sample	primary cScore	primary r2	primary ec50	primary ec50_l
SJ000024224-2	Inactive	NA	NA	NA
SJ000031311-2	Inactive	NA	NA	NA
SJ000338276-2	Inactive	NA	NA	NA
SJ000122872-2	Inactive	NA	NA	NA
SJ000460846-2	Inactive	NA	NA	NA
SJ000251743-2	Inactive	NA	NA	NA
SJ000049059-2	Inactive	NA	NA	NA
SJ000338514-2	Inverse	0.92	-3.823908741	-4.013228266
SJ000184291-2	Inverse	0.97	-3.537602002	-3.721246399
SJ000518754-2	Inverse	0.86	-3.48148606	-3.958607315
SJ000007551-2	Inverse	0.74	-3.420216403	-4
SJ000208458-2	Inverse	0.64	-3.292429824	-3.920818754
SJ000517298-2	Inverse	0.8	-3.537602002	-3.958607315
SJ000337803-2	Inverse	0.24	-3.22184875	-4.096910013
SJ000292370-3	Inverse	0.67	-3.356547324	-4.055517328
SJ000161809-3	Inverse	0.57	-3.366531544	-4
SJ000124514-2	Inverse	-2.20E-16	-6.721246399	-10.14874165
SJ000081990-2	Inverse	0.4	-4.060480747	-4.853871964
SJ000097754-2	Inverse	0.72	-4.214670165	-4.37675071
SJ000369908-2	Inverse	0.59	-3.37675071	-4
SJ000108033-2	Inverse	0.87	-4.13667714	-4.27572413
SJ000304667-2	Inverse	0.91	-3.744727495	-3.853871964
SJ000516965-2	Inverse	0.93	-3.568636236	-3.602059991
SJ000151680-2	Inverse	0.68	-3.420216403	-4.113509275
SJ000184121-2	Inverse	0.58	-3.886056648	-4.096910013
SJ000291942-2	Sigmoidal	0.98	-6.619788758	-6.853871964
SJ000370178-2	Sigmoidal	0.93	-6	-6.346787486
SJ000063181-2	Sigmoidal	0.85	-7.443697499	-7.795880017
SJ000024045-2	Sigmoidal	0.91	-8.920818754	-9.070581074
SJ000029514-2	Sigmoidal	0.97	-8.301029996	-8.443697499
SJ000026852-2	Sigmoidal	0.94	-8.173925197	-8.356547324
SJ000298151-2	Sigmoidal	0.93	-7.958607315	-8.13667714
SJ000340178-2	Sigmoidal	0.92	-7.853871964	-8.022276395
SJ000293035-2	Sigmoidal	0.96	-7.823908741	-7.958607315
SJ000055839-2	Sigmoidal	0.91	-7.744727495	-7.920818754
SJ000063028-2	Sigmoidal	0.91	-7.619788758	-7.769551079
SJ000031471-2	Sigmoidal	0.94	-7.585026652	-7.744727495
SJ000207974-2	Sigmoidal	0.93	-7.327902142	-7.48148606
SJ000208514-2	Sigmoidal	0.95	-7.292429824	-7.468521083
SJ000045485-2	Sigmoidal	0.99	-7.207608311	-7.292429824
