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Compound name
1-(2-Methylphenyl)-4-(1,2,3,4-tetrahydro-2-naphthalenyl)piperazine
11-[1-[2-[4-(quinolin-2-ylmethoxy)phenyl]ethyl]piperidin-4-ylidene]-5,6-dihydroimidazo[2,1-b]pyridine
12-Benzyl-3-methyl-1,2,3,4,6,7,12,12b-octahydroindolo[2,3-a]quinoline
2-[[[(3 <i>aS</i> ,3 <i>bR</i> ,7 <i>S</i> ,9 <i>aR</i> ,9 <i>bS</i> ,11 <i>aS</i>)-9 <i>a</i> ,11 <i>a</i> -dimethyl-2,3,3 <i>a</i> ,3 <i>b</i> ,4,6,7,8,9,9 <i>b</i> ,10,11-dodecahydronaphtho[2,1-e]pyrido[3,4-b]indole-10-ylidene]methyl]pyridine-4-ylidene]-5,6-dihydroimidazo[2,1-b]pyridine
8-(3-Chlorostyryl)caffeine
A 81834
Acitretin
AGN-190521
AGN-191659
AL 3152
Alpertine
AM 580
AMG-2674
Aminitrozole
Amolanone
Apilimod
AQ-13
Arotinoic acid (TTNPB)
ARQ736
AS-602704
Astemizole
AT-406
Aurothioglucose
AZD-3514
BAY-27-9955
Beclabuvir
BEOV (AKP-020)
BIBS 222
BILR-355
BMS-908662
BMV 20862
BTCP hydrochloride
Cepharanthine
Chloroquine
Clofazimine
CUDC-427
DDD498
Dimethylaminoparthenolide
DS-6930
EC-23 (AGN-190205)
Elopirazole
Estradiol-dinicate
Flumatinib mesylate
GDC-0152
GR 127935

GSK2578215A
Haloxon
Hanfangchin A
Ingenol mebutate
ISQ-1
JNJ-42165279
KW 8232
L 159689
Lexanopadol
LGD-1550
Licochalcone A
M-55532
MDI-101
MDI-403
MDL 28170
Metirapone
Milfasartan
MLN-3897
N-tert-Butylisoquine
NBI-30775, R-121919
NS-11394 (AN-721)
Onconoxib
ONO 5334
P-3622
Pagoclone
PF-2545920
R 82913
Remdesivir
Resiniferatoxin
RG-7314
RO 168714
RO-13-7410 (TTNPB)
RO-316930
Saripidem
SB 202190
SB-616234-A
SDZ-62-434
SL-11128
Sorivudine
SSR 149744
Stirocainide
Tamibarotene
Tazarotene
Tetrazepam
Tipifarnib
Tretinoin
Tyrphostin AG 538

	VBY-825
	WAY 141608
	WN1316
	YH-1238
	Z LVG CHN2
	Zaleplon GR
	ZK-261991
	ZK-93426

Status	Category
Preclinical	non-selective or unknown
Preclinical	non-selective or unknown
Preclinical	non-selective or unknown
Preclinical	non-selective or unknown
Preclinical	GPCR
Preclinical	5-lipoxygenase-activating protein (FLAP)
Approved (FDA)	Retinoic acid receptor agonist
Preclinical	Retinoic acid receptor agonist
Phase II	Retinoic acid receptor agonist
Preclinical	Aldose reductase inhibitor
Preclinical	Antipsychotic
Preclinical	Retinoic acid receptor agonist
Preclinical	Ion Channel Inhibitor
Preclinical	Anti-infective
Preclinical	local anesthetic
Phase II	Kinase Inhibitor
Phase II	Antimalarial
Preclinical	Retinoic acid receptor agonist
Preclinical	Kinase inhibitor
Phase I	β -sheet breaker
Approved (FDA) and withdrawn	Histamine H1 Blocker
Phase II	IAP antagonist
Preclinical	Kinase inhibitor
Phase I	Androgen receptor inhibitor
Phase II	Glucagon receptor antagonist
Phase III	Antiviral
Phase II	non-selective or unknown
Preclinical	Angiotensin II receptor antagonist
Phase II	Antiviral
Phase II	Kinase Inhibitor
Preclinical	Neuroprotective agent
Preclinical	Dopamin reuptake inhibitor
Preclinical	non-selective or unknown
Approved (FDA)	Antimalarial
Approved (FDA)	Anti-infective
Phase I	IAP antagonist
Phase I	Antimalarial
Preclinical	NF-kappa B inhibitor
Phase I	PPAR γ agonist
Phase II	Retinoic acid receptor agonist
Phase I	GPCR
Preclinical	Estrogen receptor modulator
Approved (China)	c-Abl/c-Kit/PDGRF β inhibitor
Phase I	IAP inhibitor
Phase I	GPCR

