O)\C#N  |
| 346 | CCCCC1ccc(s1)c1ccc(s1)c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(/C(=O)O)\C#N  |
| 347 | CCCCC1sc(e2c1OCCO2)c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(/C(=O)O)\C#N   |
| 348 | CCCCC1ccc(s1)c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(/C(=O)O)\C#N   |
| 349 | COc1ccc(cc1)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)OC)ccc(c1)/C=C(/C(=O)O)\C#N   |
| 350 | COc1ccc(cc1)N1c2cccc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N  |
| 351 | CCCCCCCOC1ccc(cc1)N1c2cccc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N  |
| 352 | COc1ccc(cc1)N1c2ccc(cc2Sc2c1ccc2)/C=C(/C(=O)O)\C#N  |
| 353 | N#C/C(=C\c1ccc(o1)c1ccc(cc1)N(c1ccc(cc1)N1c2cccc2Sc2c1ccc2)c1ccc(cc1)N1c2ccc2Sc2c1ccc2)/C(=O)O                            |
| 354 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)N1c2cccc2Sc2c1ccc2)c1ccc(cc1)N1c2ccc2Sc2c1ccc2)/C(=O)O                            |
| 355 | N#C/C(=C\c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)N1c2cccc2Sc2c1ccc2)c1ccc(cc1)N1c2ccc2Sc2c1ccc2)/C(=O)O                           |
| 356 | CCN1c2ccc(cc2Sc2c1ccc2)/C=C(/C(=O)O)\C#N  |
| 357 | CC(CCOc1ccc(cc1)N1c2ccc(cc2Sc2c1ccc2)/C=C/C1=[N]=c2cc(ccc2=[N]=C1/C=C/c1ccc2c(c1)Sc1c(N2c2ccc(cc2)OCCC(C)C)ccc1)/C(=O)O)C |
| 358 | CCCCN1c2ccc(cc2Sc2c1ccc2)c1sc(e2c1OCCO2)/C=C(/C(=O)O)\C#N   |
| 359 | CCCCN1c2ccc(cc2Sc2c1ccc2)c1ccc(o1)/C=C(/C(=O)O)\C#N   |
| 360 | CCCCN1c2ccc(cc2Sc2c1ccc2)/C=C(/C(=O)O)\C#N  |
| 361 | N#C/C(=C\c1ccc(cc1)N1c2cccc2Sc2c1ccc2)/C(=O)O   |
| 362 | COCCOCCOCCN1c2cccc2Sc2c1ccc(c2)/C=C(\C(=O)O)/C#N  |
| 363 | OCCN1c2ccc(cc2Sc2c1ccc2)/C=C(/C(=O)O)\C#N   |
| 364 | N#C/C(=C\c1ccc2c(c1)Sc1c(N2C)ccc1)/C(=O)O   |
| 365 | CCCCCN(c1cccc1)c1ccc(cc1)/C=C(/c1ccc(s1)/C=C(/C(=O)O)\C#N)\C#N  |
| 366 | CN1c2ccc(cc2S(=O)(=O)c2c1ccc(c2)c1csc2c1sc(c2)[C@@H](C(=O)O)C#N)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC                     |
| 367 | CCCCCN1c2ccc(cc2S(=O)(=O)c2c1ccc(c2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC              |
| 368 | CCCCCN1c2ccc(cc2S(=O)(=O)c2c1ccc(c2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1                       |
| 369 | CCCCCN1c2ccc(cc2S(=O)(=O)c2c1ccc(c2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1cccc1)c1cccc1                                |
| 370 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)N(c1cccc1)c1cccc1)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 371 | Cn1c2cc(sc2c2c1c1c(e3c2nsn3)c2c(n1C)cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc2c(c1)Sc1c(N2C)ccc1                             |
| 372 | CCCCCN1c2cc(sc2c2c1c1n(CCCCC)c3c(e1c1c2nsn1)sc(c3)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)Sc1c(N2CCCCC)ccc1                 |



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| 373 | <chem>Cn1c2cc(sc2c2c1c1c(c3c2nsn3)c2c(n1C)cc(s2)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)Sc1c(N2C)cccc1</chem>   |
| 374 | <chem>CCCCCCCCCCCC1(CCCCCCCCCCCC)c2cc(sc2-c2c1cc(s2)c1ccc2c(c1)Sc1c(N2CCCC)cccc1)/C=C(/C(=O)O)\C#N</chem>  |
| 375 | <chem>N#C/C(=C/c1ccc(s1)/C=C\c1ccc2c(c1)Sc1c(N2)cc(cc1)SC)/C(=O)O</chem>   |
| 376 | <chem>CCCCCc1ccc(s1)c1ccc(s1)c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(/C(=O)O)\C#N</chem>   |
| 377 | <chem>CCCCCc1ccc(s1)c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(\C(=O)O)/C#N</chem>  |
| 378 | <chem>CCCCN1c2ccc(cc2Sc2c1ccc(e2)c1ccc(cc1OCCCC)OCCCC)c1ccc(e2c1nsn2)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 379 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)N(c1ccc2c(c1)c1cccc1n2CCCC)ccc(c1)/C=C(/C(=O)O)\C#N</chem>   |
| 380 | <chem>c1cc2c(cc1/C=C(/C(=O)O)\C#N)Sc1c(cccc1)N2CCCCCN1c2cccc2Sc2c1ccc(e2)/C=C(/C(=O)O)</chem>  |
| 381 | <chem>N#C/C(=C\c1ccc2c(c1)Sc1c(N2CCCCO)c2ccc(cc2)[C@@](c2ccc(cc2)OCCCCCN2c3cccc3Se3c2ccc(c3)/C=C(\C(=O)O)/C#N)(c2ccc(cc2)OCCCCCN2c3cccc3Se3c2ccc(c3)/C=C(/C(=O)O)\C#N)C)cccc1)/C(=O)O</chem> |
| 382 | <chem>CCCCCCCCN1c2cccc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N</chem>  |
| 383 | <chem>CCCCCOc1c2cc(ccc2c(e2c1ccc(e2)/C=C(/C(=O)O)\C#N)OCCCCC)N(c1ccc2c(c1)Sc1c(N2CCCCC)cccc1)c1cccc1</chem>  |
| 384 | <chem>CCCCCOc1c2cc(ccc2c(e2c1ccc(e2)c1ccc(s1)/C=C(/C(=O)O)\C#N)OCCCCC)N(c1ccc2c(c1)Sc1c(N2CCCCC)cccc1)c1cccc1</chem>   |
| 385 | <chem>CCCCCOc1c2cc(ccc2c(e2c1cccc2)OCCCCC)N(c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(/C(=O)O)\C#N)c1cccc1</chem>  |
| 386 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(e2)c1ccc(s1)/C=C(\C(=O)O)/C#N)N(c1ccc2c(c1)c(OCCCC)ccc1)c1cccc1</chem>  |
| 387 | <chem>CCCCCOc1c2cc(ccc2c(e2c1cccc2)OCCCCC)N(c1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(\C(=O)O)/C#N)c1cccc1</chem>  |
| 388 | <chem>CCCN1c2ccc(cc2Sc2c1ccc(e2)C1=[N]=C2C(=C[CH]C=C2)N1c1cccc1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 389 | <chem>CCCN1c2ccc(cc2Sc2c1ccc(e2)C1=[N]=C2[C](N1c1cccc1)C=CC=C2)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 390 | <chem>CCCN1c2ccc(cc2Sc2c1ccc(e2)C1=[N]=C2C(=C[CH]C=C2)N1c1cccc1)c1ccc(cc1)/C=C(\C(=O)O)/C#N</chem>   |
| 391 | <chem>CCCN1c2ccc(cc2Sc2c1ccc(e2)C1=[N]=C2[C](N1c1cccc1)C=CC=C2)c1ccc(s1)c1ccc(cc1)/C=C(\C(=O)O)/C#N</chem>   |
| 392 | <chem>CCCN1c2ccc(cc2Sc2c1cccc2)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>  |
| 393 | <chem>CCCN1c2ccc(cc2Sc2c1cccc2)/C=C/c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 394 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(e2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1cccc1)c1cccc1</chem>  |
| 395 | <chem>CCCCCOc1ccc(cc1)N(c1ccc2c(c1)c1cccc1n2CCCCC)ccc(c1)/C=C(/C(=O)O)\C#N</chem>  |
| 396 | <chem>CCCCCN1c2ccc(cc2S(=O)(=O)c2c1ccc(e2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1</chem>   |

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| 397 | CCCCCN1c2ccc(cc2S(=O)(=O)c2c1ccc(e2)c1sc2c(c1)sc(e2)/C=C(/C(=O)O)\C#N)c1c<br>cc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC   |
| 398 | CCCCCN1c2ccc(cc2Sc2c1cccc2)/C=C\c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)<br>O)\C#N)c1cccc1  |
| 399 | CCCCCN1c2ccc(cc2Sc2c1cccc2)/C=C\c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)/C#N   |
| 400 | CCN1c2ccc(cc2Sc2c1cccc2)/C=C/C(=O)O   |
| 401 | CCN1c2ccc(cc2Sc2c1cccc2)/C=C(/C(=O)O)\C#N   |
| 402 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C\1/SC(=S)N(C1=O)CC(=O)O)n1c2ccc(cc2c2c1<br>ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)<br>C(C)(C)C |
| 403 | CCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C\1/SC(=S)N(C1=O)CC(=O)O)n1c2ccc(cc2c2c1ccc<br>(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C)C(<br>C)(C)C   |
| 404 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C)/C=C/<br>1\SC(=S)NCC(=O)OC1=O   |
| 405 | CCCN1c2ccc(cc2Sc2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C)/C=C/1\S<br>C(=S)N(C1=O)CC(=O)O   |
| 406 | CCCCCCCc1cc(sc1c1ccc(s1)c1sc(cc1CCCCCCC)/C=C(/C(=O)O)\C#N)c1cc2cc(n3-<br>c4c(Sc(e23)c1cccc4)c1ccc(cc1)OCCCCC  |
| 407 | CC1(C)c2cc(ccc2-c2c1cccc2)N1c2ccc(cc2Sc2c1ccc(e2)c1ccc2-c3c(C(c2c1)(C)C)cccc3)<br>c1ccc(s1)C#Cc1cc(cc(c1)[C]1C=CC=[N]=C1)[C]1C=CC=[N]=C1                            |
| 408 | OC(=O)c1cccc(c1)c1cc(C#Cc2ccc(s2)c2ccc3c(e2)Sc2c(N3[C]3[C]4[CH]C5=C([C]34)C<br>(C)(C)e3c5cccc3)ccc(e2)c2ccc3-c4c(C(c3c2)(C)C)cccc4)cc(c1)c1ccc(c1)C(=O)O            |
| 409 | OC(=O)c1ccc(cc1)C#Cc1ccc(s1)c1ccc2c(c1)Sc1c(N2c2ccc3-c4c(C(c3c2)(C)C)cccc4)cc<br>c(c1)c1ccc2-c3c(C(c2c1)(C)C)cccc3  |
| 410 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C)c1c<br>cc(s1)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N  |
| 411 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C)c1c<br>cc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 412 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C)c1c<br>cc(cc1)/C=C(/C(=O)O)\C#N  |
| 413 | CCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)N(c1ccc2c(c1)c1cccc1n2CC<br>CCCC)c1ccc2c(c1)sc2   |
| 414 | CCCCCOc1ccc(cc1)c1cc2c3n1-c1cccc1Sc3cc(e2)c1ccc(o1)/C=C(/C(=O)O)\C#N  |
| 415 | COc1ccc(cc1)c1cc2c3n1-c1cccc1Sc3cc(e2)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 416 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(C)C)cc(cc3)N1c2cccc2Sc2c1cccc2/<br>C(=O)O   |
| 417 | CCCC1(CCCC)c2cc(ccc2-c2c1cc(cc2)c1ccc(s1)/C=C(/C(=O)O)\C#N)N1c2cccc2Sc2<br>c1ccc(e2)[CH]C1=c2c(=C3C1=CC=C[CH]3)cccc2  |
| 418 | CCCCCOc1ccc(cc1)c1ccc2c(c1)Sc1c(N2CCCC)ccc(c1)c1ccc(cc1)C1=C2C(=C(N(<br>C2=O)CCCC)c2ccc(cc2)C#Cc2sc(c(e2)CCCC)/C=C(/C(=O)O)\C#N)C(=O)N1CC<br>CCCC                   |
| 419 | CCCC[C@H]1c2c(C)c(c(n2[B])(N2C(=C([C]([C@H]12)C)c1ccc2c(c1)Sc1c(N2CCC)c   |

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|     | <chem>ccc1C(F)F)C)c1ccc(o1)/C=C/1\SC(=S)N(C1=O)CC(=O)O</chem>   |
| 420 | <chem>CCCC[C@@H]1c2c(C)c(c(n2[B](N2C(=C([C]([C@H]12)C)c1ccc2c(c1)Sc1c(N2CCC)cccc1C)(F)F)C)c1ccc(o1)/C=C(\C(=O)O)/C#N</chem>   |
| 421 | <chem>CCCC[C@H]1c2c(C)c(c(n2[B](N2C(=C([C]([C@H]12)C)c1ccc2c(c1)Sc1c(N2CCC)ccc1C)(F)F)C)c1ccc(s1)/C=C\1/SC(=S)N(C1=O)CC(=O)O</chem>   |
| 422 | <chem>CCCC[C@@H]1c2c(C)c(c(n2[B](N2C(=C([C]([C@H]12)C)c1ccc2c(c1)Sc1c(N2CCC)cccc1C)(F)F)C)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>   |
| 423 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(e2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 424 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc2)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 425 | <chem>CN1c2ccc(cc2Sc2c1ccc(e2)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OC)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OC</chem>                        |
| 426 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)C#Cc1ccc(cc1)C#Cc1ccc2c(c1)Sc1c(N2CCCCC)ccc(c1)/C=C(\C(=O)O)/C#N</chem>   |
| 427 | <chem>CCCCn1c2cc(C#Cc3ccc4c(c3)Sc3e(N4CCCC)ccc(c3)/C=C(\C(=O)O)/C#N)ccc2c2c1cc(C#Cc1ccc3c(c1)Sc1c(N3CCCC)ccc(c1)/C=C(\C(=O)O)/C#N)cc2</chem>  |
| 428 | <chem>CCCC1(CCCC)c2cc(ccc2-c2c1cc(cc2)C#Cc1ccc2c(c1)Sc1c(N2CCCC)ccc(c1)/C=C(\C(=O)O)/C#N)C#Cc1ccc2c(c1)Sc1c(N2CCCC)ccc(c1)/C=C(\C(=O)O)/C#N</chem>                                    |
| 429 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)C#Cc1ccc(cc1)c1ccc(cc1)C#Cc1ccc2c(c1)Sc1c(N2CCCC)ccc(c1)/C=C(\C(=O)O)/C#N</chem>  |
| 430 | <chem>C(CCCCCN1c2cccc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)CCCCN1c2cccc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N</chem>   |
| 431 | <chem>N#C/C(=C)c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N1c2cccc2Sc2c1ccc2/C(=O)O</chem>   |
| 432 | <chem>O=C1OC(=O)/C(=C/c2ccc(cc2)N(c2ccc(cc2)N2c3cccc3Sc3c2ccc3)c2ccc(cc2)/C=C/2\SC(=S)NCC(=O)OC2=O)/SC(=S)NC1</chem>  |
| 433 | <chem>CCCCCCCCCCCCN1c2ccc(cc2Sc2c1ccc2)c1ccc(e2c1nsn2)c1ccc2c(c1)Sc1c(N2CCCCCCCC)ccc(c1)/C=C(/C(=O)O)\C#N</chem>  |
| 434 | <chem>CCC(CCCCN1c2ccc(cc2Sc2c1ccc(e2)c1ccc(e2=[N]=C(C(=[N]=e12)c1cccc1)c1cccc1)C1=CC=C(C1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc2c(c1)ccc(e2c1c(OCCCC(CC)C)C)ccc2c1ccc2)OCCCC(CC)CC</chem> |
| 435 | <chem>CCC(CCCCN1c2ccc(cc2Sc2c1ccc(e2)c1ccc(e2=[N]=C(C(=[N]=e12)c1cccc1)c1cccc1)C1=CC=C(C1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc2c(c1)ccc(e2)OCCCC(CC)CC)C</chem>                          |
| 436 | <chem>CCC(CCCCN1c2ccc(cc2Sc2c1ccc(e2)c1ccc(e2=[N]=C(C(=[N]=e12)c1cccc1)c1cccc1)C1=CC=C(C1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OCCCC(CC)CC</chem>  |
| 437 | <chem>CN1c2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)n1c2ccc(cc2c2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C</chem>                              |
| 438 | <chem>CCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)n1c2ccc(cc2c2c1ccc(e2)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C</chem>                            |
| 439 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C</chem>  |
| 440 | <chem>CCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(\C(=O)O)/C#N)n1c2ccc(cc2c2c1ccc(e2)C(C)(C)C(C)(C)C</chem>  |

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| 441 | CCCCCCCCCCCCCN1c2ccc(cc2Sc2c1ccc(e2)/C=C(/C(=O)O)\C#N)c1ccc(e2c1nsn2)c1c<br>cc2c(e1)Sc1c(N2CCCCCCCCCCCC)ccc(e1)/C=C(/C(=O)O)\C#N   |
| 442 | CCCCCSC1=C(SCCCCC)S/C(=C\c2ccc(cc2)c2ccc(cc2)c2ccc3c(e2)N(CCCC)c2c(S3<br>)ccc(e2)/C=C(/C(=O)O)\C#N)/S1   |
| 443 | CCCCCOc1cc(ecc1/C=C\1/SC(=C(S1)SCCCCC)SCCCCC)c1ccc2c(e1)N(CCCC)c<br>1c(S2)ccc(e1)/C=C(/C(=O)O)\C#N   |
| 444 | CCCN1c2cc(ccc2Sc2c1cc(cc2)/C=C(/C(=O)O)\C#N)c1ccc(cc1F)/C=C\1/SC(=C(S1)S<br>CCCCC)SCCCCC   |
| 445 | CCCN1c2cc(ccc2Sc2c1cc(cc2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)/C=C\1/SC(=C(S1)SC<br>CCCC)SCCCCC  |
| 446 | CCCN1c2cc(ccc2Sc2c1cc(cc2)/C=C(/C(=O)O)\C#N)/C=C\1\SC(=C(S1)SCCCCC)S<br>CCCCC  |
| 447 | CCCN1c2cc(ccc2Sc2c1ccc2)/C=C(/C(=O)O)\C#N  |
| 448 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccc(e2)c1ccc(o1)/C=C(/C(=O)O)\C#N)c1ccc2c(e1)<br>c1=[N]=c3cccc3=[N]=c1n2C[C@@H](CCCC)CC)CC   |
| 449 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccc(e2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc2c(e1)<br>c1=[N]=c3cccc3=[N]=c1n2C[C@@H](CCCC)CC)CC   |
| 450 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccc2)c1ccc(s1)/C=C(/C(=O)O)\C#N)CC   |
| 451 | CN1c2ccc(cc2Sc2c1ccc2)/C=C\c1cc(e2ccc(s2)/C=C(\C(=O)O)/C#N)c(cc1/C=C/c1ccc2<br>c(e1)Sc1c(N2C)cccc1)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 452 | CN1c2ccc(cc2Sc2c1ccc2)/C=C/c1cc(c(cc1c1ccc(s1)/C=C(/C(=O)O)\C#N)/C=C/c1ccc2<br>c(e1)Sc1c(N2C)cccc1)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 453 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc2)/C=C\c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#<br>N)c1ccc(cc1)/C=C/c1ccc2c(e1)Sc1c(N2CCCCCCCC)cccc1  |
| 454 | CC(Cc1cc(sc1c1sc2c(e1)c1nonc1c1c2sc(e1)c1sc(cc1CC(C)C)/C=C(/C(=O)O)\C#N)c1cc<br>c2c(e1)Sc1c(N2C)cccc1)C  |
| 455 | CCCC[C@@H]1c2c(C)c(c(n2[B](N2C(=C([C]([C@@H]12)C)c1ccc2c(e1)Sc1c(N2C<br>CC)cccc1)C)(F)F)C)/C=C(\C(=O)O)/C#N  |
| 456 | CCCC[C@H]1c2c(C)c(c(n2[B](N2C(=C([C]([C@@H]12)C)c1ccc2c(e1)Sc1c(N2CCC<br>)ccc(e1)C1=C(N2[C@H]([C]1C)[C@@H](c1n([B]2(F)F)c(c(e1C)c1ccc(o1)/C=C(/C(=O)<br>)O)\C#N)C)CCCC)C)(F)F)C)c1ccc(o1)/C=C(\C(=O)O)/C#N |
| 457 | CCCC[C@H]1c2c(C)c(c(n2[B](N2C(=C([C]([C@@H]12)C)c1ccc2c(e1)Sc1c(N2CCC<br>)ccc(e1)C1=C(N2[C@@H]([C]1C)[C@@H](c1n([B]2(F)F)c(c(e1C)/C=C(/C(=O)O)\C#<br>N)C)CCCC)C)(F)F)C)/C=C(/C(=O)O)\C#N                   |
| 458 | C[C]1c2c(c(c(n2[B](n2c1c(C)c(e2C)c1ccc(s1)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(e1)<br>Sc1c(ccc1)N2CCCCCN1c2cccc2Sc2c1ccc(e2)c1c(C)c2[C](C)c3n([B](n2c1C)(F)F)c<br>(c(c3C)/C=C(/C(=O)O)\C#N)C)C                 |
| 459 | CCCC[C]1c2c(c(c(n2[B](n2c1c(C)c(e2C)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(e1)Sc<br>1c(N2CCCCCN2c3cccc3Sc3c2ccc(e3)c2c(C)c3[C](CCCC)c4n([B](n3c2C)(F)F)c(c(<br>c4C)/C=C(/C(=O)O)\C#N)C)cccc1)C                   |
| 460 | CCCC[C]1c2c(c(c(n2[B](n2c1c(C)c(e2C)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(e1)Sc<br>1c(N2CCCC)cccc1)C  |
| 461 | CCCC[C]1c2c(c(c(n2[B](n2c1c(C)c(e2C)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(e1)Sc<br>1c(N2CCC)cccc1)C   |

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| 462 | N#C/C(=C/c1ccc2c(c1)Sc1c(N2CCCCO)c2ccc(cc2)OCCCCCN2c3cccc3Sc3c2ccc(c3)/C=C(/C(=O)O)\C#N)cccc1)/C(=O)O   |
| 463 | N#C/C(=C/c1ccc2c(c1)Sc1c(N2CCCCO)c2ccc(cc2)OCCCCCN2c3cccc3Sc3c2ccc(c3)/C=C(/C(=O)O)\C#N)cccc1)/C(=O)O   |
| 464 | c1(c(ccc1)OCCCCN1c2cccc2Sc2c1ccc(c2)/C=C(\C(=O)O)/C#N)OCCCCN1c2ccc(cc2Sc2c1cccc2)/C=C(\C(=O)O)/C#N  |
| 465 | CC1(C)c2cc(ccc2-c2c1cccc2)c1ccc2c(c1)Sc1c(N2c2ccc3c(c2)sc2c3sc3c2ccc(c3)c2cc(c(s2)/C=C(\C(=O)O)/C#N)C)ccc(c1)c1ccc2-c3c(C(c2c1)(C)C)cccc3                       |
| 466 | CCCN1c2ccc(cc2Sc2c1cccc2)C1=[N]=C2C(=C(C=C[C]2c2ccc(cc2)/C=C(/C(=O)O)\C#N)c2ccc(cc2)/C=C(/C(=O)O)\C#N)N1CCCC  |
| 467 | CCCN1c2ccc(cc2SC2=[C]C=CC=C12)C1=[N]=C2[C](N1CCCC)[C](C=C[C]2[C]S[C]([CH])[CH])/C=C(/C(=O)O)\C#N)c1ccc(s1)/C=C(/C(=O)O)\C#N.[H]                                 |
| 468 | CCCN1c2ccc(cc2Sc2c1cccc2)C1=[N]=C2[C](N1CCCC)[C](C=C[C]2c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N                                 |
| 469 | CCN1c2ccc(cc2Sc2c1ccc(c2)/C=C\1/SC(=S)N(C1=O)CC(=O)O)/C=C\1/SC(=S)N(C1=O)CC(=O)O  |
| 470 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)c1cc2c(s1)c1c(n2CCCC)ccs1   |
| 471 | COc1ccc(cc1)n1c2cc(sc2c2c1ccs2)c1ccc2c(c1)Sc1c(N2C)ccc(c1)/C=C(/C(=O)O)\C#N   |
| 472 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccc(c2)/C=C\C(=O)O)/C=C/[C]1C=C([C]2C(=O)N(CC)C(=S)N(C2=O)CC)C=C(O1)/C=C\c1ccc2c(c1)Sc1c(N2C[C@@H](CCCC)CC)ccc(c1)/C=C/C(=O)O)CC    |
| 473 | CCCC[C@H](CN1c2ccc(cc2Sc2c1ccc(c2)/C=C/C(=O)O)/C=C\C[C]1C=C([C](C#N)C#N)C=C(O1)/C=C/c1ccc2c(c1)Sc1c(N2C[C@@H](CCCC)CC)ccc(c1)/C=N\C(=O)O)CC                     |
| 474 | CCCCCCCc1cc(sc1c1ccc(s1)c1sc(cc1CCCCCCC)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)Sc1c(N2C[C@@H](CCCC)CC)ccc(c1)c1ccc(cc1)OCCCC  |
| 475 | CCCCCCCc1cc(sc1c1ccc(s1)c1sc(cc1CCCCCCC)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)Sc1c(N2C[C@@H](CCCC)CC)cccc1   |
| 476 | CCCC[C@H](CN1c2ccc(cc2Sc2c1cccc2)c1ccc(s1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)CC  |
| 477 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)/C=C\1\SC(=C(S1)SC)SC   |
| 478 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C\1\SC(=C(S1)SC)SC)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 479 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(\C(=O)O)/C#N)[C]/[NH]=C(\[C]c1ccc(cc1)OC)/c1ccc(cc1)OC.[NH]  |
| 480 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(\C(=O)O)/C#N)C1=[N]=C([C](N1)c1cccc1)c1cccc1   |
| 481 | CCCC[C@@H](CN1c2ccc(cc2Sc2c1ccc(c2)/C=C\C(=O)O)/C=C/[C]1C=C([C]2C(=O)c3c(C2=C(C#N)C#N)cccc3)C=C(O1)/C=C\c1ccc2c(c1)Sc1c(N2C[C@@H](CCCC)CC)ccc(c1)/C=C/C(=O)O)CC |
| 482 | N#C/C(=C\c1ccc2c(c1)Sc1c(N2CCCCCCCCN2c3cccc3Sc3c2ccc(c3)/C=C(/C(=O)O)\C#N)cccc1)/C(=O)O   |
| 483 | CCCN1c2ccc(cc2Sc2c1cccc2)c1ccc(s1)c1cc2c(s1)c1c(n2c2ccc3-c4c(C(c3c2)(CCCC)CCC)cccc4)cc(s1)/C=C(\C(=O)O)/C#N   |