SJ000063138-2	Sigmoidal	0.92	-7.070581074	-7.200659451
SJ000354312-2	Sigmoidal	0.96	-7.060480747	-7.229147988
SJ000017426-3	Sigmoidal	0.96	-6.958607315	-7.173925197

SJ000062591-2	Sigmoidal	0.93	-6.886056648	-7.036212173
SJ000162243-3	Sigmoidal	0.94	-6.795880017	-6.886056648
SJ000367650-2	Sigmoidal	0.9	-6.769551079	-6.958607315
SJ000063180-2	Sigmoidal	0.94	-6.769551079	-7
SJ000154298-2	Sigmoidal	0.91	-6.744727495	-7.13667714
SJ000062600-2	Sigmoidal	0.95	-6.568636236	-6.744727495
SJ000370379-2	Sigmoidal	0.95	-6.552841969	-6.769551079
SJ000444978-2	Sigmoidal	0.95	-6.537602002	-6.677780705
SJ000316928-2	Sigmoidal	0.92	-6.508638306	-6.721246399
SJ000295844-2	Sigmoidal	-1.5	-8.853871964	-44.02687215
SJ000121199-2	Sigmoidal	0.81	-8.494850022	-8.744727495
SJ000338565-2	Sigmoidal	0.82	-8.193820026	-8.431798276
SJ000056835-2	Sigmoidal	0.9	-8.148741651	-8.30980392
SJ000124445-2	Sigmoidal	0.9	-8	-8.200659451
SJ000143378-2	Sigmoidal	0.74	-7.958607315	-8.27572413
SJ000063040-2	Sigmoidal	0.85	-7.920818754	-8.102372909
SJ000518716-2	Sigmoidal	0.89	-7.886056648	-8.15490196
SJ000294921-2	Sigmoidal	0.83	-7.853871964	-8.107905397
SJ000394353-2	Sigmoidal	0.83	-7.795880017	-7.886056648
SJ000208831-2	Sigmoidal	0.83	-7.698970004	-7.958607315
SJ000007707-2	Sigmoidal	0.8	-7.552841969	-7.958607315
SJ000045486-2	Sigmoidal	0.88	-7.508638306	-7.769551079
SJ000139983-2	Sigmoidal	0.87	-7.431798276	-7.677780705
SJ000441894-2	Sigmoidal	0.82	-7.408935393	-7.585026652
SJ000161544-3	Sigmoidal	0.86	-7.408935393	-7.744727495
SJ000390741-2	Sigmoidal	0.81	-7	-7.327902142
SJ000451891-2	Sigmoidal	0.74	-6.958607315	-7.292429824
SJ000294743-2	Sigmoidal	0.87	-6.886056648	-7.494850022
SJ000208133-2	Sigmoidal	0.88	-6.638272164	-6.769551079
SJ000414020-2	Sigmoidal	0.86	-3.744727495	-4.075720714
SJ000421218-2	Sigmoidal	0.7	-3.744727495	-4.167491087
SJ000063022-2	Sigmoidal	0.8	-3.677780705	-4.22184875
SJ000339592-2	Sigmoidal	0.92	-8.050609993	-8.161150909
SJ000013778-2	Sigmoidal	0.93	-7.823908741	-7.958607315
SJ000296667-2	Sigmoidal	0.91	-7.214670165	-7.455931956