Preclinical	Kinase Inhibitor
Preclinical	Anthelmintics
Phase III	Antimalarial
Approved (FDA, <i>Topical</i>)	Kinase activator
Phase I	Antimalarial
Phase II	Fatty acid amide hydrolase (FAAH) inhibitor
Preclinical	Prostaglandin inhibitor
Preclinical	GPCR
Preclinical	GPCR
Phase II	Retinoic acid receptor agonist
Preclinical	Chalconoid
Preclinical	Factor Xa
Phase II	Retinoic acid receptor agonist
Phase III	Retinoic acid receptor agonist
Preclinical	Protease Inhibitor
Phase III	Glucocorticoid synthesis inhibitor
Phase II	GPCR
Phase II	GPCR
Phase I	Antimalarial
Phase II	CRF-1 receptor antagonist
Phase I	Benzodiazepine receptor agonist
Preclinical	Cyclooxygenase 2 inhibitor
Phase II	Protease Inhibitor
Preclinical	Cholesterol synthesis inhibitor
Phase III	Benzodiazepine receptor agonist
Phase II	Phosphodiesterase inhibitor
Phase I	Antiviral
Emergency Use Authorization (EUA) (FDA)	Antiviral
Phase II	Ion channel activator
Phase II	Vasopressin V1A receptor antagonist
Preclinical	Adrenoceptor agonist
Preclinical	Retinoic acid receptor agonist
Preclinical	Potassium channel stimulator
Preclinical	Benzodiazepine receptor agonist
Preclinical	p38 MAP kinase inhibitor
Preclinical	GPCR
Phase I	PAF inhibitor
Preclinical	Polyamine analog
Phase III	Antiviral
Phase II	Pottasium channel inhibitor
Preclinical	Antiarrhythmic agent
Approved (Japan)	Retinoic acid receptor agonist
Approved (FDA, <i>Topical</i>)	Retinoic acid receptor agonist
Preclinical	Benzodiazepine receptor agonist
Phase II	Farnesyltransferase inhibitor
Approved (FDA)	Retinoic acid receptor agonist
Preclinical	IGF-1 receptor

Phase 0	Protease Inhibitor
Phase I	GPCR
Phase I	non-selective or unknown
Phase I	Proton pump inhibitor
Preclinical	Protease Inhibitor
Phase II	Benzodiazepine receptor agonist
Preclinical	VEGF receptor antagonist
Phase I	Benzodiazepine receptor agonist

Target molecule
non-selective or unknown
non-selective or unknown
non-selective or unknown
non-selective or unknown
A2A adenosine receptor (ADORA2A)
5-lipoxygenase-activating protein (FLAP, ALOX5AP)
retinoic acid binding proteins (CRABP1)
retinoic acid receptor (RARA, RARB, RARG)
retinoid X receptor (RXRA, RXRB, RXRG)
aldose reductase (AKR1B1)
non-selective or unknown
retinoic acid receptor (RARA)
TRPV1
non-selective or unknown
non-selective or unknown
PIKfyve
non-selective or unknown
retinoic acid receptor (RARA, RARB, RARG)
B-Raf (BRAF)
amyloid- β peptide (APP)
histamine H1 receptor (HRH1, KCNH2, CYP3A4)
XIAP, cIAP1, cIAP2, BIRC2, BIRC3
PKC iota (PRKCI)
androgen receptor (AR)
glucagon receptor (GCGR)
NS5B RNA-dependent RNA polymerase
non-selective or unknown
angiotensin II receptors (AGTR1, AGTR2)
reverse transcriptase
RAF kinase (RAF1)
non-selective or unknown
neuronal dopamine transporter (DAT, SLC6A3)
non-selective or unknown
palmitoyl-protein thioesterase 1 (PPT1)
mycobacterial DNA (ABCB1)
XIAP, cIAP1, cIAP2, BIRC2, BIRC3
<i>Plasmodium falciparum</i> EF2
non-selective or unknown
PPAR γ
retinoic acid receptor (RARA, RARB, RARG)
D2 and D3 dopamine receptors (DRD2, DRD3), 5-HT1A serotonin receptor (HTR1A)
estrogen receptor (ESR1, ESR2)
c-Abl, c-Kit, PDGFR β (ABL1, KIT, PDGFRB)
XIAP, cIAP1, cIAP2, ML-IAP, BIRC2, BIRC3, BIRC7
5-HT1B/1D serotonin receptor (HTR1B, HTR1D)

Leucine-rich repeat kinase 2 (LRRK2)
non-selective or unknown
calcium channels (non-selective)
PKC delta (PRKCD)
non-selective or unknown
FAAH
prostaglandin receptors
angiotensin II receptors (AGTR1, AGTR2)
ORL-1, nociceptin receptor, opioid mu receptor (OPRL1, OPRM1)
retinoic acid receptor (RARA, RARB, RARG)
non-selective or unknown
factor Xa (F10)
retinoic acid receptor (RARA, RARB, RARG)
retinoic acid receptor (RARA, RARB, RARG)
Calpain I / II (CAPN1, CAPN2)
11-beta-hydroxylase (CYP11B1)
angiotensin II receptor type 1 (AGTR1)
C-C Motif Chemokine Receptor 1 (CCR1)
hERG potassium ion channel (KCNH2)
CRF1 receptor (CRHR1)
GABAA receptors (GABRA3, GABRA5)
COX-2 (PTGS2)
cathepsin K (CTSK)
squalene synthase (FDFT1)
GABAA receptors (GABRA1, GABRA2, GABRA3, GABRA5)
phosphodiesterase (PDE10A)
reverse transcriptase
viral RNA polymerase
TRPV1
vasopressin receptor 1A (AVPR1A)
β3 adrenoceptor (ADRB3)
retinoic acid receptor (RARA, RARB, RARG)
potassium channel (SUR2B splice variant/Kir6.2, KCNJ11, ABCC9)
GABAA receptor (GABRA1, GABRA2, GABRB2, GABRG2)
p38 MAP kinase (MAPK14)
5-HT1B serotonin receptor (HTR1B)
non-selective or unknown
non-selective or unknown
viral DNA polymerase
several ion channels
non-selective or unknown
retinoic acid receptor (RARB, RARG)
retinoic acid receptor (RARB, RARG)
type 1 and type 2 benzodiazepine site (GABRA1, GABRG2, TSPOAP1)
Protein farnesyltransferase (FNTA, FNTB)
retinoic acid receptor (RARA, RARB, RARG)
IGF-1 receptor (IGF1R)