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| 484 | CCCCCOc1cc(OCCCC)ccc1n1c2cc(sc2c2c1ccs2)c1ccc2c(c1)Sc1c(N2CCCCC)cc<br>c(c1)/C=C(/C(=O)O)\C#N  |
| 485 | CCCCCOc1cc(OCCCC)ccc1n1c2cc(sc2c2c1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc2c(c<br>1)Sc1c(N2CCCCC)cccc1  |
| 486 | CCCCCCCCCCCCN1c2ccc(cc2Sc2c1cccc2)c1ccc(c2c1nn(n2)CCCCCCC)c1ccc2c(c1<br>)Sc1c(N2CCCCCCCCCCCC)ccc(c1)/C=C(/C(=O)O)\C#N                                 |
| 487 | CCCCCCCCCCCCN1c2ccc(cc2Sc2c1cccc2)C1=[N]=C([CH]C=C1)c1ccc2c(c1)Sc1c(N<br>2CCCCCCCCCCCC)ccc(c1)/C=C(/C(=O)O)\C#N                                       |
| 488 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)[C]([N@]1[C@@<br>H]2Ce2n([B]1(F)F)c(c1c2cccc1)c1cccc1OC)c1cccc1OC                            |
| 489 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)C#Cc1ccc2c3c1ccc1c3c(cc2)c<br>cc1   |
| 490 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)C#Cc1ccc2c3c1ccc1c3c(cc<br>2)ccc1  |
| 491 | CN1c2ccc(cc2Sc2c1ccc(c2)/C=C\1/SC(=S)N(C1=O)CC(=O)O)C#Cc1ccc2c3c1ccc1c3c(c<br>c2)ccc1   |
| 492 | CCCCCN1c2ccc(cc2Sc2c1ccc(c2)C=C(C#N)C#N)C#Cc1ccc2c3c1ccc1c3c(cc2)ccc1   |
| 493 | CCCCCCCCN1c2ccc(cc2Sc2c1ccc(c2)C=C(C#N)C#N)C#Cc1ccc2c3c1ccc1c3c(cc2)ccc<br>1  |
| 494 | CN1c2ccc(cc2Sc2c1ccc(c2)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(<br>cc1)OC)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC |
| 495 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)/C=C/c1sc2c(c1)n(c1c2sc(c1)/C=C(\C(=O)O)/<br>C#N)c1ccc(cc1)N1c2cccc2Sc2c1cccc2                                   |
| 496 | CCCCN1c2ccc(cc2Sc2c1cccc2)/C=C/c1ccc(cc1)/C=C\1/SC(=S)NCC(=O)OC1=O  |
| 497 | CCCCN1c2ccc(cc2Sc2c1cccc2)/C=C\1/SC(=S)N(C1=O)CC(=O)O   |
| 498 | CCCCN1c2ccc(cc2Sc2c1cccc2)/C=C/c1ccc(cc1)/C=C(/C(=O)O)\C#N  |
| 499 | CCCC[C@@H](COc1ccc(cc1)c1ccc2c(c1)Sc1c(N2[C@H]2CC=C(C=C2)c2ccc(cc2)C(<br>=O)O)ccc(c1)c1ccc(cc1)OC[C@H](CCCC)CC)CC                                     |
| 500 | C(COc1ccc(cc1)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)C(=O)O)ccc(c1)c1ccc(cc1)OCC(C)C)(C<br>)C  |
| 501 | Cc1cc(sc1/C=C(/C(=O)O)\C#N)c1ccc(c2c1nns2)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)N(c2ccc<br>(cc2)C)c2ccc(cc2)C)cccc1   |
| 502 | CCCCCc1cc(sc1/C=C(/C(=O)O)\C#N)c1ccc(c2c1nns2)c1ccc2c(c1)Sc1c(N2[C@H](<br>CCCC)CC)cccc1   |
| 503 | CCCCCc1cc(sc1/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc2c(c1)Sc1c(N2[C@H](CCCC)<br>CC)cccc1   |
| 504 | COc1ccc(cc1)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)OC)ccc(c1)c1ccc(o1)/C=C(/C(=O)O)\C#N  |
| 505 | COc1ccc(cc1)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)OC)ccc(c1)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 506 | OC(=O)/C=C/c1ccc2c(c1)Sc1c(N2CCCCCn2c3ccc(cc3c3c2ccc(c3)C(C)(C)C(C)(C)<br>C)cccc1   |
| 507 | OC(=O)C(=Cc1ccc2c(c1)Sc1c(N2CCCCCn2c3ccc(cc3c3c2ccc(c3)C(C)(C)C(C)(C)<br>C)cccc1)C(=O)O   |
| 508 | CCCCCN1c2ccc(cc2Sc2c1cccc2)n1cc(c2c1cccc2)/C=C(/C(=O)O)\C#N   |

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| 509 | <chem>O=C(O)CN1C(=S)S/C(=C/c2ccc3c(c2)Sc2c(N3CCCCCn3c4ccc(cc4c4c3ccc(c4)C(C)(C)C)C(C)(C)C)cccc2)/C1=O</chem>  |
| 510 | <chem>N#C/C(=C/c1ccc2c(c1)Sc1c(N2CCCCN2c3ccc(cc3c3c2ccc(c3)C(C)(C)C)C(C)(C)C)cccc1)/C(=O)O</chem>   |
| 511 | <chem>CCCCCN1c2ccc(cc2Sc2c1cccc2)/C=C\1/SC(=S)N(C1=O)C(=O)O</chem>  |
| 512 | <chem>CCCCCCCN1c2cccc2c2c1ccc(c2)N1c2cccc2Sc2c1ccc(c2)/C=C\1/SC(=S)N(C1=O)C(=O)O</chem>   |
| 513 | <chem>Cn1c2cccc2c2c1ccc(c2)N1c2cccc2Sc2c1ccc(c2)/C=C\1/SC(=S)NCC(=O)OC1=O</chem>  |
| 514 | <chem>Cn1c2ccc(cc2c2c1cccc2)N1c2ccc(cc2Sc2c1cccc2)/C=C\1/SC(=S)NCC(=O)OC1=O</chem>  |
| 515 | <chem>CCCCCCCN1c2cccc2c2c1ccc(c2)N1c2cccc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N</chem>  |
| 516 | <chem>Cn1c2cccc2c2c1ccc(c2)N1c2cccc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N</chem>  |
| 517 | <chem>N#C/C(=C/c1ccc2c(c1)Sc1c(N2c2ccc3c(c2)c2cccc2n3CC)cccc1)/C(=O)O</chem>  |
| 518 | <chem>COc1ccc(cc1)N1c2ccc(cc2Sc2c1cccc2)/C=C/[C@@H]1C/C(=C(/C(=O)O)\C#N)/CC(C1)(C)C</chem>  |
| 519 | <chem>CCCCCN1c2ccc(cc2Sc2c1cccc2)c1cc(sc1c1sc(c(c1)c1ccc2c(c1)Sc1c(N2CCCCC)cccc1)c1ccc2c(c1)Sc1c(N2CCCCC)cccc1)/C=C(/C(=O)O)\C#N</chem>                               |
| 520 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(cc1)OC)c1ccc(o1)/C=C(/C(=O)O)\C#N</chem>  |
| 521 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1cccc1)c1ccc(o1)/C=C(/C(=O)O)\C#N</chem>   |
| 522 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(cc1)OC)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 523 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1cccc1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 524 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(cc1)OC)c1cc(F)c(c(c1)F)/C=C(/C(=O)O)\C#N</chem>   |
| 525 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1cccc1)c1cc(F)c(c(c1)F)/C=C(/C(=O)O)\C#N</chem>  |
| 526 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(cc1)OC)c1ccc(c(c1)F)/C=C(/C(=O)O)\C#N</chem>  |
| 527 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1cccc1)c1ccc(c(c1)F)/C=C(\C(=O)O)\C#N</chem>   |
| 528 | <chem>CN1c2ccc(cc2Sc2c1ccc(c2)c1ccc(cc1)OC)c1ccc(cc1)/C=C(/C(=O)O)\C#N</chem>   |
| 529 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)c1cccc1)c1ccc(cc1)/C=C(/C(=O)O)\C#N</chem>  |
| 530 | <chem>CCCCCN1c2ccc(cc2Sc2c1ccc(c2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OC</chem>   |
| 531 | <chem>N#C/C(=C/c1ccc(s1)c1ccc2c(c1)Sc1c(N2CC)cccc1)/C(=O)O</chem>   |
| 532 | <chem>N#C/C(=C/c1ccc(s1)c1ccc2c(c1)c1cccc1n2CC)/C(=O)O</chem>   |
| 533 | <chem>N#C/C(=C/c1ccc(s1)c1ccc2c(c1)Sc1c(N2CCCCCN2c3ccc(cc3c3c2cccc3)c2ccc(s2)/C=C(/C(=O)O)\C#N)cccc1)/C(=O)O</chem>   |
| 534 | <chem>N#C/C(=C/c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)/C=C/c1cc2ccc(cc2oc1=O)N(CC)CC)c1ccc(cc1)/C=C/c1cc2ccc(cc2oc1=O)N(CC)CC)/C(=O)O</chem>                         |
| 535 | <chem>N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)/C=C/c1cc2ccc(cc2oc1=O)N(CC)CC)c1ccc(cc1)/C=C/c1cc2ccc(cc2oc1=O)N(CC)CC)/C(=O)O</chem>                                  |
| 536 | <chem>CCN(c1ccc2c(c1)oc(=O)c(c2)/C=C/c1ccc(cc1)N(c1ccc(cc1)/C=C(\C(=O)O)\C#N)c1ccc(cc1)/C=C/c1cc2ccc(cc2oc1=O)N(CC)CC)CC</chem>                                       |
| 537 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc(c2c1OCC(CO2)(CCCC)CCCC)C1=[N]=C2C(=[N])=C(S2)c2sc(c3c2OCC(CO3)(CCCC)CCCC)c2ccc(s2)/C=C(/C(=O)O)\C#N)S1</chem> |
| 538 | <chem>O=C(O)CN1C(=S)S/C(=C/c2ccc(cc2)N(c2ccc(cc2)N2c3cccc3Sc3c2cccc3)c2ccc(cc2)N2c3cccc3Sc3c2cccc3)/C1=O</chem>   |

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| 539 | CCCCCN1e2ccc(cc2S(=O)(=O)c2c1ccc(c2)c1csc2c1sc(c2)[C@@H](C(=O)O)C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC   |
| 540 | CCCCCN1e2ccc(cc2S(=O)(=O)c2c1ccc(c2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC  |
| 541 | CCCCCN1e2ccc(cc2S(=O)(=O)c2c1ccc(c2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 542 | CCCCCN1e2ccc(cc2S(=O)(=O)c2c1ccc(c2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 543 | CCCCCN1e2ccc(cc2Sc2c1ccc(c2)N(c1cccc1)c1cccc1)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 544 | CCCCCN1e2cc(sc2c2c1c1c(c3c2nsn3)c2c(n1CCCCC)cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 545 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1ccc2c(c1)c1cccc1n2CC)/C(=O)O  |
| 546 | N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)c1ccc(cc1n2CC)c1ccc(s1)/C=C(/C(=O)O)\C#N)/C(=O)O                            |
| 547 | CCCCCCCCN1e2ccc(cc2Sc2c1cccc2)/C=C/c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)/C=C/c1ccc2c(c1)Sc1c(N2CCCCCCC)cccc1   |
| 548 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)c1ccc(cc1n2CC)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)/C(=O)O |
| 549 | N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1ccc2c(c1)c1cccc1n2CC)/C(=O)O   |
| 550 | N#C/C(=C/c1en(c2c1cccc2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 551 | CCCCCOc1cc(OCCCCC)cccc1c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCCCCC)OCCCCC)c1ccc(cc1)/C=C/1\SC(=[N]=C1c1cccc1)[C](C(=O)O)C#N   |
| 552 | N#C/C(=C\c1ccc(cc1)N(c1cccc1)c1ccc(cc1)/C=N/c1ccc2c(c1)c1cccc1n2CC)/C(=O)O  |
| 553 | CCCCCN1e2ccc(cc2c2c1ccc(c2)/C=C(/C(=O)O)\C#N)/C=N\c1ccc2c(c1)c1cccc1n2CC  |
| 554 | CCCCCCCCCCCCc1cc(sc1c1sc2c(c1)sc(c2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 555 | CCCCCCCCCCCCc1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 556 | N#C/C(=C\c1ccc(s1)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 557 | N#C/C(=C\c1cc2c(s1)cc(s2)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 558 | CCCCCCCCc1cc(sc1c1cc(c(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)CCCCCCC)c1ccc(c2c1nsn2)c1cc(c(s1)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N)CCCCCCC   |
| 559 | O=C(O)CN1C(=S)S/C(=C\c2ccc(s2)c2sc(c3c2OCCO3)c2ccc(cc2)N(c2cccc2)c2cccc2)/C1=O  |
| 560 | N#C/C(=C\c1ccc(s1)c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 561 | CCCCCCCCc1cc(sc1c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)CCCCC)c1ccc(cc1)CCCCC)c  |



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|     | 1ccc(c2c1nsn2)c1sc(c(c1)CCCCCCC)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 562 | CCCCC[C@@H](C1cc(sc1c1cc2c(s1)c1sc(cc1c1c2non1)c1sc(cc1C[C@H](CCCCC)CCCC)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1)CCCC  |
| 563 | CCCCn1c2cc(ccc2c2c1cc(cc2)c1ccc(s1)c1ccc2n1[B](F)(F)n1c(ccc1[C]2c1ccc(s1)/C=C(/C1=CC=[N]=C[CH]1)\C#N)c1ccc(s1)c1ccc2c(c1)n(CCCC)c1c2ccc(c1)N(c1cccc1)c1cccc1)N(c1cccc1)c1cccc1 |
| 564 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O   |
| 565 | N#C/C(=C\c1cc2c(s1)cc(s2)c1ccc(s1)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O  |
| 566 | N#C/C(=C\c1ccc(cc1)c1ccc(s1)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O  |
| 567 | N#C/C(=C\c1sc(e2c1OCC(CO2)(C)C)c1sc(e2c1OCC(CO2)(C)C)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 568 | CCCCn1c2cc(ccc2c2c1cc(cc2)c1ccc(s1)c1ccc2n1[B](F)(F)n1c(ccc1[C]2c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc2c(c1)n(CCCC)c1c2ccc(c1)N(c1cccc1)c1cccc1)N(c1ccc(cc1)c1cccc1)        |
| 569 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O  |
| 570 | CCCCCSc1ccc(cc1)N(c1ccc(cc1)SCCCCC)c1ccc(cc1)c1sc(e2c1OCC(CO2)(CCCC)CCCC)C1=[N]=C2C(=[N]=C(S2)c2sc(e3c2OCC(CO3)(CCCC)CCCC)c2ccc(s2)/C=C(/C(=O)O)\C#N)S1                        |
| 571 | CCCCCCCCc1cc(sc1c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(e2c1nsn2)c1cc(c(s1)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N)CCCCCCCC  |
| 572 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)c1ccc(c2c1nsn2)c1ccc(s1)/C=C(\C(=O)O)/C#N   |
| 573 | CCCCCc1cc(sc1c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2   |
| 574 | N#C/C(=C\c1ccc(cc1)[C]1C=[N]=C(e2c1nsn2)c1ccc(s1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 575 | N#C/C(=C\c1cc2c(s1)cc(s2)c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O   |
| 576 | N#C/C(=C\c1ccc(s1)c1cc2c(s1)c1c(s2)cc(s1)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O   |
| 577 | N#C/C(=C\c1cc2c(s1)cc(s2)c1cc2c(s1)c1c(s2)cc(s1)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O  |
| 578 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2c(c1)N(c1cccc1)[C@H]1[C@@H]2[C@@H]2CC[C@H]1C2)/C(=O)O   |
| 579 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc2c(c1)N(c1cccc1)[C@H]1[C@@H]2[C@@H]2CC[C@H]1C2)/C(=O)O  |
| 580 | CCCCCc1cc(sc1c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc2c(c1)N(c1cccc1)[C@@H]1[C@H]2[C@H]2CC[C@@H]1C2  |
| 581 | CCCCCc1cc(sc1c1ccc(s1)/C=C/1\SC(=S)N(C1=O)CC(=O)O)c1ccc2c(c1)N(c1cccc1)[C@H]1[C@@H]2[C@@H]2CC[C@H]1C2  |
| 582 | CCCCCCCCCCCCc1cc(sc1c1ccc(s1)/C=C/1\SC(=S)N(C1=O)CC(=O)O)c1ccc2c(c1)N(   |

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|     | c1cccc1)[C@H]1[C@@H]2[C@H]2CC[C@@H]1C2  |
| 583 | N#C/C(=C\c1ccc(s1)c1sc(e2c1OCCO2)c1ccc2c(c1)N(c1cccc1)[C@@H]1[C@H]2[C@H]2CC[C@@H]1C2)/C(=O)O            |
| 584 | N#C/C(=C\c1ccc(s1)c1cc2c(s1)cc(s2)c1ccc2c(c1)N(c1cccc1)[C@H]1[C@@H]2[C@@H]2CC[C@H]1C2)/C(=O)O           |
| 585 | N#C/C(=C/c1cc2c(s1)cc(s2)c1ccc(s1)c1ccc(cc1)N1c2cccc2[C@@H]2[C@H]1[C@H]1CC[C@@H]2C1)/C(=O)O             |
| 586 | N#C/C(=C/c1ccc(cc1)c1ccc(s1)c1ccc(cc1)N1c2cccc2[C@@H]2[C@H]1[C@@H]1CC[C@H]2C1)/C(=O)O                   |
| 587 | O=C1OC(=O)/C(=C/c2ccc(s2)c2ccc(s2)c2ccc(s2)c2ccc(cc2)N2c3cccc3[C@@H]3[C@H]2[C@@H]2CC[C@H]3C2)/SC(=S)NC1 |
| 588 | CCCCC1cc(sc1c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N1c2cccc2[C@@H]2[C@H]1[C@H]1CC[C@@H]2C1                |
| 589 | CCCCC1cc(sc1c1sc2c(c1)sc(c2)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N1c2cccc2[C@H]2[C@@H]1[C@@H]1CC[C@H]2C1         |
| 590 | CCCCC1cc(sc1c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N1c2cccc2[C@@H]2[C@H]1[C@H]1CC[C@@H]2C1               |
| 591 | CCCCC1cc(sc1c1ccc(s1)/C=C/1\SC(=S)N(C1=O)CC(=O)O)c1ccc(cc1)N1c2cccc2[C@H]2[C@@H]1[C@@H]1CC[C@H]2C1      |
| 592 | CCCCCCCCCCCC1cc(sc1c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N1c2cccc2[C@@H]2[C@H]1[C@H]1CC[C@@H]2C1         |
| 593 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O                                  |
| 594 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 595 | N#C/C(=C\c1cc2c(s1)cc(s2)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O                                   |
| 596 | N#C/C(=C\c1ccc(cc1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 597 | N#C/C(=C\c1ccc(cc1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O                                |
| 598 | CCCCC1cc(sc1c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1                                      |
| 599 | CCCCC1cc(sc1c1sc2c(c1)sc(c2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1                               |
| 600 | CCCCC1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)/C=C(/C(=O)O)\C#N                                     |
| 601 | CCCCC1cc(sc1c1ccc(s1)/C=C/1\SC(=S)N(C1=O)CC(=O)O)c1ccc(cc1)N(c1cccc1)c1cccc1                            |
| 602 | CCCCCCCCCCCC1cc(sc1c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1                               |
| 603 | N#C/C(=C\c1ccc(cc1)c1sc(e2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O                                   |
| 604 | N#C/C(=C\c1sc2c(c1)sc(c2)c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O                            |
| 605 | CCCCCCCCCCCC1cc(sc1c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N1c2cccc2[C@@H]2[C@H]1[C@H]1CC[C@@H]2C1        |
| 606 | CCCCCCCCCCCC1cc(sc1c1ccc(s1)/C=C/1\SC(=S)NCC(=O)OC1=O)c1ccc(cc1)N1c2cccc2[C@H]2[C@@H]1[C@@H]1CC[C@H]2C1 |
| 607 | N#C/C(=C\c1ccc(s1)c1sc(e2c1OCCO2)c1ccc(cc1)N1c2cccc2[C@H]2[C@@H]1[C@@H]1CC[C@H]2C1)/C(=O)O              |
| 608 | N#C/C(=C/c1cc2c(s1)cc(s2)c1sc(e2c1OCCO2)c1ccc(cc1)N1c2cccc2[C@@H]2[C@H]1                                |

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|     | <chem>I[C@H]1CC[C@@H]2C1)/C(=O)O</chem>   |
| 609 | <chem>N#C/C(=C\c1ccc(s1)c1cc2c(s1)sc(e2)c1ccc(cc1)N1c2cccc2[C@@H]2[C@H]1[C@@H]1CC[C@H]2C1)/C(=O)O</chem>                          |
| 610 | <chem>N#C/C(=C\c1ccc(cc1)c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 611 | <chem>N#C/C(=C\c1ccc(cc1)c1cc2c(s1)c1c(s2)cc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 612 | <chem>OC(=O)CN1C(=S)S/C(=C\c2ccc(s2)c2ccc(s2)c2ccc(cc2)N(c2ccc3c(c2)OCCO3)c2ccc3c(c2)OCCO3)/C1=O</chem>                           |
| 613 | <chem>N#C/C(=C\c1ccc(cc1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O</chem>                           |
| 614 | <chem>CCCCC1c1cc(sc1c1sc2c(c1)sc(c2)/C=C(/C(=O)O)/C#N)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2</chem>                        |
| 615 | <chem>N#C/C(=C\c1ccc(s1)c1sc2c1sc(c2)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O</chem>                                 |
| 616 | <chem>N#C/C(=C\c1ccc(cc1)c1sc2c(c1)sc(c2)c1ccc(cc1)[N]c1ccc2c(c1)OCCO2)/C(=O)O.S1[C@H]C2=C(C=C1)OCCO2</chem>                      |
| 617 | <chem>N#C/C(=C\c1ccc(cc1)c1sc(c2c1OCCO2)c1ccc2c(c1)N(c1cccc1)[C@H]1[C@@H]2[C@@H]2CC[C@H]1C2)/C(=O)O</chem>                        |
| 618 | <chem>CCCCCCCCCCCCc1cc(sc1c1sc2c(c1)sc(c2)/C=C(/C(=O)O)/C#N)c1ccc(cc1)N1c2cccc2[C@@H]2[C@@H]1[C@@H]1CC[C@H]2C1</chem>             |
| 619 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)c1ccc(c2c1nsn2)/C=C(/C(=O)O)/C#N</chem>                      |
| 620 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)c1ccc(c2c1nsn2)c1ccc(cc1)/C=C(/C(=O)O)/C#N</chem>            |
| 621 | <chem>N#C/C(=C\c1ccc(s1)C1=C2C(=[N]=C(S2)C)[C](C=C1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>                                    |
| 622 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(c2=[N]=C(C(=[N]=c12)c1cccc1)c1cccc1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>                 |
| 623 | <chem>N#C/C(=C\c1ccc(cc1F)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 624 | <chem>N#C/C(=C\c1ccc(c(c1)F)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 625 | <chem>N#C/C(=C/c1cc2c(-c3c(C2(CC)CC)cc(s3)c2ccc(cc2)N(c2ccc(cc2)N(C)C)c2ccc(cc2)N(C)C)s1)/C(=O)O</chem>                           |
| 626 | <chem>N#C/C(=C\c1cc2c(-c3c(C2(CC)CC)cc(s3)c2ccc(cc2)N(c2cccc2)c2cccc2)s1)/C(=O)O</chem>   |
| 627 | <chem>N#C/C(=C\c1cc2c(-c3c(C2(CC)CC)cc(s3)c2sc(c3c2OCCO3)c2ccc(cc2)N(c2cccc2)c2cccc2)s1)/C(=O)O</chem>                            |
| 628 | <chem>N#C/C(=C\c1ccc(s1)[C]1C=CC(=C2C1=[N]=C(S2)C)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>                                      |
| 629 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(cc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 630 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)[C@]12OCCOC1=C(SC2)c1ccc(c2c1nsn2)/C=C(/C(=O)O)/C#N</chem>                     |
| 631 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)[C@]12OCCOC1=C(SC2)c1ccc(c2c1nsn2)c1ccc(cc1)/C=C(/C(=O)O)/C#N</chem>           |
| 632 | <chem>OC(=O)c1ccc2=[N]=C(C(=[N]=c2c1)c1ccc(cc1)/C=C\c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)/C=C\c1ccc(cc1)N(c1cccc1)c1cccc1</chem> |

