**Table S1.** Preliminary screening bioactive compounds that inhibit ZIKV infection in SNB-19 cells

| No. | Name | Target | Inhibition rate (%) | Brief introduction |
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| 1 | Pazopanib HCl | VEGFR, PDGFR, c-Kit | 95 | Pazopanib (GW786034) is a novel multi-target inhibitor of VEGFR1, VEGFR2, VEGFR3, PDGFR, FGFR, c-Kit and c-Fms with IC50 of 10 nM, 30 nM, 47 nM, 84 nM, 74 nM, 140 nM and 146 nM, respectively. |
| 2 | Axitinib | VEGFR, PDGFR, c-Kit | 95 | Axitinib is a multi-target inhibitor of VEGFR1, VEGFR2, VEGFR3, PDGFRβ and c-Kit with IC50 of 0.1 nM, 0.2 nM, 0.1-0.3 nM, 1.6 nM and 1.7 nM, respectively. |
| 3 | Plinabulin (NPI-2358) | VDA | 95 | Plinabulin (NPI-2358) is a vascular disrupting agent (VDA) against tubulin-depolymerizing with IC50 of 9.8~18 nM in tumor cells. Phase 1/2. |
| 4 | Mitoxantrone | Topoisomerase | 95 | Mitoxantrone is a type II topoisomerase inhibitor with IC50 of 2.0 μM, 0.42 mM for HepG2 and MCF-7/wt cells, respectively |
| 5 | Doxorubicin (Adriamycin) | Topoisomerase | 95 | Doxorubicin (Adriamycin) is an antibiotic agent that inhibits DNA topoisomerase II and induces DNA damage and apoptosis. |
| 6 | Epirubicin HCl | Topoisomerase | 95 | Epirubicin HCl, a semisynthetic L-arabino derivative of doxorubicin, is an antineoplastic agent by inhibiting Topoisomerase. |
| 7 | Beta-Lapachone | Topoisomerase | 95 | Beta-Lapachone is a selective DNA topoisomerase I inhibitor, exhibiting no inhibitory activities against DNA topoisomerase II or ligase. Phase 2. |
| 8 | Pirarubicin | Topoisomerase | 95 | Pirarubicin is an anthracycline antibiotic, and also a DNA/RNA synthesis inhibitor by intercalating into DNA and interacts with topoisomerase II, used as an antineoplastic agent. |
| 9 | Fludarabine | STAT, DNA/RNA Synthesis | 95 | Fludarabine is a STAT1 activation inhibitor and a DNA synthesis inhibitor in Vascular smooth muscle cells. |
| 10 | Cryptotanshinone | STAT | 95 | Cryptotanshinone (CPT) is a STAT3 inhibitor with IC50 of 4.6 μM, strongly inhibits phosphorylation of STAT3 Tyr705, with a small effect on STAT3 Ser727, but none against STAT1 nor STAT5. |
| 11 | Saracatinib (AZD0530) | Src, Bcr-Abl | 95 | Saracatinib (AZD0530) is a potent Src inhibitor with IC50 of 2.7 nM, and potent to c-Yes, Fyn, Lyn, Blk, Fgr and Lck; less active for Abl and EGFR (L858R and L861Q). Phase 1/2. |
| 12 | Bosutinib (SKI-606) | Src | 95 | Bosutinib (SKI-606) is a novel, dual Src/Abl inhibitor with IC50 of 1.2 nM and 1 nM, respectively. |
| 13 | Ouabain | Sodium Channel | 95 | Ouabain is a selective Na+/K+, -ATPase inhibitor, binds to α2 /α3 subunit with Ki of 41 nM/15 nM. |
| 14 | Sorafenib | Raf | 95 | Sorafenib is a multikinase inhibitor of Raf-1, B-Raf and VEGFR-2 with IC50 of 6 nM, 22 nM and 90 nM, respectively. |

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| 15 | Pantoprazole sodium | Proton Pump | 95 | Pantoprazole is a proton pump inhibitor drug that inhibits gastric acid secretion. It works on gastric parietal cells to irreversibly inhibit (H+/K+)-ATPase function and suppress the production of gastric acid. |
| 16 | Zinc Pyrithione | Proton Pump | 95 | Zinc pyrithione is an antifungal and antibacterial agent disrupting membrane transport by blocking the proton pump. |
| 17 | Esomeprazole Magnesium | Proton Pump | 95 | Esomeprazole Magnesium is a proton pump inhibitor to reduce gastric acid secretion. |
| 18 | Danoprevir (ITMN-191) | Proteasome, HCV Protease | 95 | Danoprevir(ITMN-191) is a peptidomimetic inhibitor of the NS3/4A protease of hepatitis C virus (HCV) with IC50 of 0.2-3.5 nM, inhibition effect for HCV genotypes 1A/1B/4/5/6 is ~10-fold higher than 2B/3A. Phase 2. |
| 19 | CEP-18770 (Delanzomib) | Proteasome | 95 | CEP-18770 is an orally active inhibitor of the chymotrypsin-like activity of proteasome with IC50 of 3.8 nM, with only marginal inhibition of the tryptic and peptidylglutamyl activities of the proteosome. Phase 1/2. |
| 20 | Carfilzomib (PR-171) | Proteasome | 95 | Carfilzomib (PR-171) is an irreversible proteasome inhibitor with IC50 of <5 nM, displayed preferential in vitro inhibitory potency against the ChT-L activity in the β5 subunit, but little or no effect on the PGPH and T-L activities. |
| 21 | Epoxomicin | Proteasome | 95 | Epoxomicin is a selective proteasome inhibitor with anti-inflammatory activity, inhibits primarily the CH-L activity of the 20S proteasome, while T-L and PGPH catalytic activities are also inhibited at 100- and 1000-fold reduced rate. |
| 22 | MG-132 | Proteasome | 95 | MG-132 is an inhibitor of proteasome with IC50 of 100 nM, and also inhibits calpain with IC50 of 1.2 μM. |
| 23 | ONX-0914 (PR-957) | Proteasome | 95 | ONX-0914 (PR-957) is a potent and selective immunoproteasome inhibitor with minimal cross-reactivity for the constitutive proteasome. |
| 24 | MLN2238 | Proteasome | 95 | MLN2238 inhibits the chymotrypsin-like proteolytic (β5) site of the 20S proteasome with IC50 and Ki of 3.4 nM and 0.93 nM, respectively, also inhibits the caspase-like (β1) and trypsin-like (β2) proteolytic sites, with IC50 of 31 and 3500 nM. |
| 25 | MLN9708 | Proteasome | 95 | MLN9708 immediately hydrolyzed to MLN2238, the biologically active form, on exposure to aqueous solutions or plasma. MLN2238 inhibits the chymotrypsin-like proteolytic (β5) site of the 20S proteasome with IC50/Ki of 3.4 nM/0.93 nM, less potent to β1 and little activity to β2. Phase 3. |
| 26 | Hexachlorophene | potassium channel | 95 | Hexachlorophene is a potent KCNQ1/KCNE1 potassium channel activator with EC50 of 4.61 ± 1.29 μM; It can also attenuate Wnt/beta-catenin signaling through the Siah-1-mediated beta-catenin degradation. |
| 27 | PIK-75 | PI3K, DNA-PK | 95 | PIK-75 is a p110α inhibitor with IC50 of 5.8 nM (200-fold more potently than p110β), isoform-specific mutants at Ser773, and |