SJ000293006-2	Sigmoidal	0.93	-7.207608311	-7.508638306
SJ000433644-2	Sigmoidal	0.91	-6.823908741	-7.075720714
SJ000368630-2	Sigmoidal	0.96	-5.958607315	-6.13667714
SJ000007499-2	Sigmoidal	0.83	-8.346787486	-8.619788758
SJ000154959-2	Sigmoidal	0.78	-8.096910013	-8.397940009
SJ000297687-2	Sigmoidal	0.86	-8.091514981	-8.292429824
SJ000290800-2	Sigmoidal	0.83	-7.823908741	-8.119186408
SJ000121296-3	Sigmoidal	0.84	-7.795880017	-8.031517051
SJ000207559-2	Sigmoidal	0.9	-7.200659451	-7.443697499

SJ000105009-2	Single-Point	NA	NA	NA
SJ000449712-2	Single-Point	NA	NA	NA
SJ000106942-2	Single-Point	NA	NA	NA
SJ000338685-2	Single-Point	NA	NA	NA
SJ000195722-2	Single-Point	NA	NA	NA
SJ000208919-2	Single-Point	NA	NA	NA
SJ000339517-2	Super Active	NA	-9	NA
SJ000294876-2	Super Active	NA	-9	NA
SJ000157784-2	Super Active	NA	-9	NA
SJ000338428-2	Super Active	NA	-9	NA
SJ000286673-2	Supplement	NA	NA	NA
SJ000287098-9	Supplement	NA	NA	NA
SJ000286237-8	Supplement	NA	NA	NA
SJ000821588-2	Supplement	NA	NA	NA

primary ec50_u	zebrafish_assay @1uM	supplier	supplierID
NA	inactive	CHEMBRIDGE	5570428
NA	inactive	CHEMDIV	4789-3815
NA	inactive	CHEMBRIDGE	9034936
NA	inactive	CHEMBRIDGE	5699405
NA	inactive	ENAMINE	Z1003723306
NA	inactive	CHEMDIV	K405-3423
NA	inactive	CHEMDIV	8005-8705
-3.552841969	inactive	CHEMBRIDGE	9040360
-3.366531544	inactive	CHEMBRIDGE	7376081
-3.48148606	inactive	CHEMBRIDGE	14235531
-3.420216403	inactive	CHEMDIV	2043-2122
-3.301029996	inactive	CHEMBRIDGE	9016978
-3.318758763	inactive	CHEMBRIDGE	91560538
-3.22184875	inactive	CHEMBRIDGE	7985706
-3.356547324	inactive	CHEMBRIDGE	5246216
-3.207608311	inactive	CHEMBRIDGE	6201133
-4.124938737	inactive	CHEMDIV	C226-0962
-4.060480747	inactive	CHEMDIV	C720-0233
-3.721246399	inactive	CHEMDIV	E141-0526
-3.193820026	inactive	ENAMINE	Z19456130
-3.958607315	inactive	CHEMDIV	E722-1335
-3.602059991	toxic	CHEMBRIDGE	51137717
-3.508638306	toxic	CHEMBRIDGE	91880890
-3.420216403	toxic	CHEMBRIDGE	5691489
-3.522878745	toxic	CHEMBRIDGE	7367629
-6.30980392	active	CHEMBRIDGE	6204620
-5.744727495	active	ENAMINE	Z19757816