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| 633 | <chem>N#CC(=c1s/c(=C\c2ccc(cc2)N(c2ccccc2)c2ccccc2)/c(=O)[nH]1)C#N</chem>   |
| 634 | <chem>N#CC(=c1[nH]c(=O)/c(=C/c2ccc(cc2)N(c2ccc(cc2)/C=c/2\sc(=C(C#N)C#N)[nH]c2=O)c2ccccc2)/s1)C#N</chem>  |
| 635 | <chem>N#CC(=c1s/c(=C/c2ccc(cc2)N(c2ccc(cc2)/C=c/2\sc(=C(C#N)C#N)[nH]c2=O)c2ccc(cc2)/C=c/2\sc(=C(C#N)C#N)[nH]c2=O)/c(=O)[nH]1)C#N</chem>                     |
| 636 | <chem>N#CC(=c1[nH]c(=O)/c(=C/c2ccc(s2)c2ccc(cc2)N(c2ccccc2)c2ccccc2)/s1)C#N</chem>  |
| 637 | <chem>N#CC(=c1[nH]c(=O)/c(=C/c2ccc(s2)c2ccc(cc2)N(c2ccc(cc2)c2ccc(s2)/C=c/2\sc(=C(C#N)C#N)[nH]c2=O)c2ccccc2)/s1)C#N</chem>                                  |
| 638 | <chem>CCCCCCCCOe1cc2c3cc(se3c3e(c2cc1OCCCCCCCC)cc(s3)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC</chem>   |
| 639 | <chem>CCCCCCCCOe1cc2c3cc(se3c3e(c2cc1OCCCCCCCC)cc(s3)/C=C(\C(=O)O)/C#N)c1sc(c2e1OCCO2)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC</chem>                          |
| 640 | <chem>CCCCCCCCOe1cc2c3cc(se3c3e(c2cc1OCCCCCCCC)cc(s3)C[C@H](C(O)O)CN)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC</chem>   |
| 641 | <chem>N#C/C(=C\c1ccc(c(s1)c1sc(cc1C)c1ccc(cc1)N(c1ccccc1)c1ccccc1)C)/C(=O)O</chem>  |
| 642 | <chem>CCCCCc1cc(se1c1se(cc1CCCCC)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccccc1)c1ccccc1</chem>   |
| 643 | <chem>CCCCCn1c2cc(ccc2n(c1=S)CCCCC)N(c1ccc2c(c1)n(CCCCC)c(=S)n2CCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>                                   |
| 644 | <chem>CCCCCn1c2cc(ccc2n(c1=S)CCCCC)N(c1ccc2c(c1)n(CCCCC)c(=S)n2CCCCC)c1ccc(cc1)c1cc(c(s1)c1sc(cc1C)/C=C(\C(=O)O)/C#N)C</chem>                               |
| 645 | <chem>CCCCCc1cc(se1c1se(cc1CCCCC)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc2c(c1)n(CCCCC)c(=S)n2CCCCC)c1ccc2c(c1)n(CCCCC)c(=S)n2CCCCC</chem>                       |
| 646 | <chem>CCCCCCn1c2ccc(cc2c2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)c1ccccc1</chem>  |
| 647 | <chem>CCCCCCn1c2ccc(cc2c2c1ccc(c2)c1ccc(o1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)c1ccccc1</chem>  |
| 648 | <chem>CCCCCn1c2ccc(cc2c2c1ccc(c2)c1ccc(o1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccccc1)c1ccccc1</chem>  |
| 649 | <chem>N#C/C(=C\c1ccc(o1)c1ccc2c(c1)c1cc(ccc1n2CCCC(C)C)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>   |
| 650 | <chem>N#C/C(=C\c1ccc(o1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 651 | <chem>CCCCC1(CCCCC)COe2c(OC1)c(sc2C1=[N]=C2C(=[N]=C(S2)c2sc(c3c2OCC(CO3)(CCCC)CCCC)c2ccc(s2)/C=C(\C(=O)O)/C#N)S1)c1ccc(cc1)N(c1ccccc1)c1ccccc1</chem>       |
| 652 | <chem>CCCCC1(CCCCC)COe2c(OC1)c(sc2C1=[N]=C2C(=[N]=C(S2)c2sc(c3c2OCC(CO3)(CCCC)CCCC)c2sc(c3c2OCCO3)/C=C(\C(=O)O)/C#N)S1)c1ccc(cc1)N(c1ccccc1)c1ccccc1</chem> |
| 653 | <chem>CC1(C)COe2c(OC1)c(sc2C1=[N]=C2C(=[N]=C(S2)c2sc(c3c2OCC(CO3)(C)C)c2ccc(s2)/C=C(\C(=O)O)/C#N)S1)c1ccc2c(c1)Sc1c(N2c2ccc(cc2)OC)cccc1</chem>             |
| 654 | <chem>N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 655 | <chem>CCCCOe1cc(OCCCC)ccc1c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCCCC)OCCCC)c1ccc(cc1)/C=C\c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>                                       |
| 656 | <chem>CCCCCCCCN1C(=O)C2=C(N(C(=O)C2=C1C1=[N]=C[C](C=C1)c1ccc(cc1)N(c1ccccc1</chem>  |

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|     | 1)c1cccc1)CCCCCCCC)C1=[N]=C[C](C=C1)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 657 | CCCCCc1cc(se1c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(e2c1nsn2)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OC[C@H](CCCC)CC)c1ccc(cc1)OC[C@@H](CCCC)CC   |
| 658 | CCCCCCC1=C(S/C(=C\2/SC(=C(N2)CCCCC)c2ccc(s2)/C=C(/C(=O)O)\C#N)/N1)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 659 | CCCCCCC1=[N]=C(S[C]1C#Cc1ccc(cc1)N(c1cccc1)c1cccc1)C1=[N]=C([C](S1)c1ccc(s1)/C=C(/C(=O)O)\C#N)CCCCC   |
| 660 | N#C/C(=C\c1ccc(n1c1c(F)c(F)c(c1F)F)/C=C\c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 661 | C=Cc1ccc(cc1)N(c1cccc1)c1ccc(cc1)/C=C\1/SC(=S)NCC(=O)OC1=O  |
| 662 | C=Cc1ccc(cc1)N(c1cccc1)c1ccc(cc1)/C=C/C=C\1/SC(=S)N(C1=O)CC(=O)O  |
| 663 | OC(=O)CN1C(=S)S/C(=C/c2ccc(cc2)N(c2cccc2)c2cccc2)/C1=O  |
| 664 | CCCCCCCCOe1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(e2c1nsn2)c1ccc(cc1)C(=O)O)c1ccc(cc1)c1ccc(cc1)OCCCCCCC   |
| 665 | CCCCCCOe1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(e1)C1=[N]=c2cccc(e2=[N]=C1e1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC                      |
| 666 | CCCCCCOe1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(e2=[N]=C(C(=[N]=c12)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC |
| 667 | N#CSc1cn(e2c1cc(cc2)c1cc(e(s1)/C=C(/C(=O)O)\C#N)C)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C   |
| 668 | N#C/C(=C\c1sc(cc1C)c1ccc2c(c1)cn2c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)/C(=O)O  |
| 669 | CCCC[C@H](CN1C(=C2C(=C(N(C2=O)C[C@H](CCCC)CC)C2=[N]=C[C](C=C2)e2ccc(s2)/C=C(\C(=O)O)/C#N)C1=O)C1=[N]=C[C](C=C1)c1ccc(cc1)N(c1cccc1)c1cccc1)CC   |
| 670 | CCCCCc1cc(se1c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(e2c1nsn2)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)OC[C@H](CCCC)CC)c1ccc(cc1)c1ccc(cc1)OC[C@H](CCCC)CC  |
| 671 | CCCCCCC1=[N]=C(S[C]1c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)C1=[N]=C([C](S1)c1ccc(s1)/C=C(/C(=O)O)\C#N)CCCCC  |
| 672 | CCCCCCC1=[N]=C(S[C]1c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)C1=[N]=C([C](S1)c1ccc(cc1)/C=C(/C(=O)O)\C#N)CCCCC   |
| 673 | CCCCCCC1=[N]=C(S[C]1c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)C1=[N]=C([C](S1)C#Cc1ccc(cc1)/C=C(/C(=O)O)\C#N)CCCCC  |
| 674 | CCCCCc1cc(se1[C]1C=[N]=C(e2c1nsn2)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 675 | CCCCCOe1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)C1=[N]=C[C](e2c1nsn2)c1sc(cc1CCCCC)c1sc(c1)CCCCC)/C=C(/C(=O)O)\C#N   |
| 676 | CCCCCc1cc(se1[C]1C=[N]=C(e2c1nsn2)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 677 | CCCCCc1cc(se1C1=[N]=C[C](e2c1nsn2)c1sc(cc1CCCCC)c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC   |

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| 678 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)C1=[N]=C[C](c2c1nns2)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 679 | O=C(O)CN1C(=O)c2ccc(c3c2c(C1=O)ccc3)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 680 | O1C(=O)CNC(=O)c2ccc(c3c2c(C1=O)ccc3c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 681 | CCCOc1ccc(c(c1)OCCCC)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)OCCCC)OCCCC)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 682 | CCCOc1cc(OCCCC)ccc1c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 683 | CCCCc1c(sc(c1CCCC)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 684 | CCCCc1c(sc(c1CCCC)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1cc2c(s1)c1c(s2)cc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 685 | N#C/C(=C\c1ccc(s1)c1ccc(c2c1nns2)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 686 | N#C/C(=C\c1ccc(s1)c1ccc(c2c1nns2)c1ccc(s1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 687 | N#C/C(=C\c1ccc(s1)c1ccc(c2c1nns2)c1ccc(s1)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 688 | CCCC[C@@H](COc1ccc(cc1)N(c1ccc(cc1)OC[C@H](CCCC)CC)c1ccc(cc1)c1ccc(s1)c1ccc(c2c1nns2)c1ccc(s1)/C=C(/C(=O)O)\C#N)CC  |
| 689 | CCCCCCCCN1C(=O)C2=C(N(C(=O)C2=C1C1=[N]=C[C](C=C1)c1ccc(cc1)N(c1ccc(c1)OC)c1ccc(cc1)OC)CCCCCCC)C1=[N]=C[C](C=C1)c1ccc(s1)/C=C(/C(=O)O)\C#N                 |
| 690 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)c1ccc(o1)/C=C(/C(=O)O)\C#N   |
| 691 | COc1ccc(c(c1)OC)N(c1ccc(cc1)OC)OC)c1ccc(cc1)c1ccc(o1)/C=C(/C(=O)O)\C#N  |
| 692 | N#C/C(=C/c1ccc(o1)c1ccc(cc1)N(c1ccc(c(c1)OC)OC)c1ccc(c(c1)OC)OC)/C(=O)O   |
| 693 | N#C/C(=C\c1ccc(o1)c1ccc(cc1)N(c1ccc2c(c1)OCCO2)c1ccc2c(c1)OCCO2)/C(=O)O   |
| 694 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)/C=C\C(=C(/C(=O)O)\C#N)\c1cc(OC)ccc1OC   |
| 695 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)/C=C/C(=C(\C(=O)O)/C#N)/c1cc(OCCC)ccc1OCCC   |
| 696 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)/C=C\C(=C(/C(=O)O)\C#N)c1cc(OC)ccc1OC  |
| 697 | N#C/C(=C\c1cc(OC)c(cc1OC)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 698 | N#C/C(=C\c1cc(OC)c(cc1OC)/C=C/c1cc(OC)c(cc1OC)N(c1cccc1)c1cccc1)/C(=O)O   |
| 699 | N#C/C(=C/c1cc(OC)c(cc1OC)/C=C/c1cc(OC)c(cc1OC)/C=C/c1cc(OC)c(cc1OC)N(c1cccc1)c1cccc1)/C(=O)O  |
| 700 | N#C/C(=C\c1ccc(n1c1ccc(cc1)C#N)/C=C\c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 701 | OC(=O)CN1C(=S)S/C(=C/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)/C1=O  |
| 702 | CCCC[C@@H](CN1C(=C2C(=C(N(C2=O)C[C@@H](CCCC)CC)C2=[N]=C[C](C=C2)c2ccc(s2)/C=C(/C(=O)O)\C#N)C1=O)C1=[N]=C[C](C=C1)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)CC |

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| 703 | CC(COc1ccc(cc1)N(c1ccc(cc1)OCCC)c1ccc(cc1)c1ccc(s1)c1ccc(c2c1nsn2)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N)C  |
| 704 | CCCC1(CCC)COc2c(OC1)c(sc2c1ccc(cc1)N(c1cccc1)c1cccc1)c1sc(c2c1OCC(CO2)(CCC)CCC)/C=C(/C(=O)O)\C#N  |
| 705 | CCCCCCC1(CCCCC)COc2c(OC1)c(sc2c1sc(c2c1OCC(CO2)(CCCC)CCCC)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 706 | N#C/C(=C/c1sc2-c3c([Si](c2c1)(c1cccc1)c1cccc1)cc(s3)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 707 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)c1sc2-c3c([Si](c2c1)(c1cccc1)c1cccc1)cc(s3)/C=C(\C(=O)O)\C#N  |
| 708 | N#C/C(=C/c1ccc(cc1)/C=C/c1cccc(c1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 709 | N#C/C(=C/c1ccc(cc1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 710 | N#C/C(=C/c1cccc(c1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 711 | N#C/C(=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 712 | OC(=O)c1ccc(cc1)/C=C/c1cccc(c1)N(c1cccc1)c1cccc1  |
| 713 | OC(=O)c1ccc(cc1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 714 | OC(=O)c1cccc(c1)N(c1cccc1)c1cccc1   |
| 715 | OC(=O)Cc1ccc(cc1)N(c1cccc1)c1cccc1  |
| 716 | N#C/C(=C/c1ccc(o1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 717 | N#C/C(=C/c1ccc(o1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc1)c1cccc1)/C(=O)O  |
| 718 | N#C/C(=C/c1ccc(o1)/C=C/c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc1)c1cccc1)/C(=O)O  |
| 719 | CCCCCCCCN1C(=O)C2=C(N(C(=O)C2=C1c1ccc(cc1)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)CCCCCCC)c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)\C#N         |
| 720 | CCCCCCCCN1C(=O)C2=C(N(C(=O)C2=C1c1ccc(cc1)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)CCCCCCC)c1ccc(cc1)c1ccc(cc1)/C=C(\C(=O)O)\C#N        |
| 721 | OC(=O)c1ccc2c(c1)N[C]1N2C(=O)c2c3c1cccc3c(cc2)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 722 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)c1ccc2c3c1cccc3[C]1N(C2=O)c2c(N1)cc(cc2)C(=O)O  |
| 723 | COc1ccc(cc1)N1c2ccc(cc2Sc2c1cccc2)/C=C/C1=[N]=c2cc(ccc2=[N]=C1/C=C/c1ccc2c(c1)Sc1c(N2c2ccc(cc2)OC)cccc1)C(=O)O                                    |
| 724 | Cc1cc(sc1/C=C(\C(=O)O)\C#N)c1sc2c(c1)c1nn(nc1c1c2sc(c1)c1ccc(cc1)N(c1cccc1)c1cccc1)CC(C)C   |
| 725 | CCCC[C@@H](Cn1nc2c(n1)c1ccc(sc1c1c2cc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(s1)/C=C(\C(=O)O)\C#N)CC  |
| 726 | CCCC[C@@H](CN1Nc2c(N1)c1cc(sc1c1c2cc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C=C(/C(=O)O)\C#N)CC  |
| 727 | CCCCCCCCOc1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)OCCCCCCC)c1ccc(cc1)c1ccc(c2c1nsn2)C#Cc1sc2c(c1)c(OCCCCCCC)c1c(c2OCCCCCCC)cc(s1)c1ccc(s1)C(=O)O |
| 728 | CCCCCCCCOc1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)OCCCCCCC)c1ccc(cc1)c1ccc(c2c1nsn2)C#Cc1sc2c(c1)c(OCCCCCCC)c1c(c2OCCCCCCC)cc(s1)c1ccc(cc1)      |

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|     | C(=O)O   |
| 729 | COc1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(e2c1nsn2)C#Cc1ccc(cc1)C(=O)O)c1ccc(cc1)c1ccc(cc1)OC  |
| 730 | CC(CCOc1ccc(cc1)N(c1ccc(cc1)OCCC(C)C)c1ccc(cc1)/C=C/C1=[N]=c2cc(ccc2=[N]=C1/C=C/c1ccc(cc1)N(c1ccc(cc1)OCCC(C)C)c1ccc(cc1)OCCC(C)C(=O)O)C                                 |
| 731 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)/C=C/C1=[N]=c2cc(ccc2=[N]=C1/C=C/c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)C(=O)O   |
| 732 | COc1ccc(cc1)N(c1ccc2-c3c(C(e2c1)(C)C)c1-c2cccc2C(c1c1-c2c(C(e31)(C)C)cccc2)(C)C)c1ccc(cc1)c1cc2c(s1)c1c(n2C)c(es1)/C=C(\C(=O)O)/C#N                                      |
| 733 | CCCCCCCCC1(CCCCCC)c2cc(C#CC#Cc3ccc(cc3)N(e3cccc3)e3cccc3)ccc2-c2c1cc(cc2)/C=C(\C(=O)O)/C#N   |
| 734 | CCCCCOc1ccc(cc1)N(c1ccc2-c3c(C(e2c1)(CCCC)CCCC)c1-c2cccc2C(c1c1-c2c(C(e31)(CCCC)CCCC)cccc2)(CCCC)CCCC)c1ccc(cc1)c1cc2c(s1)c1c(n2c2ccc(cc2)OCCCCC)c(es1)/C=C(\C(=O)O)/C#N |
| 735 | CCCC[C@H](Cc1cc(sc1c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(e2c1nsn2)c1cc(c(s1)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N)C[C@H](CCCC)CC)CC                                  |
| 736 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)N(c1ccc2-c3c(C(e2c1)(C)C)c1-c2cccc2C(c1c1-c2c(C(e31)(C)C)cccc2)(C)C)c1ccc(cc1)c1cc2c(s1)c1c(n2C)cc(s1)/C=C(/C(=O)O)\C#N             |
| 737 | Cn1c2cc(sc2c2c1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc2-c3c(C(e2c1)(C)C)c1-c2cccc2C(c1c1-c2c(C(e31)(C)C)cccc2)(C)C)c1ccc(cc1)N(c1cccc1)c1cccc1                         |
| 738 | COc1cccc(c1)[C]1C=CC(=C2C1=[N]=C(N2)c1ccc(cc1)N(c1ccc(cc1)[CH][C](C(=O)O)[N]#[C])c1ccc(cc1)Br)c1cccc(c1)OC   |
| 739 | COc1cccc(c1)C1=C2C(=[N]=C(N2)e2ccc(cc2)N(e2ccc(cc2)e2cccc(e2)N(C)C)e2ccc(cc2)[CH][C](C(=O)O)[N]#[C])[C](C=C1)c1cccc(c1)OC  |
| 740 | COc1cccc(c1)c1ccc(cc1)N(c1ccc(cc1)[CH][C](C(=O)O)[N]#[C])c1ccc(cc1)C1=[N]=C2C(=C(C=C[C]2c2cccc(e2)OC)e2cccc(e2)OC)N1   |
| 741 | CCCCCc1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)CCCCC)c1ccc(cc1)/C=C\1/SC(=S)N(C1=O)CC(=O)O   |
| 742 | CCCCCc1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)CCCCC)c1ccc(cc1)/C=C(\C(=O)O)/C#N   |
| 743 | N#C/C(=C/c1ccc(s1)c1ccc(s1)C1=[N]=C([C](S1)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)OC)/C(=O)O  |
| 744 | N#C/C(=C\c1ccc(s1)C1=[N]=C([C](S1)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)OC)/C(=O)O   |
| 745 | N#C/C(=C/c1ccc(s1)[C]1NC(=C(S1)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)OC)/C(=O)O  |
| 746 | CCCCCn1nc2c(n1)[C](c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1c([C]2c2ccc(cc2)N(e2ccc(cc2)OCCCCC)e2ccc(cc2)OCCCCC)cccc1   |
| 747 | CCCCCn1nc2c(n1)[C](c1ccc(s1)/C=C(/C(=O)O)\C#N)c1c([C]2c2ccc(cc2)N(e2ccc(cc2)OCCCCC)e2ccc(cc2)OCCCCC)cccc1  |
| 748 | N#C/C(=C\c1ccc(s1)[C]1c2cccc2[C](e2c1nsn2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 749 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)[C]1c2cccc2[C](e2c1nsn2)c   |



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|     | 1ccc(cc1)/C=C(/C(=O)O)\C#N  |
| 750 | CC1(C)c2cc(ccc2-c2c1cc(cc2)/C=C(/C(=O)O)\C#N)C#C[Pt]([P](CC)(CC)CC)([P](CC)(CC)CC)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1  |
| 751 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)[C]1c2ccccc2[C](c2c1nsn2)c1ccc(s1)/C=C(/C(=O)O)\C#N                  |
| 752 | CCCCCc1ccc(cc1)N(c1ccc(cc1)/C=C/1\SC(=S)NCC(=O)OC1=O)c1ccc(cc1)/C=N/N(c1cccc1)CCCCCCCC                            |
| 753 | CCCCCCCCCN(c1cccc1)/N=C/c1ccc(cc1)N(c1ccc(cc1)/C=C/1\SC(=S)NCC(=O)OC1=O)c1ccc(cc1)C                               |
| 754 | COc1ccc(cc1)N(c1ccc(cc1)/C=C/1\SC(=S)NCC(=O)OC1=O)c1ccc(cc1)/C=N/N(c1cccc1)c1cccc1                                |
| 755 | Cc1ccc(cc1)N(c1ccc(cc1)/C=C/1\SC(=S)NCC(=O)OC1=O)c1ccc(cc1)/C=N/N(c1cccc1)c1cccc1                                 |
| 756 | O1C(=O)CNC(=S)S/C(=C\c2ccc(cc2)N(c2ccc(cc2)/C=N/N(c2ccccc2)c2ccccc2)c2ccccc2)/C1=O                                |
| 757 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O |
| 758 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O |
| 759 | N#C/C(=C\c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O          |
| 760 | N#C/C(=C/c1ccc(o1)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)c1ccc(cc1)C(C)(C)C)/C(=O)O              |
| 761 | N#C/C(=C/c1se(c2e1OCCO2)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)c1ccc(cc1)C(C)(C)C)/C(=O)O        |
| 762 | N#C/C(=C/c1ccc(s1)c1ccc(s1)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)c1ccc(cc1)C(C)(C)C)/C(=O)O     |
| 763 | N#C/C(=C/c1ccc(s1)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)c1ccc(cc1)C(C)(C)C)/C(=O)O              |
| 764 | CCCCCCCCCCCC1(CCCCCCCCCC)c2cc(sc2-c2c1cc(s2)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC)/C=C(\C(=O)O)/C#N       |
| 765 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc2c(c1)c1cc(sc1c(e2OCC)CCCC)OCCCCC)/C=C(/C(=O)O)\C#N              |
| 766 | N#C/C(=C\1/C=C(/C=C/c2ccc(cc2)N(c2ccc(cc2)n2c3ccccc3c3c2cccc3)c2ccc(cc2)n2c3ccccc3c3c2cccc3)CC(C1)(C)C)/C(=O)O    |
| 767 | N#C/C(=C\1/C=C(/C=C/c2ccc(cc2)N(c2ccc(cc2)N(c2ccccc2)c2ccccc2)c2ccc(cc2)N(c2ccccc2)c2ccccc2)CC(C1)(C)C)/C(=O)O    |
| 768 | N#C/C(=C\1/C=C(/C=C/c2ccc(cc2)N(c2ccc(cc2)N(c2ccccc2)c2ccccc2)c2ccccc2)CC(C1)(C)C)/C(=O)O                         |
| 769 | N#C/C(=C\1/C=C(/C=C/c2ccc(cc2)N(c2ccccc2)c2ccccc2)CC(C1)(C)C)/C(=O)O  |
| 770 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1cc2c(s1)c1c(n2CCCC)cs1)/C=C(/C(=O)O)\C#N                           |
| 771 | N#C/C(=C\c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |

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| 772 | CCCCCOc1c(OCCCCC)c(e2ccc(s2)/C=C(/C(=O)O)\C#N)c2c(c1c1ccc(cc1)N(c1cccc1)c1cccc1)nsn2   |
| 773 | COc1c(OC)c(e2ccc(s2)/C=C(/C(=O)O)\C#N)c2c(c1c1ccc3-c4c(C(c3c1)(C)C)cc(cc4)N(c1cccc1)c1cccc1)nsn2   |
| 774 | CCCCCOc1c(OCCCCC)c(e2ccc(s2)/C=C(/C(=O)O)\C#N)c2c(c1C#Cc1ccc(cc1)N(c1cccc1)c1cccc1)nsn2  |
| 775 | O=C1OC(=O)/C=C/c2ccc(cc2)N(e2ccc(cc2)C=C(e2cccc2)c2cccc2)/SC(=S)NC1  |
| 776 | CCCCCOc1c(OCCCCC)c(e2ccc(s2)/C=C(/C(=O)O)\C#N)c2c(c1c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)nsn2  |
| 777 | CCCCCOc1c(e2ccc(s2)c2ccc(cc2)N(c2ccc(cc2)OC)c2ccc(cc2)OC)c2nsnc2c(c1OCCCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 778 | N#C/C(=C\c1ccc(s1)c1ccc(c2c1nsn2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 779 | N#C/C(=C\c1ccc(s1)[C]1C=[N]=C(c2c1nsn2)c1ccc(s1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 780 | CCCCCN1C(=C2C(=C(N(C2=O)CCCCC)c2ccc(cc2)c2ccc(cc2)/C=C(/C(=O)O)\C#N)C1=O)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC   |
| 781 | CCCCCN1C(=C2C(=C(N(C2=O)CCCCC)c2ccc(cc2)/C=C(/C(=O)O)\C#N)C1=O)c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC   |
| 782 | CCCCCN1C(=O)C2=C(N(C(=O)C2=C1c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC)CCCCC)c1ccc(cc1)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 783 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc2c(c1)sc(c2)c1sc2c(c1)sc(c2)/C=C(\C(=O)O)/C#N   |
| 784 | Cc1c(/C=C(\C(=O)O)/C#N)sc2c1sc1c2sc2c1sc(c2C)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 785 | Cc1c(/C=C(\C(=O)O)/C#N)sc2c1sc1c2sc2c1sc(c2C)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 786 | Cc1c(sc2c1sc1c2sc2c1sc(c2C)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 787 | Cc1c(sc2c1sc1c2sc2c1sc(c2C)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(s1)/C=C(\C(=O)O)/C#N   |
| 788 | N#C/C(=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 789 | N#C/C(=C/c1ccc(cc1)N(c1cccc1)c1ccc(cc1)C1=[N]=C([C](N1)c1cccc1)c1cccc1)/C(=O)O   |
| 790 | N#C/C(=C/c1ccc(cc1)N(c1cccc1)c1ccc(cc1)C1=[N]=C2[C](N1)c1cccc1-c1c2cccc1)/C(=O)O   |
| 791 | CCCCCCCCC1(CCCCCC)c2cc(/C=C/c3ccc(cc3)N(c3cccc3)c3cccc3)ccc2-c2c1cc(cc2)/C=C(\C(=O)O)/C#N  |
| 792 | CCCCCc1c(sc1CCCCC)c1ccc(c(s1)c1cc(c(s1)c1ccc2c3c1cccc3c1=[N]=C3C(=C[C]H)C=C3)n1c2=O)CCCCC)CCCCC)c1ccc(c(s1)c1cc(c(s1)c1ccc(cc1)N(c1ccc(cc1)C(=O)O)c1ccc(cc1)C(=O)O)CCCCC)CCCCC |
| 793 | N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc(cc1)[CH]C1=c2c(=C3)[C]1C=CC=C3)cccc2)c1cccc1)/C(=O)O   |
| 794 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc(cc1)[CH]C1=c2c(=C3[C]1C=CC=C3)cccc2)c1cccc1)/C(=O)O   |

