

Computational screening of putative small-molecule binders of *Mycobacterium tuberculosis* Pup using pharmacophore modelling, molecular docking and molecular dynamics simulation

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Supplementary data

SMILES	ID	Formula	MW
<chem>COc1c(cc(cc1)F)[C@H]([C@H]1C[C@@H](C1)O)NC(=O)Cn1c(nnn1)N</chem>	MolPort-038-398-937	C15H19FN6O3	350.35
<chem>CC(C)[C@@H](C(=O)N[C@@H](C(=O)O)c1cccc1)n1c(=O)[nH]c2ccccc2c1=O</chem>	MolPort-002-529-779 2134977 ChemDiv-Y040-2781 LN00345054 MCULE-2918641678 PubChem-1789998 ZINC000002134977	C21H21N3O5	395.41
<chem>OC(=O)[C@H](Cc1c[nH]c2ccccc12)NCc1c(ccc1)C(=O)O</chem>	MolPort-005-910-189 LN00383804 MCULE-1104946603 MCULE-9142924304 PubChem-17158766 PubChem-17158767 PubChem-49953754	C19H18N2O4	338.36
<chem>Cc1nc(C)c(CC(=O)N[C@@H](Cc2cncnc2)[C@@H]2C[C@H](C2)O)c(=O)[nH]1</chem>	MolPort-038-425-041	C19H24N4O3	356.42
<chem>C/C(=N/NS(=O)(=O)c1ccc(cc1)F)/c1c(cc(cc1)O)O</chem>	MolPort-008-292-658 17066375 LN01856114 PubChem-135647711 ZINC000017066375	C14H13FN2O4S	324.33
<chem>Cc1ccc(cc1)S(=O)(=O)N/N=C\c1ccc(c(c1)O)O</chem>	MolPort-006-386-862 32561922 PubChem-135641595 ZINC000032561922 ZINC32561922	C14H22N4O3S	326.34
<chem>C1[C@@H]([C@H](CN1CCO)NC(=O)CCCS(=O)(=O)N)c1cccc1</chem>	MolPort-027-866-714 MolPort-047-500-235 91563311 MCULE-3639799162 MCULE-5312604739 PubChem-154897903 PubChem-86283209 ZINC000091563311	C16H25N3O4S	355.45
<chem>Clc1c(cccc1)[C@@H]1[C@@H](C(=O)NCc2c[nH]n2)OCC(=O)N1</chem>	MolPort-046-518-765 1529144001 MCULE-1063296143 ZINC001529144001	C15H15ClN4O3	334.76
<chem>CN(Cc1c2c(CCCC2)[nH]n1)C(=O)N[C@H](c1ccc(cc1)O)C(=O)O</chem>	MolPort-042-643-060 426707369 MCULE-8015381574 PubChem-121512626 ZINC000426707369	C18H22N4O4	358.39
<chem>Cc1cc(C)n(c(=O)n1)CC(=O)N[C@@H](Cc1cccn1)[C@H]1C[C@@H](C1)O</chem>	MolPort-038-404-767	C19H24N4O3	356.42
<chem>CC[C@H](C)[C@H](CO)NC(=O)[C@H](c1ccc1)n1cnn1</chem>	MolPort-042-665-059 MCULE-1664963063 PubChem-121239617	C15H21N5O2	303.36
<chem>CN1[C@@H]([C@@H](C(=O)NCCCCCO)OCC1=O)c1c(C)cccc1</chem>	MolPort-046-525-192 1529173612 MCULE-3756567970 PubChem-134709411 ZINC001529173612	C18H26N2O4	334.41
<chem>Cc1nc(c[nH]1)C(=O)N[C@]1(CCNC[C@H]1O)c1cccc1</chem>	MolPort-051-706-507	C16H20N4O2	300.36

<chem>COc1ccc(cc1F)S(=O)(=O)NC[C@]1(CCOC1)OCCO</chem>	MolPort-046-064-691 CSC087038491 MCULE-8557270980 PubChem-132451042	C14H20FNO6S	349.38
<chem>N1(C(=O)CCC1=O)OC(=O)[C@@H](NC(=O)N1CC(=Nc2ccccc12)O)Cc1ccccc1</chem>	MolPort-000-823-378 MCULE-1984885349	C22H20N4O6	436.42
<chem>CC(=O)Nc1ccc(cc1)NC(=O)C[C@@H]1C(=O)OCCN1Cc1ccccc1</chem>	MolPort-002-674-766 LN00806628 MCULE-1726522086 PubChem-16459799	C21H23N3O4	381.43
<chem>CN(CCC(=O)N[C@H](Cc1ccccc1)[C@H]1C[C@H](C1)O)S(=O)(=O)C</chem>	MolPort-038-411-531	C16H25N3O4S	355.45
<chem>Cc1ccc(cc1)S(=O)(=O)NNC(=O)CCC(=O)Nc1ccc(C)c(C)c1</chem>	MolPort-001-520-409 ChEMBL1441336 LN01165911 MCULE-772728827 PubChem-4331685 ZINC04588478	C19H23N3O4S	389.47
<chem>NC(=O)c1ccc[n+](CC(=O)Nc2c(cccc2)C(=O)O)c1</chem>	MolPort-003-700-915 MolPort-047-117-910 ChEMBL1541066 ChEMBL1624816 ChemDiv-0173-0023 MCULE-4042253049 MCULE-4706568945 PubChem-24762083 PubChem-3568257 ZINC000001920128	C15H14N3O4+	300.29
<chem>CS(=O)(=O)Nc1c(cccc1)C(=O)N1CC(=O)Nc2c1ccccc2</chem>	MolPort-000-123-504 4937985 MCULE-6432080147 PubChem-6459751 ZINC000004937985 ZINC04937985	C16H15N3O4S	345.37
<chem>Cc1c(c(c(c1)CO)/C=N/NS(=O)(=O)Cc1ccccc1)O</chem>	MolPort-002-963-165 MolPort-046-845-088 4703517 PubChem-135613427 PubChem-163327920 ZINC000004703517 ZINC04703517	C15H17N3O4S	335.38
<chem>CC1(C)C(=O)N(C(=O)N1)CC(=O)N[C@@H]([C@H]1C[C@@H](C1)O)c1cccs1</chem>	MolPort-038-393-834 ChEMBL4932816	C16H21N3O4S	351.42
<chem>Cc1cc(c(cc1)OC)S(=O)(=O)NCc1csc(n1)N</chem>	MolPort-037-611-454 74801433 MCULE-2572820493 PubChem-110718084 ZINC000074801433	C12H15N3O3S2	313.4
<chem>CN(CCC(=O)N[C@H](Cc1ccccc1)[C@H]1C[C@H](C1)O)S(=O)(=O)C</chem>	MolPort-038-405-276	C16H25N3O4S	355.45
<chem>O[C@@H]1CNCC[C@@]1(c1ccccc1)NC(=O)c1cc(C(F)F)[nH]n1</chem>	MolPort-051-711-515	C16H18F2N4O2	336.34
<chem>Cc1c(c(nc1)O)O)NS(=O)(=O)c1ccccc1</chem>	MolPort-002-013-037 ChEMBL1426677 MCULE-7091954658	C11H11N3O4S	281.29
<chem>Cc1enc(cc1)C1(CCN(CC1)C(=O)c1c(cccc1)c1nn[nH]1)O</chem>	MolPort-019-892-900 67713069 MCULE-7616683782 ZINC000067713069	C19H20N6O2	364.4
<chem>Cc1cc(ccc1)[C@@H](C(=O)O)NC(=O)c1cc(C(C)C)nc(n1)N</chem>	MolPort-035-856-693 MCULE-7863431113 PubChem-90650027	C17H20N4O3	328.37
<chem>CC[C@@H](C)[C@@H](C(=O)O)NC(=O)[C@@]1(CCN(CC1)C(=O)[C@@H]1CCCN1)c1ccccc1</chem>	MolPort-000-793-859 MolPort-002-532-996 LN00388138 PubChem-16405259 PubChem-44664679	C23H33N3O4	415.53
<chem>Cc1nc(CNC(=O)[C@@H]2[C@@H](c3c(cccc3)Cl)NC(=O)CO2)n[nH]1</chem>	MolPort-046-515-373 1529114576 MCULE-5849624017 PubChem-134699616 ZINC001529114576	C15H16ClN5O3	349.77
<chem>c1cc(cc(c1)O)CN1CCC[C@H](C1)NS(=O)(=O)c1cc2c(cc1)oc(=O)[nH]2</chem>	MolPort-044-695-395 MolPort-047-512-139 MCULE-5753101071 MCULE-7117059803 PubChem-131917513 PubChem-154909762	C19H21N3O5S	403.45
<chem>Cc1ccc(cc1)S(=O)(=O)Nc1c(O)nc(O)nc1C</chem>	MolPort-006-779-905 ChemDiv-5842-8710 MCULE-4332306821	C12H13N3O4S	295.31
<chem>n1(CCC(=O)N[C@@H](Cc2ccccc2)C(=O)O)c(=O)c2ccccc2[nH]c1=O</chem>	MolPort-002-529-009 2130930 LN00355525 MCULE-6294444102 PubChem-1786321 ZINC000002130930	C20H19N3O5	381.38
<chem>COc1ccc(cc1NC(=O)Cc1ccccc1C(=O)O)C(=O)N</chem>	MolPort-009-097-577 44980264 LN00394604 MCULE-9073148957 PubChem-45835374 Z812953880 ZINC000044980264	C17H16N2O5	328.32
<chem>CC(C)C[C@@H](C(=O)N)NC(=O)CNS(=O)(=O)c1c(C)cc(C)cc1</chem>	MolPort-016-608-676 55212071 MCULE-8278085214 PubChem-50964323 ZINC000055212071 ZINC55212071	C16H25N3O4S	355.45