cathepsins B, L, S and V (CTSB, CTSL, CTSS, CTSV)
Vasopressin receptor 2 (AVPR2)
non-selective or unknown
H,K-ATPase (ATP4A, ATP4B)
cysteine proteinase produced by group A streptococci
GABAA receptors, BZ Site 1 (GABRA1, TSPOAP1)
VEGFR-2 (KDR)
benzodiazepine receptor (TSPOAP1)

Smiles
<chem>Cc1cccc1N1CCN(CC1)C1CCc2c(C1)cccc2</chem>
<chem>OC(=O)c1cnc2n1CCc1c(C2=C2CCN(CC2)CCc2ccc(cc2)OCc2ccc3c(n2)cccc3)ccc</chem>
<chem>CC1CCC2N(C1)CCc1c2n(Cc2cccc2)c2c1cccc2</chem>
<chem>CCN(CCO[C@H]1CC[C@]2(C(=CC[C@@H]3[C@@H]2CC[C@]2([C@H]3CCO2)C)C</chem>
<chem>ClC1=CC(/C=C/C(N3C)=NC2=C3C(N(C)C(N2C)=O)=O)=CC=C1</chem>
<chem>OC(=O)CO/N=C/C(Cc1c(SC(C)(C)C)c2c(n1Cc1ccc(cc1)Cl)ccc(c2)OCc1ccc2c(n1)cccc</chem>
<chem>COc1cc(C)c(c(c1C)C)/C=C/C(=C/C=C/C(=C/C(=O)O)/C)/C</chem>
<chem>O=C(c1cc2c(cc1C)C(C)(C)CCC2(C)C)Oc1ccc(cc1)C(=O)O</chem>
<chem>C/C(=C\c1ccc(s1)C(=O)O)/c1cc2c(cc1C)C(C)(C)CCC2(C)C</chem>
<chem>COc1cc(F)cc2c1c1ccc(cc1C12NC(=O)NC1=O)F</chem>
<chem>CCOC(=O)c1nc2c(c1CCN1CCN(CC1)c1cccc1)cc(c(c2)OC)OC</chem>
<chem>O=C(c1ccc2c(c1)C(C)(C)CCC2(C)C)Nc1ccc(cc1)C(=O)O</chem>
<chem>OCC(c1cnc(c(c1)Cl)N1CCN([C@@H](C1)C)c1nc2c([nH]1)cc(cc2c1cc(F)c(c(c1)F)F)C(F</chem>
<chem>CC(=O)Nc1ncc(s1)[N+](=O)[O-]</chem>
<chem>CCN(CCC1(c2cccc2)C(=O)Oc2c1cccc2)CC</chem>
<chem>Cc1cccc(c1)/C=N/Nc1nc(OCc2ccccn2)nc(c1)N1CCOCC1</chem>
<chem>CCN(CCCNc1ccnc2c1ccc(c2)Cl)CC</chem>
<chem>C\C(=C/C1=CC=C(C=C1)C(O)=O)C1=CC=C2C(=C1)C(C)(C)CCC2(C)C</chem>
<chem>Cn1ccc(n1)S(=O)(=O)N1CCCC(C1)Nc1nccc(n1)c1c(nc2n1cco2)c1cccc(c1)OCOP(=O)(</chem>
<chem>CC(C[C@@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N)CC(=O)O)Cc1cc</chem>
<chem>COc1ccc(cc1)CCN1CCC(CC1)Nc1nc2c(n1Cc1ccc(cc1)F)cccc2</chem>