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| 795 | <chem>N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc(cc1)[CH]C1=c2cccc2=C2[C]1C=CC=C2)c1ccc(cc1)[CH]C1=c2cccc2=C2[C]1C=CC=C2)/C(=O)O</chem>                |
| 796 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc(cc1)[CH]C1=c2c(=C3[C]1C=CC=C3)cccc2)c1ccc(cc1)[CH]C1=c2c(=C3[C]1C=CC=C3)cccc2)/C(=O)O</chem> |
| 797 | <chem>N#CC(=Cc1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1cccc1)C#N</chem>  |
| 798 | <chem>N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 799 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 800 | <chem>N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)/C(=O)O</chem>                                |
| 801 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)/C(=O)O</chem>                       |
| 802 | <chem>c1cc(ccc1)N(c1cccc1)c1ccc(cc1)c1ccc(s1)[C](C(=O)O)C#N</chem>  |
| 803 | <chem>c1cc(ccc1)N(c1cccc1)c1ccc(cc1)c1sc(/C=C/c2ccc(s2)/C=C(/C#N)\C(=O)O)cc1</chem>   |
| 804 | <chem>c1cc(ccc1)N(c1cccc1)c1ccc(cc1)/C=C/c1sc(/C=C/c2ccc(s2)/C=C(/C#N)\C(=O)O)cc1</chem>  |
| 805 | <chem>CCCCC1cc(sc1c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1sc(cc1CCCC)sc(cc1CCCC)/C=C(/C(=O)O)\C#N</chem>                              |
| 806 | <chem>CCCCC1=C[C](c2sc([C]3S[C@@](C=C3CCCC)(C=O)/C=C(/C(=O)O)\C#N)cc2CCCC)S[C@@H]1c1cc2c(s1)cc(cc2)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3</chem> |
| 807 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 808 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 809 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>                                    |
| 810 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 811 | <chem>CCCCC1(CCCCC)c2cc(ccc2-c2c1cc(cc2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)OCCCC</chem>  |
| 812 | <chem>CCCCC1(CCCCC)c2cc(sc2-c2c1cc(s2)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)OCCCC)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>  |
| 813 | <chem>OC(=O)CN1C(=S)S/C(=C\c2ccc(cc2)N(c2ccc(cc2)/C=C\2/SC(=S)NCC(=O)OC2=O)c2cccc2)/C1=O</chem>   |
| 814 | <chem>O1C(=O)CNC(=S)S/C(=C\c2ccc(cc2)N(c2ccc(cc2)/C=C\2/SC(=S)N(C2=O)CC(=O)O)c2ccc(cc2)/C=C\2/SC(=S)N(C2=O)CC(=O)O)/C1=O</chem>                                       |
| 815 | <chem>CCCCC1cc(sc1c1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)OCCCC)c1ccc(e2c1nsn2)c1sc(c1)CCCC)c1ccc(cc1)/C=C(\C(=O)O)/C#N</chem>  |
| 816 | <chem>CCCCC1cc(sc1c1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)OCCCC)c1ccc(e2c1nsn2)c1sc(c1)CCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 817 | <chem>N#C/C(=C\c1ccc(s1)[C]1C=[N]=C(c2c1nsn2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 818 | <chem>N#C/C(=C\c1ccc(cc1)[C]1C=[N]=C(c2c1nsn2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |

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|     | O   |
| 819 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1ccc(o1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OCCCCC<br>C  |
| 820 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(o1)c1ccc(o1)/C=C(/C(=O)O)\C#N  |
| 821 | COc1cc(/C=C(\C(=O)O)/C#N)c(cc1N1[N]N=C([CH]1)c1ccc(cc1)N(c1ccc(cc1)C1=N[N]N([CH]1)c1cc(OC)c(cc1OC)/C=C(\C(=O)O)/C#N)c1ccccc1)OC                         |
| 822 | CCCCN1C(=C2C(=C(N(C2=O)CCCC)c2ccc(cc2)c2ccc(cc2)/C=C(/C(=O)O)\C#N)C1=O)c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC                                  |
| 823 | CCCCN1C(=O)C2=C(N(C(=O)C2=C1c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)CCCC)c1ccc(cc1)c1ccc(o1)/C=C(/C(=O)O)\C#N                                   |
| 824 | CCCCN1C(=O)C2=C(N(C(=O)C2=C1c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)CCCC)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N                                   |
| 825 | N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(=O)c2c1)cc(cc3)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)/C(=O)O   |
| 826 | CCC(CCCOe1ccccc1N(c1ccccc1OCCCC(CC)CC)c1ccc(cc1)c1ccc2-c3c(C(=O)c2c1)cc(cc3)c1ccc(s1)/C=C(\C(=O)O)/C#N)CC   |
| 827 | N#C/C(=C\c1cc2c(-c3c(C2=O)cc(s3)c2sc(c3c2OCCO3)c2ccc(cc2)N(c2ccc(cc2)C)c2ccc(cc2)C)s1)/C(=O)O   |
| 828 | N#C/C(=C\c1cc2c(-c3c(C2=O)cc(s3)c2ccc(s2)c2ccc(cc2)N(c2ccc(cc2)C)c2ccc(cc2)C)s1)/C(=O)O   |
| 829 | N#C/C(=C\c1cc2c(-c3c(C2=O)cc(s3)c2ccc(cc2)N(c2ccc(cc2)C)c2ccc(cc2)C)s1)/C(=O)O  |
| 830 | CCCCCOc1cc(OCCCCC)cc2c1-c1ccc(cc1C2(C)C)N(c1ccc2-c3c(C(c2c1)(C)C)cc(cc3OCCCCC)OCCCCC)c1ccc(cc1)c1cc2c(s1)c1c(n2C(CCCCC)CCCCC)cc(s1)/C=C(/C(=O)O)\C#N    |
| 831 | CCCCCOc1cc(OCCCCC)ccc1c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCCCCC)OCCCCC)c1ccc(cc1)c1cc2c(s1)c1c(n2C(CCCCC)CCCCC)cc(s1)/C=C(/C(=O)O)\C#N                      |
| 832 | CCCCOe1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)c1sc(c2c1OCCO2)c1sc(c2c1OCCO2)/C=C(/C(=O)O)\C#N  |
| 833 | CCCCOe1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)c1ccc(s1)c1sc(c2c1OCCO2)/C=C(/C(=O)O)\C#N  |
| 834 | N#C/C(=C\c1ccc(s1)C1=[N]=C2C(=C[C](C=C2)N(c2ccccc2)c2ccccc2)C1(C)C)/C(=O)O  |
| 835 | N#C/C(=C\c1ccc(n1C)C1=[N]=C2C(=C[C](C=C2)N(c2ccccc2)c2ccccc2)C1(C)C)/C(=O)O   |
| 836 | CCCCCN1c(/C=C/c2ccc(cc2)N(c2ccccc2)c2ccccc2)ccc1/C=C(/C(=O)O)\C#N   |
| 837 | N#C/C(=C\c1ccc(n1CCCCCOe1ccc(cc1)C(=O)OC)/C=C\c1ccc(cc1)N(c1ccccc1)c1ccc(cc1)/C(=O)O  |
| 838 | N#C/C(=C\c1ccc(n1CCCCCOe1ccc(cc1)C(=O)OC(C)(C)C)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O  |
| 839 | COC(=O)c1cc(OCCCCCN2c(/C=C\C3ccc(cc3)N(c3ccccc3)c3ccccc3)ccc2/C=C(/C(=O)O)\C#N)cc(c1)OCCCCCN1c(/C=C/c2ccc(cc2)N(c2ccccc2)c2ccccc2)ccc1/C=C(/C(=O)O)\C#N |

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| 840 | CCCCCc1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)c1cc(c(s1)/C=C(\C(=O)O)/C#N)CCCC   |
| 841 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc(cc1CCCCC)c1cc(c(s1)[CH][C](C(=O)O)C#N)OCCCCC  |
| 842 | CCCCCc1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc2c(c1)c(c1ccc(cc1)C(C)(C)C)c1c(e2c2ccc(cc2)C(C)(C)C)cc(cc1)c1sc(c(e1)OCCCC)/C=C(\C(=O)O)/C#N                    |
| 843 | CCCCCc1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)/C=C(/C(=O)O)\C#N  |
| 844 | CCCCCc1cc(sc1c1ccc(s1)c1sc(cc1CCCCC)c1ccc(cc1)N(c1cccc1)c1cccc1)c1sc(c(e1)CCCCC)c1ccc(s1)c1sc(cc1CCCCC)/C=C(\C(=O)O)/C#N                                      |
| 845 | CCCCCc1cc(sc1c1ccc(s1)c1sc(cc1CCCCC)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 846 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 847 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(e2c(sc(e2c2ccc(cc2)N(c2ccc(cc2)OC)c2ccc(cc2)OC)c2ccsc2c2ccc(s2)c2ccc(s2)/C=C(\C(=O)O)/C#N)c2ccc(c3ccc(s3)c3cccs3)s2)cc1      |
| 848 | CCCN1C(=C2C(=C(N(C2=O)CCCC)c2ccc(s2)c2ccc(s2)/C=C(/C(=O)O)\C#N)C1=O)c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC   |
| 849 | COc1ccc(cc1)c1c2cc(ccc2c(e2c1ccc(e2)c1cc(c(s1)/C=C(\C(=O)O)/C#N)OC)c1ccc(cc1)OC)c1cc(c(s1)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)C                             |
| 850 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc(cc1CCCCC)c1ccc2c(c1)c(c1ccc(cc1)C(C)(C)C)c1c(e2c2ccc(cc2)C(C)(C)C)cc(cc1)c1cc(c(s1)/C=C(\C(=O)O)/C#N)OCCCCC |
| 851 | CCCCCc1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc2c(c1)c(c1ccc(cc1)OCCCCC)c1c(e2c2ccc(cc2)OCCCCC)cc(cc1)c1sc(c(e1)OCCCC)/C=C(\C(=O)O)/C#N                        |
| 852 | N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc(e1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1cccc1)/C(=O)O  |
| 853 | CCCCCCCCN1/C(=C/[C]2C(=C(C2=O)/C=C\2/N(CC)c3c(C2(C)C)cccc3O)/C(e2c1ccc(e2)C(=O)O)(C)C   |
| 854 | N#C/C(=C\c1ccc(cc1)N(=O)=O)/c1ccc(cc1)N(c1ccc(cc1)/C=C(/c1ccc(cc1)N(=O)=O)\C#N)c1ccc(cc1)/C=C\C(=O)O  |
| 855 | N#C/C(=C\c1ccc(cc1)N(=O)=O)/c1ccc(cc1)N(c1ccc(cc1)/C=C\C(=O)O)c1ccc(cc1)/C=C\C(=O)O   |
| 856 | CCCCCc1cc(sc1c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)c1c(OCCCCC)c(OCCCCC)c(c2=[N]=c3c(=[N]=c12)c1cccc1c1c3cccc1)c1sc(c(e1)CCCCC)/C=C(/C(=O)O)\C#N               |
| 857 | CCCCCOc1c(OCCCCC)c(c2sc(c(e2)CCCCC)/C=C(/C(=O)O)\C#N)c2=[N]=c3c(=[N]=c2c1c1sc(c(e1)CCCCC)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)c1c(e2c3cccc2)cccc1              |
| 858 | CCCCCOc1c(OCCCCC)c(c2sc(c(e2)CCCCC)/C=C(/C(=O)O)\C#N)c2=[N]=c3c(=[N]=c2c1c1sc(c(e1)CCCCC)c1ccc(cc1)N(c1cccc1)c1cccc1)c1c(e2c3cccc2)cccc1                      |
| 859 | N#C/C(=C/c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 860 | CCCCCOc1c(OCCCCC)c(c2ccc(o2)/C=C(/C(=O)O)\C#N)c2=[N]=C(C(=[N]=c2c1c1ccc(o1)c1ccc(cc1)N(c1cccc1)c1cccc1)C)C  |
| 861 | COc1c(OC)c(c2ccc(s2)/C=C(/C(=O)O)\C#N)c2=[N]=C(C(=[N]=c2c1c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)C)C  |

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| 862 | CCCCC1c1cc(sc1/C=C(\C(=O)O)/C#N)c1ccc2-c3c(C4(c2c1)c1cccc1-c1c4cccc1)cc(cc3)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 863 | CCCCC1c1cc(sc1/C=C(\C(=O)O)/C#N)c1ccc2c(c1)n(CC)c1c2ccc(c1)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 864 | N#C/C(=C/c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 865 | CCCCC1c1cc(/C=C(\C(=O)O)/C#N)c(cc1N1NN=C([CH]1)c1ccc(cc1)N(c1cccc1)c1cccc1)OCCCCC   |
| 866 | COc1cc(/C=C(\C(=O)O)/C#N)c(cc1N1[N]N=C([CH]1)c1ccc(cc1)N(c1ccc(cc1)C1=N[N]N([CH]1)c1cc(OC)c(cc1OC)/C=C(\C(=O)O)/C#N)c1ccc(cc1)C1=N[N]N([CH]1)c1cc(OC)c(cc1OC)/C=C(\C(=O)O)/C#N)OC |
| 867 | CCCCC1c1cc(ccc2n(c1=S)CCCC)N(c1ccc2c(c1)n(CCCCC)c(=S)n2CCCC)c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 868 | CCCCC1c1cc(sc1c1sc(cc1C)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc2c(c1)n(CCCCC)c(=S)n2CCCC)c1ccc2c(c1)n(CCCCC)c(=S)n2CCCC   |
| 869 | CCCCC1c1cc(sc1c1ccc(s1)/C=C(\C(=O)O)/C#N)/C=C/c1ccc(cc1)N(c1ccc2c(c1)n(CCCCC)c(=S)n2CCCC)c1ccc2c(c1)n(CCCCC)c(=S)n2CCCC   |
| 870 | CCCCC1c1cc(ccc2n(c1=S)CCCC)N(c1ccc2c(c1)n(CCCCC)c(=S)n2CCCC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N   |
| 871 | N#C/C(=C\c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)c1cccs1)c1ccc(cc1)c1cccs1)/C(=O)O  |
| 872 | N#C/C(=C\c1ccc(s1)c1ccc2c(c1)c1cc(ccc1n2CC)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1cccs1)c1ccc(cc1)c1cccs1)/C(=O)O   |
| 873 | CCCCC1c1cc2cc3c(cc2c(=O)c2c1ccc(e2)c1ccc(cc1)N(c1cccc1)c1cccc1)n(CCCCC)c1c(c3=O)cc(cc1)c1ccc(o1)/C=C(\C(=O)O)/C#N   |
| 874 | CCCCC1c1cc2cc3c(=O)c4cc(ccc4n(c3cc2c(=O)c2c1ccc(e2)/C=C\c1ccc(cc1)N(c1cccc1)c1cccc1)CCCC)C1ccc(o1)/C=C(/C(=O)O)/C#N   |
| 875 | CCCCC1c1cc2cc3c(=O)c4cc(ccc4n(c3cc2c(=O)c2c1ccc(e2)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)CCCC)C1ccc(o1)/C=C(\C(=O)O)/C#N  |
| 876 | CCCCO1c1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)c1ccc(s1)c1ccc2-c3c(C4(C5(c2c1)OCCO5)OCCO4)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 877 | CCCCC1c1cc2ccc(cc2CCc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)c1cccc1   |
| 878 | OCCCCC1c1cc2ccc(cc2CCc2c1ccc(c2)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 879 | N#C/C(=C\c1ccc(s1)c1ccc2c(c1)CCc1c(N2CCCCCOc2ccc(cc2)C(=O)O)ccc(c1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 880 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(s1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 881 | O=C1OC(=O)[C](SC(=S)NC1)[CH]c1cc(e2ccs2)c(cc1c1cccs1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 882 | O=C(O)CN1C(=S)S/C(=C/c2cc(Cl)c(cc2Cl)/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)/C1=O   |
| 883 | O1C(=O)CNC(=S)S/C(=C/c2cc(Br)c(cc2Br)/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)/C1=O   |

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| 884 | <chem>O=C(O)CN1C(=S)S/C(=C/c2ccc(cc2)/C=C/c2ccc(cc2)N(c2ccccc2)c2ccccc2)/C1=O</chem>  |
| 885 | <chem>N#C/C(=C\C1ccc(C#N)c(cc1C#N))/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 886 | <chem>N#C/C(=C\C1ccc(c2cccs2)c(cc1c1cccs1)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>   |
| 887 | <chem>N#C/C(=C\C1ccc(Cl)c(cc1Cl)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>   |
| 888 | <chem>N#C/C(=C\C1ccc(Br)c(cc1Br)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>   |
| 889 | <chem>N#C/C(=C\C1ccc(cc1)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 890 | <chem>CCCCC1c1cc(sc1/C=C\C1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)/C=C(/C(=O)O)\C#N</chem>   |
| 891 | <chem>N#C/C(=C\C1ccc(c(s1)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)C)/C(=O)O</chem>   |
| 892 | <chem>N#C/C(=C\C1ccc(c(s1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)C)/C(=O)O</chem>  |
| 893 | <chem>O1C(=O)CNC(=S)S/C(=C/c2ccc(cc2)N(c2ccccc2)c2ccc(cc2)/C=C/c2ccc(cc2)N(c2ccccc2)c2ccccc2)/C1=O</chem>   |
| 894 | <chem>N#C/C(=C\C1ccc(cc1)c1ccc(s1)c1ccc(n1c1c(cccc1C(C)C)C(C)C)c1ccc(s1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 895 | <chem>N#C/C(=C\C1ccc(n(c1c1ccc(s1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)c1c(cccc1C(C)C)C(C)C)c1ccc(s1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 896 | <chem>COc1cc(C#Cc2ccc(cc2)N(c2ccccc2)c2ccccc2)c(cc1C#Cc1ccc(cc1)/C=C(\C(=O)O)/C#N)OC</chem>   |
| 897 | <chem>COc1cc(C#Cc2ccc(cc2)N(c2ccccc2)c2ccccc2)c(cc1C#Cc1ccc(cc1)C(=O)O)OC</chem>  |
| 898 | <chem>N#C/C(=C\C1ccc(cc1)C#Cc1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 899 | <chem>OC(=O)c1ccc(cc1)C#Cc1ccc(cc1)N(c1ccccc1)c1ccccc1</chem>   |
| 900 | <chem>N#C/C(=C\C1ccc2c(s1)c1c(s2)cc(s1)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 901 | <chem>CCCCO1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)c1ccc2-c3c(C4(C5(c2c1)OCCO5)OCCO4)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 902 | <chem>N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 903 | <chem>c1(ccc(cc1)C1(c2ccc(cc2)C)c2cc3-c4cc5Cc6c(-e5cc4C(c3cc2-c2c1cc1-e3ccc(cc3C(c1c2)(C)C)N(c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C)(c1ccc(cc1)C)c1ccc(cc1)C)ccc(c6)/C=C(/C(=O)O)\C#N)C</chem> |
| 904 | <chem>N#C/C(=C\C1sc(c(c1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>   |
| 905 | <chem>N#C/C(=C/c1ccc(s1)c1sc(c(c1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>  |
| 906 | <chem>N#C/C(=C/c1ccc(s1)c1ccc(s1)c1sc(c(c1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>   |
| 907 | <chem>OC(=O)C(=Cc1ccc(cc1)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)C(=O)O</chem>  |
| 908 | <chem>CCOC(=O)/C(=C\C1ccc(cc1)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O</chem>   |
| 909 | <chem>N#C/C(=C\C1ccc(cc1)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/S([O])([O])O</chem>  |
| 910 | <chem>O/N=C/C(=C/c1ccc(cc1)/C=C/c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C#N</chem>   |
| 911 | <chem>CCCCCCCCN1c2cc(ccc2/C(=C\2/c3ccc(cc3N(C2=O)CCCCCCCC)c2ccc(s2)/C=C(\C(=O)O)/C#N)/C1=O)c1ccc(cc1)N(c1ccccc1)c1ccccc1</chem>   |
| 912 | <chem>CCCCCCCCN1c2cc(ccc2/C(=C\2/c3ccc(cc3N(C2=O)CCCCCCCC)c2ccc(o2)/C=C(\C(=O)O)/C#N)/C1=O)c1ccc(cc1)N(c1ccccc1)c1ccccc1</chem>   |
| 913 | <chem>CCCCCCCCN1c2cc(ccc2/C(=C\2/c3ccc(cc3N(C2=O)CCCCCCCC)c2ccc(cc2)/C=C(/C(=O)O)\C#N)/C1=O)c1ccc(cc1)N(c1ccccc1)c1ccccc1</chem>  |

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| 914 | CCN1c2cc(ccc2/C(=C/2\C(=O)N(c3c2ccc(c3)c2ccc(s2)/C=C(\C(=O)O)/C#N)C)/C1=O)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC   |
| 915 | CCCCCCCCN1c2cc(ccc2/C(=C/2\C(=O)N(c3c2ccc(c3)c2ccc(o2)/C=C(\C(=O)O)/C#N)CCCCCCCC)/C1=O)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC                              |
| 916 | CCCCCCCCN1c2cc(ccc2/C(=C/2\C(=O)N(c3c2ccc(c3)c2ccc(cc2)/C=C(/C(=O)O)\C#N)CCCCCCCC)/C1=O)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC                             |
| 917 | CCCCCCCCC1(CCCCCCCC)c2cc(ccc2-e2c1cc(cc2)/C=C(\C(=O)O)/C#N)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1   |
| 918 | CCCCCCCCC1(CCCCCCCC)c2cc(ccc2-e2c1cc(cc2)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1)C#Cc1ccc2-c3c(C(c2c1)(CCCCCCCC)CCCCCCCC)cc(cc3)/C=C(\C(=O)O)/C#N                  |
| 919 | N#C/C(=C\c1ccc(cc1)N(c1ccc(cc1)/C=C\1/SC(=C(S1)SC)SC)c1ccc(cc1)/C=C\1/SC(=C(S1)SC)SC)/C(=O)O  |
| 920 | O(c1c(/C=C/c2ccc(cc2)N(e2ccc(cc2)C)c2ccc(cc2)C)cc(cc1/C=C/c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)c1sc(c(c1)CC)/C=C(/C(=O)O)\C#N)C                            |
| 921 | O(c1c(/C=C/C=C/c2ccc(cc2)N(e2ccc(cc2)C)c2ccc(cc2)C)cc(cc1/C=C/C=C/c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)c1sc(c(c1)CC)/C=C(/C(=O)O)\C#N)C                    |
| 922 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1cc2c(s1)c1c(n2CCCCC)c2c(s1)c1c(n2CCCCC)cc(s1)/C=C(/C(=O)O)\C#N   |
| 923 | CCCCCOc1ccc(cc1)n1c2cc(se2c2e1e1c(s2)e2c(n1e1ccc(cc1)OCCCCC)cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC                         |
| 924 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1cc2c(s1)c1c(n2CCCCC)c2c(s1)/C=C(\C(=O)O)/C#N   |
| 925 | CCCCCc1cc(sc1e1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)c1ccc2-c3c(C(=O)e2c1)cc(cc3)c1cc(c(s1)C=C(C#N)C#N)CCCCC  |
| 926 | CCCCCc1cc(sc1e1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)c1ccc2c(c1)C(=C1[C]2C=CC(=C1)c1cc(c(s1)/C=C(\C(=O)O)/C#N)CCCCC)[C](C#N)C#N                               |
| 927 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1cccs1)c1ccc(cc1)c1cccs1)/C(=O)O   |
| 928 | CCCCCc1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc(s1)CCCCC   |
| 929 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccccc1)c1ccc(cc1)c1ccccc1)/C(=O)O   |
| 930 | N#C/C(=C/c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccccc1)/C(=O)O   |
| 931 | CCCCCCCCN1C(=S)S/C(=c\2/s/c(=C/c3ccc(cc3)N(c3ccc(cc3)/C=C/3\S/C(=C\4/SC(=S)N(C4=O)CCCCCCCC)/NCC(=O)OC3=O)c3ccccc3)/c(=O)n2CC(=O)O)/C1=O                   |
| 932 | CCCCCCCCN1C(=S)S/C(=C\2/S/C(=C\c3ccc(cc3)N(c3ccc(cc3)C)c3ccccc3)/C(=O)OC(=O)CN2)/C1=O   |
| 933 | CCCCCCCCN1C(=S)S/C(=c\2/s/c(=C\c3ccc(cc3)N(c3ccc(cc3)/C=c/3\s/c(=C\4/SC(=S)N(C4=O)CCCCCCCC)/n(c3=O)CC(=O)O)c3ccccc3)/c(=O)n2CC(=O)O)/C1=O                 |
| 934 | N#C/C(=C/c1ccc(cc1)[C]1NN[C](O1)c1ccc(cc1)N(c1ccc(cc1)C(C)C)c1ccc(cc1)C(C)C)/C(=O)O   |
| 935 | CCCCCc1cc(sc1e1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)c1ccc2-c3c(C(=O)e2c1)cc(cc3)c1cc(c(s1)/C=C(/C(=O)O)\C#N)CCCCC  |
| 936 | N1(C(=S)S/C(=c\2/s/c(=C/c3ccc(cc3)N(c3ccc(cc3)/C=c/3\s/c(=C\4/SC(=S)N(C4=O)C)/n(c3=O)CC(=O)O)c3ccc(cc3)/C=c/3\s/c(=C\4/SC(=S)N(C4=O)C)/n(c3=O)CC(=O)O)/c( |



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|     | <chem>=O)n2CC(=O)O/C1=O)C</chem>   |
| 937 | <chem>N#C/C(=C\c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 938 | <chem>N#C/C(=C\c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C(=O)O</chem>  |
| 939 | <chem>N#C/C(=C\c1cc2c(s1)cc(s2)c1cc(OC)c(cc1OC)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C(=O)O</chem>  |
| 940 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc2c(c1)sc(c2)/C=C(/C(=O)O)\C#N</chem>  |
| 941 | <chem>N#C/C(=C\1/CCCC(=C1)/C=C/c1ccc(cc1)N(c1ccc(cc1)n1c2cccc2c2c1cccc2)c1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O</chem>  |
| 942 | <chem>OC1=[N]=c2ccc(cc2=[N]=C1O)c1ccc(cc1)N(c1cccc1)c1cccc1</chem>   |
| 943 | <chem>OC1=[N]=c2ccc(cc2=[N]=C1O)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1</chem>  |
| 944 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1cc2c(s1)c1c(n2c2ccc(cc2)N(c2ccc(cc2)OCCCCC)c2ccc(cc2)OCCCCC)cc(s1)/C=C(/C(=O)O)\C#N</chem>                                      |
| 945 | <chem>O(c1ccc(cc1)N(c1cc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)C</chem>         |
| 946 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 947 | <chem>O=C1OC(=O)/C=C/c2ccc(cc2)N(c2ccc(cc2)c2ccc3c(c2)[nH]c2c3cccc2)c2cccc2)/SC(=S)NC1</chem>  |
| 948 | <chem>O=C1OC(=O)/C=C/c2ccc(cc2)N(c2ccc(cc2)c2ccc3c(c2)[nH]c2c3cccc2)c2ccc(cc2)/C=C\2/SC(=S)N(C2=O)CC(=O)O)/SC(=S)NC1</chem>  |
| 949 | <chem>O1C(=O)CNC(=S)S/C=C/c2ccc(cc2)N(c2ccc(cc2)c2ccc3c(c2)[nH]c2c3cccc2)c2ccc(cc2)c2ccc3c(c2)[nH]c2c3cccc2)/C1=O</chem>   |
| 950 | <chem>CCCC[C@H](Cn1nc2c(n1)[C](C=C[C]2/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1)CC</chem>  |
| 951 | <chem>CCCC[C@H](CN1Nc2c(N1)c1cc(sc1c1e2cc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C=C(/C(=O)O)\C#N)CC</chem>   |
| 952 | <chem>CCCCCN1[C@@H]2C[C@H](S[C@@H]2[C@H]2[C@@H]1[C@@H]1N(CCCCC)[C@@H]3[C@H]([C@@H]1[C@H]1[C@@H]2NN(N1)C[C@@H](CCCC)CC)S[C@H](C3)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1</chem> |
| 953 | <chem>OC(=O)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1</chem>  |
| 954 | <chem>O(c1ccc(cc1)c1c2cc(ccc2c(c2c1ccc(e2)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(c1)OC)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)C</chem>   |
| 955 | <chem>CCCCCOc1ccc(cc1)c1c2cc(ccc2c(c2c1ccc(e2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OCCCCC)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC</chem>                              |
| 956 | <chem>CCCCCOc1ccc(cc1)c1c2cc(ccc2c(c2c1ccc(e2)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OCCCCC)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC</chem>                              |
| 957 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 958 | <chem>CCCOc1c2Cc3cc(cc(Cc4cc(cc(Cc5c(c(Cc1cc(e2)C(C)(C)C)cc(e5)C(C)(C)C)OCCC)c4O)C(C)(C)C)c3OCCCC(=O)CO)c1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)/C=C(\C(=O)O)/C#N)C(C)(C)C</chem>        |
| 959 | <chem>CCCOc1c2Cc3cc(cc(Cc4cc(cc(Cc5c(c(Cc1cc(e2)C(C)(C)C)cc(e5)C(C)(C)C)OCCCC(</chem>  |