<chem>CO[C@@]1(CNS(=O)(=O)c2cn(C)cn2)CCN(C(C1)C(=O)[C@@H](C)O</chem>	MolPort-051-752-747	C14H24N4O5S	360.43
<chem>Cc1cc(cc(=O)[nH]1)C(=O)N[C@H](CC(=O)O)c1ccccc1</chem>	MolPort-035-762-036 MCULE-1255781410 PubChem-86285574	C16H16N2O4	300.31
<chem>Cc1cc(ccc1)[C@H](C(=O)O)NC(=O)CCn1ccc(=O)[nH]c1=O</chem>	MolPort-035-858-927 MCULE-7161641204 PubChem-90652252	C16H17N3O5	331.32
<chem>O=C(CC[C@@H]1C(=O)Nc2c(C(=O)N1)cccc2)NCc1nnnn1c1ccccc1</chem>	MolPort-039-347-056 LN01764769 MCULE-5898529823 PubChem-110210421	C20H19N7O3	405.41
<chem>CN1[C@@H]([C@@H](C(=O)NCCCCO)OCC1=O)c1c(C)ccccc1</chem>	MolPort-046-528-084 1529189324 MCULE-7642883033 PubChem-134712289 ZINC001529189324	C16H22N2O4	306.36
<chem>Cc1c(c(C)nc(n1)N)CC(=O)N[C@H]([C@@H]1C[C@H](C1)O)c1ccccc1</chem>	MolPort-038-404-964 ChEMBL4916839	C18H23N5O2	341.41
<chem>Cc1cc(cc(O)n1)C(=O)N[C@H]1[C@@H]2CN3C[C@]1(CN(C2)CC3)c1ccccc1</chem>	MolPort-045-921-037 MCULE-7093713404	C22H26N4O2	378.47
<chem>OC(=O)[C@H](c1ccccc1)NS(=O)(=O)c1cc2OCC(=O)Nc2cc1Cl</chem>	MolPort-006-327-533 MCULE-7301435016 PubChem-43915021	C16H13CIN2O6S	396.8
<chem>C1[C@H](C[C@H]1O)[C@@H](c1cc2ccccc2nc1)NC(=O)CN1C(=O)CNC1=O</chem>	MolPort-038-399-185 MCULE-5479924676 PubChem-91768467	C19H20N4O4	368.39
<chem>OC(=O)[C@H](Cc1ccccc1)NC(=O)CCc1c[nH]nc1</chem>	MolPort-042-635-703 426537798 MCULE-4807094822 PubChem-121505308 ZINC000426537798	C15H17N3O3	287.31
<chem>N1(c2ccccc2C(=O)NN)C(=O)[C@]2(N(Cc3c4c([nH]c23)ccccc4)C1=O)C</chem>	MolPort-002-521-133 LN00341490 MCULE-4465050028 PubChem-6569500	C21H19N5O3	389.41
<chem>c1(c2c([nH]cn2)nc(n1)Cl)N[C@H](Cc1ccccc1)C(=O)O</chem>	MolPort-028-605-706 LN05037460 MCULE-3258517857	C14H12CIN5O2	317.73
<chem>NC(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc1ccccc1)C(=O)O</chem>	MolPort-045-946-665 739168103 MCULE-1364937763 PubChem-131904184 ZINC000739168103	C15H19N3O4	305.33
<chem>Cc1c(CN2CCN(C(=O)N[C@@H](CC(C)C)C(=O)O)[C@@H](Cc3ccccc3)C2=O)[nH]cn1</chem>	MolPort-046-788-442 34630977 ChEMBL3218390 MCULE-9954585219	C23H31N5O4	441.52
<chem>C1[C@H]([C@H](C(=O)N1)C(=O)N/N=C\c1c(c(ccc1)O)c1ccccc1</chem>	MolPort-016-586-452 PubChem-5911131	C18H17N3O3	323.35
<chem>Nc1nc(nc(c1)O)CCNC(=O)CN1CCOc2c(C1)ccc2</chem>	MolPort-035-856-635 220058904 MCULE-8876503536 ZINC000220058904	C17H21N5O3	343.38
<chem>OC(=O)[C@H](Cc1ccccc1)NC(=O)CCN1c(=O)[nH]c2ccccc2c1=O</chem>	MolPort-002-527-544 2126962 ChemDiv-Y040-8637 LN00343820 PubChem-1781580 ZINC000002126962	C21H21N3O5	395.41
<chem>Cc1cc(c(C)cc1)S(=O)(=O)NC[C@]1(CCOC1)OCCO</chem>	MolPort-046-064-688 CSC102078439 MCULE-9236569401 PubChem-132451039	C15H23NO5S	329.41
<chem>Cc1ccc(cc1)S(=O)(=O)NNC(=O)c1ccc(cc1)NC(=O)C1CC1</chem>	MolPort-001-530-052 ChEMBL1462295 LN01189174 MCULE-8746875532 PubChem-1013377 ZINC00674445	C18H19N3O4S	373.43
<chem>COc1c(cc(/C=C\c2c(c(C)no2)NC(=O)C)cc1)S(=O)(=O)NC(C)C</chem>	MolPort-007-977-375 ChemDiv-L991-0732 PubChem-46394112 ZINC000033170654 ZINC33170654	C18H23N3O5S	393.46
<chem>CC(=O)Nc1ccc(cc1)C(=O)N[C@H](CC(=O)O)c1ccc(cc1)Cl</chem>	MolPort-002-724-454 ChEMBL1462533 ChemDiv-8015-2866 MCULE-8427236050 PubChem-4051185	C18H17CIN2O4	360.79
<chem>COc1c(cc(cc1)F)[C@H]([C@H]1C[C@H](C1)O)NC(=O)c1cc(O)no1</chem>	MolPort-038-417-141	C16H17FN2O5	336.31
<chem>OC(=O)[C@H](Cc1c[nH]c2ccccc12)NS(=O)(=O)c1ccc(cc1)Br</chem>	MolPort-005-335-847 896684 CSC046173794 LN01886485 MCULE-2895184073 PubChem-1150308 ZINC000000896684	C17H15BrN2O4S	423.28
<chem>Cc1cc(C)c(cc1)S(=O)(=O)N/N=C\c1c(c(ccc1)O)O</chem>	MolPort-008-266-240 32575618 LN01856074 PubChem-135647613 ZINC000032575618 ZINC32575618	C15H16N2O4S	320.36

<chem>C/C(=N/NS(=O)(=O)c1c(C)cc(C)cc1)/c1cc(cc1)O</chem>	MolPort-008-266-344 17068808 PubChem-20182317 ZINC000017068808 ZINC17068808	C16H18N2O4S	334.39
<chem>Cc1c(enc(N)n1)C(=O)NC[C@@H](c1cccn1)N1CCOCC1</chem>	MolPort-035-373-138 MCULE-8970180745 PubChem-77083986	C17H22N6O2	342.4
<chem>NS(=O)(=O)CCCC(=O)N[C@@H]1[C@H]2CN3C[C@@]1(CN(C2)CC3)c1ccccc1</chem>	MolPort-045-938-696 MolPort-047-514-913 MCULE-2718430166 MCULE-7736152651 PubChem-131896746 PubChem-154912554	C19H28N4O3S	392.52
<chem>S(=O)(=O)(NC[C@H]1N([C@H](CC1)CC(=O)NC)C)c1oc(cc1)c1[nH]nc(c1C)C</chem>	MolPort-051-627-491 MCULE-8020739257	C18H27N5O4S	409.5
<chem>Cc1cc(=O)n(CC(=O)N[C@@H](Cc2ccccc2)[C@@H]2C[C@H](C2O)nc1C</chem>	MolPort-038-402-103	C20H25N3O3	355.43
<chem>NC(=O)c1cc[n+](CC(=O)Nc2c(cccc2)C(=O)O)cc1</chem>	MolPort-003-700-916 MolPort-047-117-911 ChemDiv-0173-0024 MCULE-7864006948 MCULE-9478395871 PubChem-126475976 PubChem-5031053 ZINC000001920129	C15H14N3O4+	300.29
<chem>[C@]12([C@H]3[C@@H]([C@@H](Cc4ccc(c4)O)N2)C(=O)N(C(C)(C)C)C3=O)c2cc(cc2NC1=O)F</chem>	MolPort-002-654-321 LN00744096 MCULE-6174761149 PubChem-17578605	C24H24FN3O5	453.46
<chem>CN(Cc1ccccc1)C(=O)C[C@H]1[C@@H]([C@@H]([C@@H]([C@@H](CNC(=O)Nc2cc(ccc2)F)O1)O)O</chem>	MolPort-001-747-906 12603597 MCULE-2153109101 PubChem-25390214 ZINC000012603597 ZINC12603597	C22H26FN3O5	431.46
<chem>COc1ccc(cc1)NC(=O)O[C@@H]1CO[C@@H]2[C@H](CO[C@H]12)NS(=O)(=O)Cc1ccccc1</chem>	MolPort-001-751-179	C21H24N2O7S	448.49
<chem>OC(=O)[C@H](Cc1c[nH]c2ccccc12)NS(=O)(=O)c1ccccc1</chem>	MolPort-002-346-978 ChEMBL1547750 CSC046194047 MCULE-2230467300 PubChem-22917069 PubChem-4574798 Z45636973	C17H16N2O4S	344.38
<chem>Cc1ccc(cc1)S(=O)(=O)Nc1nc(C)cc(NN)n1</chem>	MolPort-001-887-147 270459 ChEMBL1412308 MCULE-7532721404 PubChem-778494 ZINC000000270459	C12H15N5O2S	293.34
<chem>O=C(c1c(cccc1)n1cncn1)NCc1cc2CNCCn2n1</chem>	MolPort-023-325-910 MolPort-047-498-201 82137395 MCULE-1741314245 MCULE-5076460654 PubChem-154896240 PubChem-70766452 ZINC000082137395	C16H17N7O	323.35
<chem>CC[C@]1(CCC[C@@H]2CN(C[C@H]12)C(=O)c1c(cccc1)c1nn[nH]1)O</chem>	MolPort-046-576-961 MCULE-7783083813	C18H23N5O2	341.41
<chem>O[C@H]1C[C@](CNC(=O)c2cncn2)(COc2ccnc2)C[C@H]1O</chem>	MolPort-027-852-663 MolPort-047-149-373 ZINC000107430651	C17H20N4O4	344.37
<chem>Cc1ccc(cc1)S(=O)(=O)N/N=C/c1cc(ccc1)O</chem>	MolPort-001-493-280 5415746 LN01847102 PubChem-9653993 ZINC000005415746 ZINC05415746	C14H14N2O3S	290.34
<chem>Cn1cc(cn1)[C@H]([C@@H]1C[C@H](C1)O)NC(=O)Cc1c(C)non1</chem>	MolPort-038-428-046	C14H19N5O3	305.33
<chem>CN1[C@@H]([C@@H](C(=O)NCc2cc[nH]n2)OCC1=O)c1c(C)ccccc1</chem>	MolPort-046-528-530 1529190682 MCULE-2916806421 ZINC001529190682	C17H20N4O3	328.37
<chem>CN(C)CCNC(=O)c1ccc2c(c1)sc(n2)NS(=O)(=O)c1ccccc1</chem>	MolPort-005-911-792 9421037 LN00799154 PubChem-16425929 ZINC000009421037	C18H20N4O3S2	404.51
<chem>C[C@@H](C(=O)N1CC[C@@H](CC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)O)N</chem>	MolPort-002-529-044 2131020 LN00339840 MCULE-8104657088 PubChem-1786453 ZINC000002131020	C18H25N3O4	347.41
<chem>COc1c(CN2CCNC(=O)[C@@H]2CC(=O)N[C@@H]2CC[C@@H](CC2)O)ccccc1</chem>	MolPort-005-066-589 MCULE-9466988702	C20H29N3O4	375.46
<chem>Cc1ccccc1N(CC(=O)NCC1(CO)CCOCC1)S(=O)(=O)C</chem>	MolPort-046-586-173 MCULE-5303801101 PubChem-135118761 ZINC001704353592	C17H26N2O5S	370.46
<chem>Cc1c(c(c(cn1)CO)CN[C@H]1[C@H]2CN3C[C@@]1(CN(C2)CC3)c1ccccc1)O</chem>	MolPort-045-941-802 MCULE-2661801337 PubChem-131917194	C23H30N4O2	394.51