-7.017728767	active	CHEMDIV	C226-3140
-8.769551079	inactive	CHEMBRIDGE	5935313
-8.173925197	inactive	CHEMDIV	4530-7241
-8	inactive	CHEMDIV	4340-0686
-7.795880017	inactive	CHEMBRIDGE	5347647
-7.619788758	inactive	CHEMBRIDGE	9091914
-7.698970004	inactive	CHEMBRIDGE	6073715
-7.522878745	inactive	CHEMDIV	8016-2491
-7.537602002	inactive	CHEMDIV	C226-2456
-7.397940009	inactive	CHEMDIV	4813-0675
-7.187086643	inactive	CHEMBRIDGE	9013027
-7.13076828	inactive	CHEMBRIDGE	9017637
-7.124938737	inactive	CHEMDIV	7610-2363
-6.920818754	inactive	CHEMDIV	C226-3024
-6.920818754	inactive	CHEMBRIDGE	62726111
-6.744727495	inactive	CHEMBRIDGE	5245599

-6.769551079	inactive	CHEMDIV	C226-0235
-6.638272164	inactive	CHEMBRIDGE	6224143
-6.619788758	inactive	ENAMINE	Z1106665833
-6.522878745	inactive	CHEMDIV	C226-3138
-6.124938737	inactive	CHEMBRIDGE	5813384
-6.408935393	inactive	CHEMDIV	C226-0252
-6.102372909	inactive	ENAMINE	Z1106859828
-6.337242168	inactive	ENAMINE	Z145341032
-6.086186148	inactive	CHEMDIV	F264-0031
-4.602059991	inactive	CHEMBRIDGE	5255387
-8.22184875	inactive	CHEMBRIDGE	5701537
-8	inactive	CHEMBRIDGE	9083529
-7.958607315	inactive	CHEMDIV	8017-9848
-7.744727495	inactive	CHEMDIV	C226-0392
-7.602059991	inactive	CHEMBRIDGE	5265701
-7.657577319	inactive	CHEMDIV	C226-2476
-7.508638306	inactive	CHEMBRIDGE	79722939
-7.602059991	inactive	CHEMBRIDGE	6097929
-7.602059991	inactive	ENAMINE	Z18373059
-7.346787486	inactive	CHEMBRIDGE	9020985
-7.065501549	inactive	CHEMDIV	2054-0030
-7.086186148	inactive	CHEMDIV	7610-2364
-7.200659451	inactive	CHEMBRIDGE	7977589
-6.958607315	inactive	ENAMINE	Z281772932
-7.008773924	inactive	CHEMBRIDGE	6188444
-6.366531544	inactive	ENAMINE	Z1106859880
-6.420216403	inactive	ENAMINE	Z1037584322
-6.193820026	inactive	CHEMBRIDGE	5220999
-6.251811973	inactive	CHEMBRIDGE	9014002
-3.744727495	inactive	ENAMINE	Z111906406
-3.744727495	inactive	ENAMINE	Z19758643
-3.698970004	inactive	CHEMDIV	C226-2442
-7.920818754	toxic	CHEMBRIDGE	9085609
-7.721246399	toxic	CHEMDIV	3156-0424
-6.920818754	toxic	CHEMBRIDGE	5307485