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|     | <chem>=O)COc1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)/C=C(\C(=O)O)/C#N)c4OCCC)C(C)(C)C)c3OCCCCC(=O)COc1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)/C=C(\C(=O)O)/C#N)C(C)(C)C</chem>               |
| 960 | <chem>N#C/C(=C/c1ccc(c1)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1)C#C)/C(=O)O</chem>  |
| 961 | <chem>N#C/C(=C\c1ccc(c1)C#C)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 962 | <chem>N#C/C(=C\c1ccc(c1)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 963 | <chem>CCCCCc1cc(sc1c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC)[C]1C=C[ NH](C=C1)CC(=O)[O]</chem>  |
| 964 | <chem>[O]C(=O)C[NH]1C=C[C](C=C1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1</chem>  |
| 965 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1ccc([se]1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCC CCC</chem>  |
| 966 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc([se]1)c1ccc([se]1)/C=C (/C(=O)O)\C#N</chem>   |
| 967 | <chem>N#C/C(=C\c1ccc(s1)c1cc2c(s1)cc(cc2)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C( c2c1)(C)C)cccc3)/C(=O)O</chem>   |
| 968 | <chem>N#C/C(=C/c1ccc(s1)/C=C/c1cc2c(s1)cc(cc2)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c 3c(C(c2c1)(C)C)cccc3)/C(=O)O</chem>  |
| 969 | <chem>c1(ccc(cc1)C1(c2ccc(cc2)C)c2cc3-c4ccc(cc4C(c3cc2-c2c1cc1-c3cc4Cc5c(-c4cc3C(c1c2 ))(c1ccc(cc1)C)c1ccc(cc1)C)ccc(c5)/C=C(/C(=O)O)\C#N)(C)C)N(c1ccc(cc1)C)c1ccc(cc 1)C)C</chem> |
| 970 | <chem>c1(ccc(cc1)C1(c2ccc(cc2)C)c2cc3-c4cc5c(-c6c(C5(C)C)cc(cc6)N5c6cccc6Sc6c5cccc6) cc4C(c3cc2-c2c1cc1-c3c(Cc1c2)cc(cc3)/C=C(/C(=O)O)\C#N)(c1ccc(cc1)C)c1ccc(cc1)C )C</chem>      |
| 971 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(c2c1nns2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 972 | <chem>N#C/C(=C/c1ccc(s1)[C]1C=CC(=C2C1=N[Se]N2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(= O)O</chem>   |
| 973 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(c2c1nns2)c1ccc(s1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 974 | <chem>N#C/C(=C/c1ccc(s1)c1ccc(c2c1n[se]n2)c1ccc(s1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 975 | <chem>N#C/C(=C\c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C( c2c1)(C)C)cccc3)/C(=O)O</chem>   |
| 976 | <chem>N#C/C(=C\c1ccc(s1)c1e2cccc2c(c2c1cccc2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 977 | <chem>N#C/C(=C/c1ccc(cc1)/C=C\c1e2cccc2c(c2c1cccc2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C (=O)O</chem>   |
| 978 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OCCCCC C</chem>   |
| 979 | <chem>CCCCCCCCC1(CCCCCCCC)c2cc(ccc2-c2c1cc(cc2)/C=C/c1ccc(cc1)N(c1cccc1)c1ccc cc1)/C=C\c1ccc2-c3c(C(c2c1)(CCCCCCC)CCCCCCC)cc(cc3)/C=C(/C(=O)O)\C#N</chem>                          |
| 980 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc 1)c1cccc1)/C(=O)O</chem>  |
| 981 | <chem>N#C/C(=C\c1cc2c(-c3c(C2(C)C)cc(s3)e2ccc(s2)e2ccc(cc2)N(c2cccc2)c2cccc2)s1)/C( =O)O</chem>  |
| 982 | <chem>O=C(O)CN1C(=S)S/C(=C/c2ccc(cc2)N(c2cccc2)c2cccc2)/C1=O</chem>  |

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| 983  | N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)C(=O)O)/C(=O)O  |
| 984  | CCCCCc1cc(sc1c1sc(c(c1)CCCCC)c1ccc(cc1)N(c1ccc(cc1)C(=O)O)c1ccc(cc1)C(=O)O)c1sc(c(c1CCCCC)CCCCC)c1sc(c(c1)CCCCC)c1sc(c(c1)CCCCC)C=C(C#N)C#N  |
| 985  | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 986  | N#C/C(=C/1\C[C@@H]/C=C/c2ccc(cc2)N(c2ccccc2)c2ccccc2)CC(C1)(C)C)/C(=O)O  |
| 987  | N#C/C(=C/1\C[C@@H]/C=C/c2ccc(cc2)N(c2ccccc3c2ccccc3)c2ccccc2)CC(C1)(C)C)/C(=O)O  |
| 988  | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)/C=C/[C@H]1C/C(=C(/C(=O)O)\C#N)/CC(C1)(C)C  |
| 989  | CC(COc1cc(OCC(C)C)ccc1c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCC(C)C)OCC(C)C)c1ccc(cc1)c1sc(c2e1OCCO2)c1ccc(e2=[N]=C(C(=[N]=c12)c1ccccc1)c1ccccc1)c1ccc(cc1)/C=C(\C(=O)O)/C#N)C                                |
| 990  | CC(C[C@]1(CCC(C)C)c2cc(sc2-c2c1cc(s2)[C]1C=C[C](C2=[N]=C(C(=[N]=C12)c1ccc(cc1)c1ccccc1)c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCC(C)C)OCC(C)C)c1ccc(cc1)c1ccc(cc1OCC(C)C)OCC(C)C)C |
| 991  | CCCCCn1nc2c(n1)c(ccc2c1ccc(o1)/C=C(/C(=O)O)\C#N)c1ccc(o1)c1ccc(cc1)N(c1ccc(cc1)/C(=C\C)/C=C  |
| 992  | CC(COc1cc(OCC(C)C)ccc1c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCC(C)C)OCC(C)C)c1ccc(cc1)c1ccc(s1)c1ccc(e2=[N]=C(C(=[N]=c12)c1ccccc1)c1ccccc1)c1ccc(cc1)/C=C(\C(=O)O)/C#N)C                                      |
| 993  | N#C/C(=C\c1ccc(cc1)c1ccc(cc1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O   |
| 994  | N#C/C(=C\c1ccc(cc1)c1ccc(cc1)c1ccc(cc1)N(c1cccc2c1cccc2)c1ccccc1)/C(=O)O   |
| 995  | N#C/C(=C\c1ccc(cc1)c1ccc(s1)c1ccc(cc1)N(c1cccc2c1cccc2)c1ccccc1)/C(=O)O  |
| 996  | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc2c1cccc2)c1ccccc1)/C(=O)O   |
| 997  | N#C/C(=C\c1ccc(cc1)c1c2ccccc2c(c2c1cccc2)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O   |
| 998  | N#C/C(=C/c1ccc(s1)/C=C/c1c2ccccc2c(c2c1cccc2)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O   |
| 999  | N#C/C(=C\c1ccc(s1)C#Cc1c2ccccc2c(c2c1cccc2)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O   |
| 1000 | N#C/C(=C\c1ccc(cc1)C#Cc1c2ccccc2c(c2c1cccc2)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C(=O)O  |
| 1001 | N#C/C(=C\c1ccc(s1)C#Cc1c2ccccc2c(c2c1cccc2)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C(=O)O   |
| 1002 | N#C/C(=C\c1ccc(cc1)c1c2ccccc2c(c2c1cccc2)C#Cc1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O  |
| 1003 | N#C/C(=C\c1ccc(cc1)c1c2ccccc2c(c2c1cccc2)C#Cc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C(=O)O  |
| 1004 | N#C/C(=C\c1ccc(cc1)/C=C\c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O  |
| 1005 | N#C/C(=C\c1ccc(cc1)C#Cc1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O  |
| 1006 | N#C/C(=C\c1ccc(cc1)/C=C/c1c2ccccc2c(c2c1cccc2)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O  |

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| 1007 | <chem>N#C/C(=C\c1ccc(cc1)C#Cc1c2ccccc2c(e2c1cccc2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 1008 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 1009 | <chem>COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)c1ccc(s1)c1sc(e(c1)c1ccc(s1)c1cc(se1c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem> |
| 1010 | <chem>N#C/C(=C\c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc1)c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1011 | <chem>N#C/C(=C\c1ccc(cc1)N(c1cccc2c1cccc2)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O</chem>  |
| 1012 | <chem>N#C/C(=C\c1ccc2c(c1)c1cccc1n2c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)n1c2ccccc2c2c1cccc2)/C(=O)O</chem>  |
| 1013 | <chem>N#C/C(=C\c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1cccc1)/C(=O)O</chem>   |
| 1014 | <chem>N#CC(=C1C=C(/C=C/c2ccc(cc2)N(c2ccccc2)c2ccccc2)CC(C1)(C)C)C#N</chem>   |
| 1015 | <chem>N#C/C(=C/c1ccc(cc1)N(c1ccc(cc1)N1CCc2c1cccc2)c1ccc(cc1)N1CCc2c1cccc2)/C(=O)O</chem>  |
| 1016 | <chem>N#C/C(=C/c1ccc(cc1)N(c1ccc(cc1)N1[C@@H](C)Cc2c1cccc2)c1ccc(cc1)N1[C@H](C)Cc2c1cccc2)/C(=O)O</chem>   |
| 1017 | <chem>CCCCCec1cc(se1c1ccc(cc1)N(c1cccc1)c1cccc1)C1=C[CH]N(C=C1)CC(=O)O</chem>  |
| 1018 | <chem>CCCCCec1cc(se1c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)C1=C[CH]N(C=C1)CC(=O)O</chem>  |
| 1019 | <chem>CCN1C(=S)S/C(=C\2/S/C(=C/c3ccc(s3)C3=CN4[CH]C(=[N]=C4C(=C3)c3ccc(cc3)N(c3ccccc3)c3ccccc3)C)/[NH](C2=O)CC(=O)[O])/C1=O</chem>   |
| 1020 | <chem>CCO[Si](c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)(OCC)OCC</chem>  |
| 1021 | <chem>CCO[Si](c1ccc(s1)c1ccc(s1)c1ccc2c(s1)cc(cc2)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)(OCC)OCC</chem>  |
| 1022 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O</chem>  |
| 1023 | <chem>N#C/C(=C\c1ccc2-c3c(C(c2c1)(C)C)cc(cc3)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1024 | <chem>N#C/C(=C/c1ccc2-c3c(C(c2c1)(C)C)cc(cc3)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 1025 | <chem>N#C/C(=C/c1ccc2-c3c(C(c2c1)(C)C)cc(cc3)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1026 | <chem>CCCCCCCc1cc(se1c1sc(e(c1)CCCCCCC)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc2-c3c(C(c2c1)(C)C)cc(cc3)/C=C(/C(=O)O)\C#N</chem>  |
| 1027 | <chem>N#C/C(=C\c1ccc2-c3c(C(c2c1)(C)C)cc(cc3)c1sc(e2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 1028 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1sc(e2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 1029 | <chem>N#C/C(=C\c1ccc2-c3c(C(c2c1)(C)C)cc(cc3)c1ccc(s1)c1sc(e2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |

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| 1030 | CCCCCn1nc2c(n1)c(ccc2c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1031 | CCCCCn1nc2c(n1)c(ccc2c1ccc([se]1)/C=C(/C(=O)O)\C#N)c1ccc([se]1)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1032 | CCCCCn1nc2c(n1)[C](C=C[C]2c1sc(c1)CCCCC)c1ccc(cc1)N(c1cccc1)c1cccc1c1sc(c1)CCCCC/C=C(\C(=O)O)/C#N  |
| 1033 | N#C/C(=C\c1ccc(s1)c1c(F)c(F)c(c2c1n[nH]n2)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1034 | CCCCCCCCC1=[N]=C(S[C]1c1ccc(cc1)N(c1cccc1)c1cccc1)C1=[N]=C([C](S1)c1ccc(s1)/C=C(/C(=O)O)\C#N)CCCCCCCC  |
| 1035 | N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1ccc2c(-c3cccc3C2(C)C)c1)c1ccc2c(-c3cccc3C2(C)C)c1)/C(=O)O  |
| 1036 | N#C/C(=C/c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc2c(-c3cccc3C2(C)C)c1)c1ccc2c(-c3cccc3C2(C)C)c1)/C(=O)O   |
| 1037 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)/C=C/C1=C[CH]N(C=C1)CC(=O)O   |
| 1038 | CCCCCOc1ccc(cc1)N(c1cc2c3ccc(cc3n(e2cc1OCCCCC)CCCCC)c1cc2c(s1)c1c(n2c2cccc(e2)OCCCCC)cc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OCCCCC  |
| 1039 | COc1cccc(c1)n1c2ccse2c2c1cc(s2)c1ccc(cc1)N(c1cc2c(cc1OC)n(c1c2cc(cc1)c1sc2c(c1)n(c1c2sc(c1)/C=C(\C(=O)O)/C#N)c1cccc(c1)OC)c1ccc(cc1)c1sc2c(c1)n(c1c2sc(c1)cccc(c1)OC |
| 1040 | CCCCCOc1ccc(cc1)N(c1cc2c3cccc3n(e2cc1OCCCCC)CCCCC)c1ccc(cc1)c1cc2c(s1)c1c(n2c2cccc2OCCCCC)cc(s1)/C=C(/C(=O)O)\C#N  |
| 1041 | COc1cc2n(C)c3c(c2cc1N(c1ccc(cc1)c1cc2c(s1)c1c(n2c2cccc2OC)cc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1cc2c(s1)c1c(n2c2cccc2OC)ccs1)cccc3                                     |
| 1042 | N#C/C(=C/c1sc(c2c1[C@@H]1CC[C@H]2C=C1)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O  |
| 1043 | N#C/C(=C\c1sc(c2c1[C@@H]1CC[C@H]2C=C1)c1sc(c2c1[C@H]1CC[C@@H]2C=C1)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O                     |
| 1044 | N#C/C(=C\c1sc(c2c1cccc2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O  |
| 1045 | N#C/C(=C\c1ccc(cc1)N(c1cccc1)c1ccc(cc1)c1cc2CCCN3c2c(c1)CCC3)/C(=O)O   |
| 1046 | O=C1OC(=O)/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)/SC(=S)NC1  |
| 1047 | O=C(O)CN1C(=S)S/C(=C\c2ccc(cc2)N(c2ccc(cc2)c2cc3CCCN4c3c(c2)CCC4)c2cccc2)/C1=O   |
| 1048 | CCCCCOc1cc(OCCCCC)ccc1n1c2cc(sc2c2c1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc2c(c1)sc1c2sc1)c1ccc2c(c1)sc1c2sc1  |
| 1049 | CCCCCOc1cc(OCCCCC)ccc1n1c2cc(sc2c2c1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc2c(c1)sc2)c1ccc2c(c1)sc2  |
| 1050 | CCCCCOc1cc(OCCCCC)ccc1n1c2cc(sc2c2c1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)c1cc2c(s1)ccs2)c1ccc(cc1)c1cc2c(s1)ccs2  |
| 1051 | CCCCCOc1cc(OCCCCC)ccc1n1c2cc(sc2c2c1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)c1cccs1)c1ccc(cc1)c1cccs1  |
| 1052 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc2c(c1)n(c1c2sc(c1)/C=C(\  |

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|      | /C(=O)O\C#N)c1ccc(cc1OCCCCC)OCCCCC  |
| 1053 | CCCCCOc1ccc(cc1)N(c1ccc2e(c1)sc1e2sc1)c1ccc(cc1)c1sc2e(c1)n(c1e2sc(c1)/C=C(/C(=O)O)\C#N)c1ccc(cc1OCCCCC)OCCCCC  |
| 1054 | CCCCCn1e2ccc(cc2e2e1ccc2)N(c1ccc(c(e1)C(=O)OC)c1cc2c(s1)c1c(n2CCCCC)cc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc2-c3c(C(c2e1)(CCCCC)CCCCC)c1-e2cccc2C(c1e1-c2c(C(c31)(CCCCC)CCCCC)cccc2)(CCCCC)CCCCC |
| 1055 | CCCCCn1e2ccc(cc2e2e1ccc2)N(c1ccc(cc1)c1cc2c(s1)c1c(n2CCCCC)cc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc2-c3c(C(c2e1)(CCCCC)CCCCC)c1-e2cccc2C(c1e1-c2c(C(c31)(CCCCC)CCCCC)cccc2)(CCCCC)CCCCC          |
| 1056 | CCCCC1(CCCCC)c2cc(ccc2-e2e1cc(cc2)c1ccc(cc1)n1c(/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)ccc1/C=C(/C(=O)O)\C#N)c1ccc(cc1)n1c(/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)ccc1/C=C(/C(=O)O)\C#N                     |
| 1057 | CCCCCn1e2cc(ccc2e2e1cc(cc2)c1ccc(cc1)n1c(/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)ccc1/C=C(/C(=O)O)\C#N)c1ccc(cc1)n1c(/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)ccc1/C=C(/C(=O)O)\C#N                            |
| 1058 | CCCCCOc1cc(c(cc1e1ccc(cc1)n1c(/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)ccc1/C=C(/C(=O)O)\C#N)OCCCCC)c1ccc(cc1)n1c(/C=C/c2ccc(cc2)N(c2cccc2)c2cccc2)ccc1/C=C(/C(=O)O)\C#N                                |
| 1059 | CCCCCc1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)c1cc(c(s1)/C=C(/C(=O)O)\C#N)CCCC   |
| 1060 | CCCC[C@@H](CN1c2cc(ccc2/C=C/2\C(=O)N(c3e2ccc(c3)e2ccc(s2)/C=C(\C(=O)O)\C#N)C[C@@H](CCCC)C)/C1=O)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC)CC  |
| 1061 | N#C/C(=C\c1ccc(s1)C1=[N]=C[C](c2e1nns2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1062 | N#C/C(=C\c1ccc(s1)C1=[N]=C[C](c2e1nns2)c1ccc(cc1)N(c1ccc2-c3c(C(c2e1)(C)C)ccc(c3)c1ccc2-c3c(C(c2e1)(C)C)cccc3)/C(=O)O   |
| 1063 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)[C]1C=[N]=C(c2e1nns2)c1ccc(s1)/C=C(/C(=O)O)\C#N  |
| 1064 | CCCC[C@H](Cn1e2cc(sc2e2e1cc(s2)/C=C(\C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1)CC   |
| 1065 | N#C/C(=C\c1c(F)cc(cc1F)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1066 | CCCCCOc1ccc(cc1)n1e2cc(sc2e2e1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1067 | N#C/C(=C\c1cc(c(s1)c1sc(c(e1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1068 | C=Cc1ccc(cc1)N(c1cccc1)c1ccc(cc1)/C=C(\C(=O)O)\C#N  |
| 1069 | C=Cc1ccc(cc1)N(c1cccc1)c1ccc(cc1)/C=C\C=C(/C(=O)O)\C#N  |
| 1070 | N#C/C(=C\c1sc(e2e1OCCO2)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1071 | N#C/C(=C\c1sc(e2e1OCCO2)c1ccc(s1)c1ccc(cc1)N(c1ccc2c(e1)OCCO2)c1ccc2c(e1)OCCO2)/C(=O)O  |
| 1072 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)c1sc(e2e1OCCO2)/C=C(/C(=O)O)\C#N  |
| 1073 | CCCCCCCN1C(=O)c2c(cc3c4c2c(C1=O)cc(c4C(=O)N(C3=O)CCCCCCC)c1ccc(s1)/C=C(\C(=O)O)\C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1  |

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| 1074 | CCCCCc1cc(sc1c1sc(cc1CCCCC)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1ccc1   |
| 1075 | CCCCCc1cc(sc1c1ccc(cc1)N(c1cccc1)c1cccc1)c1sc(cc1CCCCC)/C=C(/C(=O)O)\C#N  |
| 1076 | CCCCCc1cc(sc1c1cc(c(s1)/C=C(/C(=O)O)\C#N)CCCCC)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 1077 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(=O)c2c1)cc(cc3)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1078 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)n1c2cccc2c2c1ccc2)c1ccc(cc1)n1c2cccc2c2c1ccc2)/C(=O)O   |
| 1079 | CCCCCCn1c2ccc(cc2c2c1ccc(c2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1080 | CCCCCCn1c2ccc(cc2c2c1ccc(c2)/C=C\c1ccc(cc1)N(c1ccc(cc1)/C=C/c1ccc2c(c1)c1ccc(cc1n2CCCCC)/C=C(/C(=O)O)\C#N)c1cccc1/C=C(\C(=O)O)/C#N  |
| 1081 | N#C/C(=C\c1ccc(s1)[C]1C=[N]=C(c2c1n[se]n2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1082 | CCCCCn1c2ccc(cc2c2c1cccc2)C1=[N]=C[C](c2c1nsn2)c1ccc(cc1)/C=C(\C(=O)O)/C#N  |
| 1083 | CCCCCn1c2ccc(cc2c2c1cccc2)C1=[N]=CC(=C2C1=N[Se]N2)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 1084 | Cc1ccc(cc1)C1(c2ccc(cc2)C)c2cc(ccc2-c2c1cc(s2)c1ccc(c2c1nsn2)c1ccc(cc1)C(=O)O)N(c1ccc(cc1)C)c1ccc(cc1)C   |
| 1085 | Cc1ccc(cc1)C1(c2ccc(cc2)C)c2cc(sc2-c2c1cc(cc2)N(c1ccc(cc1)C)c1ccc(cc1)C)c1c(F)c(F)c(c2c1nsn2)c1ccc(cc1)C(=O)O   |
| 1086 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCCC  |
| 1087 | N#C[C@@H](c1cc2c(s1)c1c(s2)cc(s1)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)C(=O)O   |
| 1088 | COc1cc(OC)ccc1c1ccc(cc1)N(c1ccc(cc1)C1=[N]=C[C](C2=[N]=C(C=[N]=C12)c1cccc1)c1cccc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc(cc1OC)OC  |
| 1089 | Cn1c2ccc(cc2c2c1ccc(c2)/C=C/c1ccc(cc1)N(c1ccc(cc1)/C=C/c1ccc2c(c1)c1ccc(cc1n2C)/C=C(\C(=O)O)/C#N)c1ccc(cc1)/C=C/c1ccc2c(c1)c1ccc(cc1n2C)/C=C(/C(=O)O)\C#N/C=C(\C(=O)O)/C#N              |
| 1090 | N#C/C(=C\c1c(F)cc(cc1F)/C=C/c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O  |
| 1091 | N#C/C(=C\c1sc(c2c1OCCO2)c1ccc(cc1)N(c1ccc(cc1)n1c2cccc2c2c1cccc2)c1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O   |
| 1092 | C1(C)(c2c3-c4ccc(cc4C(c3c3-c4c(C(c3c2-c2c1cccc2)(C)C)cccc4)(C)C)N(c1ccc(cc1)N(c1ccc2c(-c3cccc3C2(C)C)c1)c1ccc2c(-c3cccc3C2(C)C)c1)c1ccc(cc1)c1cc2c(s1)c1c(n2C)cc(s1)/C=C(/C(=O)O)\C#N)C |
| 1093 | CN(c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)c1-c2cccc2C(c1c1-c2c(C(c31)(C)C)cccc2)(C)C)c1ccc(cc1)c1cc2c(s1)c1c(n2C)cc(s1)/C=C(/C(=O)O)\C#N)C  |
| 1094 | Cn1c2ccsc2c2c1cc(s2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)c1-c2cccc2C(c1c1-c2c(C(c31)(C)C)cccc2)(C)C)c1ccc(cc1)c1sc2c(c1)n(c1c2sc(c1)/C=C(/C(=O)O)\C#N)C                                   |
| 1095 | Cn1c2cc(sc2c2c1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc2-c3c([C@@](c2c1)(C)CC)c1-c2cccc2C(c1c1-c2c(C(c31)(C)C)cccc2)(C)C)c1ccc(cc1)n1c2ccsc2c2c1ccs2                                   |

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| 1096 | COc1ccc(c(c1)OC)c1cc(ccc1N(c1ccc2-c3c(C(c2c1)(C)C)cc(s3)c1c(F)c(F)c(c2c1nsn2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(cc1OC)OC)c1ccc(cc1OC)OC                            |
| 1097 | COc1ccc(c(c1)OC)c1cc(ccc1N(c1ccc2-c3c(C(c2c1)(C)C)cc(s3)c1ccc(c2c1nsn2)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(cc1OC)OC)c1ccc(cc1OC)OC                                  |
| 1098 | COc1ccc(c(c1)OC)c1cc(ccc1N(c1ccc2-c3c(C(c2c1)(C)C)cc(s3)C1=[N]=C[C](C2=[N]=C(C(=[N]=C12)c1cccc1)c1cccc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(cc1OC)OC)c1ccc(cc1OC)OC |
| 1099 | CCN1C(=S)S[C]([C]2S/C(=C/c3ccc4c(c3)[C@@H]3CCC[C@H]3N4c3ccc(cc3)C=C(c3cccc3)c3cccc3)/C(=O)N2CC(=O)O)C1=O   |
| 1100 | CCCCCCCn1nc2c(n1)[C](c1ccc(s1)/C=C(/C(=O)O)\C#N)C1=[N]=C(C(=[N]=C1[C]2c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1cccc1)c1cccc1   |
| 1101 | N#C/C(=C\c1ccc(cc1F)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1102 | N#C/C(=C\c1ccc(cc1)/C=C/c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O   |
| 1103 | N#C/C(=C\c1ccc(cc1F)/C=C/c1ccc(cc1)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O  |
| 1104 | N#C/C(=C\c1sc2-c3c([Si](c2c1)(c1cccc1)c1cccc1)cc(s3)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1105 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc2-c3c([Si](c2c1)(c1cccc1)c1cccc1)cc(s3)/C=C(/C(=O)O)\C#N  |
| 1106 | CCCCCOc1cc(OCCCCC)ccc1n1c2cc(sc2c2c1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 1107 | N#C/C(=C\c1ccc(cc1)c1ccc(c2c1nsn2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1108 | N#C/C(=C\c1ccc(s1)c1sc2c(c1C[C@@H](CC(C)(C)C)sc1c2sc2c1sc(c2C[C@H](CC(C)(C)C)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1109 | CCCCCCCCc1c(sc2c1sc1c2sc2c1sc(c2CCCCCCCC)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 1110 | Cc1c(sc2c1sc1c2sc2c1sc(c2C)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 1111 | N#C/C(=C\c1ccc(s1)c1cc2cc(ccc2oc1=O)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1112 | N#C/C(=C/c1ccc(s1)c1ccc(s1)c1cc2cc(ccc2oc1=O)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1113 | N#C/C(=C\c1ccc(cc1)c1ccc(s1)c1cc2cc(ccc2oc1=O)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1114 | CCCCCOc1cc(OCCCCC)ccc1n1c2cc(sc2c2c1cc(s2)c1sc2c(c1)n(c1c2sc(c1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1cc(OCCCCC)cc(c1)OCCCCC)/C=C(/C(=O)O)\C#N                                     |
| 1115 | CCCCCCCn1nc2c(n1)[C](c1ccc(cc1)/C=C(/C(=O)O)\C#N)C1=[N]=C(C(=[N]=C1[C]2c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1cccc1)c1cccc1  |
| 1116 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1cc2c(s1)c1c(n2CCCCC)cc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc2-c3c(C(c2c1)(CCCC)CCCC)c1-c2cccc2C(c1c1-c2c(C(c31)(CCCC)CCCC)cccc2)(CCCC)CCCC    |
| 1117 | CCCCC1=[N]=c2c3cc(sc3c3c(c2=[N]=C1CCCC)cc(s3)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1118 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc2c(c1)c1=[N]=C(CCCC)C(=[N]=c1c1c2sc(c1)/C=C(/C(=O)O)\C#N)CCCC   |