<chem>CN[C@H](C(=O)N[C@H]1CN(CC[C@@H]2N(C1=O)[C@@H](CC2)C(=O)NC(c1cccc1)c1cccc</chem>
<chem>C(C1C(C(C(C(O1)[S-])O)O)O)O.[Au+]</chem>
<chem>CC(=O)N1CCN(CC1)CCOc1ccc(cc1)C1CCN(CC1)C1=Nn2c(CC1)nnc2C(F)(F)F</chem>
<chem>CCCc1c(cc(c(c1c1ccc(cc1)F)C(O)C)C(C)C)C(C)C</chem>
<chem>COc1ccc2c(c1)[C@@H]1C[C@@]1(Cn1c2c(C2CCCC2)c2c1cc(cc2)C(=O)NS(=O)(=O)N(C)C)C(=O</chem>
<chem>CCc1occc(=O)c1O[V](=O)Oc1c(=O)ccoc1CC</chem>
<chem>CCCCc1nc2c(n1Cc1ccc(cc1)NC(=O)c1c(Cl)ccc(c1C(=O)O)Cl)cc(cc2)N(C(=O)NC)CC</chem>
<chem>CCn1c2ncc(cc2c(=O)n(c2c1nccc2)C)CCOc1cc[n+](c2c1cccc2)[O-]</chem>
<chem>COC(=O)Nc1nc2c(n1)cc(cc2)C1(O)c2cccc2C(=O)N1Cc1cccc1</chem>
<chem>CN1c2cccc2CNc2c1nnc2</chem>
<chem>C1CCC(CC1)(C2=CC3=CC=CC=C3S2)N4CCCCC4.Cl</chem>
<chem>COc1cc2CCN([C@H]3c2cc1Oc1c2c(CCN([C@H]2Cc2ccc(Oc4cc(C3)ccc4OC)cc2)C)cc2c</chem>
<chem>CCN(CCCC(Nc1ccnc2c1ccc(c2)Cl)C)CC</chem>
<chem>Clc1ccc(cc1)Nc1cc2nc3cccc3n(c2c/c/1=N\C(C)C)c1ccc(cc1)Cl</chem>
<chem>CN[C@H](C(=O)N[C@H](C(=O)N1CCC[C@H]1C(=O)Nc1sc(nc1c1cccc1)c1ncco1)C1C</chem>
<chem>Fc1ccc2c(c1)c(cc(n2)c1ccc(cc1)CN1CCOCC1)C(=O)NCCN1CCCC1</chem>
<chem>CN(C[C@@H]1C(=O)O[C@H]2[C@H]1CC/C(=C/CC[C@@]1([C@@H]2O1)C)/O</chem>
<chem>Fc1ccc(cc1)Oc1cc(cnc1Nc1ccc(c1)C1nnnn1)Sc1cccc1</chem>
<chem>OC(=O)c1ccc(cc1)C#Cc1ccc2c(c1)C(C)(C)CCC2(C)C</chem>
<chem>Fc1ccc(cc1)c1ccc([nH]1)CN1CCN(CC1)c1cccc2c1occ2</chem>
<chem>O=C(c1ccnc1)O[C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CCc2c1ccc(c2)OC(=O</chem>
<chem>CN1CCN(CC1)Cc1ccc(cc1C(F)(F)F)C(=O)Nc1cnc(c(c1)Nc1nccc(n1)c1ccnc1)C</chem>
<chem>CN[C@H](C(=O)N[C@H](C(=O)N1CCC[C@H]1C(=O)Nc1snnc1c1cccc1)C1CCCC</chem>
<chem>CC1=C(C(=CC(=C1)C2=NOC(=N2)C)C3=CC=C(C=C3)C(=O)NC4=CC(=C(C=C4)OC)N5CCN(</chem>