-6.744727495	toxic	CHEMBRIDGE	6233047
-6.657577319	toxic	ENAMINE	Z1171615156
-5.744727495	toxic	ENAMINE	Z104483252
-8.107905397	toxic	CHEMDIV	2042-2748
-7.769551079	toxic	CHEMBRIDGE	5853438
-7.886056648	toxic	CHEMBRIDGE	5331317
-7.431798276	toxic	CHEMBRIDGE	5142125
-7.552841969	toxic	CHEMDIV	1000-0399
-7.013228266	toxic	CHEMBRIDGE	9010587

NA	inactive	CHEMDIV	E596-0010
NA	inactive	ENAMINE	Z101340260
NA	inactive	CHEMDIV	E676-2829
NA	inactive	CHEMBRIDGE	9083857
NA	inactive	CHEMBRIDGE	7848005
NA	inactive	CHEMBRIDGE	9022135
NA	inactive	CHEMBRIDGE	9087412
NA	inactive	CHEMBRIDGE	6028799
NA	inactive	CHEMBRIDGE	6021190
NA	inactive	CHEMBRIDGE	9035557
NA	toxic	CAYMAN	10739
NA	inactive	SELLECK	S2380
NA	inactive	SANTA_CRUZ	sc-3529
NA	inactive	TCI_AMERICA	H0955

molsmiles
Fc1ccc(cc1)C(=O)N2CCN(CC2)c3ccccc3;Fc1ccc(cc1)C(=O)N2CCN(CC2)c3ccccc3
CCN(CC)CCCNc1ncnc2sc3CC(C)CCc3c12;CCN(CC)CCCNc1ncnc2sc3CC(C)CCc3c12
CCC1CCc2nc3sc(C(=O)O)c(N)c3cc2C1;CCC1CCc2nc3sc(C(=O)O)c(N)c3cc2C1
NC(=O)c1ccccc1NS(=O)(=O)c2cc(Cl)ccc2Cl;NC(=O)c1ccccc1NS(=O)(=O)c2cc(Cl)ccc2Cl
Fc1ccccc1NC(=O)CCN2C=Nc3scc(c4ccc(Br)cc4)c3C2=O;Fc1ccccc1NC(=O)CCN2C=Nc3scc(c4ccc(Br)cc4)c3C2=O
Cc1ccc(Cl)cc1n2ncc3c(NCCO)ncnc23;Cc1ccc(Cl)cc1n2ncc3c(NCCO)ncnc23
O=C(Nc1ccccc1C#N)c2cccs2;O=C(Nc1ccccc1C#N)c2cccs2
CCC1CCc2nc3sc(C(=O)C)c(N)c3cc2C1;CCC1CCc2nc3sc(C(=O)C)c(N)c3cc2C1
CC1CCN(CC1)c2ncnc3c2cnn3c4ccc(Cl)cc4;CC1CCN(CC1)c2ncnc3c2cnn3c4ccc(Cl)cc4
Cc1csc2c(ncnc12)c3ccc4OCCOc4c3;Cc1csc2c(ncnc12)c3ccc4OCCOc4c3
Fc1ccc(NC(=O)c2sc3ccccc3c2Cl)c(F)c1;Fc1ccc(NC(=O)c2sc3ccccc3c2Cl)c(F)c1
Fc1ccccc1c2onc(n2)c3ccc4OCOc4c3;Fc1ccccc1c2onc(n2)c3ccc4OCOc4c3
Nc1nc(NCc2ccccc2)nc(n1)c3cnc4ccccc4c3;Nc1nc(NCc2ccccc2)nc(n1)c3cnc4ccccc4c3
CCOC(=O)c1sc2nc3ccc(OC)cc3cc2c1N;CCOC(=O)c1sc2nc3ccc(OC)cc3cc2c1N
O=C(Nc1nc2ccccc2s1)c3ccc(cc3)c4ccccc4;O=C(Nc1nc2ccccc2s1)c3ccc(cc3)c4ccccc4
Cc1ccc(OCC(=O)Nc2ccc(Cl)cn2)c(C)c1;Cc1ccc(OCC(=O)Nc2ccc(Cl)cn2)c(C)c1
COc1ccccc1c2onc(c2)C(=O)Nc3cccc(Cl)c3;COc1ccccc1c2onc(c2)C(=O)Nc3cccc(Cl)c3
CC1=CC2=NC=C(C(=O)Nc3ccc(C)c(C)c3)C(=O)N2C=C1;CC1=CC2=NC=C(C(=O)Nc3ccc(C)c(C)c3)C(=O)N2C=C1