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| 1119 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc(c2c1OCCO2)c1sc2c(c1)c1=[N]=C(CCCCC)C(=[N]=c1c1e2sc(c1)/C=C(/C(=O)O)\C#N)CCCCC  |
| 1120 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(c2c1nsn2)c1sc2c(c1)c1=[N]=C(CCCCC)C(=[N]=c1c1e2sc(c1)/C=C(/C(=O)O)\C#N)CCCCC  |
| 1121 | CN1[C]([CH][CH])C(c2c1ccc(e2)C(=O)O)(C)C.c1(ccc(cc1)N(c1cccc1)c1cccc1)I  |
| 1122 | CC1(C)c2cc(ccc2-c2c1cccc2)N(c1ccc2-c3c(C(c2c1)(C)C)ccc3)c1ccc2c(c1)sc1c2sc2c1c cc(e2)c1ccc(c(s1)/C=C(\C(=O)O)/C#N)C  |
| 1123 | CCCCN1C(=[N]=C2C1=C(C=C[C]2c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1124 | CCCCN1C(=[N]=C2[C]1[C](C=C[C]2c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 1125 | CCCCN1C(=[N]=C2C1=C(C=C[C]2c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1126 | N#CC(=CC(=C(C#N)C#N)c1ccc(cc1)N(c1cccc1)c1cccc1)C#N  |
| 1127 | N#CC(=C[C](c1ccc([C](C#N)C#N)cc1)c1ccc(cc1)N(c1cccc1)c1cccc1)C#N   |
| 1128 | Cn1nc2c(n1)[C](c1ccc(s1)C(=O)O)C1=[N]=C(C(=[N]=C1[C]2c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1cccc1)c1cccc1  |
| 1129 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)C1=[N]=C[C](C=C1)/C=C(/C(=O)O)\C#N  |
| 1130 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCCC  |
| 1131 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)[C]1S[C](C2=[N]=C(C(=[N]=C12)c1ccc(cc1)C(=O)O)c1ccc(cc1)C(=O)O)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC                    |
| 1132 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)c1ccc(s1)C1=C2C(=C(N(C2=O)CC(C)C)c2ccc(c2)c2ccc(cc2)/C=C(\C(=O)O)/C#N)C(=O)N1CC(C)C   |
| 1133 | CCCCCOc1ccc(OCCCCC)cc(c1)c1ccc(cc1)N(c1ccc(cc1)c1cc(OCCCCC)cc(c1)/C=C/C(CCCC)c1ccc(cc1)/C=C(\C(=O)O)/C#N   |
| 1134 | CCCCC[C]1c2c(c(c(n2[B])(n2c1c(C)c(e2C)c1ccc(o1)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(c1)Oc1c(N2CCC)cccc1)C  |
| 1135 | N#C/C(=C\c1ccc(s1)c1cc2c3c(c1)C(c1ccc(cc1)C)(c1ccc(cc1)C)c1e4N3c3c(C2(c2ccc(cc2)C)c2ccc(cc2)C)cccc3C(c4ccc1)(c1ccc(cc1)C)c1ccc(cc1)C)/C(=O)O                                 |
| 1136 | CCCCCc1ccc(s1)c1cc2c3c(c1)C(c1ccc(cc1)C)(c1ccc(cc1)C)c1e4N3c3c(C2(c2ccc(cc2)C)c2ccc(cc2)C)ccc(cc3C(c4ccc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)(c1ccc(cc1)C)c1ccc(cc1)C)c1ccc(s1)CCCCC |
| 1137 | CCCCCc1ccsc1c1cc2c3c(c1)C(c1ccc(cc1)C)(c1ccc(cc1)C)c1e4N3c3c(C2(c2ccc(cc2)C)c2ccc(cc2)C)ccc(cc3C(c4ccc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)(c1ccc(cc1)C)c1ccc(cc1)C)c1sc1CCCCC       |
| 1138 | CCCCCCCn1nc2c(n1)[C](c1ccc(cc1)C(=O)O)C1=[N]=C(C(=[N]=C1[C]2c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1cccc1)c1cccc1   |
| 1139 | N#C/C(=C\c1ccc(cc1)c1cc2c3c(c1)C(c1ccc(cc1)C)(c1ccc(cc1)C)c1e4N3c3c(C2(c2ccc(cc2)C)c2ccc(cc2)C)cccc3C(c4ccc1)(c1ccc(cc1)C)c1ccc(cc1)C)/C(=O)O                                |
| 1140 | N#C/C(=C\c1ccc(o1)c1cc2c3c(c1)C(c1ccc(cc1)C)(c1ccc(cc1)C)c1e4N3c3c(C2(c2ccc(cc2)C)c2ccc(cc2)C)cccc3C(c4ccc1)(c1ccc(cc1)C)c1ccc(cc1)C)/C(=O)O                                 |

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| 1141 | [C@H]1(C)c2cc(ccc2-c2c1c1-c3ccc(cc3C(c1c1-c3c(C(e21)(C)C)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#N)(C)C)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1                |
| 1142 | CC1(C)c2cc(ccc2-c2c1c1-c3ccc(cc3C(c1c1-c3c(C(e21)(C)C)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#N)(C)C)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1                    |
| 1143 | CC1(C)c2cc(ccc2-c2c1c1-c3ccc(cc3C(c1c1-c3c(C(e21)(C)C)cc(cc3)c1ccc(cc1)N(c1cccc1)c1cccc1)(C)C)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(s1)/C=C\1/SC(=S)N(O)CC(=O)O            |
| 1144 | COc1ccc(cc1)[C@H]1N=C(N[C@@H]1c1ccc(cc1)OC)c1ccc(cc1)N(c1ccc(cc1)/C=C(\C(=O)O)\C#N)c1cccc1   |
| 1145 | N#C/C(=C/c1ccc(cc1)N(c1cccc1)c1ccc(cc1)C1=N[C@@H]([C@H](N1)c1ccc(cc1)c1cccs1)c1ccc(cc1)c1cccs1)/C(=O)O   |
| 1146 | N#C/C(=C/c1ccc(cc1)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc(cc1)c1cccc1)/C(=O)O  |
| 1147 | N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc(cc1)c1cccc1)/C(=O)O   |
| 1148 | N#C/C(=C/c1ccc(o1)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc(cc1)c1cccc1)/C(=O)O   |
| 1149 | CCCCC1(CCCC)c2cc(ccc2-c2c1cccc2)n1c2cc(sc2c2c1cc(s2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C=C(\C(=O)O)\C#N  |
| 1150 | CCCCC1(CCCC)c2cc(ccc2-c2c1cc(cc2)N(c1cccc1)c1cccc1)c1sc2c(c1)n(c1c2sc(c1)/C=C(\C(=O)O)\C#N)c1ccc2-c3c(C(c2c1)(CCCC)CCCC)cccc3  |
| 1151 | Cc1ccc(s1)C1=[N]=c2c(ccc(c2=[N]=C1c1ccc(s1)C)c1ccc(cc1)/C=C(\C(=O)O)\C#N)c1cc(c(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)C   |
| 1152 | CCCCCCCc1ccc(s1)C1=[N]=c2c3cc(sc3c3c(c2=[N]=C1c1ccc(s1)CCCCCCC)cc(s3)c1ccc(cc1)/C=C(\C(=O)O)\C#N)c1ccc(c(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)CCCCCCC                        |
| 1153 | Cc1ccc(s1)C1=[N]=C2[C](S[C](C2=[N]=C1c1ccc(s1)C)c1ccc(cc1)/C=C(\C(=O)O)\C#N)c1ccc(c(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)C   |
| 1154 | c1(c(/C=C/c2ccc(cc2)N(c2ccc(cc2)C)c2ccc(cc2)C)cc(cc1)/C=C/c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)c1ccc(s1)c1c(F)c(F)c(c2c1nsn2)c1ccc(cc1)C(=O)O)OC                        |
| 1155 | CCCCCCCn1nc2c(n1)[C](c1ccc(cc1)N(c1cccc1)c1cccc1)C1=[N]=C(C(=[N]=C1[C]2c1ccc(s1)/C=C(/C(=O)O)\C#N)c1cccc1)c1cccc1  |
| 1156 | CCCCCCCn1nc2c(n1)[C](c1ccc(cc1)N(c1cccc1)c1cccc1)C1=[N]=C(C(=[N]=C1[C]2c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1cccc1)c1cccc1   |
| 1157 | CCCCCCCn1nc2c(n1)[C](c1ccc(cc1)N(c1cccc1)c1cccc1)C1=[N]=C(C(=[N]=C1[C]2c1ccc(s1)C(=O)O)c1cccc1)c1cccc1   |
| 1158 | CCCCCCCn1nc2c(n1)[C](c1ccc(cc1)N(c1cccc1)c1cccc1)C1=[N]=C(C(=[N]=C1[C]2c1ccc(cc1)C(=O)O)c1cccc1)c1cccc1  |
| 1159 | CC(CN1C(=C2C(=C(N(C2=O)CC(C)C)c2ccc(s2)c2ccc(cc2)C(=O)O)C1=O)c1ccc(s1)c1cc(/C=C/c2ccc(cc2)N(c2ccc(cc2)C)c2ccc(cc2)C)c(c1)/C=C/c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)OC)C |
| 1160 | COC(=O)[C]1C(=[N]=C2N1C=C(C=C2c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(s1)/C=C(\C(=O)O)\C#N)C   |
| 1161 | N#C/C(=C/c1ccc(s1)C1=CN2[CH]C(=[N]=C2C(=C1)c1ccc(cc1)N(c1cccc1)c1cccc1)  |

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|      | C)/C(=O)O   |
| 1162 | CCCCCCC1(CCCCCC)c2cc(ccc2-c2c1cc(cc2)c1sc2c(c1)n(c1c2sc(c1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)c1sc2c(c1)n(c1c2sc(c1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C            |
| 1163 | CC1(C)c2cc(ccc2-c2c1c1-c3ccc(cc3C(c1c1-c3c(C(c21)(C)C)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#C)(C)C)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC   |
| 1164 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)/C(=O)O   |
| 1165 | CCCCC1(CCCC)c2cc(ccc2-c2c1cc(cc2)/C=C(/C(=O)O)\C#N)N(c1cccc1)c1cccc1  |
| 1166 | CCCCC1(CCCC)c2cc(ccc2-c2c1cc(cc2)/C=C(/C(=O)O)\C#N)N(c1ccc(cc1)OC)c1ccc(cc1)OC  |
| 1167 | CC1(C)c2cc(ccc2-c2c1cc(cc2)/C=C(/C(=O)O)\C#N)N(c1ccc(cc1)OCCOC(C(F)(F)F)(C(F)(F)F)C(F)(F)F)c1ccc(cc1)OCCOC(C(F)(F)F)(C(F)(F)F)C(F)(F)F)C(F)(F)F   |
| 1168 | N#C/C(=C\c1ccc2-c3c(C(c2c1)(CCOC(C(F)(F)F)(C(F)(F)F)C(F)(F)F)CCCOC(C(F)(F)F)(C(F)(F)F)C(F)(F)F)cc(cc3)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1169 | N#C/C(=C\c1ccc2-c3c(C(c2c1)(CCOC(C(F)(F)F)(C(F)(F)F)C(F)(F)F)CCCOC(C(F)(F)F)(C(F)(F)F)C(F)(F)F)cc(cc3)N(c1ccc(cc1)OCCOC(C(F)(F)F)(C(F)(F)F)C(F)(F)F)c1ccc(cc1)OCCOC(C(F)(F)F)(C(F)(F)F)C(F)(F)F)/C(=O)O |
| 1170 | CCCCC1(CCCC)c2cc(ccc2-c2c1cc(cc2)C(=O)O)N(c1cccc1)c1cccc1   |
| 1171 | c1ccc(cc1)N(c1cccc1)c1ccc(cc1)[CH][N]/N=C/1\C]2C=CC=[N]=C2C2=[N]=C[CH]C=C12   |
| 1172 | N#C/C(=C/c1ccc(s1)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc(cc1)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O  |
| 1173 | N#C/C(=C/c1cc(c(s1)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc(cc1)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O   |
| 1174 | CCCCCOCc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 1175 | CCCCCOCc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(c2c1nsn2)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 1176 | CCCCCCCCC1=[N]=c2c(ccc(c2=[N]=C1CCCCC)C)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1177 | Cc1ccc(s1)C1=[N]=c2c(=[N]=C1c1ccc(s1)C)c(ccc2c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 1178 | CCCCCCCCc1sc2c(c1)c1cc(sc1c1=[N]=c3c(=[N]=c21)c(ccc3c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)CCCCCCCC  |
| 1179 | CCCCCec1cc(sc1/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc(c1)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C=C(\C(=O)O)/C#N   |
| 1180 | N#C/C(=C\c1ccc(s1)c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O   |
| 1181 | N#C/C(=C\c1sc(e2c1OCCO2)c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O   |
| 1182 | CCCCCCCCCCCC1=[N]=C(S[C]1c1ccc(cc1)N(c1ccc(cc1)C)c1cccc1)C1=[N]=C([C](S1)c1ccc(s1)/C=C(/C(=O)O)\C#N)CCCCCCCC  |

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| 1183 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(=O)c2c1)cc(cc3)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)/C(=O)O                              |
| 1184 | N#C/C(=C\c1ccc(cc1)/C=C/c1cc2CCc3ccc(CCc1cc2)cc3/C=C/c1ccc(cc1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O                         |
| 1185 | COc1cc(/C=C/e2ccc(cc2)N(c2cccc2)c2cccc2)c(cc1/C=C/c1cc2ccc1CCc1ccc(CC2)c(c1)/C=C/c1cc(OC)c(cc1OC)/C=C(/C(=O)O)\C#N)OC           |
| 1186 | N#C/C(=C\c1ccc(s1)c1cc2CCc3ccc(CCc1cc2)cc3c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1187 | CCCCCCC1(CCCCCC)c2cc(sc2-c2c1cc(s2)C1=CC2=[N]=C(C(=C[C]2C=C1)/C=C(\C(=O)O)/C#N)Cl)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC |
| 1188 | CCCCCCC1(CCCCCC)c2cc(sc2-c2c1cc(s2)c1ccc2c(c1)[nH]c(=O)c(c2)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC     |
| 1189 | CCCCCCC1(CCCCCC)c2cc(sc2-c2c1cc(s2)c1ccc2c(c1)[nH]c(=O)c(c2)C=C(C#N)C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC           |
| 1190 | CCCCCCC1(CCCCCC)c2cc(sc2-c2c1cc(s2)c1ccc2c(c1)[nH]c(=O)c(c2)C(=O)O)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC                |
| 1191 | CCCCCCC1(CCCCCC)c2cc(sc2-c2c1cc(s2)C1=CC2=[N]=C(C(=C[C]2C=C1)C(=O)O)Cl)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC            |
| 1192 | CCCCCCC1(CCCCCC)c2cc(sc2-c2c1cc(s2)c1ccc2c(c1)[nH]c(=O)c(c2)C=O)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC                   |
| 1193 | N#C/C(=C\c1ccc(s1)c1cc2c(o1)cc(cc2)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O                          |
| 1194 | N#C/C(=C/c1ccc(s1)/C=C/c1cc2c(o1)cc(cc2)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O                     |
| 1195 | N#C/C(=C\c1ccc(cc1)c1nnc(o1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1196 | N#C/C(=C/c1ccc(cc1)c1nnc(o1)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)/C(=O)O   |
| 1197 | N#C/C(=C/c1ccc(cc1)c1nnc(o1)c1ccc(cc1)N(c1ccc(cc1)CC)c1ccc(cc1)CC)/C(=O)O   |
| 1198 | N#C/C(=C\c1ccc(cc1)c1nnc(o1)c1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C(=O)O   |
| 1199 | N#C/C(=C\c1sc(c1c1ccc(cc1)N(c1cccc1)c1cccc1)c1cccc(c1)N(c1cccc1)c1cccc1)/C=C(/C(=O)O)\C#N)/C(=O)O                               |
| 1200 | N#C/C(=C/c1ccc(cc1)N(c1ccc(cc1)/C=C\c1cccc1)c1ccc(cc1)/C=C\c1cccc1)/C(=O)O  |
| 1201 | Cc1ccc(cc1)C1(c2ccc(cc2)C)c2cc(ccc2-c2c1cc(s2)c1ccc(s1)c1ccc(cc1)C(=O)O)N(c1ccc(cc1)C)c1ccc(cc1)C                               |
| 1202 | COc1cc(OC)ccc1c1ccc(cc1)N(c1ccc2c(c1)sc1c2sc(c1)[C@]1(CC=C(S1)c1ccs1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(cc1OC)OC                 |
| 1203 | CCCCCOc1cc(OCCCCC)ccc1c1ccc(cc1)N(c1ccc2c(c1)sc1c2sc(c1)c1cc2c(s1)cc(s2)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(cc1OCCCCC)OCCCCC      |
| 1204 | COc1cc(OC)ccc1c1ccc(cc1)N(c1ccc2c(c1)sc1c2sc(c1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(cc1OC)OC                                      |
| 1205 | N#C/C(=C\c1ccc(s1)c1ccc2c(c1)c1cccc1n2c1ccc(cc1)N(c1ccc(cc1)n1c2cccc2c2c1ccc2)c1ccc(cc1)n1c2cccc2c2c1cccc2)/C(=O)O              |
| 1206 | O1C(=O)CNC(=S)S/C(=C\c2ccc(s2)c2ccc3c(c2)c2cccc2n3c2ccc(cc2)N(c2ccc(cc2)n2c3cccc3c3c2cccc3)/C1=O                                |

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| 1207 | <chem>Cc1ccc(cc1)C1(c2ccc(cc2)C)c2cc(ccc2-c2c1cc(s2)c1ccc(s1)c1ccc(c2c1nsn2)c1ccc(cc1)C(=O)O)N(c1ccc(cc1)C)c1ccc(cc1)C</chem>  |
| 1208 | <chem>CCCC[C@@H](CN1C(=O)C2=C(N(C(=O)C2=C1c1ccc(s1)c1sc2-c3c(C(c2c1)(c1ccc(cc1)C)c1ccc(cc1)C)cc(cc3)N(c1ccc(cc1)C)c1ccc(cc1)C)C[C@@H](CCCC)CC)c1ccc(s1)c1ccc(cc1)C(=O)O)CC</chem>            |
| 1209 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)C1=[N]=C2C(=C(C(=C[C]2c2ccc(s2)/C=C(\C(=O)O)/C#N)c2ccc(s2)/C=C(/C(=O)O)\C#N)N1CCCCC</chem>                                       |
| 1210 | <chem>COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)C1=[N]=C2C(=C(C(=C[C]2c2cc(c(s2)/C=C(\C(=O)O)/C#N)C)c2cc(c(s2)/C=C(/C(=O)O)\C#N)C)N1C</chem>  |
| 1211 | <chem>COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)C1=[N]=C2C(=C(C(=C[C]2c2ccc(s2)e2sc(c(c2)C)/C=C(/C(=O)O)\C#N)c2ccc(s2)e2sc(c(c2)C)/C=C(/C(=O)O)\C#N)N1C</chem>                                    |
| 1212 | <chem>CCCCCCn1c2cc(/C=C/c3ccc(cc3)N(c3cccc3)c3cccc3)ccc2c2c1ccc(c2)/C=C(/C(=O)O)\C#N</chem>  |
| 1213 | <chem>Cn1c2ccc(cc2c2c1cc(/C=C/c1ccc(cc1)N(c1ccc(cc1)/C=C\c1ccc3c(c1)n(C)c1c3cc(cc1)/C=C(\C(=O)O)/C#N)c1cccc1)cc2)/C=C(/C(=O)O)\C#N</chem>  |
| 1214 | <chem>Cn1c2cc(/C=C/c3ccc(cc3)N(c3ccc(cc3)/C=C\c3ccc4c(c3)n(C)c3c4cc(cc3)/C=C(\C(=O)O)/C#N)c3ccc(cc3)/C=C\c3ccc4c(c3)n(C)c3c4cc(cc3)/C=C(\C(=O)O)/C#N)ccc2c2c1ccc(c2)/C=C(\C(=O)O)/C#N</chem> |
| 1215 | <chem>OC(=O)CN1C(=S)S/C(=C\c2ccc(s2)c2ccc(cc2)N(c2ccc(cc2)n2c3ccc(cc3c3c2ccc(c3)C(C)(C)C(C)(C)C)c2ccc(cc2)n2c3ccc(cc3c3c2ccc(c3)C(C)(C)C)C(C)(C)C)/C1=O</chem>                               |
| 1216 | <chem>CCCC[C]1c2e(c(c(n2[B](n2c1c(C)c(c2C)c1ccc(o1)/C=C(/C(=O)O)\C#N)(F)F)C)c1ccc2c(c1)n(CCC)c1c2cc(cc1)OC)C</chem>  |
| 1217 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)[CH]C1=c2ccc(cc2=C2[C]1C=CC(=C2)N(c1ccc(cc1)OC)c1ccc(cc1)OC)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C(=O)O</chem>  |
| 1218 | <chem>COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc2c(c1)C1=CC(=C[CH]C1=C2[CH]c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)N(c1ccc(cc1)OC)c1ccc(cc1)OC</chem>  |
| 1219 | <chem>N#C/C(=C/c1ccc(s1)[CH]C1=c2c(=C3[C]1C=CC(=C3)N(c1ccc(cc1)OC)c1ccc(cc1)OC)cc(cc2)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C(=O)O</chem>   |
| 1220 | <chem>N#C/C(=C\c1cc(c(s1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1221 | <chem>N#C/C(=C\c1cc(c(s1)c1sc(cc1c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 1222 | <chem>N#C/C(=C\c1cc(c(s1)c1sc(cc1c1ccc(cc1)N(c1cccc1)c1cccc1)c1sc(c(c1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1223 | <chem>COc1cc(OC)ccc1c1ccc(cc1)N(c1ccc2c(c1)sc1c2sc(c1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(cc1)OC)OC</chem>  |
| 1224 | <chem>CCCCCc1cc(sc1c1ccc(s1)[CH]C1=c2ccc(cc2=C2[C]1C=CC(=C2)N(c1cccc1)c1cccc1)N(c1cccc1)c1cccc1)/C=C(/C(=O)O)\C#N</chem>   |
| 1225 | <chem>CCCCCc1cc(sc1c1ccc(s1)[CH]C1=c2ccc(cc2=C2[C]1C=CC(=C2)N(c1ccc(cc1)OC)c1ccc(cc1)OC)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C=C(/C(=O)O)\C#N</chem>   |
| 1226 | <chem>Cc1cc(sc1c1ccc(s1)[CH]C1=c2ccc(cc2=C2[C]1C=CC(=C2)N(c1ccc(cc1)OC)c1ccc(cc1)OC)N(c1ccc(cc1)OC)c1ccc(cc1)OC)/C=C(\C(=O)O)/C#N</chem>   |
| 1227 | <chem>N#C/C(=C/c1ccc(s1)[C]1C=CC(=C2C1=N[Se]N2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=</chem>   |

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| 1228 | CCCCCCCCOe1ccc(cc1)N(c1ccc(cc1)OCCCCCCC)c1ccc(cc1)c1ccc(c2c1n[se]n2)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 1229 | CCCCCCCCOe1ccc(cc1)N(c1ccc(cc1)OCCCCCCC)c1ccc(cc1)c1ccc(c2c1n[se]n2)c1ccc(cc1)/C=C(\C(=O)O)/C#N   |
| 1230 | CCCCCOe1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCCC   |
| 1231 | CCCCCOe1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCCC   |
| 1232 | CCCCCOe1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCCC  |
| 1233 | COe1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)/C=C/c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC   |
| 1234 | COe1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)/C=C\c1ccc(cc1)/C=C\c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC                                      |
| 1235 | Cn1e2cccc2e2c1ccc(c2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)c1-e2cccc2C(c1e1-c2c(C(c31)(C)C)cccc2)(C)C)c1ccc(cc1)c1sc2-c3c(C(c2c1)(C)C)cc(s3)/C=C(/C(=O)O)\C#N                          |
| 1236 | CN1e2ccc(cc2Sc2e1cccc2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)c1-e2cccc2C(c1e1-c2c(C(c31)(C)C)cccc2)(C)C)c1ccc(cc1)c1sc2-c3c(C(c2c1)(C)C)cc(s3)/C=C(/C(=O)O)\C#N                        |
| 1237 | CCCCCOe1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc2-c3c(C(c2c1)(CCCC)CCCC)cc(s3)/C=C(/C(=O)O)\C#N  |
| 1238 | N#C/C(=C\c1cc(OCCC(C)C)c(cc1OCCC(C)C)/C=C/c1ccc(cc1)N(c1ccc2c(-c3cccc3C2(C)C)c1)c1ccc2c(-c3cccc3C2(C)C)c1)/C(=O)O   |
| 1239 | N#C/C(=C\c1cc(OCCC(C)C)c(cc1OCCC(C)C)/C=C\c1cc(OCCC(C)C)c(cc1OCCC(C)C)/C=C/c1ccc(cc1)N(c1ccc2c(-c3cccc3C2(C)C)c1)c1ccc2c(-c3cccc3C2(C)C)c1)/C(=O)O                                  |
| 1240 | N#C/C(=C\c1cc(OCCC(C)C)c(cc1OCCC(C)C)/C=C/c1cc(OCCC(C)C)c(cc1OCCC(C)C)/C=C/c1cc(OCCC(C)C)c(cc1OCCC(C)C)/C=C/c1ccc(cc1)N(c1ccc2c(-c3cccc3C2(C)C)c1)c1ccc2c(-c3cccc3C2(C)C)c1)/C(=O)O |
| 1241 | N#C/C(=C\c1ccc(cc1)c1ccc(n1C)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1242 | N#C/C(=C\c1ccc(s1)c1ccc(n1C)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1243 | N#C/C(=C\c1ccc(s1)c1ccc(n1C)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1244 | N#C/C(=C\c1ccc(s1)c1ccc(n1C)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O  |
| 1245 | CCCCCN1e2ccc(cc2e2c1ccc(e2)N(c1cccc1)c1cccc1)c1ccc(n1C)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 1246 | N#C/C(=C\c1ccc(n1C)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1247 | N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O  |
| 1248 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1cccc2c1cccc2)c1cccc1)/C(=O)O   |