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| | | | | also potently inhibits DNA-PK with IC50 of 2 nM. |
| 28 | Veliparib (ABT-888) | PARP | 95 | Veliparib (ABT-888) is a potent inhibitor of PARP1 and PARP2 with Ki of 5.2 nM and 2.9 nM, respectively. It is inactive to SIRT2. Phase 1/2. |
| 29 | Rucaparib (AG-014699,PF-01367338) | PARP | 95 | Rucaparib (AG-014699, PF-01367338) is an inhibitor of PARP with Ki of 1.4 nM for PARP1, also showing binding affinity to eight other PARP domains. Phase 1/2. |
| 30 | Tenovin-1 | p53 | 95 | Tenovin-1 protects against MDM2-mediated p53 degradation, which involves ubiquitination, and acts through inhibition of protein-deacetylating activities of SirT1 and SirT2. |
| 31 | Baicalein | P450 | 95 | Baicalein is a CYP2C9 and prolyl endopeptidase inhibitor. |
| 32 | Avasimibe | P450 | 95 | Avasimibe inhibits ACAT with IC50 of 3.3 μM, also inhibits human P450 isoenzymes CYP2C9, CYP1A2 and CYP2C19 with IC50 of 2.9 μM, 13.9 μM and 26.5 μM, |
| 33 | Gambogic Acid | Others | 95 | Gambogic Acid activates caspases with EC50 of 0.78-1.64 μM and competitively inhibits Bcl-X<sub>L</sub>, Bcl-2, Bcl-W, Bcl-B, Bfl-1 and Mcl-1 with IC50 of 1.47, 1.21, 2.02, 0.66, 1.06 and 0.79 μM, respectively. |
| 34 | Gemcitabine | Others | 95 | Gemcitabine(Gemzar) belongs to the group of medicines called antimetabolites.Phase 3. |
| 35 | Telmisartan | Others | 95 | Telmisartan (Micardis) is an angiotensin II receptor antagonist (ARB) used in the management of hypertension. |
| 36 | Mycophenolate Mofetil | Others | 95 | Mycophenolate Mofetil is a non-competitive, selective and reversible inhibitor of inosine monophosphate dehydrogenase I/II with IC50 of 39 nM and 27 nM, respectively. |
| 37 | Nevirapine | Others | 95 | Nevirapine(Viramune) is a non-nucleoside reverse transcriptase inhibitor (NNRTI) used to treat HIV-1 infection and AIDS. |
| 38 | Domiphen Bromide | Others | 95 | Domiphen bromide is a quaternary ammonium antiseptic with actions as a cationic surfactant. |
| 39 | Mitoxantrone HCl | Others | 95 | Mitoxantrone HCl is a classic folic acid antagonist. |
| 40 | Halofuginone | Others | 95 | Halofuginone is the competitively inhibitor of prolyl-tRNA synthetase with Ki of 18.3 nM.It could also down-regulate Smad3 and blocked TGF-β signaling at 10 ng/ml in mammal. |
| 41 | Teniposide | Others | 95 | Teniposide(Vumon)is a chemotherapeutic medication mainly used in the treatment of childhood acute lymphocytic leukemia (ALL). |
| 42 | Adapalene | Others | 95 | Adapalene is a third-generation topical retinoid primarily used in the treatment of acne. |
| 43 | Cetylpyridinium Chloride | Others | 95 | Cetylpyridinium chloride is a cationic quaternary ammonium compound used as oropharyngeal antiseptic. |
| 44 | NH125 | Others | 95 | NH125 is a selective eEF-2 kinase inhibitor with IC50 of 60 |

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| | | | | nM, >125-fold selectivity over PKC, PKA, and CaMKII, and also a potent histidine kinase inhibitor. |
| 45 | Mycophenolic acid | Others | 95 | Mycophenolic acid is an immunosuppressant agent used to prevent rejection in organ transplantation. |
| 46 | AI-10-49 | Others | 95 | AI-10-49 is a selective inhibitor of the binding of CBFβ-SMMHC to RUNX1 with IC50 of 260 nM. |
| 47 | PTC-209 | Others | 95 | PTC-209 is a potent and selective BMI-1 inhibitor with IC50 of 0.5 μM, and results in irreversible reduction of cancer-initiating cells (CICs). |
| 48 | MK-886 (L-663,536) | others | 95 | MK-886 is an inhibitor of leukotriene biosynthesis, inhibiting 5-lipoxygenase-activating protein (FLAP). It is also a moderately potent PPARα antagonist. |
| 49 | Dp44mT | Others | 95 | Dp44mT is a potent iron chelator, which shows selective antitumor activity. |
| 50 | Ethacridine lactate monohydrate | Others | 95 | Ethacridine lactate monohydrate is an aromatic organic compound based on acridine used as an antiseptic agent. |
| 51 | Crystal Violet | Others | 95 | Crystal violet is a triarylmethane dye. |
| 52 | Methylene Blue | others | 95 | Methylene Blue is used as a dye in chromoendoscopy. It Inhibits tau filament formation with IC50 of 1.9μM. Also it inhibits soluble guanylyl cyclase. |
| 53 | Dapson | others | 95 | Dapsone, also known as diaminodiphenyl sulfone (DDS), is an antibiotic commonly used in combination with rifampicin and clofazimine for the treatment of leprosy. |
| 54 | Prednisolone | Others | 95 | Prednisolone(Hydroretrocortine) is a synthetic glucocorticoid with anti-inflammatory and immunomodulating properties. |
| 55 | i-Inositol | others | 95 | i-Inositol, also known as myo-inositol, is a chemical compound which is sugar alcohol. i-Inositol is involved in a number of biological processes including insulin signal transduction, cytoskeleton transduction and so on. |
| 56 | Thiabendazole | Others | 95 | Thiabendazole inhibites the mitochondrial helminth-specific enzyme, fumarate reductase, with anthelminthic property. |
| 57 | Rifabutin | Others | 95 | Rifabutin(Mycobutin) is a semisynthetic ansamycin antibiotic with potent antimycobacterial properties. |
| 58 | TRx 0237 (LMTX™) mesylate | others | 95 | TRx 0237 (LMTX™) mesylate is a second-generation tau protein aggregation inhibitor for the treatment of Alzheimer's disease (AD) and frontotemporal dementia. |
| 59 | Guaifenesin | Others | 95 | Guaifenesin(Guaiphenesin) is thought to act as an expectorant. |
| 60 | Nicotinic Acid | Others | 95 | Nicotinic Acid is a water-soluble vitamin belonging to the vitamin B family. |
| 61 | Ropivacaine HCl | Others | 95 | Ropivacaine HCl is an anaesthetic agent and blocks impulse conduction in nerve fibres through inhibiting sodium ion influx |