<chem>Cc1ccc(c(C(=O)NCC(=O)N)c1)NS(=O)(=O)C</chem>	MolPort-051-598-155 ZINC000263949172	C11H15N3O4S	285.32
<chem>Cc1cc(=O)n(CC(=O)N[C@@H]([C@H]2C[C@@H](C2)O)c2ccccc2)nc1C</chem>	MolPort-038-393-772	C18H22N4O3	342.39
<chem>C[C@]1(CCOC2(CCN(CC2)C(=O)c2c(cccc2)c2nnn[nH]2)[C@H]1O)O</chem>	MolPort-046-579-163 MCULE-7079882588	C18H23N5O4	373.41
<chem>Cc1cc(c(C)c(c1/C=N\NC(=O)[C@H]1[C@@H](CNC1=O)c1ccccc1)O)O</chem>	MolPort-002-966-251 LN00952343 PubChem-135643660	C20H21N3O4	367.4
<chem>CCc1ccc(cc1)S(=O)(=O)N/N=C\c1c(c(ccc1)O)O</chem>	MolPort-008-266-352 17055269 LN01856491 PubChem-135647701 ZINC000017055269	C15H16N2O4S	320.36
<chem>O=C(c1c(cccc1)c1nnn[nH]1)N1CCNC(=O)[C@H]1Cc1ccccc1</chem>	MolPort-030-060-057 MCULE-9772450108	C19H18N6O2	362.39
<chem>Cc1c2c(c(cc(=O)o2)CC(=O)N[C@H](C(=O)O)c2ccccc2)ccc1O</chem>	MolPort-002-520-271 LN00352083 MCULE-7953787740 PubChem-5926315	C20H17NO6	367.35
<chem>c1ccc(c(c1)c1nnn[nH]1)C(=O)NCC1CCNCC1</chem>	MolPort-044-718-041 MolPort-047-513-506 MCULE-3752623391 MCULE-3902117887	C14H18N6O	286.33
<chem>CCCCNC(=O)[C@H]1C[C@H]2CCCN2[C@@]21C(=O)Nc1c2ccccc1</chem>	MolPort-051-503-925 MCULE-8469255863 PubChem-164699196	C18H23N3O3	329.39
<chem>CNC(=O)c1cc(ccc1)NC(=O)C[C@H]1C(=O)Nc2c(C(=O)N1)cccc2</chem>	MolPort-035-700-972 LN00386073 MCULE-9398748511 PubChem-91637624 ZINC000217776177	C19H18N4O4	366.37
<chem>NC(=O)CCNC(=O)C[C@H]1N(Cc2ccc(cc2)c2ccccc2)CCNC1=O</chem>	MolPort-020-203-876 MCULE-2219266625 PubChem-56895540	C22H26N4O3	394.47
<chem>Cc1c(ccc(c1)S(=O)(=O)NCC(=O)N[C@@H]1CC[C@H](C1)N)F</chem>	MolPort-019-892-550 MolPort-047-490-460 67691981 MCULE-2938245184 MCULE-6535347300 PubChem-154888780 PubChem-56750183 ZINC000067691981	C14H20FN3O3S	329.39
<chem>CS(=O)(=O)Nc1c(cccc1)C(=O)C[C@]1(C(=O)Nc2c1ccccc2)O</chem>	MolPort-005-287-564 MCULE-7585695001 PubChem-16805405	C17H16N2O5S	360.38
<chem>Cn1c2c(en1)c(=O)[nH]c(CN(CCO)Cc1nccs1)n2</chem>	MolPort-039-038-735 MCULE-2925578666 PubChem-136663733	C13H16N6O2S	320.37
<chem>C([C@@H](C(=O)O)NCc1ccccc1)C(=O)Nc1c(cc(cc1)O</chem>	MolPort-000-466-693 LN01111995 MCULE-3269749370 PubChem-2954734	C17H18N2O4	314.34
<chem>c1(c2ccccc2c(nn1)O)CC(=O)N[C@@H](Cc1c(cccc1)C(=O)O</chem>	MolPort-000-853-175 LN01773877 MCULE-9964279881	C19H17N3O4	351.36
<chem>NC(=O)[C@@H]1CCN(CC1)C(=O)N[C@H](Cc1ccccc1)C(=O)O</chem>	MolPort-002-518-426 4046046 LN00347714 MCULE-2769339814 PubChem-907384 ZINC000004046046	C16H21N3O4	319.36
<chem>Cc1cc(C)n(c(=O)n1)CC(=O)N[C@@H](Cc1ccncc1)[C@H]1C[C@@H](C1)O</chem>	MolPort-038-421-304	C19H24N4O3	356.42
<chem>CN1[C@H]([C@H](C[C@@]1(C)C(=O)O)C(=O)N[C@H]1CC[C@@H](CC1)O)c1ccc(cc1)Cl</chem>	MolPort-019-888-846 244626645 MCULE-6111348172 ZINC000102378480 ZINC000244626645	C20H27CIN2O4	394.89
<chem>O=C(/C=C/c1ccc(O)c(O)c1)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)O</chem>	MolPort-049-227-825 ChEMBL2392128 PubChem-15228042	C20H18N2O5	366.37
<chem>CC(=O)N[C@H]1CCN(C1)C(=O)N[C@H](c1ccc(cc1)O)C(=O)O</chem>	MolPort-044-699-875 534646491 MCULE-8073101570 PubChem-122564991 ZINC000534646491	C15H19N3O5	321.33
<chem>Nc1ncc(cc1)C(=O)N[C@H]1[C@@H]2CN3C[C@]1(CN(C2)CC3)c1ccccc1</chem>	MolPort-045-954-793 MolPort-047-515-781 MCULE-5271579576 MCULE-9771255764 PubChem-131909203 PubChem-154913420	C21H25N5O	363.46
<chem>CN1[C@H]([C@H](C[C@@]1(C)C(=O)O)C(=O)NCCO)c1ccc(cc1)Cl</chem>	MolPort-019-897-995 67880406 MCULE-6658204428 PubChem-56755614 ZINC000067880406	C16H21CIN2O4	340.8

<chem>COC[C@H]1CCCN1[C@@H]1[C@@H](CNS(=O)(=O)c2ccccc2)O[C@H](CO)[C@H]1O</chem>	MolPort-005-952-298 MolPort-047-148-466 20465297 ChEMBL4905552 MCULE-2418115818 MCULE-3939468266 PubChem-146118715 PubChem-28961810 ZINC000020465297	C18H28N2O6S	400.49
<chem>CC(=O)Nc1ccc(cc1)S(=O)(=O)N[C@@H](Cc1ccccc1)C(=O)O</chem>	MolPort-002-346-958 CSC046207525 LN05037375 MCULE-6728755459 PubChem-3677765 PubChem-77760141 Z45636836	C17H18N2O5S	362.4
<chem>COC(=O)c1c(cccc1)S(=O)(=O)N[C@@H]1CO[C@@H]2[C@H](CO[C@H]12)O</chem>	MolPort-047-377-434	C14H17NO7S	343.35
<chem>O=C(CS(=O)(=O)c1ccccc1)Nc1ccc2C(=O)NC(=O)c2c1</chem>	MolPort-003-131-379 4496377 MCULE-7165387460 PubChem-7254446 ZINC000004496377 ZINC04496377	C16H12N2O5S	344.34
<chem>O=C(C1(Cc2ccccc2)CN(c2c3c(ncn2)[nH]cc3)C1)NC[C@@H](O)CO</chem>	MolPort-051-628-794 MCULE-9971977946	C20H23N5O3	381.43
<chem>c1ccc(cc1)S(=O)(=O)NC(=O)CCCCN</chem>	MolPort-047-903-601 MCULE-3451472040 MCULE-4667791176 PubChem-113801090 PubChem-146673312	C11H16N2O3S	256.32
<chem>Cc1ccc(cc1)S(=O)(=O)N/N=C(\C)/C(=N/O)/C</chem>	MolPort-049-243-816 56683338 PubChem-135822518	C11H15N3O3S	269.32
<chem>CC(C)N1[C@H]([C@@H](C(=O)NCc2cc(nen2)O)OCC1=O)c1ccccc1</chem>	MolPort-046-528-768 1529191045 MCULE-8014285185 ZINC001529191045	C19H22N4O4	370.4
<chem>O[C@H]1CCCCC[C@H]1NC(=O)c1c(ccc1)c1nn[nH]1</chem>	MolPort-047-390-724 MCULE-4700784210	C16H21N5O2	315.37
<chem>CN(C)CCNC(=O)c1ccccc1n1cc(CN)cn1</chem>	MolPort-046-984-989 257201699 MCULE-2947195742 MCULE-4319423603 PubChem-110121751 ZINC000257201699	C15H21N5O	287.36
<chem>COc1ccc(cc1)S(=O)(=O)NNC(=O)C(=O)NNc1ccccc1</chem>	MolPort-003-702-976 ChemDiv-1193-0125 MCULE-6630589543 PubChem-3396843 ZINC01921375	C15H16N4O5S	364.38
<chem>Cc1cnc(en1)CNC(=O)N(CCCO)Cc1ccccc1</chem>	MolPort-042-572-024 426575015 MCULE-2981431721 PubChem-119069634 ZINC000426575015	C17H22N4O2	314.38
<chem>OC[C@H]([C@@H](O)c1ccccc1)NC(=O)CCc1c[nH]nc1</chem>	MolPort-030-048-679 97468226 MCULE-8083088657 PubChem-74235360 ZINC000097468226 ZINC97468226	C16H21N3O3	303.36
<chem>C1CN(C[C@]1(CO)O)C(=O)NCc1nc(Cc2ccccc2)no1</chem>	MolPort-044-712-671 MCULE-9182493510 PubChem-122569732	C16H20N4O4	332.35
<chem>Cc1cc2c(cc1S(=O)(=O)N[C@@H](Cc1ccccc1)C(=O)O)OCC(=O)N2</chem>	MolPort-015-136-230 MCULE-6814983019 PubChem-44121921	C18H18N2O6S	390.41
<chem>n1(CCCC(=O)N[C@@H](c2ccccc2)C(=O)O)c(=O)c2ccccc2[nH]c1=O</chem>	MolPort-002-527-682 2127440 ChemDiv-Y040-8636 LN00360706 MCULE-3674926971 PubChem-1782126 ZINC000002127440	C20H19N3O5	381.38
<chem>CNC(=O)c1ccc(cc1)S(=O)(=O)N[C@H](Cc1ccccc1)C(=O)O</chem>	MolPort-046-188-165 MCULE-5855404768 PubChem-132421619	C17H18N2O5S	362.4
<chem>Cn1cc(en1)S(=O)(=O)NNC(=O)c1cc(ccc1)O</chem>	MolPort-019-907-453 LN00442745 MCULE-9773894365 PubChem-56761508 ZINC71284716	C11H12N4O4S	296.3
<chem>OCCCN(Cc1c2ccccc2ccc1)C(=O)c1c(C(=O)O)nc[nH]1</chem>	MolPort-035-373-741 MCULE-2626320143	C19H19N3O4	353.37
<chem>OC(=O)[C@H](Cc1c[nH]c2ccccc12)NS(=O)(=O)c1ccc(cc1)Cl</chem>	MolPort-002-508-259 3886295 CSC000761128 LN00818300 MCULE-2705216700 MCULE-5912140049 PubChem-982211 ZINC000003886295	C17H15ClN2O4S	378.83
<chem>Oc1cc(CNC(=O)[C@H]2C[C@H]3CCCN3[C@@H]2)C(=O)Nc2c3ccccc2)ncn1</chem>	MolPort-051-464-721 2356161419 MCULE-1887396016	C20H21N5O3	379.41