Cc1c(nnn1c2ccc(Br)cc2)C(=O)Nc3ccccc3;Cc1c(nnn1c2ccc(Br)cc2)C(=O)Nc3ccccc3
Clc1ccccc1CSc2oc(nn2)c3ccc4OCOc4c3;Clc1ccccc1CSc2oc(nn2)c3ccc4OCOc4c3
Cc1ccc(NC(=O)C2=Cc3sc(C)c(C)c3CS2)cc1C;Cc1ccc(NC(=O)C2=Cc3sc(C)c(C)c3CS2)cc1C
COc1cccc(c1)[C@@H](C)NC(=O)C2=CN(C=C(C(=O)NCC(C)C)C2=O)C3CCCC3;COc1cccc(c1)[C@@H](C)NC(=O)C2=Cl
COc1cc(nc(N)n1)c2cccc(OC(C)C)c2;COc1cc(nc(N)n1)c2cccc(OC(C)C)c2
Cc1cn2cc(nc2s1)c3ccc(I)cc3;Cc1cn2cc(nc2s1)c3ccc(I)cc3
CC(C)(C)c1ccc(cc1Br)C(=O)N2CCc3ccccc23;CC(C)(C)c1ccc(cc1Br)C(=O)N2CCc3ccccc23
CCc1ccc(OCC(=O)Nc2ccc(F)c(c2)[N+](=O)[O-])cc1;CCc1ccc(OCC(=O)Nc2ccc(F)c(c2)[N+](=O)[O-])cc1
Cc1ccsc1C(=O)OCC(=O)Nc2ccc(OC(F)F)cc2;Cc1ccsc1C(=O)OCC(=O)Nc2ccc(OC(F)F)cc2
CC(C)Cc1onc(c1)C(=O)Nc2ccc(F)c(Cl)c2;CC(C)Cc1onc(c1)C(=O)Nc2ccc(F)c(Cl)c2
Clc1ccc(cc1)c2csc(Nc3ncccn3)n2;Clc1ccc(cc1)c2csc(Nc3ncccn3)n2
Cc1ccc(cc1)C(=O)C2=C(O)C(=O)N(C2c3ccc(F)cc3)c4nc5ccccc5s4;Cc1ccc(cc1)C(=O)C2=C(O)C(=O)N(C2c3ccc(F)cc3)c
COC(=O)c1sc(NC(=O)c2ccc(Cl)cc2)nc1C;COC(=O)c1sc(NC(=O)c2ccc(Cl)cc2)nc1C
Cc1ccc(cc1)C(=O)Nc2ccc(Cl)cc2C;Cc1ccc(cc1)C(=O)Nc2ccc(Cl)cc2C
COC(=O)c1sc(NC(=O)c2csc3ccccc23)nc1C;COC(=O)c1sc(NC(=O)c2csc3ccccc23)nc1C
Cc1ccccc1CNC(=O)CN(c2ccc(Oc3ccccc3)cc2)S(=O)(=O)C;Cc1ccccc1CNC(=O)CN(c2ccc(Oc3ccccc3)cc2)S(=O)(=O)C
Cc1cccc(c1)C(=O)Nc2nc3ccc(F)cc3s2;Cc1cccc(c1)C(=O)Nc2nc3ccc(F)cc3s2
Oc1ccccc1c2onc(c2)C(=O)Nc3ccc(F)c(Cl)c3;Oc1ccccc1c2onc(c2)C(=O)Nc3ccc(F)c(Cl)c3
[O-][N+](=O)c1ccc(cc1)c2noc(n2)c3ccc(Cl)cc3Cl;[O-][N+](=O)c1ccc(cc1)c2noc(n2)c3ccc(Cl)cc3Cl
Clc1ccccc1OCC(=O)Nc2ccc(Br)cn2;Clc1ccccc1OCC(=O)Nc2ccc(Br)cn2
COc1cc(ccc1OCc2ccc(Cl)c(Cl)c2)C(=O)N;COc1cc(ccc1OCc2ccc(Cl)c(Cl)c2)C(=O)N
CC1CCN(CC1)C(=O)c2cc(on2)c3ccc(C)cc3;CC1CCN(CC1)C(=O)c2cc(on2)c3ccc(C)cc3
CCCc1onc(c1)C(=O)Nc2ccc(CC)cc2;CCCc1onc(c1)C(=O)Nc2ccc(CC)cc2
COC(=O)CCNC(=O)c1csc2nc(cn12)c3ccccc3Cl;COC(=O)CCNC(=O)c1csc2nc(cn12)c3ccccc3Cl
Cc1ccc(NC(=O)c2cccs2)cc1C;Cc1ccc(NC(=O)c2cccs2)cc1C

CC1CCN(CC1)C(=O)c2cc(on2)c3ccc(F)cc3;CC1CCN(CC1)C(=O)c2cc(on2)c3ccc(F)cc3
Cc1ccc(NC(=O)CN(c2ccc(Oc3ccccc3)cc2)S(=O)(=O)C)cc1;Cc1ccc(NC(=O)CN(c2ccc(Oc3ccccc3)cc2)S(=O)(=O)C)cc1