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| | | | | reversibly. |
| 62 | Triptolide (PG490) | Others | 95 | Triptolide is a diterpene triepoxide, immunosuppresive agent extracted from the Chinese herb Tripterygium wilfordii. |
| 63 | Iopamidol | others | 95 | Iopamidol is a non-ionic, water-soluble radiographic contrast agent. |
| 64 | Triclosan | others | 95 | Triclosan is a diphenyl ether derivative used in cosmetics and toilet soaps as an antiseptic. It has some bacteriostatic and fungistatic action. |
| 65 | Nitrofurantoin | others | 95 | Nitrofurantoin is an antibiotic used to treat bladder infections.It inhibits bacterial DNA, RNA, and cell wall protein synthesis. |
| 66 | JTC-801 | Opioid Receptor | 95 | JTC-801 is a selective opioid receptor-like1 (ORL1) receptor antagonist with IC50 of 94 nM, weakly inhibits receptors δ, κ, and μ. |
| 67 | Rapamycin (Sirolimus) | mTOR | 95 | Rapamycin (Sirolimus, AY-22989, WY-090217) is a specific mTOR inhibitor with IC50 of ~0.1 nM. |
| 68 | Temsirolimus (CCI-779, NSC 683864) | mTOR | 95 | Temsirolimus (CCI-779) is a specific mTOR inhibitor with IC50 of 1.76 μM. |
| 69 | IMD 0354 | IKK | 95 | IMD-0354 is an IKKβ inhibitor and blocks IκBα phosphorylation in NF-κB pathway. |
| 70 | VER-50589 | HSP (e.g. HSP90) | 95 | VER-50589 is a potent HSP90 inhibitor with IC50 of 21 nM for HSP90β. |
| 71 | BIIB021 | HSP | 95 | BIIB021 is an orally available, fully synthetic small-molecule inhibitor of HSP90 with Ki and EC50 of 1.7 nM and 38 nM, respectively. |
| 72 | VER-49009 | HSP | 95 | VER-49009 is a potent HSP90 inhibitor with IC50 of 47 nM for HSP90β. |
| 73 | Ganetespib (STA-9090) | HSP | 95 | Ganetespib is an HSP90 inhibitor with IC50 of 4 nM in OSA 8 cells, induces apoptosis of OSA cells while normal osteoblasts are not affected; active metabolite of STA-1474. |
| 74 | 17-AAG (Tanespimycin) | HSP | 95 | 17-AAG is a potent HSP90 inhibitor with IC50 of 5 nM, having a 100-fold higher binding affinity for HSP90 derived from tumour cells than HSP90 from normal cells. |
| 75 | 17-DMAG (Alvespimycin) HCl | HSP | 95 | 17-DMAG is a potent, water-soluble HSP90 inhibitor with IC50 of 62 nM. |
| 76 | CUDC-907 | HDAC, PI3K | 95 | CUDC-907 is a dual PI3K and HDAC inhibitor for PI3Kα and HDAC1/2/3/10 with IC50 of 19 nM and 1.7 nM/5 nM/1.8 nM/2.8 nM, respectively. Phase 1. |
| 77 | Givinostat (ITF2357) | HDAC | 95 | Givinostat (ITF2357) is a potent HDAC inhibitor for HDAC2, HDAC1B and HDAC1A with IC50 of 10 nM, 7.5 nM and 16 nM. Phase 1/2. |
| 78 | CAY10603 | HDAC | 95 | CAY10603 is a potent and selective HDAC6 inhibitor |

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| | | | | with IC50 of 2 pM, >200-fold selectivity over other HDACs. |
| 79 | Lapatinib (GW-572016) Ditosylate | EGFR, HER2 | 95 | Lapatinib Ditosylate (GW572016, GW2016) is a potent EGFR and ErbB2 inhibitor with IC50 of 10.8 and 9.2 nM, respectively. |
| 80 | AZD3759 | EGFR | 95 | AZD3759 is a potent, oral active, CNS-penetrant EGFR inhibitor with IC50 of 0.3 nM, 0.2 nM, and 0.2 nM for EGFR (WT), EGFR (L858R), and EGFR (exon 19Del), respectively. Phase 1. |
| 81 | Tyrphostin 9 | EGFR | 95 | Tyrphostin 9 is firstly designed as an EGFR inhibitor with IC50 of 460 μM, but is also found to be more potent to PDGFR with IC50 of 0.5 μM. |
| 82 | PR-619 | DUB | 95 | PR-619 is a non-selective, reversible inhibitor of the deubiquitinylating enzymes (DUBs) with EC50 of 1-20 μM. |
| 83 | PP121 | DNA-PK, mTOR, PDGF | 95 | PP-121 is a multi-targeted inhibitor of PDGFR, Hck, mTOR, VEGFR2, Src and Abl with IC50 of 2 nM, 8 nM, 10 nM, 12 nM, 14 nM and 18 nM, also inhibits DNA-PK with IC50 of 60 nM. |
| 84 | Fludarabine Phosphate | DNA/RNA Synthesis | 95 | Fludarabine Phosphate is an analogue of adenosine and deoxyadenosine, which is able to compete with dATP for incorporation into DNA and inhibit DNA synthesis. |
| 85 | Clofarabine | DNA/RNA Synthesis | 95 | Clofarabine inhibits the enzymatic activities of ribonucleotide reductase (IC50 = 65 nM) and DNA polymerase. |
| 86 | MG-101 (ALLN) | Cysteine Protease | 95 | MG-101 (ALLN) is a cell-permeable and potent inhibitor of cysteine proteases including calpains and lysosomal cathepsins. |
| 87 | Salicylic acid | COX | 95 | Salicylic acid is a beta hydroxy acid that occurs as a natural compound in plants which is an inhibitor of ethylene biosynthesis and cyclooxygenase activity. |
| 88 | BMS-794833 | c-Met, VEGFR | 95 | BMS-794833 is a potent ATP competitive inhibitor of Met/VEGFR2 with IC50 of 1.7 nM/15 nM, also inhibits Ron, Axl and Flt3 with IC50 of <3 nM; a prodrug of BMS-817378. Phase 1. |
| 89 | AZD7762 | Chk | 95 | AZD7762 is a potent and selective inhibitor of Chk1 with IC50 of 5 nM. It is equally potent against Chk2 and less potent against CAM, Yes, Fyn, Lyn, Hck and Lck. Phase 1. |
| 90 | R547 | CDK | 95 | R547 is a potent ATP-competitive inhibitor of CDK1/2/4 with Ki of 2 nM/3 nM/1 nM. It is less potent to CDK7 and GSK3α/β, while inactive to other kinases. |
| 91 | AT7519 | CDK | 95 | AT7519 is a multi-CDK inhibitor for CDK1, 2, 4, 6 and 9 with IC50 of 10-210 nM. It is less potent to CDK3 and little active to CDK7. Phase 1. |
| 92 | Flavopiridol HCl | CDK | 95 | Flavopiridol competes with ATP to inhibit CDKs including CDK1, CDK2, CDK4 and CDK6 with IC50 of ~ 40 nM. It is 7.5-fold more selective for CDK1/2/4/6 than CDK7. Flavopiridol |