<chem>Cc1cc(c2c(C)c(CC(=O)N[C@@H](Cc3ccccc3)C(=O)O)c(=O)oc2c1)O</chem>	MolPort-002-525-421 20610077 LN00354321 MCULE-8639883523 PubChem-6851271 ZINC000020610077	C22H21NO6	395.41
<chem>Cc1cc(c(cc1)OCC(=O)N/N=C/c1ccc[nH]1)[N+](=O)[O-]</chem>	MolPort-002-947-970 PubChem-135643258 ZINC00523012	C14H14N4O4	302.29
<chem>Cc1nc(CNC(=O)N(C[C@@H]2CCC(=O)N2)C c2cnccc2)no1</chem>	MolPort-044-688-019 534592211 MCULE-1760170433 PubChem-122560652 ZINC000534592211	C16H20N6O3	344.37
<chem>n1(CCC(=O)N[C@H](Cc2ccccc2)C(=O)O)c(=O)c2ccccc2nc1O</chem>	MolPort-000-816-611 MCULE-6607615288	C20H19N3O5	381.38
<chem>CN1C(=O)[C@@H](c2ccccc2C=N1)NC(=O)N C(=O)[C@H](c1cc(cc(c1)F)F)O</chem>	MolPort-046-418-500 203556813 MCULE-1503458535 MCULE-5722268116 PubChem-66577058 ZINC000203556813	C19H16F2N4O4	402.35
<chem>Cc1c(ccc(c1)S(=O)(=O)NCC(=O)N1C[C@@H][C[C@H](C1)O)O)F</chem>	MolPort-051-469-296 2356166910 MCULE-2107216937 PubChem-162635447	C14H19FN2O5S	346.37
<chem>C/C(=N\NS(=O)(=O)c1ccccc1)/c1c(cc(C)oc1=O)O</chem>	MolPort-001-543-117 101160202 ChEMBL3208635 LN00990321 PubChem-135543351 ZINC000101160202	C14H14N2O5S	322.34
<chem>Cn1c(c(cn1)S(=O)(=O)NNC(=O)c1cc(ccc1)O)C</chem>	MolPort-019-908-500 LN00434904 MCULE-1123634102 PubChem-56762463 ZINC71286381	C12H14N4O4S	310.33
<chem>CCCNC(=O)N1C[C@@H]2[C@H](C1)Oc1ccc ccc1S(=O)(=O)NC[C@@H](CN2C)O</chem>	MolPort-046-152-853 1534612685 MCULE-6027174751 PubChem-137954923 ZINC001534612685	C18H28N4O5S	412.5
<chem>OC1(CCN(CC1)C(=O)c1c(cccc1)c1nnn[nH]1) c1ccccc1</chem>	MolPort-030-058-071 97694777 MCULE-9767535586 ZINC000097694777	C19H19N5O2	349.39
<chem>Cc1cc(C)c(c(C)c1)S(=O)(=O)Nc1c(O)nc(O)nc 1C</chem>	MolPort-001-009-973 ChEMBL1522080 MCULE-1685589445	C14H17N3O4S	323.37
<chem>O=C(CCN(C(=O)[C@@H](c1cnccc1)N1CCOC C1)Nc1ccccc1</chem>	MolPort-030-053-643 MCULE-9688634137 PubChem-74240302	C20H24N4O3	368.43
<chem>Cn1cc(cn1)[C@H]([C@H]1C[C@@H](C1)O) NC(=O)c1c(c(C)on1)CO</chem>	MolPort-038-427-071	C15H20N4O4	320.34
<chem>n1([nH]c(=O)c(c1C)CCO)S(=O)(=O)c1ccccc cnc12</chem>	MolPort-002-861-027 4089438 MCULE-3546214453 PubChem-3810782 ZINC000004089438	C15H15N3O4S	333.36
<chem>OC(=O)[C@@H](Cc1ccccc1)NC(=O)Cn1c(=O) [nH]c2ccccc2c1=O</chem>	MolPort-002-533-711 3985238 LN00340670 PubChem-7068615 ZINC000003985238	C19H17N3O5	367.36
<chem>OC(=O)[C@H](c1cc(c(cc1)Cl)Cl)NC(=O)c1cc (=O)[nH]cc1</chem>	MolPort-051-735-895	C14H10Cl2N2O4	341.15
<chem>c1ccc(cc1)CNC(=O)CC(=O)N/N=C\c1ccccc1C (=O)O</chem>	MolPort-001-962-609 PubChem-6184487	C18H17N3O4	339.35
<chem>Cc1cc(=O)[nH]c(CCNC(=O)[C@@H]2Cc3c(c ccc3)S(=O)(=O)N2)n1</chem>	MolPort-038-417-998 MCULE-1943114514 PubChem-136665397	C16H18N4O4S	362.4
<chem>CCNc1ncc(cn1)C(=O)N[C@@H](CC(=O)O)c 1ccc(cc1)F</chem>	MolPort-028-592-592 MCULE-437233332 PubChem-72913914	C16H17FN4O3	332.33
<chem>Oc1ccc(CCNC(=O)C[C@H]2C(=Nc3c(C(=O) N2)cccc3)O)cc1</chem>	MolPort-023-281-458 MCULE-4718722348	C19H19N3O4	353.37
<chem>S(=O)(=O)(c1ccccc2ccccc12)NNC(=O)c1ccc(O) cc1</chem>	MolPort-019-839-241 LN01937053 MCULE-2253880794 PubChem-51703062	C17H14N2O4S	342.37
<chem>Nc1ccc(CC(=O)N[C@H]([C@@H](c2ccccc2) O)C(=O)O)cc1</chem>	MolPort-002-510-185 LN00352816 MCULE-2330938980 PubChem-3846381	C17H18N2O4	314.34
<chem>Cc1n[nH]c([C@H]2CCN(CC2)C(=O)[C@H]2 Cc3c(cccc3)S(=O)(=O)N2)n1</chem>	MolPort-035-763-597 MCULE-7479016300	C17H21N5O3S	375.45
<chem>OC(=O)[C@H](Cc1ccccc1)NC(=O)Cn1c(=O)[nH]c2ccccc2c1=O</chem>	MolPort-002-534-358 2130507 LN00369602 PubChem-1785742 ZINC000002130507	C19H17N3O5	367.36
<chem>O=C(ON1C(=O)CCC1=O)[C@H](Cc1ccccc1) NC(=O)N1CC(=O)Nc2c1cccc2</chem>	MolPort-002-658-125 101367039 LN00733603 PubChem-17579231 ZINC000101367039	C22H20N4O6	436.42

<chem>COc1ccc(cc1)S(=O)(=O)Nc1ccc(CCC(=O)NCc2ccc(cc2)F)n1</chem>	MolPort-009-730-891 16848516 MCULE-9747040068 PubChem-27376809 XHCIYIJSKXJUMX-UHFFFAOYSA-N ZINC000016848516 ZINC16848516	C20H20FN3O4S 2	449.52
<chem>OC(=O)[C@@H](Cc1c[nH]c2ccccc12)Nc1c(c(c1)C(F)(F)F)[N+](=O)[O-]</chem>	MolPort-000-758-842 5590123 LN01791994 MCULE-3252930196 MCULE-4470046126 PubChem-40547602 PubChem-44661204 ZINC000005590123	C18H14F3N3O4	393.32
<chem>NC(=O)c1nc(ccc1)C(=O)N[C@H](C(=O)c1ccc(cc1)F)O</chem>	MolPort-001-846-750 ChemDiv-Y070-0195 LN01053134 MCULE-8747941295 PubChem-4263588	C15H12FN3O4	317.27
<chem>COc1c(cc(cc1)F)[C@H]([C@H]1C[C@@H](C1)O)NC(=O)CS(=O)(=O)C(C)C</chem>	MolPort-038-391-506	C17H24FNO5S	373.44
<chem>C1C[C@@H](CN(C1)CCNS(=O)(=O)c1c[nH]nc1)CO</chem>	MolPort-044-707-137 MCULE-6515511157 PubChem-131933475	C11H20N4O3S	288.37
<chem>CC1(C(=O)N(C(=O)N1)CC(=O)N[C@@H]([C@@H]1C[C@H](C1)O)c1cc2c(cc1)OCC2)C</chem>	MolPort-038-408-264 MCULE-3816156740 PubChem-91778640	C20H25N3O5	387.43
<chem>C[C@@H](C(=O)O)NC(=O)[C@H](Cc1ccccc1)NC(=O)N1CC(=Nc2c1ccccc2)O</chem>	MolPort-000-818-016 MCULE-6202884807	C21H22N4O5	410.42
<chem>Cc1cc(=O)n(CC(=O)N[C@H]([C@H]2C[C@@H](C2)O)c2cccs2)nc1C</chem>	MolPort-038-400-755	C17H21N3O3S	347.43
<chem>Cc1c(c2c(CCCC2=O)[nH]1)C(=O)N[C@@H](c1ccccc1)C(=O)O</chem>	MolPort-042-633-803 426509591 MCULE-5231590198 PubChem-121503420 ZINC000426509591	C18H18N2O4	326.35
<chem>CC(C)[C@@H](C(=O)N1CC[C@@H](CC1)C(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)O)N</chem>	MolPort-002-528-303 4082731 LN00341334 MCULE-7851699746 PubChem-7093292 ZINC000004082731	C22H30N4O4	414.5
<chem>Cc1cc(nc(n1)NS(=O)(=O)c1ccc(cc1)Cl)NN</chem>	MolPort-001-954-704 270450 ChEMBL1347345 LN00431025 MCULE-6631707002 PubChem-778488 ZINC000000270450	C11H12ClN5O2 S	313.76
<chem>c1ccc(c(c1)c1nn[nH]1)C(=O)N[C@@H]1CC=CC[C@H]1C(=O)N</chem>	MolPort-044-718-715 MCULE-9976629721	C15H16N6O2	312.33
<chem>CN1C[C@H](CNS(=O)(=O)c2ccccc2O[C@H]2CN(C[C@@H]12)C(=O)Nc1ccccc1)O</chem>	MolPort-046-152-852 1534613875 MCULE-8465232589 PubChem-137954922 ZINC001534613875	C21H26N4O5S	446.52
<chem>C[C@@H]1CNCCN1C(=O)NCc1nc(Cc2cccs2)no1</chem>	MolPort-045-954-722 825012747 MCULE-6966302735 PubChem-131906359 ZINC000825012747	C14H19N5O2S	321.4
<chem>Cc1ccc(cc1)S(=O)(=O)NC(=O)COc1c(cccc1)C(=O)N</chem>	MolPort-002-274-751 ChEMBL1451956 MCULE-2610258615 PubChem-829972	C16H16N2O5S	348.37
<chem>CO[C@H]1C[C@H](CC[C@@H]1NS(=O)(=O)c1c(C)onc1C)C(=O)NCCN(C)C</chem>	MolPort-047-393-449 1857692943 MCULE-3234625065 PubChem-145938721	C17H30N4O5S	402.51
<chem>O[C@@H]1C[C@H](C1)[C@@H](c1cc2c(OC2)cc1)NC(=O)Cc1cnc[nH]c1=O</chem>	MolPort-038-400-355	C19H21N3O4	355.39
<chem>CC[C@H](C)[C@@H](C(=O)O)NC(=O)[C@]1(CCN(CC1)C(=O)[C@@H]1CSCN1)c1ccccc1</chem>	MolPort-000-809-872 MolPort-002-533-060 LN00368831 PubChem-16405282 PubChem-44666508	C22H31N3O4S	433.56
<chem>C/C(=N)NS(=O)(=O)c1ccccc1/c1cc(ccc1)N</chem>	MolPort-002-185-078 5090805 LN01849722 PubChem-9586375 ZINC000005090805 ZINC05090805	C14H15N3O2S	289.35
<chem>C/C(=N)NC(=O)[C@H](c1ccccc1)O/c1ccc(cc1)NC(=O)C1CC1</chem>	MolPort-001-501-862 PubChem-6070911	C20H21N3O3	351.4
<chem>NC(=O)CC[C@@H]1N[C@@]2([C@@H]3[C@H]1C(=O)N(C3=O)c1c(cccc1)F)C(=O)Nc1c2ccccc1</chem>	MolPort-019-706-523 MCULE-7990349277 PubChem-4895292	C22H19FN4O4	422.41
<chem>COc1nc(cc(=O)[nH]1)[C@@H]1C[C@H](C1)NS(=O)(=O)c1c(cccc1)C#N</chem>	MolPort-038-391-294 MCULE-9949907696 ZINC000218251406	C17H18N4O4S	374.41