O=C(NC1CCCCCCC1)c2ccc(cc2)C#N;O=C(NC1CCCCCCC1)c2ccc(cc2)C#N
CCc1ccc(NC(=O)c2cc(CC(C)C)on2)cc1;CCc1ccc(NC(=O)c2cc(CC(C)C)on2)cc1
Cc1cccnc1NC(=O)COc2ccc(Br)cc2;Cc1cccnc1NC(=O)COc2ccc(Br)cc2
CC1CCCCN1C(=O)c2cc(on2)c3ccc(F)cc3;CC1CCCCN1C(=O)c2cc(on2)c3ccc(F)cc3
Fc1ccccc1OCC(=O)Nc2ccc3CCCc3c2;Fc1ccccc1OCC(=O)Nc2ccc3CCCc3c2
COc1ccc(cc1)c2nc(C)c(s2)C(=O)N3CCN(CC3)c4ccc(cc4)C(=O)C;COc1ccc(cc1)c2nc(C)c(s2)C(=O)N3CCN(CC3)c4ccc(c
Cc1ccc(cc1)C2=CC(=O)c3cc(NC(=O)c4occc4)ccc3O2;Cc1ccc(cc1)C2=CC(=O)c3cc(NC(=O)c4occc4)ccc3O2
CC(=O)Nc1ccc2oc(nc2c1)c3ccc(Cl)cc3;CC(=O)Nc1ccc2oc(nc2c1)c3ccc(Cl)cc3
CCOC(=O)c1sc(NC(=O)c2cccc(Cl)c2)nc1C;CCOC(=O)c1sc(NC(=O)c2cccc(Cl)c2)nc1C
Fc1ccc(NC(=O)c2ccc(cc2)N3CCCCC3)cc1;Fc1ccc(NC(=O)c2ccc(cc2)N3CCCCC3)cc1
CCc1ccc(NC(=O)c2sc3nc(C)c(C)c(C)c3c2N)cc1;CCc1ccc(NC(=O)c2sc3nc(C)c(C)c(C)c3c2N)cc1
Clc1ccc(cc1)c2onc(c2)C(=O)Nc3cccc(Cl)c3;Clc1ccc(cc1)c2onc(c2)C(=O)Nc3cccc(Cl)c3
Brc1ccccc1NC(=O)c2ccc(cc2)c3ccccc3;Brc1ccccc1NC(=O)c2ccc(cc2)c3ccccc3
CC(=O)c1cccc(NC(=O)c2cc(on2)c3ccccc3O)c1;CC(=O)c1cccc(NC(=O)c2cc(on2)c3ccccc3O)c1
CN(C)C(=O)c1cccc(c1)c2nc3ccc(Cl)cc3s2;CN(C)C(=O)c1cccc(c1)c2nc3ccc(Cl)cc3s2
Clc1ccc(NC(=S)NC(=O)c2cccs2)c(Cl)c1;Clc1ccc(NC(=S)NC(=O)c2cccs2)c(Cl)c1
Cc1ccc2nc(sc2c1)c3ccc(NC(=O)COC(=O)c4ccc(cc4)C#N)cc3;Cc1ccc2nc(sc2c1)c3ccc(NC(=O)COC(=O)c4ccc(cc4)C#N
Cc1ccc(NC(=O)C(=O)c2c[nH]c3ccccc23)cc1C;Cc1ccc(NC(=O)C(=O)c2c[nH]c3ccccc23)cc1C
CC(C)(C)c1ccc(cc1)C(=O)Nc2ccc(Cl)cc2Cl;CC(C)(C)c1ccc(cc1)C(=O)Nc2ccc(Cl)cc2Cl
CC1CCCCN1C(=O)c2cc(on2)c3ccc(C)cc3;CC1CCCCN1C(=O)c2cc(on2)c3ccc(C)cc3
CC(C)(C)c1ccc(cc1)C(=O)Nc2cccc(NC(=O)COc3ccccc3Cl)c2;CC(C)(C)c1ccc(cc1)C(=O)Nc2cccc(NC(=O)COc3ccccc3Cl)
Clc1cc(ccc1OCc2cc(on2)c3ccccc3)C#N;Clc1cc(ccc1OCc2cc(on2)c3ccccc3)C#N
CCOc1ccc(NC(=O)CN(c2ccc(Oc3ccccc3)cc2)S(=O)(=O)C)cc1;CCOc1ccc(NC(=O)CN(c2ccc(Oc3ccccc3)cc2)S(=O)(=O)C
O=C(Nc1ccc2CCCc2c1)c3ccc(cc3)C#N;O=C(Nc1ccc2CCCc2c1)c3ccc(cc3)C#N
CCc1ccc(cc1)c2nc(NC3CC3)sc2C;CCc1ccc(cc1)c2nc(NC3CC3)sc2C
Fc1ccccc1C(=O)Nc2ccc(Cl)cc2Cl;Fc1ccccc1C(=O)Nc2ccc(Cl)cc2Cl
CCC(=O)NCc1ccc(cc1)c2oc3ccccc3n2;CCC(=O)NCc1ccc(cc1)c2oc3ccccc3n2