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| | | | | is initially found to inhibit EGFR and PKA. Phase 1/2. |
| 93 | Dinaciclib (SCH727965) | CDK | 95 | Dinaciclib (SCH727965) is a novel and potent CDK inhibitor for CDK2, CDK5, CDK1 and CDK9 with IC50 of 1 nM, 1 nM, 3 nM and 4 nM, respectively. It also blocks thymidine (dThd) DNA incorporation. Phase 3. |
| 94 | AZD5438 | CDK | 95 | AZD5438 is a potent inhibitor of CDK1/2/9 with IC50 of 16 nM/6 nM/20 nM. It is less potent to CDK5/6 and also inhibits GSK3β. Phase 1. |
| 95 | SNS-032 (BMS-387032) | CDK | 95 | SNS-032 has firstly been described as a selective inhibitor of CDK2 with IC50 of 48 nM and is 10- and 20-fold selective over CDK1/CDK4. It is also found to be sensitive to CDK7/9 with IC50 of 62 nM/4 nM, with little effect on CDK6. Phase 1. |
| 96 | Lercanidipine (hydrochloride) | Calcium Channel | 95 | Lercanidipine is a calcium channel blocker of the dihydropyridine class. |
| 97 | Ponatinib (AP24534) | Bcr-Abl, VEGFR, FGFR, PDGFR, Flt | 95 | Ponatinib (AP24534) is a novel, potent multi-target inhibitor of Abl, PDGFRα, VEGFR2, FGFR1 and Src with IC50 of 0.37 nM, 1.1 nM, 1.5 nM, 2.2 nM and 5.4 nM, respectively. |
| 98 | DCC-2036 (Rebastinib) | Bcr-Abl | 95 | DCC-2036 is a conformational control Bcr-Abl inhibitor for Abl1(WT) and Abl1(T315I) with IC50 of 0.8 nM and 4 nM, also inhibits SRC, LYN, FGR, HCK, KDR, FLT3, and Tie-2, and low activity to seen towards c-Kit. Phase 1/2. |
| 99 | AT101 | Bcl-2 | 95 | AT101, the R-(-) enantiomer of Gossypol acetic acid, binds with Bcl-2, Bcl-xL and Mcl-1 with Ki of 0.32 μM, 0.48 μM and 0.18 μM; does not inhibit BIR3 domain and BID. Phase 1/2. |
| 100 | ABT-199 (GDC-0199) | Bcl-2 | 95 | ABT-199 (GDC-0199) is a Bcl-2-selective inhibitor with Ki of <0.01 nM, >4800-fold more selective versus Bcl-xL and Bcl-w, and no activity to Mcl-1. Phase 2. |
| 101 | Alisertib (MLN8237) | Aurora Kinase | 95 | Alisertib (MLN8237) is a selective Aurora A inhibitor with IC50 of 1.2 nM. It has >200-fold higher selectivity for Aurora A than Aurora B. Phase 3. |
| 102 | FCCP | ATPase | 95 | FCCP is a potent uncoupler of oxidative phosphorylation in mitochondria that disrupts ATP synthesis by transporting protons across cell membranes. |
| 103 | CGK 733 | ATM/ATR | 95 | CGK 733 is a potent and selective inhibitor of ATM/ATR with IC50 of ~200 nM. |
| 104 | MK-2866 (GTx-024) | Androgen Receptor | 95 | MK-2866 (GTx-024) is a selective androgen receptor modulator (SARM) with Ki of 3.8 nM, and is tissue-selective for anabolic organs. Phase 3. |
| 105 | GSK690693 | Akt | 95 | GSK690693 is a pan-Akt inhibitor targeting Akt1/2/3 with IC50 of 2 nM/13 nM/9 nM, also sensitive to the AGC kinase family: PKA, PrkX and PKC isozymes. Phase 1. |
| 106 | Formoterol Hemifumarate | Adrenergic Receptor | 95 | Formoterol hemifumarate is a potent, selective and long-acting β2-adrenoceptor agonist to β2 and β1 receptors with pKd of |