<chem>Cc1ccc(cc1)[C@H](C(=O)O)NC(=O)[C@@H]1CCCN(CC(=O)N)C1</chem>	MolPort-045-966-854 MCULE-8554944856 PubChem-131942306	C17H23N3O4	333.38
<chem>NC(=O)CN1CCC[C@H](C1)C(=O)N[C@H](C(=O)O)c1cc(ccc1)F</chem>	MolPort-045-960-137 MCULE-8267014051 PubChem-131950338	C16H20FN3O4	337.35
<chem>FCCNC(=O)c1cccc(c1)S(=O)(=O)NCC(=O)N1CCNCC1</chem>	MolPort-035-368-398 214949436 MCULE-5570675369 PubChem-77078559 ZINC000214949436	C15H21FN4O4S	372.42
<chem>CC(C)C[C@@H](C(=O)N[C@@H](C(=O)O)c1cccc1)NC(=O)N1CC(=Nc2c1cccc2)O</chem>	MolPort-000-823-454 MCULE-3567836089	C23H26N4O5	438.48
<chem>Oc1ccc(C[C@H](C(=O)NCc2n[nH]c(=O)[nH]2)c2cccc2)cc1</chem>	MolPort-045-923-617 MCULE-6992876737 PubChem-137177428	C18H18N4O3	338.36
<chem>Cc1c(ccc(c1)F)S(=O)(=O)NCC(=O)N1CCCC[C@H]1CCCO</chem>	MolPort-038-402-584 MCULE-1267567288 PubChem-91772890	C17H25FN2O4S	372.45
<chem>COc1cc(c(cc1)S(=O)(=O)N/N=C\c1cc(c(c(c1)OC)O)OC)OC</chem>	MolPort-008-292-778 32577083 PubChem-135624689 ZINC000032577083 ZINC32577083	C17H20N2O7S	396.41
<chem>Oc1cccc(c1)C(=O)NNC1=NS(=O)(=O)c2c1ccc c2</chem>	MolPort-001-620-080 ChemDiv-8008-1056 MCULE-2774680898 PubChem-829138 ZINC00350917	C14H11N3O4S	317.32
<chem>OCOC[C@@]1(CNS(=O)(=O)c2c(cc(cc2)F)F)CCOC1</chem>	MolPort-046-064-689 CSC102078426 MCULE-3383329549 PubChem-132451040	C13H17F2NO5S	337.34
<chem>O=C([C@H]1OCC(=O)N[C@@H]1c1cccc1)NCc1c2c(CCCC2)[nH]n1</chem>	MolPort-046-523-439 1529168605 MCULE-2908623045 PubChem-134707659 ZINC001529168605	C20H24N4O3	368.43
<chem>COCc1cc(CNC(=O)[C@@H]2[C@@H](c3c(C)cccc3)N(C(=O)CO2)C)n[nH]1</chem>	MolPort-046-516-355 MCULE-7319521169	C19H24N4O4	372.42
<chem>O[C@H]1C[C@](CNC(=O)c2cncn2)(COc2ccc2)[C@H]1O</chem>	MolPort-027-852-632 MolPort-047-149-360 ZINC000107430599	C18H21N3O4	343.38
<chem>CC(C)Oc1c(cc(cc1)C(=O)N)NC(=O)Cc1c(cccc1)C(=O)O</chem>	MolPort-019-909-693 70666444 LN00376069 MCULE-1084895945 PubChem-56763548 ZINC000070666444	C19H20N2O5	356.37
<chem>CC(=O)Nc1ccc(CN[C@@H]2CO[C@H](CNS(=O)(=O)c3cccc3)[C@H]2O)cc1</chem>	MolPort-023-275-149 77264640 MCULE-2386933438 PubChem-75536685 ZINC000077264640	C20H25N3O5S	419.49
<chem>CC(C)CC(=O)N[C@H]1C[C@H](c2nc(C)n[nH]2)N(C1)C(=O)c1c(c(C)on1)CN(C)C</chem>	MolPort-046-608-571 MCULE-5744577518	C20H31N7O3	417.51
<chem>OC(=O)[C@H]1CCCN1C(=O)[C@H](Cc1ccc cc1)NC(=O)N1CC(=O)Nc2c1cccc2</chem>	MolPort-002-533-497 LN00346031 MCULE-7315421502 PubChem-16405443	C23H24N4O5	436.46
<chem>COC(=O)[C@]1(C)C[C@@H]([C@H](c2c(cc cc2)Cl)N1C)C(=O)NC(C)(C)CO</chem>	MolPort-005-148-707 55386013 MCULE-5941177654 PubChem-42464034 ZINC000055386013 ZINC55386013	C19H27ClN2O4	382.88
<chem>COc1cccc(c1)S(=O)(=O)NCc1c2CNC(=O)[C@H](C(C)C)n2nn1</chem>	MolPort-047-140-069 MCULE-5250668595 PubChem-146070929	C16H21N5O4S	379.43
<chem>CC(C)(C)NS(=O)(=O)c1cccc1c1cn(CC(=O)N)Cnc1</chem>	MolPort-042-634-817 426521523 MCULE-6629810261 PubChem-121504429 ZINC000426521523	C16H22N4O3S	350.44
<chem>OC(=O)[C@@H](Cc1c[nH]c2cccc12)NS(=O)(=O)c1ccc(cc1)Cl</chem>	MolPort-000-473-688 ChEMBL1545762 CSC000682244 LN01063568 MCULE-6356237452 PubChem-2787483 Z45636969	C17H15ClN2O4S	378.83
<chem>Oc1cccc(/C=N\NS(=O)(=O)c2ccc(cc2)Cl)c1O</chem>	MolPort-008-266-161 17066888 PubChem-135647544 ZINC000017066888 ZINC17066888	C13H11ClN2O4S	326.76
<chem>CN1[C@H]([C@H](C[C@@]1(C)C(=O)O)C(=O)NC(CO)CO)c1ccc(cc1)Cl</chem>	MolPort-019-900-665 67947987 MCULE-3002288933 PubChem-56758278 ZINC000067947987	C17H23ClN2O5	370.83
<chem>Cn1c(=O)c(=O)[nH]c2cc(CCC(=O)N[C@@H](Cc3cccc3)C(=O)O)ccc12</chem>	MolPort-035-705-234 218416270 LN00416343 MCULE-8130686944 PubChem-91641219 ZINC000218416270	C21H21N3O5	395.41

<chem>OCc1cc2c(OCCN(CCC(=O)Nc3c(C(=O)O)sc3)C2)cc1</chem>	MolPort-039-040-989 252499388 MCULE-2021527347 PubChem-91835826 ZINC000252499388	C18H20N2O5S	376.43
<chem>Cn1c(=O)[nH]cc(CC(=O)N[C@@H](CC(=O)O)c2ccccc2)c1=O</chem>	MolPort-035-760-940 MCULE-1504623404 PubChem-86284888	C16H17N3O5	331.32
<chem>C/C(=N/NS(=O)(=O)c1ccccc1)/c1cc(cc(c1)O)O</chem>	MolPort-008-266-299 17031310 PubChem-20181828 ZINC000017031310 ZINC17031310	C14H14N2O4S	306.34
<chem>Cc1ccc(cc1)S(=O)(=O)CC(=O)NNC(=O)Nc1ccccc1</chem>	MolPort-006-755-662 MCULE-5702129733 PubChem-4083103 ZINC02582177	C16H17N3O4S	347.39
<chem>Cc1ccc(cc1)S(=O)(=O)NC[C@H]1[C@@H]([C@@H](CO1)NCc1ccc[nH]1)O</chem>	MolPort-023-275-180 77264810 MCULE-3424664965 PubChem-75536716 ZINC000077264810	C16H22N4O4S	366.44
<chem>CN1[C@H]([C@H](C[C@@]1(C)C(=O)O)C(=O)NCCO)c1c(ccc1)Cl</chem>	MolPort-019-891-233 67872510 MCULE-2364895497 PubChem-56748873 ZINC000067872510	C16H21ClN2O4	340.8
<chem>OCc1ccc(CNC(=O)[C@H]2OCC(=O)N(C3CC3)[C@@H]2c2cnccc2)cc1</chem>	MolPort-046-529-178 1529191700 MCULE-3397006277 PubChem-134713378 ZINC001529191700	C21H23N3O4	381.43
<chem>CN1[C@H]([C@H](C[C@@]1(C)C(=O)O)C(=O)NCCc1c[nH]cn1)c1ccc(cc1)Cl</chem>	MolPort-019-893-849 67742760 CHEMBL5014544 MCULE-7386039262 ZINC000067742760	C19H23ClN4O3	390.86
<chem>COC[C@]1(CNS(=O)(=O)c2ccc(cc2)F)C[C@@H]([C@@H](C1)O)O</chem>	MolPort-027-852-694 ZINC000107430730	C14H20FNO5S	333.38
<chem>COc1c(ccc(c1)[C@@H]1[C@@H]([C@](C(F)(F)F)(O)NC(=O)N1)C(=O)c1cnccc1)O</chem>	MolPort-000-681-096 CSC026537015 LN01969646 MCULE-1891748448 PubChem-2918376 Z56781941	C18H16F3N3O5	411.33
<chem>CCOc1c(CN2CCNC(=O)[C@H]2CC(=O)NCC(C)(C)CO)cccc1</chem>	MolPort-005-136-734 MCULE-2687709819 PubChem-45238624	C20H31N3O4	377.48
<chem>CC(C)C(=O)Nc1cccc(c1)C(=O)N[C@H](C(=O)O)c1cc(C)ccc1</chem>	MolPort-045-926-139 MCULE-8226662461 PubChem-131923160	C20H22N2O4	354.4
<chem>N1(CC(=O)Nc2ccccc12)C(=O)NCC(=O)N[C@@H](c1ccccc1)C(=O)O</chem>	MolPort-002-660-964 CHEMBL1579719 LN00756428 MCULE-8485792282 PubChem-7693219	C19H18N4O5	382.37
<chem>CC(=O)Nc1ccc(cc1)S(=O)(=O)N/N=C/c1c[nH]c2c1cccc2</chem>	MolPort-016-735-117 PubChem-135719331 ZINC40570793	C17H16N4O3S	356.4
<chem>CC(C)[C@@H](C(=O)N[C@H](C(=O)O)c1ccc1)NC(=O)N1CC(=O)Nc2c1cccc2</chem>	MolPort-002-659-169 9128647 CHEMBL1718705 LN00749389 MCULE-6764160085 PubChem-17579945 ZINC000009128647	C22H24N4O5	424.45
<chem>Cc1cc(ccc1)[C@H](C(=O)O)NC(=O)CCNC(=O)C</chem>	MolPort-042-634-144 MCULE-8355609022 PubChem-121503759	C14H18N2O4	278.3
<chem>CC(C)CCN1C[C@H](CNS(=O)(=O)c2ccccc2)OC[C@]2(C[C@H]([C@@H](C2)O)O)C1O</chem>	MolPort-039-100-572 ZINC000253403210	C21H34N2O6S	442.57
<chem>CC(=O)Nc1ccc(cc1)S(=O)(=O)N[C@@H](C(=O)O)c1ccccc1</chem>	MolPort-027-837-522 266598 ChemDiv-Y041-4710 LN01888111 MCULE-1271192379 PubChem-776661 ZINC000000266598	C16H16N2O5S	348.37
<chem>C[C@@H](c1cnenn1C)NC(=O)N(CCCO)Cc1ccc(cc1)Cl</chem>	MolPort-044-718-489 MCULE-9269983249 PubChem-124218478	C16H22ClN5O2	351.83
<chem>O=C([C@H]1OCC(=O)N[C@@H]1c1ccccc1)NCc1cc(C2CC2)[nH]n1</chem>	MolPort-046-522-990 MCULE-9334577613	C18H20N4O3	340.38
<chem>NCCCCCNS(=O)(=O)c1ccccc1[N+](=O)[O-]</chem>	MolPort-008-268-329 MolPort-039-337-817 44075728 LN01740111 MCULE-1175427413 MCULE-3521071856 PubChem-12042300 PubChem-22719658 ZINC000044075728	C12H19N3O4S	301.36
<chem>CC(=O)N[C@H]1CCN(C1)C(=O)N[C@H](Cc1ccccc1)C(=O)O</chem>	MolPort-042-636-399 322344662 MCULE-7867792164 PubChem-121505999 ZINC000322344662	C16H21N3O4	319.36