CC(OC(=O)c1ccccc1O)C(=O)Nc2sccc2C#N;CC(OC(=O)c1ccccc1O)C(=O)Nc2sccc2C#N
CC(=O)c1cccc(NC(=O)COC(=O)c2sccc2C)c1;CC(=O)c1cccc(NC(=O)COC(=O)c2sccc2C)c1
Oc1ccccc1c2onc(c2)C(=O)NCC=C;Oc1ccccc1c2onc(c2)C(=O)NCC=C
Cc1ccc(s1)C(=O)Nc2ccc(Br)cn2;Cc1ccc(s1)C(=O)Nc2ccc(Br)cn2
COc1ccc(cc1Br)C(=O)Nc2ccc3OCCOc3c2;COc1ccc(cc1Br)C(=O)Nc2ccc3OCCOc3c2
Clc1cccc(c1)C(=O)Nc2ccc(Br)cn2;Clc1cccc(c1)C(=O)Nc2ccc(Br)cn2
COc1cc(NC(=O)c2ccc(Cl)cc2Cl)cc(OC)c1;COc1cc(NC(=O)c2ccc(Cl)cc2Cl)cc(OC)c1
Fc1ccc(F)c(c1)C(=O)Nc2ccc(cc2)c3nccs3;Fc1ccc(F)c(c1)C(=O)Nc2ccc(cc2)c3nccs3
OC(=O)c1ccccc1NCCC2=CCCCC2;OC(=O)c1ccccc1NCCC2=CCCCC2
Fc1cccc(c1)C(=O)Nc2nc3ccccc3s2;Fc1cccc(c1)C(=O)Nc2nc3ccccc3s2
Fc1ccc(Cc2cnc(NC(=O)c3ccccc3)s2)cc1;Fc1ccc(Cc2cnc(NC(=O)c3ccccc3)s2)cc1
COc1ccc(C)cc1NC(=O)COc2ccc(C)cc2Br;COc1ccc(C)cc1NC(=O)COc2ccc(C)cc2Br
COc1ccc(cc1)C(=O)Nc2sc3CCCCc3c2C(=O)N;COc1ccc(cc1)C(=O)Nc2sc3CCCCc3c2C(=O)N
Fc1ccccc1C(=O)Nc2sc3CCCCc3c2C#N;Fc1ccccc1C(=O)Nc2sc3CCCCc3c2C#N
CNC(=O)COc1ccccc1C(=O)Nc2ccc(cc2)c3ccccc3;CNC(=O)COc1ccccc1C(=O)Nc2ccc(cc2)c3ccccc3

CN1C(=O)c2sccc2n3c(CCCC(=O)Nc4ccccc4)nnc13;CN1C(=O)c2sccc2n3c(CCCC(=O)Nc4ccccc4)nnc13
COc1ccc(cc1C(=O)Nc2ccc3Cc4ccccc4c3c2)[N+](=O)[O-];COc1ccc(cc1C(=O)Nc2ccc3Cc4ccccc4c3c2)[N+](=O)[O-]
CCN(CC)CCN(C(=O)c1occc1)c2nc3ccc(C)cc3s2;CCN(CC)CCN(C(=O)c1occc1)c2nc3ccc(C)cc3s2
Cc1c(Cl)cccc1NC(=O)Cc2noc(n2)c3ccccc3Cl;Cc1c(Cl)cccc1NC(=O)Cc2noc(n2)c3ccccc3Cl
COc1c(C)cc(Br)cc1C(=O)Nc2cccc(F)c2;COc1c(C)cc(Br)cc1C(=O)Nc2cccc(F)c2
CC(C)Oc1cccc(c1)C(=O)N(C)c2ccccc2;CC(C)Oc1cccc(c1)C(=O)N(C)c2ccccc2
Fc1ccc2c(Cl)c(sc2c1)C(=O)Nc3ccc(Cl)cn3;Fc1ccc2c(Cl)c(sc2c1)C(=O)Nc3ccc(Cl)cn3
CC(C)C(=O)Nc1ccc2oc(nc2c1)c3ccc(Cl)cc3;CC(C)C(=O)Nc1ccc2oc(nc2c1)c3ccc(Cl)cc3
CC(C)C(=O)Nc1ccc(cc1)c2oc3cc(C)c(C)cc3n2;CC(C)C(=O)Nc1ccc(cc1)c2oc3cc(C)c(C)cc3n2
CCC1CCc2nc3sc(C(=O)OC)c(N)c3cc2C1;CCC1CCc2nc3sc(C(=O)OC)c(N)c3cc2C1
COc1ccc(cc1O)C2=CC(=O)c3c(O)cc(O)cc3O2
Oc1ccc(cc1)C2=CC(=O)c3c(O)cc(O)cc3O2
Oc1ccc(\C=C\C(=O)c2ccc(O)cc2O)cc1
Oc1ccc(C=CC(=O)c2ccccc2)cc1

N(C=C(C(=O)NCC(C)C)C2=O)C3CCCC3

c4nc5ccccc5s4

c4)C(=O)C

l)cc3

c2

)cc1