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| | | | | 8.12 and 5.58, respectively. |
| 107 | Trihexyphenidyl hydrochloride | AChR | 95 | Trihexyphenidyl hydrochloride is an antiparkinsonian agent of the antimuscarinic class. |
| 108 | Prucalopride | 5-HT Receptor | 95 | Prucalopride is a selective, high affinity 5-HT receptor agonist for 5-HT4A and 5-HT4B receptor with Ki of 2.5 nM and 8 nM, respectively, exhibits >290-fold selectivity against other 5-HT receptor subtypes. Phase 3. |
| 109 | Sodium Monofluorophosphate | Akt | 95 | Perifosine (KRX-0401) is a novel Akt inhibitor with IC50 of 4.7 μM in MM.1S cells, targets pleckstrin homology domain of Akt. Phase 3. |
| 110 | Mizoribine | Others | 95 | Proflavine Hemisulfate is a topical antiseptic by interchelating DNA, thereby disrupting DNA synthesis and leading to high levels of mutation in the copied DNA strands. |
| 111 | Bivalirudin Trifluoroacetate | Autophagy,DNA/RNA Synthesis | 95 | Gemcitabine HCl is a DNA synthesis inhibitor with IC50 of 50 nM, 40 nM, 18 nM and 12 nM in PANC1, MIAPaCa2, BxPC3 and Capan2 cells, respectively. |
| 112 | PD0166285 | Wee1/Chk1 | 90 | PD0166285 is a potent Wee1 and Chk1 inhibitor with activity at nanomolar concentrations.PD0166285 is a novel G2 checkpoint abrogator. |
| 113 | NVP-BHG712 | VEGFR, Src, Raf, Bcr-Abl | 90 | NVP-BHG712 is a specific EphB4 inhibitor with ED50 of 25 nM that discriminates between VEGFR and EphB4 inhibition; also shows activity against c-Raf, c-Src and c-Abl with IC50 of 0.395 μM, 1.266 μM and 1.667 μM, respectively. |
| 114 | (S)-10-Hydroxycamptothecin | Topoisomerase | 90 | 10-Hydroxycamptothecin is a DNA topoisomerase I inhibitor with potent anti-tumor activity. |
| 115 | SU6656 | Src | 90 | SU 6656 is a selective Src family kinase inhibitor with IC50 of 280 nM, 20 nM, 130 nM, and 170 nM for Src, Yes, Lyn, and Fyn, respectively. |
| 116 | Vinpocetine | Sodium Channel | 90 | Vinpocetine is a selective inhibitor of voltage-sensitive sodium channel for the treatment of stroke, vascular dementia and Alzheimer's disease. |
| 117 | SGI-1776 free base | Pim | 90 | SGI-1776 is a novel ATP competitive inhibitor of Pim1 with IC50 of 7 nM, 50- and 10-fold selective versus Pim2 and Pim3, also potent to Flt3 and haspin. Phase 1. |
| 118 | GNE-317 | PI3K | 90 | GNE-317 is a potent, brain-penetrant PI3K inhibitor. |
| 119 | Linifanib (ABT-869) | PDGFR, VEGFR | 90 | Linifanib (ABT-869) is a novel, potent ATP-competitive VEGFR/PDGFR inhibitor for KDR, CSF-1R, Flt-1/3 and PDGFRβ with IC50 of 4 nM, 3 nM, 3 nM/4 nM and 66 nM respectively, mostly effective in mutant kinase-dependent cancer cells (i.e. FLT3). Phase 3. |
| 120 | Olaparib (AZD2281, | PARP | 90 | Olaparib (AZD2281, KU0059436) is a selective inhibitor of PARP1/2 with IC50 of 5 nM/1 nM, 300-times less effective |

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| | Ku-0059436) | | | against tankyrase-1. Phase 1/2. |
| 121 | NSC348884 | p53 | 90 | NSC348884, as a nucleophosmin inhibitor, inhibit cell proliferation and induce apoptosis in various cancer cell lines with IC50 values ranging from 1.4-4 ¦ÌM |
| 122 | Cetrimonium Bromide (CTAB) | Others | 90 | Cetrimonium Bromide is a known component of the broad-spectrum antiseptic cetrimide, which is a mixture of different quaternary ammonium salts. |
| 123 | Altretamine | Others | 90 | Altretamine is an anti-neoplastic agent. |
| 124 | 4E1RCat | Others | 90 | 4E1RCat is a dual inhibitor of eIF4E:eIF4G and eIF4E:4E-BP1 interaction, and inhibits the binding of eIF4G to eIF4E with IC50 of 3.2 μM. |
| 125 | Ridaforolimus (Deforolimus, MK-8669) | mTOR | 90 | Ridaforolimus (Deforolimus, MK-8669) is a selective mTOR inhibitor with IC50 of 0.2 nM in HT-1080 cell line; while not classified as a prodrug, mTOR inhibition and FKBP12 binding is similar to rapamycin. Phase 3. |
| 126 | CC-223 | mTOR | 90 | CC-223 is a potent, selective, and orally bioavailable mTOR inhibitor with IC50 of 16 nM, >200-fold selectivity over the related PI3K-α. Phase 1/2. |
| 127 | Combretastatin A4 | Microtubule Associated | 90 | Combretastatin A4 is a microtubule-targeting agent that binds β-tubulin with K<sub>d</sub> of 0.4 μM.Phase 3. |
| 128 | FLLL32 | JAK | 90 | FLLL32 is a potent JAK2/STAT3 inhibitor with IC50 of <5 μM. |
| 129 | Elvitegravir (GS-9137, JTK-303) | Integrase | 90 | Elvitegravir (EVG, JTK-303/GS-9137) is an HIV integrase inhibitor for HIV-1 IIIB, HIV-2 EHO and HIV-2 ROD with IC50 of 0.7 nM, 2.8 nM and 1.4 nM, respectively. |
| 130 | SNX-2112 (PF-04928473) | HSP | 90 | SNX-2112 selectively binds to the ATP pocket of HSP90α and HSP90β with Ka of 30 nM and 30 nM, uniformly more potent than 17-AAG. |
| 131 | AT13387 | HSP | 90 | AT13387 is a selective potent Hsp90 inhibitor with IC50 of 18 nM in A375 cells, displays a long duration of anti-tumor activity. |
| 132 | GSK1292263 | GPR | 90 | GSK1292263 is a novel GPR119 agonist, showing potential for the treatment of type 2 diabetes. Phase 2. |
| 133 | Erlotinib HCl (OSI-744) | EGFR | 90 | Erlotinib HCl (OSI-744) is an EGFR inhibitor with IC50 of 2 nM, >1000-fold more sensitive for EGFR than human c-Src or v-Abl. Phase 3. |
| 134 | Flavopiridol (Alvocidib) | CDK | 90 | Flavopiridol (Alvocidib) competes with ATP to inhibit CDKs including CDK1, CDK2, CDK4 and CDK6 with IC50 of ~ 40 nM. It is 7.5-fold more selective for CDK1, 2, 4, 6 versus CDK7. Flavopiridol is initially found to inhibit EGFR and PKA. Phase 1/2. |
| 135 | Almotriptan Malate | 5-HT Receptor | 90 | Almotriptan Malate is a selective 5-hydroxytryptamine1B/1D (5-HT1B/1D) receptor agonist, used for the treatment of Migraine attacks in adults. |