FC1=NC=CC(C2=CC=C(OCC3=CC=CC=C3)C(C(NC4=CC=CN=C4)=O)=C2)=C1
ClCCOP(=O)(Oc1ccc2c(c1)oc(=O)c(c2C)Cl)OCCCl
COc1c(OC)cc2c3c1Oc1cc4c(cc1OC)CCN([C@H]4Cc1ccc(Oc4cc(C[C@@H]3N(CC2)C)ccc
C/C=C(\C(=O)O[C@H]1C(=C[C@]23[C@]1(O)[C@H](O)C(=C[C@H](C3=O)[C@H]1[C@@H](C[C@
CCN(Cc1ccc(cc1O)Nc1ccnc2c1ccc(c2)Cl)CC
O=C(N1CCN(CC1)Cc1ccc2c(c1)OC(O2)(F)F)Nc1cnccc1Cl
CN(CCN1c2ccccc2c(c1C(=O)N1CCN(CC1)c1ccccc1Cl)C(c1ccc(cc1)O)c1ccc(cc1)O
CCCN(C(=O)c1ccccc1)c1ccc2c(c1)c(=O)n(c(n2)CCC)Cc1ccc(cc1)c1ccccc1c1[nH]n
CN[C@@]1(CC[C@]2(CC1)OCCc1c2nc2c1cc(cc2)F)c1ccccc1
C/C=C\C=C\C(=C\C(=O)O)\C)/c1cc(cc(c1)C(C)(C)C(C)(C)C
C=CC(c1cc/C=C/C(=O)c2ccc(cc2)O)c(cc1O)OC)(C)C
COCC12CN(CC(=O)N2CC2(O1)CCN(CC2)c1ccncc1)S(=O)(=O)c1ccc2c(c1)ccc(c2
O=C/C=C/C/C=C/C=C/C=C/C=C/C=C/C(C)CCCC1(C)C)\C)\C)OCC(=O)C(C)(C)C
CC(=O)COC(=O)/C=C/C=C/C=C/C=C/C=C/C=C/C=C/C(C)CCCC1(C)C)\C)\C
O=C(N[C@@H]([C@H](C)C)C(NC(CC2=CC=CC=C2)C([H])=O)=O)OCC1=CC=CC=
O=C(C(c1ccnc1)(C)C)c1ccnc1
CCCCc1nc(C)n(c(=O)c1Cc1ccc(cc1)c1ccccc1c1nnn[nH]1)Cc1sccc1C(=O)OC
Clc1ccc(cc1)C1(O)CCN(CC1(C)C)CCC=C1c2cc(ccc2OCc2c1cccn2)C(O)(C)C
Clc1ccc2c(c1)nccc2Nc1ccc(c(c1)O)CNC(C)(C)C
CCCN(c1cc(C)nc2n1nc(c2c1cnc(cc1C)N(C)C)C)CCC
N#Cc1ccccc1c1cccc(c1)n1cnc2c1ccc(c2)C(O)(C)C
Clc1ccc2c(c1)[nH]cc2C1CC(=NN1c1ccc(cc1)S(=O)(=O)N)C(F)(F)F
O=C(C1CCCCC1)N[C@@H](C(=O)C(=O)N/N=C/1\SC[C@H](N1C)C)C1CCOCC
CCN(CCOc1ccc(cc1)/C(=C/c1ccc(cc1)Cl)\CC)/C#N)CC
CC(CCC(=O)CC1N(c2ccc3c(n2)nc(cc3)Cl)C(=O)c2c1cccc2)C
Cn1nc(c(c1)c1ccncc1)c1ccc(cc1)OCc1ccc2c(n1)cccc2
CC(=CCN1Cc2cc(Cl)cc3c2n(C[C@@H]1C)c(=S)[nH]3)C
CCC(COC(=O)[C@@H](NP(=O)(Oc1ccccc1)OC[C@H]1O[C@@]([C@@H]([C@@H]1O)O)(C#N)c1
COc1cc(ccc1O)CC(=O)OCC1=C[C@H]2[C@H]3O[C@]4(O[C@]2([C@H]2[C@@]([C1](O)C(=O)C(=C2)C)[C@@H]
CN1Cc2cc(Cl)ccc2n2c(C1)nnc2C1CCC(CC1)Oc1cccn1
CC(N(C[C@@H](c1ccccc1)O)C[C@@H](c1ccccc1)O)CCc1ccc(cc1)C(=O)N
C/C(=C\C1ccc(cc1)C(=O)O)/c1ccc2c(c1)C(C)(C)CCC2(C)C
N#Cc1ccc2c(c1)c(c1cccn1)c(o2)C(C)C
CCCC(=O)N(Cc1c(nc2n1cccc2)c1ccc(cc1)Cl)C
OC1=CC=C(C=C1)C1=NC(=C(N1)C1=CC=NC=C1)C1=CC=C(F)C=C1
COc1cc2CCN(c2cc1N1C[C@H](C)N[C@@H](C1)C)C(=O)c1ccc(cc1)c1ccc(cc1C)c1nc
C1CCN(CC1)Cc1ccc(cc1)c1cc2ccccc2c2=NCCn12
CCNC/C=C\CNCCCCNCCCCNC/C=C\CNCC
Br/C=C/c1cn(c(=O)[nH]c1=O)[C@@H]1O[C@@H]([C@H]([C@H]1O)O)CO
CCCCc1oc2c(c1C(=O)c1ccc(cc1)CCCN(CCCC)CCCC)cc(cc2)C(=O)OC(C)C
CC(N(C(C)C)CCO/N=C/1\CCCC\C1=C\c1ccccc1)C
O=C(c1ccc(cc1)C(=O)O)Nc1ccc2c(c1)C(C)(C)CCC2(C)C
CCOC(=O)c1ccc(nc1)C#Cc1ccc2c(c1)C(C)(C)CCS2
Clc1ccc2c(c1)C(=NCC(=O)N2C)C1=CCCCC1
Clc1ccc(cc1)[C@](c1cncn1C)(c1ccc2c(c1)c(cc(=O)n2C)c1cccc(c1)Cl)N
C/C(=C\C=C\C(=C\C(=O)O)\C)/C=C/C1=C(C)CCCC1(C)C
C1=CC(=C(C=C1C=C(C#N)C(=O)C2=CC(=C(C=C2)O)O)O)O