<chem>CC(=O)N[C@@H](CCC(=O)N)c1ncnn1Cc1ccccc1</chem>	MolPort-044-704-546 670459239 ChEMBL4900349 MCULE-2198743482 PubChem-129619312 ZINC000670459239	C15H19N5O2	301.34
<chem>CS(=O)(=O)NCc1nc(CC(=O)N)nn1c1cc(ccc1Cl)Cl</chem>	MolPort-029-905-893 96180116 MCULE-3055238191 PubChem-72937907 ZINC000096180116 ZINC96180116	C12H13Cl2N5O3S	378.23
<chem>c1(c2c([nH]cn2)nc(N)n1)N[C@H](Cc1ccccc1)C(=O)O</chem>	MolPort-030-042-407 LN05037489 MCULE-5023265365	C14H14N6O2	298.3
<chem>S(=O)(=O)(c1ccc2c(CCC(=O)N2)c1)N[C@@H](Cc1ccccc1)C(=O)O</chem>	MolPort-006-067-411 LN00141625 MCULE-4897116197 PubChem-3450946	C18H18N2O5S	374.41
<chem>CN(CCC(=O)N[C@H](Cc1cccn1)[C@H]1C[C@H](C1)O)S(=O)(=O)C</chem>	MolPort-038-408-616	C16H25N3O4S	355.45
<chem>Cc1cc(C)n(c(=O)n1)CC(=O)N[C@@H](Cc1cccn1)[C@H]1C[C@@H](C1)O</chem>	MolPort-038-423-690	C19H24N4O3	356.42
<chem>CN(C)C(=O)CN1C(=O)N[C@@H](Cc2ccc(cc2)F)(C2CCNCC2)C1=O</chem>	MolPort-019-799-266 MolPort-047-485-772 MCULE-7996888764 MCULE-9965300480 PubChem-154884495 PubChem-56700842	C19H25FN4O3	376.43
<chem>n1(CCCC(=O)N[C@H](c2ccccc2)C(=O)O)c(=O)c2ccccc2nc1O</chem>	MolPort-000-849-992 MCULE-1838696411	C20H19N3O5	381.38
<chem>CN(C[C@@H]1[C@H]([C@H]([C@H](CCO1)NC(=O)Cc1ccc2c(c1)nn[nH]2)O)Cc1cccn1</chem>	MolPort-051-528-834 MCULE-6219146606 MCULE-6235404125	C18H22N6O4	386.41
<chem>CN1CCC(CC1)n1c(ccn1)NC(=O)[C@@H](Cc1c[nH]cn1)n1ccccc1</chem>	MolPort-046-524-047 MCULE-2700272125	C19H25N7O	367.45
<chem>N[C@@H](Cc1ccc(cc1)O)C(=O)N[C@@H](Cc1ccccc1)C(=O)O</chem>	MolPort-035-681-611 2384820 ChEMBL447844 LN02124472 MCULE-7460087797 MCULE-7595148054 PubChem-7009600 PubChem-71408632 ZINC000002384820	C18H20N2O4	328.36
<chem>Cc1cc(nc(n1)NS(=O)(=O)c1c(cccc1)Cl)NN</chem>	MolPort-001-954-722 270493 ChEMBL1491267 LN00516087 MCULE-6778524290 PubChem-778521 ZINC000000270493	C11H12ClN5O2S	313.76
<chem>Cc1cc(c2c(C)c(CC(=O)N[C@H](C(=O)O)c3ccccc3)c(=O)oc2c1)O</chem>	MolPort-002-524-600 20412611 ChemDiv-Y040-4419 LN00362758 MCULE-6201790818 PubChem-6571666 ZINC0000020412611	C21H19NO6	381.38
<chem>O[C@H]1CCN(Cc2ncc[nH]2)C[C@@]1(Cc1ccccc1)C(=O)O</chem>	MolPort-051-500-283 MCULE-9964564346 PubChem-164691200	C17H21N3O3	315.37
<chem>Cc1c(CCCNC(=O)[C@@H]2[C@H](c3ccc(c3)NC(=O)CO2)c(C)n[nH]1</chem>	MolPort-046-524-164 1529171835 MCULE-2610782724 PubChem-134708384 ZINC001529171835	C19H24N4O3	356.42
<chem>Cc1ccc(cc1)S(=O)(=O)N/N=C/c1ccc(c(c1)O)O</chem>	MolPort-001-488-702 482641 LN01847074 PubChem-135468262 ZINC000000482641	C14H14N2O4S	306.34
<chem>OCCCCNC(=O)[C@H]1OCC(=O)N[C@@H]1c1c(cccc1)Cl</chem>	MolPort-046-511-453 1529092867 MCULE-6922191288 PubChem-134695709 ZINC001529092867	C16H21ClN2O4	340.8
<chem>Cc1c(CN2CCN([C@H](C2=O)Cc2ccccc2)C(=O)N[C@@H](CC(C)C)C(=O)O)nc[nH]1</chem>	MolPort-046-761-290 MCULE-2144837958 PubChem-11539477	C23H31N5O4	441.52
<chem>CC(=O)Nc1ccc(cc1)S(=O)(=O)N/N=C/c1c[nH]nc1c1ccc(cc1)F</chem>	MolPort-001-627-821 17082161 LN01862014 ZINC000017082161 ZINC17082161	C18H16FN5O3S	401.41
<chem>CCNc1ncc(cn1)C(=O)N[C@H](CC(=O)O)c1ccco1</chem>	MolPort-028-582-670 MCULE-4144712298 PubChem-72874940	C14H16N4O4	304.3
<chem>NC(=O)CN1CCC[C@@H](C1)C(=O)N[C@H](Cc1ccc(cc1)F)C(=O)O</chem>	MolPort-045-967-429 MCULE-4471792144 PubChem-131932311	C17H22FN3O4	351.37
<chem>OCCCCNC(=O)[C@H]1OCC(=O)N[C@@H]1c1ccccc1</chem>	MolPort-046-517-095 1529126055 MCULE-6683554857 PubChem-134701333 ZINC001529126055	C16H22N2O4	306.36
<chem>CNC(=O)N1C[C@@H](CN(C)C)[C@@H](C1)NS(=O)(=O)c1ccc2cccn12</chem>	MolPort-044-356-221	C18H25N5O3S	391.49

<chem>O=C([C@H]1OCC(=O)N[C@@H]1c1ccccc1)NCc1c2c(CCC2)[nH]n1</chem>	MolPort-046-518-672 1529144164 MCULE-7750864382 PubChem-134702909 ZINC001529144164	C18H20N4O3	340.38
<chem>c1cc(ccc1C[C@@H](C(=O)O)NC(=O)/C=C\c1ccc(cc1)O</chem>	MolPort-019-937-476 49601481 MCULE-9336693077 PubChem-51136557 ZINC000049601481	C18H17NO5	327.33
<chem>CCS(=O)(=O)CC(=O)N[C@@H]([C@@H]1C[C@H](C1)O)c1c(ccc(c1)F)OC</chem>	MolPort-038-426-136	C16H22FNO5S	359.41
<chem>Cn1cc(en1)[C@H]([C@H]1C[C@@H](C1)O)NC(=O)Cc1c(C)nc(C)[nH]c1=O</chem>	MolPort-038-421-547	C17H23N5O3	345.4
<chem>O[C@@H]1C[C@H](C1)[C@H](c1cnc2ccccc2c1)NC(=O)CN1C(=O)CNC1=O</chem>	MolPort-038-398-216	C19H20N4O4	368.39
<chem>Cc1cccc(c1)[C@@H](C(=O)O)NC(=O)CCC(=O)NC1CCCCC1</chem>	MolPort-016-606-030 MCULE-6949030471 PubChem-50961767	C20H28N2O4	360.45
<chem>OC(=O)CNC(=O)[C@H](Cc1cccc1)n1c(=O)[nH]c2ccccc2c1=O</chem>	MolPort-002-529-327 9331881 LN00347764 PubChem-1787274 ZINC000009331881	C19H17N3O5	367.36
<chem>CO[C@@H]1C[C@H](CC[C@H]1Nc1c(cnc(C)n1)S(=O)(=O)C)C(=O)NC(C)C</chem>	MolPort-047-798-405 MolPort-047-798-406 1875250364 MCULE-1886175574 MCULE-4327146041 PubChem-155910936 PubChem-155972810	C17H28N4O4S	384.49
<chem>CNS(=O)(=O)CCNC(=O)[C@@H]1[C@@H](c2c(cccc2)Cl)NC(=O)CO1</chem>	MolPort-046-515-623 1529113786 MCULE-4060144533 PubChem-134699865 ZINC001529113786	C14H18ClN3O5S	375.83
<chem>OC(=O)[C@H](Cc1c[nH]c2ccccc12)NS(=O)(=O)c1ccc(cc1)F</chem>	MolPort-002-508-251 811636 CSC046093844 LN01886474 MCULE-2983160602 PubChem-1091373 ZINC000000811636	C17H15FN2O4S	362.38
<chem>Cn1c(N[C@@H](Cc2ccccc2)C(=O)O)nc2c1c(nc(=O)n2C)O</chem>	MolPort-000-789-257 MCULE-2148927037	C16H17N5O4	343.34
<chem>COc1cc(c(cc1)NS(=O)(=O)C)NC(=O)[C@H]1CC[C@H](C1)N</chem>	MolPort-021-773-696 72478225 MCULE-7831936029 PubChem-56914398 ZINC000072478225	C14H21N3O4S	327.4
<chem>Cc1nc(C)c(CC(=O)N[C@@H]([C@H]2C[C@@H](C2)O)c2ccccc2)c(=O)[nH]1</chem>	MolPort-038-405-619	C18H22N4O3	342.39
<chem>Oc1ccc(cc1)C(=O)NNS(=O)(=O)c1ccc(cc1)F</chem>	MolPort-001-886-537 CHEMBL1713869 MCULE-8678870686 PubChem-809440 ZINC00320595	C13H11FN2O4S	310.3
<chem>Oc1ccc(cc1)C(=O)NNS(=O)(=O)c1ccccc1</chem>	MolPort-001-934-541 CHEMBL1603218 MCULE-4971545008 PubChem-813058 ZINC00325219	C13H12N2O4S	292.31
<chem>O[C@@H]1[C@H](Cc2ccc(O)cc2)NS(=O)(=O)c2c1ccccc2</chem>	MolPort-005-913-777 LN00820026 MCULE-4673361477 PubChem-17591749	C15H15NO4S	305.35
<chem>CN1[C@H]([C@H](C[C@@]1(C)C(=O)O)C(=O)NCCc1c[nH]cn1)c1ccccc1</chem>	MolPort-019-887-157 67725472 MCULE-5714727556 ZINC000067725472	C19H24N4O3	356.42
<chem>CN(C)C[C@]1(CCCN(C1)C(=O)c1c(cccc1)c1nn[nH]1)O</chem>	MolPort-020-197-979 MCULE-1274964642	C16H22N6O2	330.38
<chem>O=C(C[C@H]1OCCNC1)Nc1c(cccc1)C(=O)NCc1ccccc1</chem>	MolPort-016-630-020 MCULE-1486824285 PubChem-50984925	C19H22N4O3	354.4
<chem>Cl[C@@H](C(=O)NC[C@H](CC(=O)N[C@@H](C)C(=O)O)c1ccc(cc1)Cl)N</chem>	MolPort-000-851-277 8764405 LN00375770 MCULE-4625879777 PubChem-16408594 ZINC000008764405	C16H22ClN3O4	355.82
<chem>S(=O)(=O)N[C@H](Cc1ccccc1)C(=O)O)c1cc2[nH]c(=O)c3c2c1ccc3</chem>	MolPort-000-685-213 LN01973873 MCULE-3840234982 PubChem-5183357	C20H16N2O5S	396.42
<chem>OC1=N[C@@H](CC(=O)NCCc2c[nH]cn2)C(=O)N1Cc1ccccc1</chem>	MolPort-038-431-704	C17H19N5O3	341.36
<chem>O=C(Cc1c[nH]c2c1ccccc2)NNC(=O)[C@@H](C(C)C)NS(=O)(=O)c1ccc(cc1)Cl</chem>	MolPort-000-829-028 MCULE-1840213992	C21H23ClN4O4S	462.95