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| 136 | Proflavine Hemisulfate | DNA/RNA Synthesis | 90 | Blasticidin S HCl is a nucleoside antibiotic isolated from Stretomyces girseochromogenes, and acts as a DNA and protein synthesis inhibitor, used to select transfected cells carrying bsr or BSD resistance genes. |
| 137 | Blasticidin S HCl | DNA/RNA Synthesis | 90 | Bivalirudin Trifluoroacetate is a synthetic 20 residue peptide (thrombin inhibitor) which reversibly inhibits thrombin. |
| 138 | Cabozantinib malate (XL184) | VEGFR | 85 | Cabozantinib malate is the malate of Cabozantinib, a potent VEGFR2 inhibitor with IC50 of 0.035 nM and also inhibits c-Met, Ret, Kit, Flt-1/3/4, Tie2, and AXL with IC50 of 1.3 nM, 4 nM, 4.6 nM, 12 nM/11.3 nM/6 nM, 14.3 nM and 7 nM, respectively. |
| 139 | Irinotecan | Topoisomerase | 85 | Irinotecan is a topoisomerase I inhibitor for LoVo cells and HT-29 cells with IC50 of 15.8 μM and 5.17 μM, respectively. |
| 140 | S3I-201 | STAT | 85 | S3I-201 shows potent inhibition of STAT3 DNA-binding activity with IC50 of 86 μM, and low activity towards STAT1 and STAT5. |
| 141 | Ibutilide Fumarate | Sodium Channel | 85 | Ibutilide Fumarate is a Class III antiarrhythmic agent that is indicated for acute cardioconversion of atrial fibrillation and atrial flutter of a recent onset to sinus rhythm by induction of slow inward sodium current, which prolongs action potential and refractory period of myocardial cells. |
| 142 | Tanshinone I | Phospholipase (e.g. PLA) | 85 | Tanshinone I, an active principle isolated from Salvia miltiorrhiza (Danshen), is structurally similar to tanshinone IIA and may possess similar cytotoxic effects on tumor cells. |
| 143 | BX-795 | PDK-1, IKK | 85 | BX795 is a potent and specific PDK1 inhibitor with IC50 of 6 nM, 140- and 1600-fold more selective for PDK1 than PKA and PKC, respectively. Meanwhile, in comparison to GSK3β more than 100-fold selectivity observed for PDK1. |
| 144 | BX-912 | PDK-1 | 85 | BX912 is a potent and specific PDK1 inhibitor with IC50 of 12 nM, 9- and 105- fold greater selectivity for PDK1 than PKA and PKC, respectively. In comparison to GSK3β, selectivity for PDK1 is 600-fold. |
| 145 | Imatinib Mesylate (STI571) | PDGFR, c-Kit, Bcr-Abl | 85 | Imatinib Mesylate (STI571) is an orally bioavailability mesylate salt of Imatinib, which is a multi-target inhibitor of v-Abl, c-Kit and PDGFR with IC50 of 0.6 μM, 0.1 μM and 0.1 μM, respectively. |
| 146 | NMS-873 | p97 | 85 | NMS-873 is an allosteric and specific p97 inhibitor with IC50 of 30 nM. |
| 147 | JNJ-26854165 (Serdemetan) | p53 | 85 | JNJ-26854165 acts as a HDM2 ubiquitin ligase antagonist and also induces early apoptosis in p53 wild-type cells, inhibits cellular proliferation followed by delayed apoptosis in the absence of functional p53. Phase 1. |
| 148 | Chlorquinaldol | Others | 85 | Chlorquinaldol is an antimicrobial agent used for local antisepsy. |

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| 149 | Cephalomannine | Others | 85 | Cephalomannine is an active anti-cancer agent obtained from Taxus yunnanensis and has an antineoplastic effect on tumors found in mice. |
| 150 | Benzethonium Chloride | Others | 85 | Benzethonium chloride is a potent inhibitor of nAChRs, it inhibits α4β2 nAChRs and α7 nAChRs with IC50 of 49 nM and 122 nM, respectively. |
| 151 | Penfluridol | Others | 85 | Penfluridol is a highly potent, first generation diphenylbutylpiperidine antipsychotic. |
| 152 | Xylose | Others | 85 | Xylose is a sugar first isolated from wood. |
| 153 | Sertaconazole nitrate | Others | 85 | Sertaconazole nitrate is a topical broad-spectrum antifungal that is developed to provide an additional agent for the treatment of superficial cutaneous and mucosal infections. |
| 154 | Mometasone furoate | Others | 85 | Mometasone furoate is a glucocorticosteroid used topically to reduce inflammation of the skin or in the airways. |
| 155 | (+)-MK 801 maleate | NMDAR | 85 | (+)-MK-801 is a potent, selective and non-competitive NMDA receptor antagonist with Kd of 37.2 nM in rat brain membranes |
| 156 | ABT-751 (E7010) | Microtubule Associated | 85 | ABT-751 (E7010) binds to the colchicine site on β-tubulin and inhibits polymerization of microtubules, not a substrate for the MDR transporter and is active against cell lines resistant to vincristine, doxorubicin, and cisplatin. Phase 1/2. |
| 157 | AZD8330 | MEK | 85 | AZD8330 is a novel, selective, non-ATP competitive MEK 1/2 inhibitor with IC50 of 7 nM. Phase 1. |
| 158 | AZD1480 | JAK | 85 | AZD1480 is a novel ATP-competitive JAK2 inhibitor with IC50 of 0.26 nM, selectivity against JAK3 and Tyk2, and to a smaller extent against JAK1. Phase 1. |
| 159 | AZ 960 | JAK | 85 | AZ 960 is a novel ATP competitive JAK2 inhibitor with IC50 and Ki of <3 nM and 0.45 nM, 3-fold selectivity of AZ960 for JAK2 over JAK3. |
| 160 | Rosuvastatin Calcium | HMG-CoA Reductase | 85 | Rosuvastatin Calcium is a competitive inhibitor of HMG-CoA reductase with IC50 of 11 nM. |
| 161 | Fluvastatin Sodium | HMG-CoA Reductase | 85 | Fluvastatin Sodium inhibits HMG-CoA reductase activity with IC50 of 8 nM. |
| 162 | Atorvastatin Calcium | HMG-CoA Reductase | 85 | Atorvastatin (Lipitor) is an inhibitor of HMG-CoA reductase used as a cholesterol-lowering medication that blocks the production of cholesterol. |
| 163 | Taladegib (LY2940680) | Hedgehog,Hedgehog/Smoothened | 85 | Taladegib (LY2940680) binds to the Smoothened (Smo) receptor and potently inhibits Hedgehog (Hh) signaling. Phase 1/2. |
| 164 | KW-2449 | Flt, Bcr-Abl, Aurora Kinase | 85 | KW-2449 is a multiple-targeted inhibitor, mostly for Flt3 with IC50 of 6.6 nM, modestly potent to FGFR1, Bcr-Abl and Aurora A; little effect on PDGFRβ, IGF-1R, EGFR. Phase 1. |
| 165 | PF-00562271 | FAK | 85 | PF-00562271 is the benzenesulfonate salt of PF-562271, which is a potent, ATP-competitive, reversible inhibitor of FAK |