CC[C@@H](C(=O)C(=O)NC1CC1)NC(=O)[C@H](CS(=O)(=O)CC1CC1)N[C@H](C(F)(F)F)C
Cc1ccn(n1)c1ccc(c(c1)C(F)(F)F)C(=O)N1Cc2cccnc2Nc2c1cccc2
O=C(Nc1[nH]cc(n1)c1ccccn1)CN(c1c(C)cc(cc1C)C)C
COc1cccc2c1nc(Nc1ccc(cc1C)F)nc2N1CCc2c(C1C)cccc2
[N-]=[N+]=CC(=O)CNC(=O)C(C(C)C)NC(=O)C(NC(=O)OCc1cccc1)CC(C)C
CCN(c1cccc(c1)c1ccnc2n1ncc2C#N)C(=O)C
O=C(N(C)C)Nc1nccc(c1)CNc1cccc1C(=O)Nc1ccc2c(c1)nn(c2)C
CCOC(=O)c1ncc2c(c1C)c1c(cccc1[nH]2)OC(C)C

Ranking CPE Assay (set 1)	FC CPE (set1)	Log2FC CPE (set 1)	Z-score CPE (set 1)	Ranking CPE Assay (set 2)
175	1,4450376884422	0,5311071205	0,8073310026	183
49	1,5422089139698	0,6249982119	1,094430832	106
103	1,5966353159358	0,6750348274	0,93323902421	137
60	1,6384251968503	0,7123098074	1,0500448704	3212
14	1,5096494474699	0,5942135832	ND	25
465	1,2379136725815	0,3079107099	0,63010550151	63
155	1,3425725878695	0,4250000914	0,82898018528	89
1823	1,1410519494545	0,1903644756	0,40711569975	50
435	1,329745245784	0,4111498789	0,64262220282	178
1635	1,1574766040530	0,2109830327	0,42521604301	114
929	1,1904540523787	0,2515119383	0,51018133639	20
257	1,3058239179084	0,3849603717	0,74085596492	400
105	1,5397298994974	0,6226772945	0,93038178403	60
264	1,2934384021221	0,3712113496	0,73614705744	330
125	1,4042784823907	0,4898290647	0,88761478708	121
18	1,9675915131732	0,9764307374	1,4048956757	164
8	1,9998779445868	0,9999119529	1,535414037	40
36	1,384589929	0,46945876	ND	9
198	1,5124724135625	0,5969088288	0,78995078678	39
703	1,2239268557260	0,2915173423	0,55801945283	23
15	1,7411713334425	0,8000581729	1,4253881771	59
59	1,6124970855677	0,6892965530	1,0503044899	116
35	1,387511236	0,472499454	ND	2
108	1,4972021450221	0,5822690202	0,91813276741	53
141	1,59733496707	0,6756668829	0,85879443619	1175
308	1,3111192481386	0,3907989066	0,7088507675	145
210	1,3934604060127	0,4786720100	0,78181738783	41
719	1,2336063011814	0,3028820395	0,55475091263	1255
116	1,6471128809925	0,7199394301	0,90681551874	1271
55	1,5575428641914	0,6392718673	1,0682432704	141
3361	1,0774357969025	0,1076019034	0,30358159369	92
66	1,297887596	0,376165443	ND	12
29	1,5338388896837	0,6171469539	1,2192068284	4473
2960	1,0584311156114	0,0819273795	0,3288387373	73
61	1,7179758908464	0,7807097906	1,0493021593	5020
34	1,8015474874585	0,8492366806	1,1653667545	11
63	1,5451083075458	0,6277079703	1,0332919863	11259
183	1,5247776365946	0,6085988649	0,80118412522	542
405	1,2952115295211	0,3731877331	0,65568020072	17
807	1,2076241548146	0,2721715189	0,53518344727	135
92	1,7128335451080	0,7763849556	0,9624152733	2503
145	1,5884515239699	0,6676210628	0,85006738033	1153
27	1,7887876884422	0,8389821638	1,2210493894	52
207	1,3883189554674	0,4733390539	0,78361166881	55
2	1,827190043	0,869626694	ND	50

33	1,39321019	0,47841293	ND	24
52	1,7718921167579	0,8252907667	1,0741383456	8415
7	1,9420023760665	0,9575449659	1,5674012372	462
6460	0,9691352776124	-0,0452300353	0,13949455646	32
30	1,6286997581481	0,7037206754	1,2137186097	6199
1041	1,1848602581777	0,2447169184	0,49274396145	201
70	1,5077222162220	0,5923706499	1,0151107621	342
613	1,2519847471400	0,3242169861	0,5832444763	614
142	1,4522585716877	0,5382983451	0,8559873002	206
80	1,5711555348933	0,6518260057	0,98887344013	3
3174	1,0665656330146	0,0929727472	0,31388515398	57
6410	0,9477696783254	-0,0773915888	0,14199343792	93
161	1,5457767672039	0,6283319880	0,82014632923	87
216	1,4998996856818	0,5848660155	0,77837845312	74
1	2,6274134354555	1,3936432329	ND	7
247	1,2998361551065	0,3783297823	0,74942774041	380
258	1,4792464389646	0,5648624220	0,73860821459	1667
22	1,7362662674190	0,7959882111	1,3535311713	427
13	1,6913721562455	0,7581941339	1,4495448198	138
244	1,3109546422138	0,3906177705	0,75018550541	473
259	1,3713129426414	0,4555578412	0,73850724317	428
172	1,3447955897603	0,4273868983	0,8108209806	75
56	1,6281222123104	0,7032089971	1,0681755887	8
9	1,9550159545489	0,9671803811	1,5091138143	5587
1868	1,1421380315273	0,1917370161	0,40243156046	599
6687	1,0169597989949	0,0242626497	0,12624014641	24
37	1,6467376085130	0,7196106940	1,1502540207	171
			ND	
67	1,5981357907001	0,6763899966	1,021814061	6
409	1,2938684849424	0,3716909822	0,65389039892	69
95	1,5171345856056	0,6013490733	0,95216593804	109
251	1,3325413111567	0,4141802598	0,74561520628	56
190	1,3642060408572	0,4480615561	0,795716872	65
3447	1,0714375234991	0,0995477276	0,29974309358	1464
60	1,310399367	0,390006566	ND	18
71	1,5156037991858	0,5998926613	1,0099934789	119
10	1,9222804094263	0,9428188021	1,5052235445	256
4	1,9714525608732	0,9792589952	1,667694039	8002
215	1,3914974947053	0,4766383112	0,77938550828	5
32	1,6051006176529	0,6826637372	1,1879317754	7529
66	1,6053368276847	0,6828760317	1,0274178312	1349
165	1,3339199296084	0,4156720693	0,81805685406	45
834	1,2819551934826	0,3583458381	0,53021733569	13
194	1,3618607425078	0,4455791876	0,79324732593	181
1994	1,1673994974874	0,2232983523	0,3937016753	788
102	1,4525326709147	0,5385706136	0,93374346346	33
16	1,486640682	0,572055993	ND	1