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| 1249 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)C1=CC=CCC1)/C(=O)O</chem>  |
| 1250 | <chem>CCCCCCCCN1C(=O)C2=C(N(C(=O)C2=C1c1ccc(s1)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)CCCCCCC)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>  |
| 1251 | <chem>CCCCCCCCN1C(=O)C2=C(N(C(=O)C2=C1c1ccc(s1)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(CCCCC)CCCCC)cccc3)c1ccc2-c3c(C(c2c1)(CCCCC)CCCCC)cccc3)CCCCCCC)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>            |
| 1252 | <chem>N#C/C(=C\c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1cccc1)c1cccc1)/C(=O)O</chem>                             |
| 1253 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1cccc1)c1cccc1)/C(=O)O</chem>           |
| 1254 | <chem>N#C/C(=C/c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2c(-c3ccc(cc3C2(CC)CC)C(c2cccc2)c2cccc2)c1)c1cccc1)/C(=O)O</chem>  |
| 1255 | <chem>N#C/C(=C/c1ccc(s1)c1ccc(s1)c1ccc2-c3c(C(c2c1)(CC)CC)cc(cc3)N(c1ccc2c(-c3ccc(cc3C2(CC)CC)C(c2cccc2)c2cccc2)c1)c1cccc1)/C(=O)O</chem>   |
| 1256 | <chem>CC1(c2cc(ccc2-e2c1cc(cc2)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C)C</chem>   |
| 1257 | <chem>C(C1(CC(C)C)c2cc(ccc2-e2c1cc(cc2)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C)C(C)C</chem>                                     |
| 1258 | <chem>CC1(C)c2cc(ccc2-e2c1cc(cc2)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C</chem>                               |
| 1259 | <chem>CCCC[C@H](C[C@@]1(C[C@H](CCCC)CC)c2cc(ccc2-e2c1cc(cc2)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)C)CC</chem> |
| 1260 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)C)c1cccc1)/C(=O)O</chem>  |
| 1261 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)C)c1cccc1)/C(=O)O</chem>   |
| 1262 | <chem>CCCC1(CCCC)c2cc(ccc2-e2c1cc(cc2)N(c1ccc2c(c1)c1cccc1n2CC)c1ccc2-c3c(C(c2c1)(CCCC)CCCC)cc(cc3)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>   |
| 1263 | <chem>CCCC1(CCCC)c2cc(ccc2-e2c1cc(cc2)N(c1ccc2c(c1)c1cccc1n2CC)c1ccc2-c3c(C(c2c1)(CCCC)CCCC)cc(cc3)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>                                 |
| 1264 | <chem>N#C/C(=C/c1ccc(cc1)N(c1cccc1)c1ccc(cc1)/C=C\1/SC(=C(S1)SC)SC)/C(=O)O</chem>   |
| 1265 | <chem>CSC1=C(SC)S/C(=C/c2ccc(cc2)N(c2ccc(cc2)/C=C(\C(=O)O)/C#N)c2ccc(cc2)/C=C(\C(=O)O)/C#N)/S1</chem>   |
| 1266 | <chem>OC(=O)c1cc2C(=O)C(=Cc3ccc(cc3)N(c3cccc3)c3cccc3)C(=O)c2cc1C(=O)O</chem>   |
| 1267 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)C=C1C(=O)c2c(C1=O)cc(c(c2)C(=O)O)C(=O)O</chem>   |
| 1268 | <chem>N#C/C(=C\c1ccc(cc1)N(c1ccc(cc1)c1cccc1)c1ccc(cc1)c1cccc1)/C(=O)O</chem>   |
| 1269 | <chem>N#C/C(=C\c1ccc(cc1)N(c1ccc(cc1)C#Cc1cccc1)c1ccc(cc1)C#Cc1cccc1)/C(=O)O</chem>   |
| 1270 | <chem>CCCCCCCCN1C(=O)C2=C(N(C(=O)C2=C1c1ccc(s1)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(CCCCC)CCCCC)cccc3)c1ccc2-c3c(C(c2c1)(CCCCC)CCCCC</chem>  |

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|      | C)cccc3)CCCCCCCC)c1ccc(s1)c1ccc(cc1)/C=C(/C(=O)O)\C#N   |
| 1271 | N#C/C(=C/c1ccc(s1)c1ccc(s1)c1sc(e2c1OCCO2)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O  |
| 1272 | Cc1cc(se1c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1cccc1)c1ccc(e2c1Insn2)c1cc(c(s1)c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1cccc1)C                              |
| 1273 | CCCCCCCCCCCCc1cc(se1c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1cccc1)c1cc2e(s1)c1c(s2)cc(s1)c1cc(c(s1)c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1cccc1)CCCCCCCCCCCC |
| 1274 | CCCCCCCCCCCCc1cc(se1c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1cccc1)c1sc2e(c1)sc1e2sc(c1)c1cc(c(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)CCCCCCCCCCCC                       |
| 1275 | O=C1N/C(=C\c2ccc(cc2)N(c2cccc2)c2cccc2)/C(=O)N1   |
| 1276 | O=C1S/C(=C\c2ccc(cc2)N(c2cccc2)c2cccc2)/C(=O)N1   |
| 1277 | O=C1NC(=O)/C(=C/c2ccc(cc2)N(c2ccc(cc2)/C=C/2\NC(=O)NC2=O)c2cccc2)/N1  |
| 1278 | O=C1NC(=O)/C(=C\c2ccc(cc2)N(c2ccc(cc2)/C=C/2\SC(=O)NC2=O)c2cccc2)/S1  |
| 1279 | CCN(c1ccc(cc1)/C=C/N([O])O)CC   |
| 1280 | OC(=O)/C=C\c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 1281 | ON([O])/C=C\c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1282 | OC(=O)/C=C\c1ccc(cc1)N(c1ccc(cc1)/C=C\C(=O)O)c1cccc1  |
| 1283 | ON([O])/C=C\c1ccc(cc1)N(c1ccc(cc1)/C=C\N([O])O)c1cccc1  |
| 1284 | N#C/C(=C/c1sc(e2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O   |
| 1285 | N#C/C(=C/c1sc(e2c1OCCO2)c1ccc(cc1)N(c1ccc(cc1)c1sc(e2c1OCCO2)/C=C(\C(=O)O)/C#N)c1cccc1)/C(=O)O  |
| 1286 | N#C/C(=C/c1sc(e2c1OCCO2)c1ccc(cc1)N(c1ccc(cc1)c1sc(e2c1OCCO2)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc2c(c1)[nH]c1e2cccc1)/C(=O)O   |
| 1287 | O=C1OC(=O)/C(=C/c2ccc(cc2)/C=C\c2ccc(cc2)N(c2ccc(cc2)/C=C/c2ccc(cc2)/C=C\2/SC(=S)N(C2=O)CC(=O)O)c2cccc2)/SC(=S)NC1  |
| 1288 | OC(=O)CN1C(=S)S/C(=C\c2ccc(cc2)N(c2ccc(cc2)/C=C/2\SC(=S)N(C2=O)CC(=O)O)c2cccc2)/C1=O  |
| 1289 | N#C/C(=C\c1en(cc1c1ccc(cc1)N(c1ccc(cc1)c1n(cc1/C=C(/C(=O)O)\C#N)C)c1cccc1)C)/C(=O)O   |
| 1290 | CC(CN1C(=C2C(=C(N(C2=O)CC(C)C)c2ccc(s2)c2ccc(s2)/C=C(\C(=O)O)/C#N)C1=O)c1ccc(s1)c1sc(e2c1OCCO2)c1ccc(cc1)N(c1cccc1)c1cccc1)C                                      |
| 1291 | N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc(s1)/C(=O)O   |
| 1292 | N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)/C(=O)O   |
| 1293 | CCCOc1ccc(cc1)N(c1ccc(cc1)OCCCC)c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N  |
| 1294 | CCCOc1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 1295 | N#C/C(=C/c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)/C(=O)O   |
| 1296 | N#C/C(=C\c1ccc(s1)/C=C\c1ccc(cc1)N(c1ccc(cc1)/C=C/c1ccc(s1)/C=C(/C(=O)O)\C#N)c1cccc1)/C(=O)O  |



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| 1297 | <chem>OC(=O)CN1C(=S)S/C(=C/c2ccc(s2)/C=C/c2ccc(cc2)N(c2ccc(cc2)/C=C/c2ccc(s2)/C=C\2/SC(=S)NCC(=O)OC2=O)c2ccccc2)/C1=O</chem>  |
| 1298 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>  |
| 1299 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1sc(e2c1OCCO2)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OCCCCC</chem>  |
| 1300 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1sc(e2c1OCCO2)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1sc(e2c1OCCO2)/C=C(\C(=O)O)/C#N</chem>  |
| 1301 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc2-c3c(C(c2c1)(CCCCC)CCCCC)cc(s3)/C=C(/C(=O)O)\C#N</chem>   |
| 1302 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1sc2-c3c(C(c2c1)(CCCCC)CCCCC)cc(s3)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1sc2-c3c(C(c2c1)(CCCCC)CCCCC)cc(s3)/C=C(/C(=O)O)\C#N</chem>                          |
| 1303 | <chem>CCCCCOc1ccc(cc1)N1[C@@H]2[C@@H]3S[C@@H]([C@@H]([C@@H]3[C@@H]2[C@@H]2[C@@H]1C[C@@H](S2)c1sc(cc1CCCCC)/C=C(\C(=O)O)/C#N)CCCCC)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC</chem>  |
| 1304 | <chem>CCCCCOc1ccc(cc1)N1[C@@H]2C[C@@H](S[C@@H]2[C@@H]2[C@@H]1[C@@H]1S[C@@H]([C@@H]([C@@H]1S2)CCCCC)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC</chem>               |
| 1305 | <chem>CCCCCOc1ccc(cc1)N1[C@@H]2C[C@@H](S[C@@H]2[C@@H]2[C@@H]1[C@@H]1S[C@@H]([C@@H]([C@@H]1S2)CCCCC)/C=C(/C(=O)O)\C#N)c1sc(cc1CCCCC)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC</chem> |
| 1306 | <chem>CCCCCOc1ccc(cc1)N1[C@@H]2[C@@H]3S[C@@H]([C@@H]([C@@H]3[C@@H]2[C@@H]2[C@@H]1C[C@@H](S2)/C=C(/C(=O)O)\C#N)CCCCC)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC</chem>                |
| 1307 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1)OCCCCC)OCCCCC)c1ccc(cc1)c1sc2-c3c(C(c2c1)(CCCCC)CCCCC)cc(s3)/C=C(/C(=O)O)\C#N</chem>                                  |
| 1308 | <chem>COc1cc(OC)c2-c3c(C(c2c1)(C)C)ccc(c3)N(c1ccc2-c3c(C(c2c1)(C)C)cc(cc3OC)OC)c1ccc(cc1)c1sc2-c3c(C(c2c1)(C)C)cc(s3)/C=C(\C(=O)O)/C#N</chem>   |
| 1309 | <chem>CCCC[C@@H](COc1ccc(cc1)N(c1ccc(cc1)OC[C@@H](CCCC)CC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)CC</chem>   |
| 1310 | <chem>CN1c2ccc(cc2C(/C/1=C/C=C\c1n(C)c2c(e1C)c1ccc(cc1cc2)C1=NNN([CH]1)CCN1C(=O)c2ccccc3c2c(C1=O)ccc3[C]1N[N]N=C1c1ccc(cc1)N(c1ccccc1)c1ccccc1)(C)C(=O)O.C.[I]</chem>                   |
| 1311 | <chem>CCCCCCC1(CCCCCC)c2ccc(ccc2-c2c1cc(cc2)N(c1ccc(cc1)C(=O)O)c1ccc(cc1)C(=O)O)c1ccc(s1)C=C1C(=O)N(CC)C(=S)N(C1=O)CC</chem>  |
| 1312 | <chem>CCCCCCC1(CCCCCC)c2ccc(ccc2-c2c1cc(s2)C=C(C#N)C#N)c1ccc(cc1)N(c1ccc(cc1)C(=O)O)c1ccc(cc1)C(=O)O</chem>   |
| 1313 | <chem>N#CC(=Cc1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)C=C(C#N)C#N)c1ccc(cc1)C(=O)O)C#N</chem>  |
| 1314 | <chem>N#CC(=Cc1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)C(=O)O)c1ccc(cc1)C(=O)O)C#N</chem>  |
| 1315 | <chem>N#CC(=Cc1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)C(=O)O)c1ccc(cc1)C(=O)O)C#N</chem>   |
| 1316 | <chem>N#CC(=Cc1sc(e2c1OCCO2)c1ccc(cc1)N(c1ccc(cc1)C(=O)O)c1ccc(cc1)C(=O)O)C#N</chem>  |
| 1317 | <chem>N#C/C(=C\C[C@@H]1COc2c(O1)c(sc2COCCCCCCCCOCC1sc(e2c1OC[C@@H](O2)/</chem>  |

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|      | <chem>C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 1318 | <chem>N#C/C(=C/c1sc(c2c1O[C@@H](COCCCCCCCCOC[C@@H]1COc3c(O1)c(sc3/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1)CO2)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 1319 | <chem>N#C/C(=C/[C@@H]1COc2c(O1)c(COCCCCCCCCOCc1sc(c3c1O[C@H](CO3)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1)sc2c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1320 | <chem>COC[C@@H]1COc2c(O1)c(sc2/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1</chem>  |
| 1321 | <chem>COC[C@H]1COc2c(O1)c(/C=C(/C(=O)O)\C#N)sc2c1ccc(cc1)N(c1cccc1)c1cccc1</chem>   |
| 1322 | <chem>CCCCCCC1(CCCCCC)c2cc(sc2-c2c1cc(s2)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(c1)OCCCCC)C1=[N]=C([CH]C(=C1)C(=O)O)C1=[N]=C([CH]C(=C1)C(=O)O)c1cc2c(-c3c(C2(CCCCC)CCCC)cc(s3)c2ccc(cc2)N(c2ccc(cc2)OCCCCC)c2ccc(cc2)OCCCCC)s1</chem> |
| 1323 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc2-c3c(C(c2c1)(CCCCC)CCCC)cc(s3)C1=[N]=C([C](C=C1)C(=O)O)C1=[N]=C([C](C=C1)C(=O)O)c1sc2-c3c(C(c2c1)(CCCCC)CCCC)cc(s3)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC</chem>   |
| 1324 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>   |
| 1325 | <chem>COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(c1)c1cc(ccc1c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)N(c1ccc(cc1)OC)c1ccc(cc1)OC)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>   |
| 1326 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1cc(c1s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1cc(sc1c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC</chem>   |
| 1327 | <chem>COc1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC</chem>   |
| 1328 | <chem>CN1c2ccc(cc2Sc2c1ccc(e2)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC</chem>  |
| 1329 | <chem>COc1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)ccc(c3)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>   |
| 1330 | <chem>COc1ccc(cc1)N(c1ccc2c(e1)n(C)c1c2cc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N</chem>   |
| 1331 | <chem>COc1ccc(cc1)C(c1cc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC)N(c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC)c1ccc(cc1)OC</chem>  |
| 1332 | <chem>CCCCCCC1(CCCCCC)c2cc(ccc2-c2c1cc(cc2)c1ccc(s1)C=C(C#N)C#N)N(c1ccc(cc1)C(=O)O)c1cccc1</chem>   |
| 1333 | <chem>CCCCCCC1(CCCCCC)c2cc(ccc2-c2c1cc(cc2)N(c1ccc(cc1)C(=O)O)c1cccc1)c1ccc(s1)c1ccc(s1)C=C(C#N)C#N</chem>  |
| 1334 | <chem>CCCCCCC1(CCCCCC)c2cc(ccc2-c2c1cc(cc2)N(c1ccc(cc1)C(=O)O)c1cccc1)c1ccc(s1)C=C1C(=O)N(CC)C(=S)N(C1=O)CC</chem>  |
| 1335 | <chem>CCCCC[Si]1(CCCCCC)c2cc(sc2-c2c1cc(s2)/C=C(\C(=O)O)/C#N)c1sc(c2c1OCCO2)c1ccc(cc1)N(c1ccc(cc1)OC[C@H](CCCC)CC)c1ccc(cc1)OC[C@@H](CCCC)CC</chem>   |

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| 1336 | OC(=O)N1C(=S)S/C(=C\c2ccc(s2)c2ccc(cc2)N(c2ccccc2)c2ccccc2)/C1=O  |
| 1337 | N#C[C]([C]1S/C(=C\c2ccc(s2)c2ccc(cc2)N(c2ccccc2)c2ccccc2)/C(=O)N1C)C(=O)O   |
| 1338 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)C#Cc1cc2CCc3ccc(CCCc1cc2)cc3)c1ccc(cc1)C#C[C@@]12[C@@H]3C4=CC=C2CCCC2=CC=C(CCC4)[C@H]3[C@H]12)/C(=O)O  |
| 1339 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)C#Cc1ccccc1)c1ccc(cc1)C#Cc1ccccc1)/C(=O)O  |
| 1340 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)/C=C/c1cc2CCc3ccc(CCCc1cc2)cc3)c1ccc(cc1)/C=C/c1cc2CCc3ccc(CCCc1cc2)cc3)/C(=O)O  |
| 1341 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)/C=C/c1ccccc1)c1ccc(cc1)/C=C/c1ccccc1)/C(=O)O  |
| 1342 | N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)/C(=O)O  |
| 1343 | N#C/C(=C\c1ccc(s1)c1sc(cc1c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O   |
| 1344 | N#C/C(=C\c1ccc(cc1)c1sc(cc1c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O  |
| 1345 | N#C/C(=C\c1ccc(cc1)c1sc(cc1c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O   |
| 1346 | CCCCCn1c2ccc(cc2c2c1ccc2)c1ccc(s1)c1sc(c(c1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1cc(s1)/C=C(/C(=O)O)\C#N  |
| 1347 | N#C/C(=C\c1ccc(s1)c1sc(cc1c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1ccccc1)c1ccccc1)/C(=O)O  |
| 1348 | c1ccc(cc1)N(c1ccc(cc1)C1=N[N]N([CH]1)Cc1ccc(cc1)/C=C/C1=[N]=C2C(=C[CH]C=C2)O1)c1ccc(cc1)C1=N[N]N([CH]1)Cc1ccc(cc1)[CH]/C=C\1\Ne2c(O1)cccc2  |
| 1349 | c1ccc(cc1)N(c1ccc(cc1)c1n[nH]nc1)c1ccc(cc1)C1=N[N]N([CH]1)Cc1ccc(cc1)/C=C/C1=[N]=C2[C](S1)C=CC=C2.[CH2]c1ccc(cc1)[CH]/C=C\1\Ne2c(S1)cccc2   |
| 1350 | c1ccc(cc1)N(c1ccc(cc1)C1=N[N]N([CH]1)Cc1cc(OCC2=N[N]N([CH]2)Cc2ccc(cc2)/C=C/C2=[N]=C3C(=C[CH]C=C3)O2)cc(c1)OC[C]1C=N[N]N1Cc1ccc(cc1)/C=C/C1=[N]=C2C(=C[CH]C=C2)O1)c1ccc(cc1)C1=N[N]N([CH]1)Cc1cc(OCC2=N[N]N([CH]2)Cc2ccc(cc2)/C=C/C2=[N]=C3C(=C[CH]C=C3)O2)cc(c1)OC[C]1C=N[N]N1Cc1ccc(cc1)/C=C/C1=[N]=C2C(=C[CH]C=C2)O1 |
| 1351 | c1ccc(cc1)N(c1ccc(cc1)C1=N[N]N([CH]1)Cc1cc(OCC2=N[N]N([CH]2)Cc2ccc(cc2)/C=C/C2=[N]=C3C(=C[CH]C=C3)S2)cc(c1)OC[C]1C=N[N]N1Cc1ccc(cc1)/C=C/C1=[N]=C2[C](S1)C=CC=C2)c1ccc(cc1)C1=N[N]N([CH]1)Cc1cc(OCC2=N[N]N([CH]2)Cc2ccc(cc2)/C=C/C2=[N]=C3[C](S2)C=CC=C3)cc(c1)OC[C]1C=N[N]N1Cc1ccc(cc1)/C=C/C1=[N]=C2[C](S1)C=CC=C2    |
| 1352 | [CH]1C=CC2=[N]=C(OC2=C1)/C=C/c1ccc(cc1)CN1[N]N=C([CH]1)c1ccc(cc1)N(c1ccc(cc1)C1=N[N]N([CH]1)Cc1ccc(cc1)/C=C/C1=[N]=C2C(=C[CH]C=C2)O1)c1ccc(cc1)C1=N[N]N([CH]1)Cc1ccc(cc1)/C=C/C1=[N]=C2C(=C[CH]C=C2)O1  |
| 1353 | C1=C[C]2C(=[N]=C(S2)/C=C/c2ccc(cc2)CN2[N]N=C([CH]2)c2ccc(cc2)N(c2ccc(cc2)C2=N[N]N([CH]2)Cc2ccc(cc2)/C=C/C2=[N]=C3[C](S2)C=CC=C3)c2ccc(cc2)C2=N[N]N([CH]2)Cc2ccc(cc2)/C=C/C2=[N]=C3[C](S2)C=CC=C3)C=C1   |
| 1354 | CCCCOe1cc(OCCCC)ccc1c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCCCC)OCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(s1)C1=CC(=[N]=C([CH]1)C(=O)O)C(=O)O   |

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| 1355 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)C1=[N]=C([C](N1C<br>CCCC)c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/<br>C#N                                 |
| 1356 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)c1ccc(s1)C1=[N]=C([C](N1C)c1ccc(cc1)c1cc<br>c(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N                               |
| 1357 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)C1=[N]=C2[C](N1<br>CCCCC)c1cc(sc1-c1c2cc(s1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(s1)/C=C(\C(=O)O)/<br>C#N                                  |
| 1358 | CC(Cc1ccc(s1)c1c2sc(cc2c(c2c1cc(s2)c1cc(c(s1)c1cc(c(s1)c1sc(c2c1OCCO2)/C=C(/C(<br>=O)O)\C#N)C)C)c1ccc(s1)C)c1cc(c(s1)c1cc(c(s1)c1sc(c2c1OCCO2)/C=C(/C(=O)O)\C#<br>N)C)C)C                    |
| 1359 | CCCCCN1C(=[N]=C([C]1c1ccc(cc1)c1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(<br>s1)/C=C(\C(=O)O)/C#N)c1ccc2c(c1)c1ccc1n2CCCCC   |
| 1360 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)c1ccc(s1)C1=[N]=C([C](N1C)c1ccc(cc1)c1cc<br>c(s1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 1361 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)C1=[N]=C([C](N1C<br>CCCCC)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#<br>N                                  |
| 1362 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1ccc(s1)C1=[N]=C2[C](N1<br>CCCCC)c1cc(sc1-c1c2cc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N)c1ccc(s1)/C=C(/C(=O)O)\<br>C#N                                  |
| 1363 | CCCCCn1c2ccc(cc2c2c1ccc2)C1=[N]=C([C](N1)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O<br>)\C#N)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 1364 | N#C/C(=C\c1ccc2c(-c3cc(ccc3[C@@]32c2cc(ccc2-c2c3cc(cc2)N(c2ccccc2)c2ccccc2)/C<br>=C(/C(=O)O)\C#N)N(c2ccccc2)c2ccccc2)c1)/C(=O)O  |
| 1365 | c1ccc(cc1)N(c1cccc1)c1ccc(cc1)/C=C/C1=CC=[N]=C[CH]1  |
| 1366 | CN1[CH]C=C(C=C1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1367 | c1ccc(cc1)N(c1cccc1)c1ccc(cc1)/C=C\C1=CC(=[N]=C([CH]1)/C=C/c1ccc(cc1)N(c1cc<br>ccc1)c1cccc1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1   |
| 1368 | CN1[C](/C=C/c2ccc(cc2)N(c2ccccc2)c2ccccc2)C=C(C=C1/C=C/c1ccc(cc1)N(c1cccc1)<br>c1cccc1)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1  |
| 1369 | CCc1c(C)c2n(c1C)[B](F)(F)n1c(c(c(e1[C]2c1ccc(cc1)N(c1ccc(cc1)[C]1c2c(c(c(n2[B](n<br>2c1c(C)c(c2C)CC)(F)F)C)CC)C)c1ccc(cc1)c1ccc(cc1)C(=O)O)C)CC)C  |
| 1370 | OC(=O)c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)[C]1c2ccc(n2[B](n2c1ccc2c1ccc(cc1)C(C)(C<br>)C)(F)F)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)[C]1c2ccc(n2[B](n2c1ccc2c1ccc(cc1)C(C)(C)C<br>)F)F)c1ccc(cc1)C(C)(C)C |
| 1371 | CCc1c(C)c2n(c1C)[B](F)(F)n1c(c(c(e1[C]2c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)[<br>C]1c2c(c(c(n2[B](n2c1c(C)c(c2C)CC)(F)F)C)CC)C)c1ccc(cc1)c1ccc(cc1)C(=O)O)C)C<br>C)C                      |
| 1372 | OC(=O)c1ccc(cc1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)[C]1c2ccc(n2[B](n2c1ccc2c1cccc1<br>)F)F)c1cccc1)c1ccc(cc1)c1ccc(s1)[C]1c2ccc(n2[B](n2c1ccc2c1cccc1)F)F)c1cccc1                                |
| 1373 | N#C/C(=C\c1ccc(s1)c1ccc(cc1)N(CCO[Si](C(C)(C)C)(C)C)/C(=O)O  |
| 1374 | CN(c1ccc(cc1)/C=C/c1ccc(s1)/C=C(/C(=O)O)\C#N)CCO[Si](C(C)(C)C)(C)C   |
| 1375 | N#C/C(=C\c1ccc(c2c1n2)N(c1ccc(cc1)N(CCO[Si](C(C)(C)C)(C)C)/C(=O)O  |