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| | | | | with IC50 of 1.5 nM, ~10-fold less potent for Pyk2 than FAK and >100-fold selectivity against other protein kinases, except for some CDKs. Phase 1. |
| 166 | Levosulpiride | Dopamine Receptor | 85 | Levosulpiride is a selective antagonist for D2 dopamine receptors used as an antipsychotic and prokinetic agent. |
| 167 | Raltitrexed | DNA/RNA Synthesis | 85 | Raltitrexed is a thymidylate synthase inhibitor with an IC50 of 9 nM for the inhibition of L1210 cell growth. |
| 168 | PHA-767491 | CDK | 85 | PHA-767491 is a potent ATP-competitive dual Cdc7/CDK9 inhibitor with IC50 of 10 nM and 34 nM in cell-free assays, respectively.It displays ~20-fold selectivity against CDK1/2 and GSK3-β, 50-fold selectivity against MK2 and CDK5, 100-fold selectivity against PLK1 and CHK2. |
| 169 | Vincristine sulfate | Autophagy,Microtubule Associated | 85 | Vincristine is an inhibitor of polymerization of microtubules by binding to tubulin with IC50 of 32 μM. |
| 170 | SNS-314 Mesylate | Aurora Kinase | 85 | SNS-314 Mesylate is a potent and selective inhibitor of Aurora A, Aurora B and Aurora C with IC50 of 9 nM, 31 nM, and 3 nM, respectively. It is less potent to Trk A/B, Flt4, Fms, Axl, c-Raf and DDR2. Phase 1. |
| 171 | 5-Iodotubercidin | adenosine receptor | 85 | 5-Iodotubercidin is a potent adenosine kinase inhibitor with IC50 of 26 nM. It inhibits nucleoside transporter, CK1, insulin receptor tyrosine kinase, phosphorylase kinase, PKA, CK2 and PKC. |
| 172 | Perifosine (KRX-0401) | Others | 85 | Sodium Monofluorophosphate is a competitive inhibitor of pyruvate kinase and alkaline phosphatase with Ki of 3.4 mM and 69 μM, respectively, which also irreversibly inhibits phosphorylase phosphatase with Ki of 0.5 mM. |
| 173 | RO4929097 | Y-Secretase | 80 | RO4929097 is a γ secretase inhibitor with IC50 of 4 nM, inhibiting cellular processing of Aβ40 and Notch with EC50 of 14 nM and 5 nM, respectively. Phase 2. |
| 174 | Telatinib | VEGFR, PDGFR, c-Kit | 80 | Telatinib is a potent inhibitor of VEGFR2/3, c-Kit and PDGFRβ with IC50 of 6 nM/4 nM, 1 nM and 15 nM, respectively. Phase 2. |
| 175 | Topotecan HCl | Topoisomerase | 80 | Topotecan (NSC 609699) is a topoisomerase I inhibitor for MCF-7 Luc cells and DU-145 Luc cells with IC50 of 13 nM and 2 nM, respectively. |
| 176 | Irinotecan HCl Trihydrate | Topoisomerase | 80 | Irinotecan prevents DNA from unwinding by inhibition of topoisomerase 1. |
| 177 | Stattic | STAT | 80 | Stattic, the first nonpeptidic small molecule, potently inhibits STAT3 activation and nuclear translocation with IC50 of 5.1 μM, highly selectivity over STAT1. |
| 178 | PF-4708671 | S6 Kinase | 80 | PF-4708671 is a cell-permeable inhibitor of p70 ribosomal S6 kinase (S6K1 isoform) with Ki/IC50 of 20 nM/160 nM, 400-fold greater selectivity for S6K1 than S6K2, and 4- and >20-fold |

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| | | | | selectivity for S6K1 than MSK1 and RSK1/2, respectively. First S6K1-specific inhibitor to be reported. |
| 179 | ML141 | Rho | 80 | ML141 is a potent, selective and reversible non-competitive inhibitor of Rho family GTPase cdc42 with IC50 of 200 nM. |
| 180 | UK 383367 | Procollagen C Proteinase | 80 | UK-383367 is a procollagen C-proteinase inhibitor with IC50 of 44 nM, has excellent selectivity over MMPs. |
| 181 | Rosiglitazone HCl | PPAR | 80 | Rosiglitazone HCl is a blood glucose-lowering drugs, stimulating insulin secretion by binding to the PPAR receptors in fat cells. |
| 182 | Rigosertib (ON-01910) | PLK | 80 | Rigosertib (ON-01910) is a non-ATP-competitive inhibitor of PLK1 with IC50 of 9 nM. It shows 30-fold greater selectivity against Plk2 and no activity to Plk3. Phase 3. |
| 183 | GSK461364 | PLK | 80 | GSK461364 inhibits purified Plk1 with Ki of 2.2 nM. It is more than 1000-fold selective against Plk2/3. Phase 1. |
| 184 | HMN-214 | PLK | 80 | HMN-214 is a prodrug of HMN-176, which alters the cellular spatial orientation of Plk1. |
| 185 | GSK2126458 (GSK458) | PI3K, mTOR | 80 | GSK2126458 is a highly selective and potent inhibitor of p110α/β/δ/γ, mTORC1/2 with Ki of 0.019 nM/0.13 nM/0.024 nM/0.06 nM and 0.18 nM/0.3 nM, respectively. Phase 1. |
| 186 | YM201636 | PI3K | 80 | YM201636 is a selective PIKfyve inhibitor with IC50 of 33 nM, less potent to p110α and insensitive to Fabl (yeast orthologue). |
| 187 | GSK2606414 | PERK | 80 | GSK2606414 is an orally available, potent, and selective PERK inhibitor with IC50 of 0.4 nM, displaying at least 100-fold selectivity over the other EIF2AKs assayed. |
| 188 | Roflumilast | PDE | 80 | Roflumilast is a selective inhibitor of PDE4 with IC50 of 0.2-4.3 nM. |
| 189 | A-966492 | PARP | 80 | A-966492 is a novel and potent inhibitor of PARP1 and PARP2 with K<sub>i</sub> of 1 nM and 1.5 nM, respectively. |
| 190 | Almorexant HCl | OX Receptor | 80 | Almorexant HCl is an orally active, dual orexin receptor antagonist with IC50 of 6.6 nM and 3.4 nM for OX1 and OX2 receptor, respectively. Phase 3. |
| 191 | Artesunate | Others | 80 | Artesunate is a part of the artemisinin group of agents with an IC50 of < 5 μM for small cell lung carcinoma cell line H69. |
| 192 | Mebendazole | others | 80 | Mebendazole is a synthetic benzimidazole derivate and anthelmintic agent. Mebendazole interferes with the reproduction and survival of helminths by inhibiting the formation of their cytoplasmic microtubules, thereby selectively and irreversibly blocking glucose uptake. |
| 193 | Modafinil | others | 80 | Modafinil is a mood-brightening and memory-enhancing psychostimulant which enhances wakefulness and vigilance. |
| 194 | LY2886721 | Others | 80 | LY2886721 is an BACE inhibitor used for the treatment of |