<chem>c1(cc(C)nn1C)S(=O)(=O)NC[C@@H]1CC[C@H](CC(=O)NC)N1C</chem>	MolPort-051-618-105 MCULE-7381068009	C14H25N5O3S	343.45
<chem>CCN1CCN(CC1)CC(=O)N[C@@H](c1cccc1)cnnc(N)s1</chem>	MolPort-042-558-241 MCULE-8982290931 PubChem-118763080	C17H24N6OS	360.48
<chem>Cn1cc(cn1)[C@@H]([C@H]1C[C@@H](C1)O)NC(=O)Cn1cnc2ccccc2c1=O</chem>	MolPort-038-395-960 MCULE-9717702737 PubChem-91766164	C19H21N5O3	367.4
<chem>Cc1ccc(CN2CCNC(=O)[C@@H]2CC(=O)NCc2c3c(CCC3)[nH]n2)o1</chem>	MolPort-005-072-261 MCULE-2216217613 PubChem-45206526	C19H25N5O3	371.43
<chem>CC(C)C[C@]1(C[C@@H]([C@H](c2cnccc2)N1C)C(=O)NCCNC(=O)C)C(=O)O</chem>	MolPort-019-902-308 67981932 MCULE-8003088243 PubChem-56759915 ZINC000067981932	C20H30N4O4	390.48
<chem>C[C@H](CNC(=O)N[C@@H](Cc1cccc1)C(=O)O)O</chem>	MolPort-002-528-806 LN00355077 MCULE-1555471884 PubChem-16402629	C13H18N2O4	266.29
<chem>Cc1ccc(cc1)S(=O)(=O)NCC(=O)NCC(=O)NN=C1CCCCC1</chem>	MolPort-002-694-183 MCULE-9775012159 PubChem-5025869 ZINC04416535	C17H24N4O4S	380.46
<chem>Nc1[nH]nc(c1Cl)C(=O)N[C@H](CC(=O)O)c1cccc1</chem>	MolPort-035-763-827 MCULE-9843785688	C13H13ClN4O3	308.72
<chem>Fe1ccc(cc1)S(=O)(=O)CC(=O)Nc1ccc2C(=O)NC(=O)c2c1</chem>	MolPort-003-641-449 5190365 MCULE-2454514490 PubChem-7544789 ZINC000005190365	C16H11FN2O5S	362.33
<chem>COc1ccc(cc1)S(=O)(=O)N/N=C(/C)\c1c(ccc(c1)O)O</chem>	MolPort-008-266-298 17070701 LN01856007 PubChem-135647661 ZINC000017070701 ZINC17070701	C15H16N2O5S	336.36
<chem>Cc1n[nH]c(n1)SCCNC(=O)C[C@@H]1C(=O)NCCN1C/C=C/c1cccc1</chem>	MolPort-005-020-042	C20H26N6O2S	414.52
<chem>NC(=O)CC[C@@H]1N[C@@]2([C@@H]3[C@H]1C(=O)N(C3=O)c1ccc(cc1)F)C(=O)Nc1c2cccc1</chem>	MolPort-019-706-361 MCULE-5998733853 PubChem-4896832	C22H19FN4O4	422.41
<chem>C[C@@H](C(=O)N[C@H](C(=O)O)c1cccc1)n1c(=O)[nH]c2ccccc2c1=O</chem>	MolPort-002-529-492 2133130 ChemDiv-Y040-2776 LN00361348 MCULE-7794428303 PubChem-1788480 ZINC000002133130	C19H17N3O5	367.36
<chem>OC(=O)[C@H](Cc1cccc1)NC(=O)CCc1onc(O)c1</chem>	MolPort-035-700-222 217659410 LN00377257 MCULE-8992885754 ZINC000217659410	C15H16N2O5	304.3
<chem>CNC(=O)c1cccc(c1)NC(=O)C[C@@H]1NC(=O)c2c(NC1=O)cccc2</chem>	MolPort-008-266-343 17068813 LN01855488 PubChem-135647692 ZINC000017068813 ZINC17068813	C19H18N4O4	366.37
<chem>OC(=O)[C@H](Cc1ccc(O)cc1)NC(=O)CCc1c[nH]nc1</chem>	MolPort-042-631-013 426477237 MCULE-6494021629 PubChem-121500640 ZINC000426477237	C15H17N3O4	303.31
<chem>OC(=O)[C@H](Cc1cccc1)NS(=O)(=O)c1cc2OCC(=O)Nc2cc1Cl</chem>	MolPort-015-136-256 MCULE-8788802730 PubChem-44121946	C17H15ClN2O6S	410.83
<chem>Cc1cc(=O)n(CC(=O)N[C@@H](Cc2cnccc2)[C@@H]2C[C@H](C2)O)nc1C</chem>	MolPort-038-394-185	C19H24N4O3	356.42
<chem>COc1ccc(/C=N/NS(=O)(=O)c2ccc(C)cc2)cc1O</chem>	MolPort-002-972-139 571767 LN00837469 PubChem-9558104 ZINC000000571767 ZINC00571767	C15H16N2O4S	320.36
<chem>OCCN1C(=O)N[C@@](Cc2ccc(cc2)F)(C2CCNCC2)C1=O</chem>	MolPort-019-802-144 MolPort-047-486-974 MCULE-6886305353 MCULE-8909246463 PubChem-154885550 PubChem-56703542	C17H22FN3O3	335.37
<chem>CS(=O)(=O)CCC(=O)N[C@@H](Cc1ccncc1)[C@@H]1C[C@H](C1)O</chem>	MolPort-038-396-392	C15H22N2O4S	326.41
<chem>C[C@@H](C(=O)O)NC(=O)[C@@H](Cc1ccc(c1)n1c(=O)[nH]c2ccccc2c1=O</chem>	MolPort-002-534-081 LN00355703 PubChem-7068680	C20H19N3O5	381.38
<chem>OC(=O)[C@@H](Cc1cccc1)NS(=O)(=O)c1cc2c(OCC(=O)N2)cc1</chem>	MolPort-015-136-236 MCULE-4083469232 PubChem-44121926	C17H16N2O6S	376.38
<chem>CC(C)C(=O)Nc1cccc(c1)C(=O)N[C@H](CC(=O)O)c1cccc1</chem>	MolPort-045-938-907 MCULE-5492420456 PubChem-131891598	C20H22N2O4	354.4

<chem>C[C@@H](C(=O)O)NC(=O)[C@H](Cc1ccccc1)n1c(=O)[nH]c2ccccc2c1=O</chem>	MolPort-002-529-984 2136214 LN00369179 PubChem-1791495 ZINC000002136214	C20H19N3O5	381.38
<chem>COc1cc(C[C@@H]2[C@H](c3c(cccc3)S(=O)(=O)N2)O)ccc1O</chem>	MolPort-005-914-105 LN00819178 MCULE-7002847191 PubChem-17592018	C16H17NO5S	335.37
<chem>Cc1cccc(OC[C@@]2(CNC(=O)c3cncn3)C[C@@H]([C@@H](C2)O)O)n1</chem>	MolPort-027-852-455 MolPort-047-149-256 ZINC000107430236	C18H22N4O4	358.39
<chem>CC(C)C[C@H](c1nnc2CCNCCn12)NS(=O)(=O)c1cc(ccc1)C#N</chem>	MolPort-019-807-649 MCULE-1151816798 PubChem-56708720	C18H24N6O2S	388.49
<chem>C[C@H](C(=O)O)NC(=O)[C@@H](Cc1ccccc1)NC(=O)N1CC(=O)Nc2c1ccccc2</chem>	MolPort-002-533-793 4090409 LN00359329 PubChem-7097196 ZINC000004090409	C21H22N4O5	410.42
<chem>COc1cc(C[C@@H]2[C@H](c3c(cccc3)S(=O)(=O)N2)O)cc(c1O)OC</chem>	MolPort-005-916-066 LN00762410 MCULE-1434037457 PubChem-17593647	C17H19NO6S	365.4
<chem>Cc1ccc(cc1)S(=O)(=O)NNC(=O)c1ccc(cc1)O</chem>	MolPort-001-936-666 ChEMBL1550187 MCULE-9875619149 PubChem-794693 ZINC00297742	C14H14N2O4S	306.34
<chem>Oc1cccc(C(=O)N[C@H]2[C@@H]3CN4C[C@@]2(CN(C3)CC4)c2ccccc2)n1</chem>	MolPort-045-913-263 MCULE-2584007314	C21H24N4O2	364.44
<chem>NC(=O)Cn1cc(/C=N\NS(=O)(=O)c2ccc(cc2)F)c2ccccc12</chem>	MolPort-008-294-192 15933887 ChEMBL3195246 PubChem-20408221 ZINC000015933887 ZINC15933887	C17H15FN4O3S	374.39
<chem>CC(C)[C@H]1C(=O)Nc2c(cccc2)N1C(=O)N[C@@H](Cc1ccccc1)C(=O)NCC(=O)O</chem>	MolPort-002-662-923 9130504 LN00729517 MCULE-8330702773 PubChem-17582190 ZINC000009130504	C23H26N4O5	438.48
<chem>Cc1cccc(c1)[C@H](C(=O)O)NC(=O)[C@H]1CC[C@@H](CC1)O</chem>	MolPort-035-855-146 MCULE-9217922916	C16H21NO4	291.34
<chem>Cc1cc(=O)n(CC(=O)N[C@@H](Cc2cccn2)[C@@H]2C[C@H](C2)O)nc1C</chem>	MolPort-038-394-179	C19H24N4O3	356.42
<chem>COCCOC[C@@]1(CNS(=O)(=O)c2ccc(cc2)F)C[C@@H]([C@@H](C1)O)O</chem>	MolPort-027-852-674 ZINC000107283888	C16H24FNO6S	377.43
<chem>NCCCCNS(=O)(=O)c1ccccc1[N+](=O)[O-]</chem>	MolPort-008-268-325 2529179 CSC007810599 LN01740106 MCULE-2133072636 PubChem-11323272 PubChem-53439281 ZINC000002529179	C10H15N3O4S	273.31
<chem>CN(C)C(=O)CNCc1cnc(NS(=O)(=O)c2ccccc2)nc1</chem>	MolPort-045-937-748 952972114 MCULE-5095200450 PubChem-131902032 ZINC000952972114	C15H19N5O3S	349.41
<chem>COc1ccc(cc1)[C@@H]1[C@@H](C(=O)NCc2cc(O)ncn2)OCC(=O)N1C1CC1</chem>	MolPort-047-964-601 2100556848 MCULE-8403015516	C20H22N4O5	398.41
<chem>Cc1n[nH]c([C@@H]2CCN(CC2)C(=O)N[C@@H](c2ccccc2)C(=O)O)n1</chem>	MolPort-042-630-117 MCULE-9205525523	C17H21N5O3	343.38
<chem>O[C@H]1CCCN(CC(=O)NCc2onc(Cc3ccccc3)n2)C1</chem>	MolPort-039-116-213 MCULE-2738160925 PubChem-118782255	C17H22N4O3	330.38
<chem>c1(c2c([nH]cn2)nc(N)n1)N[C@H](c1ccccc1)C(=O)O</chem>	MolPort-030-042-399 LN05037472 MCULE-7652496019	C13H12N6O2	284.27
<chem>CS(=O)(=O)N(CC(=O)N/N=C/c1c(cccc1)O)c1ccc(cc1)F</chem>	MolPort-002-186-961 PubChem-135422656 ZINC02958125	C16H16FN3O4S	365.38
<chem>Cc1cc(nc(n1)NS(=O)(=O)c1ccccc1)NN</chem>	MolPort-001-954-702 270444 ChEMBL1535836 MCULE-6100075710 PubChem-778482 ZINC000000270444	C11H13N5O2S	279.32
<chem>c12c(c(ccc1c(C)c(c(=O)o2)CC(=O)N[C@H](CO)c1ccccc1)O)O</chem>	MolPort-005-910-491 12901265 LN00357161 MCULE-3669856229 PubChem-17572065 ZINC000012901265	C20H19NO6	369.37
<chem>C[C@H](C(=O)NC[C@@H]1CC[C@@H](CC1)C(=O)N[C@@H](C(=O)O)c1ccccc1)N</chem>	MolPort-002-533-395 MolPort-009-758-610 100779218 248094296 LN00340653 MCULE-7445352975 ZINC000100779218 ZINC000248094296	C19H27N3O4	361.44