6	2,6749858996051	1,4195312868	1,5676903244	174
1104	1,1790951247023	0,2376801139	0,483388606	79
12302	0,3459527559055	-1,5313530613	-1,8629567445	12440
46	1,5421398684997	0,6249336202	1,1033697013	7
1	3,2595922796682	1,7046915188	2,5282843567	70
193	1,3212140126394	0,4018641758	0,79333527327	426
295	1,3405651118342	0,4228412933	0,71505549906	16
111	1,5356949073715	0,6188916279	0,91540368739	82

FC CPE (set2)	Log2FC CPE (set 2)	Z-score CPE (set 2)	Ranking CPE Assay based on Average Z scores (sets 1 & 2)
1,49	0,57	0,79186460209	115
1,33	0,407	0,87952260767	41
1,5	0,585	0,83677081835	71
1,12	0,165	0,38742271999	182
1,4154860771861	0,501	ND	27
1,44	0,528	0,96355517459	119
1,43	0,512	0,911986768	84
1,49	0,578	0,99740750609	198
1,35	0,428	0,79742385554	181
1,51	0,594	0,86680144362	287
1,71	0,775	1,1439904048	100
1,36	0,441	0,68776267482	188
1,65	0,726	0,96758128669	49
1,25	0,327	0,70974356373	177
1,39	0,479	0,86091052599	81
1,6	0,679	0,8097110999	23
1,54	0,627	1,0394112399	6
1,646571262	0,719	ND	10
1,67	0,739	1,0408928091	59
1,68	0,749	1,1113014241	98
1,57	0,65	0,96933933024	10
1,67	0,742	0,86291865842	46
1,821934538	0,865	ND	5
1,85	0,889	0,98700640616	47
1,3	0,382	0,54826636754	197
1,39	0,473	0,82722434101	138
1,61	0,687	1,0337551322	62
1,17	0,221	0,54000377439	577
1,29	0,37	0,53756290288	178
1,48	0,563	0,83394498991	48
1,36	0,448	0,90782636876	378
1,577672732	0,658	ND	18
1,04	0,0633	0,32141641543	136
1,69	0,755	0,94634726085	301
1,05	0,075	0,29532928007	237
1,83	0,869	1,2128947687	13
0,824	-0,28	-0,28020030221	2297
1,28	0,357	0,65139945618	173
1,72	0,786	1,1583174642	63
1,64	0,717	0,8414208844	218
1,1	0,14	0,42929396311	206
1,31	0,384	0,55009455	201
1,68	0,745	0,98852555255	24
1,85	0,887	0,98579327587	72
1,334065819	0,416	ND	6

1,419589676	0,505	ND	23
0,918	-0,123	0,11534394736	410
1,27	0,342	0,6701450146	22
1,66	0,734	1,0694682696	379
1,03	0,0419	0,23646467954	174
1,35	0,428	0,7817548058	303
1,29	0,368	0,70636343956	93
1,23	0,293	0,63903883427	368
1,36	0,443	0,77935941937	106
1,98	0,982	1,4037080334	11
1,84	0,879	0,97868447223	286
1,52	0,608	0,90756701495	726
1,53	0,615	0,91456796648	86
1,56	0,645	0,94586339464	91
1,6556270601161	0,727	ND	1
1,2470465237846	0,319	0,6948187334	179
1,25	0,324	0,49673135528	350
1,23	0,294	0,68046452859	36
1,35	0,428	0,83607372061	19
1,34	0,426	0,66737590287	193
1,22	0,282	0,68045852104	191
1,55	0,631	0,94377688056	77
1,78	0,836	1,2762929643	16
1,03	0,0362	0,26461261268	70
1,32	0,401	0,64195013461	741
1,8	0,849	1,1062240951	355
1,4915018639034	0,577	0,8018848738	45
		ND	
1,79	0,838	1,290283826	18
1,55	0,628	0,96008686076	110
1,52	0,601	0,87453895286	60
1,48	0,565	0,97943580382	90
1,51	0,593	0,96216614093	74
1,18	0,241	0,51875344224	1816
1,488285903	0,574	ND	24
1,5	0,586	0,86189915733	54
1,27	0,341	0,74579253664	20
0,9892179842318	-0,0156	0,14102630138	65
1,86	0,899	1,2992314404	32
0,96	-0,0582	0,16722310623	231
1,21	0,28	0,53175727121	127
1,48	0,564	1,0177528521	58
1,67	0,743	1,2004879527	89
1,36	0,444	0,79364240836	120
1,3217465027554	0,402	0,60246305725	907
1,55	0,628	1,0664749191	38
2,068960953	1,05	ND	2

1,38	0,47	0,80112125387	15
1,45	0,535	0,93246432256	194
0,272	-1,88	-2,0555946657	12333
1,73	0,787	1,2823381249	12
1,61	0,683	0,95913835284	1
1,24	0,311	0,68048368463	163
1,73	0,795	1,168957897	53
1,57	0,651	0,9222191307	57