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| 1376 | <chem>N#C/C(=C\c1ccc(cc1)c1ccc(e2c1nsn2)c1ccc(cc1)N(CCO[Si](C(C)(C)C)(C)C)/C(=O)O</chem>  |
| 1377 | <chem>COc1cc(OC)ccc1c1ccc(cc1)N(c1ccc2c(c1)n(C)c1c2sc(c1)c1ccc(e2c1nsn2)c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(cc1OC)OC</chem>                                     |
| 1378 | <chem>Cn1c2cc(ccc2c2c1cc(s2)c1ccc(e2c1nsn2)c1ccc(cc1)/C=C(\C(=O)O)/C#N)N(c1ccc(cc1)c1ccc(cc1OC)OC)c1ccc(cc1)c1ccc(cc1OC)OC</chem>                                       |
| 1379 | <chem>CCCCCOc1cc(OCCCCC)ccc1c1ccc(cc1)N(c1ccc(cc1)c1sc(e2c1OCCO2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc(cc1OCCCCC)OCCCCC</chem>  |
| 1380 | <chem>COc1cc(OC)ccc1c1ccc(cc1)N(c1ccc(cc1)c1sc(e2c1OCCO2)c1sc(e2c1OCCO2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)c1ccc(cc1OC)OC</chem>   |
| 1381 | <chem>CCCCCCCCCCCC1(CCCCCCCCCC)c2cc(sc2-c2c1cc(s2)c1sc(e2c1OCCO2)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCCCCC)OCCCCC)c1ccc(cc1)c1ccc(cc1OCCCCC)OCCCCC)/C=C(/C(=O)O)\C#N</chem> |
| 1382 | <chem>CC1(C)c2cc(sc2[C@@]2([C]1[CH]2)S[C]c1sc(e2c1OCCO2)c1sc(e2c1OCCO2)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OC)OC)c1ccc(cc1)c1ccc(cc1OC)OC)/C=C(/C(=O)O)\C#N</chem>           |
| 1383 | <chem>COc1cc(OC)ccc1c1ccc(cc1)N(c1ccc2c(c1)sc1c2sc(c1)c1ccc(e2c1nsn2)c1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)c1ccc(cc1OC)OC</chem>  |
| 1384 | <chem>CCCCOc1ccc(cc1)N(C1=C[C]2C(=[N]=C(C=C2)/C=C(/C(=O)O)\C#N)C=C1)c1ccc(cc1)OCCCC</chem>  |
| 1385 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(s1)c1ccc(e2=[N]=C(C(=[N]=c12)c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 1386 | <chem>CCc1ccc(cc1)N(c1ccc(cc1)CC)c1ccc(cc1)c1ccc(e2=[N]=C(C(=[N]=c12)c1cccc1)c1cccc1)c1ccc(cc1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>  |
| 1387 | <chem>N#C/C(=C\c1cc2c(s1)cc(s2)c1ccc(e2=[N]=C(C(=[N]=c12)c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>   |
| 1388 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(e2=[N]=C(C(=[N]=c12)c1cccc1)c1cccc1)c1ccc(s1)c1ccc(s1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1389 | <chem>N#C/C(=C\c1sc2c(c1)sc1c2sc(c1)c1ccc(e2=[N]=C(C(=[N]=c12)c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1390 | <chem>CCc1ccc(cc1)N(c1ccc(cc1)CC)c1ccc(cc1)c1ccc(e2=[N]=C(C(=[N]=c12)c1cccc1)c1cccc1)c1ccc(cc1)c1ccc(s1)c1ccc(s1)/C=C(/C(=O)O)\C#N</chem>                               |
| 1391 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(e2=[N]=C(C(=[N]=c12)c1cccc1)c1cccc1)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)c1ccc2-c3c(C(c2c1)(CC)CC)cccc3)/C(=O)O</chem>              |
| 1392 | <chem>N#C/C(=C\c1ccc(s1)c1ccc(e2=[N]=C(C(=[N]=c12)c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1393 | <chem>OC(=O)C1=C[C]2C(=[N]=Cc3c(O[Zn]4N2C=C2C=C(C=C[C]2O4)N(c2cccc2)c2cccc2)ccc(c3)N(c2cccc2)c2cccc2)C=C1</chem>  |
| 1394 | <chem>Cc1cc(C)cc(c1)N(C1=CC2=CN3C4=C[C](C=CC4=[N]=Cc4c(O[Zn]3O[C]2C=C1)ccc(c4)N(c1cc(C)cc(c1)C)c1cc(C)cc(c1)C(=O)O)c1cc(C)cc(c1)C</chem>                                |
| 1395 | <chem>OC(=O)c1ccc2c(c1)N1[CH]c3cc(ccc3O[Zn@@]31Oc1c([CH]N23)cc(cc1)N(c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C)N(c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C</chem>               |
| 1396 | <chem>CCCCC1ccc(cc1)N(c1ccc(cc1)CCCC)c1ccc2c(c1)C=N[C@]13C=C(C=CC1=[N]=Cc1c(O[Zn]3O2)ccc(c1)N(c1ccc(cc1)CCCC)c1ccc(cc1)CCCC)C(=O)O</chem>                               |
| 1397 | <chem>CCCCCCCCc1ccc(cc1)N(c1ccc2c(c1)C=N[C@@]13C=C(C=CC1=[N]=Cc1c(O[Zn]3O</chem>  |

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|      | 2)ccc(c1)N(c1ccc(cc1)CCCCCCC)c1ccc(cc1)CCCCCCC)C(=O)O)c1ccc(cc1)CCCC<br>CCCC  |
| 1398 | OC(=O)c1cc2N3[CH]c4cc(ccc4O[Zn]43Oc3c([CH]N4c2cc1C(=O)O)cc(cc3)N(c1cccc1<br>)c1cccc1)N(c1cccc1)c1cccc1  |
| 1399 | O=C1NC(=O)/C(=C\c2ccc(s2)c2ccc(c3c2nsn3)c2ccc(cc2)N(c2cccc2)c2cccc2)/N1   |
| 1400 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)c1ccc(c2c1nsn2)c1ccc(s1)/C=C/1\NC(=O)NC<br>1=O   |
| 1401 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)/C=C/c1sc2c(c1)n(c1c2sc(c1)/C=C(/C(=O)O)\<br>C#N)c1ccc(cc1)N1c2cccc2Sc2c1cccc2   |
| 1402 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)/C=C/c1sc2c(c1)n(c1c2sc(c1)<br>/C=C(\C(=O)O)/C#N)c1ccc2-c3c(C(c2c1)(CCC)CCC)c1-c2cccc2C(c1c1-c2c(C(c31)(C<br>CC)CCC)cccc2)(CCC)CCC           |
| 1403 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)/C=C/c1sc2c(c1)n(c1c2sc(c1)<br>/C=C(/C(=O)O)\C#N)c1ccc(cc1)OCCCCC  |
| 1404 | CCCCCCC1=[N]=C(S[C]1c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1ccc(cc1)/C=<br>C(/C(=O)O)\C#N)C1=[N]=C([C](S1)c1ccc(cc1)N(c1ccc(cc1)/C=C(/C(=O)O)\C#N)c1cc<br>c(cc1)/C=C(/C(=O)O)\C#N)CCCCC |
| 1405 | CN1C(=C=Cc2ccc(cc2)N(c2cccc2)c2cccc2)C(c2c1ccc(c2)C(=O)O)(C)C.I   |
| 1406 | CC1(C)C(=[N]=C2C1=C[C](C=C2)C(=O)O)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1.CI  |
| 1407 | CC(COc1ccc(OCC(C)C)ccc1c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCC(C)C)OCC(C)C)c1cc<br>c(cc1)c1sc2-c3c([C@@](c2c1)(C)CC(C)C)cc(s3)/C=C(/C(=O)O)\C#N)C  |
| 1408 | C(CC1(CC(C)C)c2cc(sc2-c2c1cc(s2)c1ccc(c2c1nsn2)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1<br>OCC(C)C)OCC(C)C)c1ccc(cc1)c1ccc(cc1OCC(C)C)OCC(C)C)c1ccc(cc1)/C=C(/C(=O)<br>O)\C#N)(C)C                 |
| 1409 | CC(CC1(CC(C)C)c2cc(sc2-c2c1cc(s2)c1ccc(cc1)N(c1ccc(cc1)c1ccc(cc1OCC(C)C)OCC<br>(C)C)c1ccc(cc1)c1ccc(cc1OCC(C)C)OCC(C)C)c1ccc(c2c1nsn2)c1ccc(s1)/C=C(/C(=O)<br>O)\C#N)C                    |
| 1410 | CCCCCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCCCC)c1ccc(cc1)c1ccc(s1)c1ccc(c2=[N]<br>=CC=[N]=c12)c1ccc(s1)/C=C(/C(=O)O)\C#N   |
| 1411 | CCCC[C@@H](Cn1c2cc(ccc2c2=[N]=c3c(=[N]=c12)c(ccc3c1ccc(cc1)N(c1cccc1)c1cc<br>ccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(o1)/C=C(/C(=O)O)\C#N)CC   |
| 1412 | CCCC[C@H](Cn1c2=[N]=c3c(ccc(c3=[N]=c2c2c1cc(cc2)c1ccc(s1)/C=c/1\sc(=C(C#N)<br>C#N)[nH]c1=O)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)CC                                     |
| 1413 | CCCC[C@H](Cn1c2=[N]=c3c(ccc(c3=[N]=c2c2c1cc(cc2)c1ccc(o1)/C=c/1\sc(=C(C#N)<br>C#N)[nH]c1=O)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)CC                                     |
| 1414 | CCCC[C@@H](Cn1c2cc(ccc2c2=[N]=c3c(=[N]=c12)c(ccc3c1ccc(cc1)N(c1cccc1)c1cc<br>ccc1)c1ccc(cc1)N(c1cccc1)c1cccc1)c1ccc(s1)/C=C(/C(=O)O)\C#N)CC   |
| 1415 | CCCCCN1cc(c2c1cccc2)/C=C(\c1ccc(s1)/C=N/c1ccc(cc1)C(=O)O)/C#N   |
| 1416 | c1cc(ccc1)N(c1cccc1)c1ccc(cc1)/C=C(\C#N)/C(=O)O   |
| 1417 | c1cc(ccc1)N(c1cccc1)c1ccc(cc1)/C=C/c1ccc(s1)/C=C(/C#N)\C(=O)O   |
| 1418 | COc1ccc(cc1)N(c1ccc(cc1)OC)c1ccc(cc1)c1sc(c2c1OCCO2)[C]1C(=O)/C(=C\C2=CC=<br>C3[C](N2C)C=CC(=C3)/C=C/C(=O)O)/C1=O   |
| 1419 | CN1c2ccc3c(c2C(/C/1=C\CH)/C=C\1/N(C)c2c(C1(C)C)cc(cc2)C(=O)O)(C)C)ccc(c3)C  |

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|      | <chem>#Cc1ccc(c2c1nsn2)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1.[I]</chem>  |
| 1420 | <chem>CCCCN1/C(=C/[CH]/C=C\2/N(CCCC)c3c(C2(C)C)cc(cc3)C(=O)O)/C(c2c1ccc1c2ccc(c1)C#Cc1ccc(cc1)N(c1cccc1)c1cccc1)(C)C.[I]</chem>                                 |
| 1421 | <chem>CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1sc(c2c1OCCO2)C1=C(O)/C(=C\C2=CC=C3[C](N2C)C=CC(=C3)C(=O)O)/C1=O</chem>                                     |
| 1422 | <chem>COc1ccc(cc1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1ccc(c2c1nsn2)c1ccc(s1)/C=C\1/SC(=S)[C@H](C1=O)CC(=O)O)c1ccc(cc1)c1ccc(s1)c1ccc(cc1)OC</chem>                 |
| 1423 | <chem>CC1(C)c2cc(sc2-c2c1cc(s2)c1ccc(cc1)N(c1ccc(cc1)c1ccc(s1)c1ccc(cc1)OC)c1ccc(cc1)c1ccc(s1)c1ccc(cc1)OC)/C=C\1/SC(=S)[C@H](C1=O)CC(=O)O</chem>               |
| 1424 | <chem>COc1ccc(cc1)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)c1sc(c2c1OCCO2)/C=C\1/SC(=S)N(C1=O)CC(=O)O)c1ccc(cc1)c1ccc(s1)c1ccc(cc1)OC</chem>                              |
| 1425 | <chem>CCCC[C@H](CN1C(=C2C(=C(N(C2=O)C)[C@@H](CCCC)CC)c2ccc(cc2)c2ccc(o2)/C=C(/C(=O)O)\C#N)C1=O)c1ccc(s1)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC)CC</chem> |
| 1426 | <chem>N#C/C(=C\C1=CC2=C3CCCC3=C3[C@@])([C@@]2(S1)C)(C)SC(=C3)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)/C(=O)O</chem>  |
| 1427 | <chem>N#C/C(=C\C1sc(c1)C1=C(CCC1)c1cc(sc1C)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1)C)/C(=O)O</chem>  |
| 1428 | <chem>OC(=O)C1=CC2=C3CCCC3=C3[C@@])([C@@]2(S1)C)(C)SC(=C3)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1</chem>   |
| 1429 | <chem>Cc1sc(cc1C1=C(CCC1)c1cc(sc1C)C(=O)O)/C=C/c1ccc(cc1)N(c1cccc1)c1cccc1</chem>   |
| 1430 | <chem>N#C/C(=C/c1c(F)cc(cc1F)c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O</chem>                               |
| 1431 | <chem>N#C/C(=C/c1ccc(cc1F)c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O</chem>                                  |
| 1432 | <chem>N#C/C(=C/c1ccc(cc1)c1cc2c(s1)cc(s2)c1ccc(cc1)N(c1ccc2-c3c(C(c2c1)(C)C)cccc3)c1ccc2-c3c(C(c2c1)(C)C)cccc3)/C(=O)O</chem>                                   |
| 1433 | <chem>OC(=O)CN1C(=S)S/C(=C\c2ccc(cc2)N(c2ccc(cc2)/C=C/2\C(=O)N(C(=S)S2)CC(=O)O)c2ccc(cc2)c2cccc3c2[nH]c2c3cccc2)/C1=O</chem>                                    |
| 1434 | <chem>OC(=O)CN1C(=S)S/C(=C\c2ccc(cc2)N(c2cccc2)c2cccc2)/C1=O</chem>   |
| 1435 | <chem>CCCCCN1c2cc(sc2c2c1cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1</chem>   |
| 1436 | <chem>CCCCCN1c2cc(ccc2c2c1c1c(s2)c2c(n1CCCCC)cc(s2)/C=C(/C(=O)O)\C#N)c1ccc(cc1)N(c1cccc1)c1cccc1</chem>   |
| 1437 | <chem>CCCCCc1cc(sc1c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC)c1ccc2c(c1)n(CCCCC)c1c2sc2c1n(CCCCC)c1e2sc(c1)/C=C(/C(=O)O)\C#N</chem>                         |
| 1438 | <chem>CCCCCN1c2cc(ccc2c2c1c1n(CCCCC)c3c(c1s2)sc(c3)/C=C(\C(=O)O)/C#N)c1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)OCCCCC</chem>                                       |
| 1439 | <chem>CCCCC[C@H](COc1ccc(cc1)N(c1ccc2c3c1cccc3c1c3c2ccc(c3ccc1)C#Cc1ccc(c2c1es)c2)c1ccc(cc1)C(=O)O)c1ccc(cc1)OC[C@@H](CCCCC)CCCC</chem>                         |
| 1440 | <chem>CCCCC[C@@H](COc1ccc(cc1)N(c1ccc2c3c1cccc3c1c3c2ccc(c3ccc1)C#Cc1ccc(s1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OC[C@@H](CCCCC)CCCC</chem>                              |
| 1441 | <chem>CC(COc1ccc(cc1)N(c1ccc2c3c1cccc3c1c3c2ccc(c3ccc1)C#Cc1ccc(cc1)/C=C(\C(=O)O)/C#N)c1ccc(cc1)OCC(C)C</chem>  |

|      |  |
|------|--|
| 1442 | CCCCC[C@@H](COc1ccc(cc1)N(c1ccc2c3c1cccc3c1c3c2ccc(c3ccc1)C#Cc1ccc(s1)C(=O)O)c1ccc(cc1)OC[C@H](CCCCC)CCCC)CCCC |
| 1443 | CCCCC[C@H](COc1ccc(cc1)N(c1ccc2c3c1cccc3c1c3c2ccc(c3ccc1)C#Cc1ccc(cc1)C(=O)O)c1ccc(cc1)OC[C@H](CCCCC)CCCC)CCCC |
| 1444 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1c2ccccc2c(c2c1cccc2)C#Cc1ccc(cc1)C(=O)O                         |
| 1445 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1c2ccccc2c(c2c1cccc2)C#CC#Cc1ccc(cc1)/C=C(/C(=O)O)\C#N           |
| 1446 | CCCCCOc1ccc(cc1)N(c1ccc(cc1)OCCCCC)c1ccc(cc1)c1c2ccccc2c(c2c1cccc2)C#CC#Cc1ccc(cc1)C(=O)O                      |

**Table S2. Descriptors of all the features used as input in the model.**

| Molecular orbital-related descriptors     |                       |                                       |                                      |  |   |
|---|-----------------------|---------------------------------------|--------------------------------------|--|---|
| Orbital energy (eV)                       | $E^L$                 | $E^{L+1}$                             | $E^{L+2}$                            | $E^{L+3}$                                | $E^{L+4}$                               |
|   | $E^H$                 | $E^{H-1}$                             | $E^{H-2}$                            | $E^{H-3}$                                | $E^{H-4}$                               |
| Orbital energy difference (eV)            | $\Delta E^H-E^L $     | $\Delta E^H-E^{L+1} $                 | $\Delta E^H-E^{L+2} $                | $\Delta E^H-E^{L+3} $                    | $\Delta E^H-E^{L+4} $                   |
|   | $\Delta E^{H-1}-E^L $ | $\Delta E^{H-1}-E^{L+1} $             | $\Delta E^{H-1}-E^{L+2} $            | $\Delta E^{H-1}-E^{L+3} $                | $\Delta E^{H-1}-E^{L+4} $               |
|   | $\Delta E^{H-2}-E^L $ | $\Delta E^{H-2}-E^{L+1} $             | $\Delta E^{H-2}-E^{L+2} $            | $\Delta E^{H-2}-E^{L+3} $                | $\Delta E^{H-2}-E^{L+4} $               |
|   | $\Delta E^{H-3}-E^L $ | $\Delta E^{H-3}-E^{L+1} $             | $\Delta E^{H-3}-E^{L+2} $            | $\Delta E^{H-3}-E^{L+3} $                | $\Delta E^{H-3}-E^{L+4} $               |
|   | $\Delta E^{H-4}-E^L $ | $\Delta E^{H-4}-E^{L+1} $             | $\Delta E^{H-4}-E^{L+2} $            | $\Delta E^{H-4}-E^{L+3} $                | $\Delta E^{H-4}-E^{L+4} $               |
| Geometry structure-related descriptors    |                       |                                       |                                      |  |   |
| Molecular volume ( $\text{\AA}^3$ )       | $V$                   |                                       |                                      |  |   |
| Molecular surface area ( $\text{\AA}^2$ ) | $S$                   |                                       |                                      |  |   |
| Molecular planarity ( $\text{\AA}$ )      | MPP                   |                                       | SDP                                  |  |   |
| Electronic structure-related descriptors  |                       |                                       |                                      |  |   |
| Molecular polarity                        | MPI (kcal/mol)        | Polar surface area ( $\text{\AA}^2$ ) | Proportion of polar surface area (%) | Nonpolar surface area ( $\text{\AA}^2$ ) | Proportion of nonpolar surface area (%) |

In the table, H and L represent the highest occupied molecular orbital and the lowest unoccupied molecular orbital.

### S3. Deep learning code used in the work

```
from sklearn.model_selection import train_test_split, KFold
import numpy as np
import pandas as pd
```



```

import tensorflow as tf
import tensorflow.keras as keras
from tensorflow.keras.models import load_model
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Dropout, BatchNormalization
from sklearn.metrics import mean_squared_error
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import r2_score
from sklearn.metrics import mean_absolute_percentage_error
from sklearn.preprocessing import MinMaxScaler
from sklearn.decomposition import PCA

# -----data_reader-----
fold = 10
test_size = 0.1
DF_data = pd.read_excel(r'C:\Users\Desktop\new\Jsc.xlsx')
DF_data = np.array(DF_data)

#normalization
scaler = MinMaxScaler()
dt = scaler.fit_transform(DF_data[:, :44])

#PCA
x=dt
pca = PCA(n_components=16) # dimensionality reduction
pca.fit(x)
# dimensionality reduction
x = pca.transform(x)

length_dt_x = dt.shape[0]
dt_x = x
dt_y = DF_data[:, -1]

dt_train_x, dt_test_x, dt_train_y, dt_test_y = train_test_split(dt_x, dt_y, random_state=24,
test_size=test_size)

length_train_x = dt_train_x.shape[0]
data_train_length = length_train_x // fold

kfolder = KFold(n_splits=fold, shuffle=True, random_state=42)
kfold = kfolder.split(dt_train_x, dt_train_y)

j = 0
k_train_pearson = []

```

```

k_val_pearson = []
k_train_MSE = []
k_val_MSE = []
k_train_R2 = []
k_val_R2 = []

# -----network-----
for train_index, val_index in kfold:
    k_x_train = dt_train_x[train_index] # training set
    k_y_train = dt_train_y[train_index] # Tag of training set tag
    k_x_vali = dt_train_x[val_index] # Testing set
    k_y_vali = dt_train_y[val_index] # Tag of testing set

    init = keras.initializers.he_normal(seed=42)
    model = Sequential() # initialization
    model.add(Dense(256, activation='relu', input_shape=(16,), kernel_initializer=init)) # Get a
fully connected layer
    model.add(BatchNormalization())
    model.add(Dropout(0.3))
    model.add(Dense(256, activation='relu', kernel_initializer=init)) # Get a fully connected
layer
    model.add(BatchNormalization())
    model.add(Dropout(0.3))
    model.add(Dense(128, activation='relu', kernel_initializer=init)) # Get a fully connected
layer
    model.add(Dense(128, activation='relu', kernel_initializer=init)) # Get a fully connected
layer
    model.add(Dense(1, activation='linear')) # Output layer

    filepath = r'C:\Users\Desktop\new\Jsc.h5'
    ## Once lifted, it covers once.
    checkpoint = keras.callbacks.ModelCheckpoint(filepath, monitor='val_loss', verbose=1,
save_best_only=True,
                                                mode='min',
save_weights_only=False, period=1)
    callbacks_list = [checkpoint]
    model.compile(optimizer=tf.keras.optimizers.Adam(lr=0.001, decay=4e-7), loss='mse',
metrics=['mae'])
    model.fit(k_x_train.astype(np.float32), k_y_train.astype(np.float32), batch_size=32,
epochs=500,
            validation_data=(k_x_vali.astype(np.float32), k_y_vali.astype(np.float32)),
callbacks=callbacks_list)

    y_pred_train = model.predict(k_x_train.astype(np.float32))

```

```

y_pred_valid = model.predict(k_x_vali.astype(np.float32))
print(y_pred_train.shape, np.corrcoef(k_y_train.astype(np.float32).T, y_pred_train.T,
rowvar=0).shape)
model = model.save(r'C:\Users\Desktop\new\Jsc.h5')
print('No.' + str(j + 1) + ' cross validation')
print('Pearson Coefficient of training set:',np.corrcoef(k_y_train.astype(np.float32),
y_pred_train, rowvar=0)[0][1])#r
k_train_pearson.append(np.corrcoef(k_y_train.astype(np.float32), y_pred_train,
rowvar=0)[0][1])
print('Pearson Coefficient of testing set:',np.corrcoef(k_y_vali.astype(np.float32),
y_pred_valid, rowvar=0)[0][1])#r
k_val_pearson.append(np.corrcoef(k_y_vali.astype(np.float32), y_pred_valid,
rowvar=0)[0][1])
print('MSE of training set:',mean_squared_error(k_y_train.astype(np.float32),
y_pred_train))#MSE
k_train_MSE.append(mean_squared_error(k_y_train.astype(np.float32), y_pred_train))
print('MSE of testing set:',mean_squared_error(k_y_vali.astype(np.float32), y_pred_valid))
# MSE
k_val_MSE.append(mean_squared_error(k_y_vali.astype(np.float32), y_pred_valid))
print('R2 of training set:',r2_score(k_y_train.astype(np.float32), y_pred_train))#R2
k_train_R2.append(r2_score(k_y_train.astype(np.float32), y_pred_train))
print('R2 of testing set:',r2_score(k_y_vali.astype(np.float32), y_pred_valid)) # R2
k_val_R2.append(r2_score(k_y_vali.astype(np.float32), y_pred_valid))

j+=1

```

```

model = load_model(r'C:\Users\Desktop\new\Jsc.h5')
y_pred_train = model.predict(dt_train_x.astype(np.float32))
y_pred_test = model.predict(dt_test_x.astype(np.float32))

train_score = []
test_score = []
print('Pearson Coefficient of training set:',np.corrcoef(dt_train_y.astype(np.float32), y_pred_train,
rowvar=0)[0][1])
train_score.append(np.corrcoef(dt_train_y.astype(np.float32), y_pred_train, rowvar=0)[0][1])
print('Pearson Coefficient of testing set:',np.corrcoef(dt_test_y.astype(np.float32),y_pred_test,
rowvar=0)[0][1])
test_score.append(np.corrcoef(dt_test_y.astype(np.float32),y_pred_test, rowvar=0)[0][1])
print('MSE of training set:',mean_squared_error(dt_train_y.astype(np.float32),
y_pred_train))#MSE
train_score.append(mean_squared_error(dt_train_y.astype(np.float32), y_pred_train))
print('MSE of testing set:',mean_squared_error(dt_test_y.astype(np.float32), y_pred_test)) #
MSE
test_score.append(mean_squared_error(dt_test_y.astype(np.float32), y_pred_test))

```

```

print('R2 of training set:',r2_score(dt_train_y.astype(np.float32), y_pred_train))#R2
train_score.append(r2_score(dt_train_y.astype(np.float32), y_pred_train))
print('R2 of testing set:',r2_score(dt_test_y.astype(np.float32), y_pred_test)) # R2
test_score.append(r2_score(dt_test_y.astype(np.float32), y_pred_test))

k_score = np.concatenate((
    np.array(k_train_pearson).reshape(1, fold),
    np.array(k_val_pearson).reshape(1, fold),
    np.array(k_train_MSE).reshape(1, fold),
    np.array(k_val_MSE).reshape(1, fold),
    np.array(k_train_R2).reshape(1, fold),
    np.array(k_val_R2).reshape(1, fold)), axis=0)

all_score = np.concatenate((
    np.array(train_score).reshape(1,3),
    np.array(test_score).reshape(1,3)),axis=0)
k_score = pd.DataFrame(k_score)
all_score = pd.DataFrame(all_score)
dt_train_y= pd.DataFrame(dt_train_y)
y_pred_train = pd.DataFrame(y_pred_train)
dt_test_y= pd.DataFrame(dt_test_y)
y_pred_test = pd.DataFrame(y_pred_test)
train=pd.concat([dt_train_y],axis=1)
test=pd.concat([dt_test_y],axis=1)

train.to_excel(r'C:\Users\Desktop\new\train.xlsx', header=False, index=False)
test.to_excel(r'C:\Users\Desktop\new\test.xlsx', header=False, index=False)
k_score.to_excel(r'C:\Users\Desktop\new\k_score.xlsx', header=False, index=False)
all_score.to_excel(r'C:\Users\Desktop\new\score.xlsx', header=False, index=False)
y_pred_train.to_excel(r'C:\Users\Desktop\new\y_pred_train.xlsx', header=False, index=False)
y_pred_test.to_excel(r'C:\Users\Desktop\new\y_pred_test.xlsx', header=False, index=False)

```