<chem>CC(=O)Nc1ccc(cc1)NS(=O)(=O)c1c(cc(C)cc1)[N+](=O)[O-]</chem>	MolPort-002-275-654 613862 CSC048052505 MCULE-8128793294 PubChem-973301 ZINC000000613862 ZINC00613862	C15H15N3O5S	349.36
<chem>CC1(C)C(=O)Nc2ccc(cc12)S(=O)(=O)N[C@H](Cc1ccccc1)C(=O)O</chem>	MolPort-015-136-319 MCULE-8669357935 PubChem-44122002	C19H20N2O5S	388.44
<chem>COc1ccc(/C=N/NS(=O)(=O)c2ccccc2)cc1O</chem>	MolPort-001-543-184 3526618 LN01852507 PubChem-6908568 ZINC000003526618 ZINC03526618	C14H14N2O4S	306.34
<chem>CC(C)[C@@H](C(=O)N[C@@H](Cc1ccccc1)C(=O)O)NC(=O)N1CC(=O)Nc2c1ccccc2</chem>	MolPort-002-534-308 ChEMBL1534138 LN00347447 PubChem-16406491	C23H26N4O5	438.48
<chem>Cc1c(C)cc(cc1)S(=O)(=O)Nc1c(O)nc(O)nc1C</chem>	MolPort-002-011-943 ChEMBL1510444 MCULE-9520503086	C13H15N3O4S	309.34
<chem>Cc1cn2c(c(cn2)C(=O)N[C@H](Cc2ccccc2)[C@@H]2C[C@H](C2)O)nc1</chem>	MolPort-038-413-641	C19H21N5O2	351.4
<chem>O[C@H]1C[C@@H](C1)[C@H](Cc1ccccc1)NC(=O)c1cncn1</chem>	MolPort-038-425-144	C16H18N4O2	298.34
<chem>CC(C)C[C@@H](C(=O)N[C@H](C(=O)O)c1ccccc1)NC(=O)N1CC(=O)Nc2c1ccccc2</chem>	MolPort-002-534-379 ChEMBL1314859 LN00365492 PubChem-16406542	C23H26N4O5	438.48
<chem>C[C@@H](C(=O)O)NC(=O)[C@]1(CCN(CC1)C(=O)[C@@H]1Cc2c(CN1)ccccc2)c1ccccc1</chem>	MolPort-000-810-351 MolPort-002-531-868 12884188 LN00367096 MCULE-1339885321 MCULE-3904888925 PubChem-16404534 PubChem-44666545 ZINC000012884188	C25H29N3O4	435.52
<chem>C/C(=N)NS(=O)(=O)c1ccc(C)cc1/C[C@@]1(C(=O)Nc2c1ccccc2)O</chem>	MolPort-020-180-580 PubChem-45926853	C18H19N3O4S	373.43
<chem>N[C@@H](Cc1c[nH]c2ccccc12)C(=O)N1CC[C@H](CC1)C(=O)N[C@@H](C(=O)O)c1ccccc1</chem>	MolPort-002-526-290 8952566 LN00350192 MCULE-5160664460 PubChem-16401614 ZINC000008952566	C25H28N4O4	448.51
<chem>O/N=C\c1ccc[n+](CC(=O)Nc2c(cccc2)C(=O)O)c1</chem>	MolPort-027-719-288 252677925 MCULE-2067209175 MCULE-6658070470 PubChem-1589726 PubChem-75062733 ZINC000252677925	C15H14N3O4+	300.29
<chem>O=C([C@@H]1Cc2c(cccc2)S(=O)(=O)N1)NCc1c2c(CCC2)[nH]n1</chem>	MolPort-035-370-230 MCULE-3732035526 PubChem-77080680	C16H18N4O3S	346.4
<chem>CC(C)C[C@]1(C[C@@H]([C@H](c2cnccc2)N1C)C(=O)NCC(C)(C)CO)C(=O)O</chem>	MolPort-019-886-699 67714182 MCULE-2008819043 PubChem-56744352 ZINC000067714182	C21H33N3O4	391.5
<chem>Cc1cc(C)n(c(=O)n1)CC(=O)N[C@@H](Cc1ccncc1)[C@H]1C[C@@H](C1)O</chem>	MolPort-038-391-233	C19H24N4O3	356.42
<chem>COC(CNC(=O)C[C@@H]1C(=O)NCCN1S(=O)(=O)c1ccccc1)OC</chem>	MolPort-008-315-644 LN00845288 MCULE-1425831497 PubChem-45492107	C16H23N3O6S	385.44
<chem>O=C([C@@H]1Cc2c(cccc2)S(=O)(=O)N1)N1CC[C@H](CC1)c1ncc[nH]1</chem>	MolPort-021-766-338 MCULE-6354266546 PubChem-70759660	C17H20N4O3S	360.43
<chem>CCNC(=O)N1CCC[C@@](CNS(=O)(=O)c2c(C)n(CC)nc2)(CC1)O</chem>	MolPort-020-198-001 MCULE-2097938281 PubChem-56891097	C16H29N5O4S	387.5
<chem>CC(=O)NCc1cn2ccccc2C(=O)NCCN2CCOC2)nc1</chem>	MolPort-046-984-948 257267767 MCULE-1502366754 PubChem-110121696 ZINC000257267767	C19H25N5O3	371.43
<chem>CC(=O)Nc1ccc(cc1)S(=O)(=O)N[C@@H](CC(=O)O)c1ccc(cc1)Cl</chem>	MolPort-002-728-019 CSC048903916 MCULE-3662821967 PubChem-4917666	C17H17ClN2O5S	396.85
<chem>OC[C@H]1CCCCN1C(=O)NCc1nncn1CCc1ccccc1</chem>	MolPort-045-914-342 MCULE-3189806907 PubChem-131945970	C18H25N5O2	343.42
<chem>CC(=O)Nc1ccccc1)NC(=O)N[C@@H](Cc1ccccc1)C(=O)O</chem>	MolPort-002-652-204 5307766 LN00760035 MCULE-6199555348 PubChem-7623388 ZINC000005307766	C18H19N3O4	341.36
<chem>NC(=O)CCNC(=O)C[C@H]1N(Cc2ccc3ccccc3c2)CCNC1=O</chem>	MolPort-020-196-003 MCULE-5576289256 PubChem-56889585	C20H24N4O3	368.43

<chem>CN(CCc1c(C)[nH]nc1C)C(=O)[C@H]1Cc2c(ccc2)S(=O)(=O)N1</chem>	MolPort-035-380-318 MCULE-4374686880 PubChem-77092323	C17H22N4O3S	362.45
<chem>Cc1c(ccc(c1)S(=O)(=O)NCC(=O)N1C[C@@H]2CNC(=O)[C@@H]2C1)F</chem>	MolPort-051-466-903 2356163952 MCULE-2544899050 PubChem-162634751	C15H18FN3O4S	355.38
<chem>C[C@@H](C(=O)N1CC[C@H](CC1)n1c(ccn1)NS(=O)(=O)Cc1cccc1)O</chem>	MolPort-019-881-586 MCULE-6910108709 PubChem-56739247	C18H24N4O4S	392.47
<chem>Oc1cccc(/C=N/NS(=O)(=O)c2cccc2)c1</chem>	MolPort-001-493-274 3575029 PubChem-6910117 ZINC000003575029 ZINC03575029	C13H12N2O3S	276.31
<chem>CC(C)[C@H](C(=O)O)NC(=O)[C@H](Cc1ccc1)n1c(=O)[nH]c2cccc2c1=O</chem>	MolPort-002-532-731 LN00374604 PubChem-7068509	C22H23N3O5	409.44
<chem>CCCC(=O)Nc1cccc(c1)C(=O)N[C@H](C(=O)O)c1c(C)[nH]nc1C</chem>	MolPort-016-610-437 MCULE-8417818526 PubChem-50966018	C18H22N4O4	358.39
<chem>c1(ccc(C[C@H](C(=O)O)NS(=O)(=O)c2cc3c(c2)OCC(=O)N3)cc1)F</chem>	MolPort-002-027-995 CSC047537761 ChemDiv-8017-5522 LN00938184 MCULE-8084942922 PubChem-5299552	C17H15FN2O6S	394.37
<chem>Cc1ccc(cc1)S(=O)(=O)NC(=O)NCCNC(=O)OC(C)(C)C</chem>	MolPort-002-888-616 MCULE-6885902371 PubChem-2795699 ZINC000003078751 ZINC03078751	C15H23N3O5S	357.43
<chem>COc1cc(c(cc1)S(=O)(=O)N/N=C\c1cc(ccc1)O)OC</chem>	MolPort-008-294-131 32577588 PubChem-20182359 ZINC000032577588 ZINC32577588	C15H16N2O5S	336.36
<chem>Oc1cc(O)c(/C=N\NC(=O)[C@H]2[C@@H](CNC2=O)c2cccc2)cc1</chem>	MolPort-002-322-830 LN01038002 PubChem-135646951	C18H17N3O4	339.35
<chem>C[C@@H](C(=O)O)NC(=O)[C@@H](Cc1ccc1)n1c(=O)[nH]c2cccc2c1=O</chem>	MolPort-002-533-591 LN00396964 PubChem-6851376	C20H19N3O5	381.38
<chem>Cc1c(O)nc(/C=N/NS(=O)(=O)c2ccc(C)cc2)n1c1cccc1</chem>	MolPort-004-949-203 1057534 PubChem-9618217 ZINC000001057534	C18H18N4O3S	370.43
<chem>Cc1cc(ccc1)[C@H](C(=O)O)NC(=O)CCCc1c[nH]nc1</chem>	MolPort-042-641-318 MCULE-1115429892 PubChem-121510892	C16H19N3O3	301.34
<chem>COc1c(cc(cc1)[C@@H]1[C@@H](C(=O)NCc2cc(C3CC3)[nH]n2)OCC(=O)N1)OC</chem>	MolPort-047-963-934 MolPort-047-963-935 MCULE-1185632486	C20H24N4O5	400.43
<chem>Cc1c(cc(cc1)S(=O)(=O)NC[C@]1(CCOC1)OCO)Cl</chem>	MolPort-046-065-419 CSC102078891 MCULE-6197287757 PubChem-132451507	C14H20ClNO5S	349.83
<chem>Cc1cc(C)c(cc1)NC(=O)CCC(=O)NNC(=O)c1c(cccc1)C(=O)O</chem>	MolPort-000-690-328 LN00939114 MCULE-8457354344 PubChem-1632382	C20H21N3O5	383.4
<chem>OCc1cccc(CNC(=O)[C@H]2OCC(=O)N(C3C3)[C@@H]2c2cnccc2)c1</chem>	MolPort-046-523-454 1529168811 MCULE-8670349165 PubChem-134707674 ZINC001529168811	C21H23N3O4	381.43
<chem>Cc1c(ccc(c1)S(=O)(=O)NCC(=O)N1CC[C@H](CO)[C@@H](C1)O)F</chem>	MolPort-051-530-390 MCULE-3046693714 MCULE-7923258203 PubChem-165418391 PubChem-166598613	C15H21FN2O5S	360.4
<chem>c12ccc(c3cccc(c(=O)n2C)c13)S(=O)(=O)NNC(=O)c1ccc(cc1)O</chem>	MolPort-019-845-573 LN01937096 MCULE-4218146227 PubChem-52100348	C19H15N3O5S	397.4
<chem>Oc1cccc(c1)[C@H]1Nc2cccc2C(=O)N1NS(=O)(=O)c1cccc1</chem>	MolPort-001-583-912 ChEMBL1424043 ChemDiv-6267-0059 MCULE-6671540696 PubChem-4402103	C20H17N3O4S	395.43
<chem>C1[C@@H]([C@H](CN1CCO)NC(=O)CCCS(=O)(=O)N)c1cccc1</chem>	MolPort-027-866-714 MolPort-047-500-235 91563311 MCULE-3639799162 MCULE-5312604739 PubChem-154897903 PubChem-86283209 ZINC000091563311	C16H25N3O4S	355.45