Average FC of CPE (sets 1 & 2)	Average Z-score CPE (sets 1 & 2)	Reconfirmation concentration (μM)	% Viral Inhibition (Reconfirmation)
1,46503686032962	0,79959780234	2,5	42,811
1,43404123537869	0,98697671984	1	50,2755
1,54833308149808	0,88500492128	1	54,2995
1,37966256222761	0,71873379519	2,5	40,604
1,46256776232806	ND	2,5	57
1,33998018401058	0,79683033805	2,5	41,9555
1,38427956814464	0,87048347664	2,5	40
1,31708218318505	0,70226160292	1	49,807
1,33774128373833	0,72002302918	2,5	44,925
1,33349399668833	0,64600874331	1	52
1,45064514774941	0,82708587059	1	52,8046666666667
1,33169983774209	0,71430931987	2,5	41,062
1,59712226216926	0,94898153536	2,5	69,5
1,2737448152796	0,72294531059	2,5	41,802
1,39923243573528	0,87426265653	2,5	52,834
1,78457356697699	1,1073033878	2,5	93,8
1,77238074873719	1,2874126384	2,5	53,3
1,5155805955	ND		42,6
1,59048758384685	0,91542179793	2,5	56,813
1,45205338466007	0,83466043848	2,5	56,854
1,65533108003809	1,1973637537	2,5	51,8
1,64261484745073	0,95661157416	1	54,0145
1,604722887	ND	2,5	44,1645
1,67423212622402	0,95256958678	2,5	49,7875
1,45035469962844	0,70353040187	1	52,7865
1,34962888091998	0,76803755426	2,5	54,56
1,50154762621758	0,90778626002	2,5	41,046
1,19940257842492	0,54737734351	1	44,477
1,469808873981	0,72218921081	2,5	43,555
1,51729298466057	0,95109413016	1	40,3346666666667
1,22075613993009	0,60570398122	2,5	42,1245
1,437780164	ND	2,5	52,73
1,2893433380523	0,77031162194	2,5	40,6055
1,37295601249	0,63759299908	1	48,714
1,38567065256124	0,67231571968	2,5	49,351
1,81412476052857	1,1891307616	1	42,181
1,18446558384468	0,37654584204	1	45,7975
1,40280778007332	0,7262917907	2,5	40,824
1,50982982820379	0,90699883245	2,5	70,333
1,42561278183937	0,68830216583	1	56,113
1,40720128265248	0,6958546182	2,5	67,6
1,44684581389933	0,70008096517	2,5	46,2025
1,7323760400668	1,104787471	2,5	42,4335
1,61887330221275	0,88470247234	2,5	42,158
1,580627931	ND	2,5	41,8785

1,406399933	ND	2,5	42,07733333333333
1,34493326969673	0,5947411465	2,5	46,5285
1,60461066688887	1,1187731259	2,5	88,9
1,3159852633273	0,60448141303	1	47,4225
1,32907446073318	0,72509164463	2,5	44,41
1,26508438642863	0,63724938362	2,5	40,7905
1,39907833188523	0,86073710084	2,5	55,3
1,23877074345841	0,61114165529	1	54,285
1,40594426068248	0,81767335978	2,5	45,862
1,77314952574695	1,1962907368	1	61,6
1,4526400222602	0,6462848131	2,5	52,3005
1,23594459546383	0,52478022643	2,5	49,2705
1,53857858557158	0,86735714785	2,5	44,0895
1,53208137347018	0,86212092388	2,5	55,7915
2,14152024778586	ND	2,5	95,4
1,27344133944557	0,72212323691	2,5	46,365
1,3655560553032	0,61766978494	2,5	66,4835
1,48112331732177	1,0169978499	2,5	65,4
1,51825882372922	1,1428092702	2,5	54,9
1,32717387851777	0,70878070414	1	60,004
1,29342668812718	0,7094828821	2,5	47,8655
1,44687728364539	0,87729893058	1	40,8745
1,70640209617128	1,1722342765	2,5	87,2
1,49020777154574	0,88686321347	2,5	50,499
1,23150457625476	0,52219084753	2,5	42,9
1,40937010721262	0,61623212076	2,5	46,6695
1,56911973620824	0,97606944724	2,5	79,1
	ND	2,5	97,1
1,69261048776758	1,1560489435	1	53,23133333333333
1,41961578357317	0,80698862984	2,5	52,625
1,51683542008501	0,91335244545	2,5	45,596
1,40613194061833	0,86252550505	2,5	41,1
1,43611371561579	0,87894150646	2,5	50,86466666666667
1,12680792439137	0,40924826791	2,5	43,5105
1,399342635	ND	2,5	54,6445
1,50849431230994	0,93594631814	2,5	76,5
1,59438893567763	1,1255080406	2,5	70,5
1,48033527255253	0,90436017017	2,5	81,8
1,6278668748309	1,0393084743	1	52,6385
1,2827894887809	0,67757744082	2,5	40,84266666666667
1,40994685342873	0,77958755119	2,5	59,643
1,40597509662265	0,91790485309	2,5	48,1
1,47793878052861	0,86535264419	1	49,9
1,36112935855071	0,79344486715	2,5	48,379
1,24457300012142	0,49808236627	2,5	42,5625
1,49912058841954	1,0001091913	1	42,1
1,7778008175	ND	2,5	55,15666666666667

2,0298853947134	1,1844057891	2,5	94,9
1,31391940801243	0,70792646428	2,5	59,5395
0,309190667644798	-1,9592757051	1	50,7195
1,63382619848675	1,1928539131	2,5	63,1
2,43273900243683	1,7437113548	1	95,8
1,28078473763181	0,73690947895	1	42,1
1,53759628024691	0,94200669804	2,5	40,6
1,55278916971863	0,91881140905	1	40,5616666666667