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| | | | | Alzheimer's Disease. |
| 195 | Nicardipine HCl | Others | 80 | Nicardipine is a dihydropyridine calcium-channel blocking agent used for the treatment of vascular disorders. |
| 196 | Cepharanthine | Others | 80 | Cepharanthine is a biscoclaurine alkaloid inhibiting tumor necrosis factor (TNF)-α-mediated NFκB stimulation, plasma membrane lipid peroxidation and platelet aggregation and suppressing cytokine production. |
| 197 | Albendazole | Others | 80 | Albendazole is a member of the benzimidazole compounds used as a drug indicated for the treatment of a variety of worm infestations. |
| 198 | Triclabendazole | Others | 80 | Triclabendazole is a benzimidazole, it binds to tubulin impairing intracellular transport mechanisms and interferes with protein synthesis. |
| 199 | Sal003 | Others | 80 | Sal003 is a potent and cell-permeable eIF-2α phosphatase inhibitor. |
| 200 | Ambrisentan | Others | 80 | Ambrisentan, a highly selective antagonist of the endothelin-1 type A receptor with IC50 of 18 nM, is indicated for the treatment of pulmonary arterial hypertension (PAH). |
| 201 | ADL5859 HCl | Opioid Receptor | 80 | ADL5859 HCl is a δ-opioid receptor agonist with Ki of 0.8 nM, selectivity against opioid receptor κ, μ, and weak inhibitory activity at the hERG channel. Phase 2. |
| 202 | Mestranol | NULL | 80 | Mestranol is the 3-methyl ether of ethinylestradiol. It was the estrogen used in many of the first oral contraceptives. |
| 203 | Caffeic Acid Phenethyl Ester | NF-κB | 80 | Caffeic acid phenethyl ester is a potent and specific inhibitor of NF-κB activation, and also displays antioxidant, immunomodulatory and antiinflammatory activities. |
| 204 | Voxtalisib (XL765, SAR245409) | mTOR,PI3K | 80 | Voxtalisib (SAR245409, XL765) is a dual inhibitor of mTOR/PI3K, mostly for p110γ with IC50 of 9 nM; also inhibits DNA-PK and mTOR. Phase 1/2. |
| 205 | PP242 | mTOR | 80 | PP242 is a selective mTOR inhibitor with IC50 of 8 nM; targets both mTOR complexes with >10- and 100-fold selectivity for mTOR than PI3Kδ or PI3Kα/β/γ, respectively. |
| 206 | INK 128 (MLN0128) | mTOR | 80 | INK 128 is a potent and selective mTOR inhibitor with IC50 of 1 nM; >200-fold less potent to class I PI3K isoforms, superior in blocking mTORC1/2 and sensitive to pro-invasion genes (vs Rapamycin). Phase 1. |
| 207 | Epothilone A | Microtubule Associated | 80 | Epothilone A is a Taxol-like microtubule-stabilizing agent with EC0.01 of 2 μM. |
| 208 | Docetaxel | Microtubule Associated | 80 | Docetaxel, an analog of taxol, is an inhibitor of depolymerisation of microtubules by binding to stabilized microtubules. |
| 209 | Pacritinib (SB1518) | JAK | 80 | Pacritinib (SB1518) is a potent and selective inhibitor of Janus Kinase 2 (JAK2) and Fms-Like Tyrosine Kinase-3 (FLT3) with IC50s of 23 and 22 nM, respectively. |

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| 210 | Tyrphostin AG 879 | HER2 | 80 | Tyrphostin AG 879 potently inhibits HER2/ErbB2 with IC50 of 1 μM, 100- and 500-fold higher selective to ErbB2 than PDGFR and EGFR. |
| 211 | Mubritinib (TAK 165) | HER2 | 80 | Mubritinib (TAK-165) is a potent inhibitor of HER2/ErbB2 with IC50 of 6 nM; no activity to EGFR, FGFR, PDGFR, JAK1, Src and Blk. |
| 212 | CUDC-101 | HDAC, EGFR, HER2 | 80 | CUDC-101 is a potent multi-targeted inhibitor against HDAC, EGFR and HER2 with IC50 of 4.4 nM, 2.4 nM, and 15.7 nM, and inhibits class I/II HDACs, but not class III, Sir-type HDACs. Phase 1. |
| 213 | M344 | HDAC | 80 | M344 is a potent HDAC inhibitor with IC50 of 100 nM and able to induce cell differentiation. |
| 214 | SKF38393 HCl | Dopamine Receptor | 80 | SKF38393 HCl is a selective dopamine D1/D5 receptor agonist. |
| 215 | Floxuridine | DNA/RNA Synthesis | 80 | Floxuridine is a prodrugs of floxuridine and an oncology agent with an GI50 of 5.1 μM for the inhibition of MDCK/PEPT1. |
| 216 | Fluorouracil (5-Fluoracil, 5-FU) | DNA/RNA Synthesis | 80 | Fluorouracil (5-Fluoracil, 5-FU) is an DNA/RNA synthesis inhibitor, which interrupts nucleotide synthetic by inhibiting thymidylate synthase (TS). |
| 217 | Methotrexate | DHFR | 80 | Methotrexate is an antimetabolite and antifolate drug, which acts by inhibiting the metabolism of folic acid. |
| 218 | JNJ-38877605 | c-Met | 80 | JNJ-38877605 is an ATP-competitive inhibitor of c-Met with IC50 of 4 nM, 600-fold selective for c-Met than 200 other tyrosine and serine-threonine kinases. Phase 1. |
| 219 | AT7519 HCl | CDK | 80 | AT7519 HCl is a multi-CDK inhibitor for CDK1, 2, 4, 6 and 9 with IC50 of 10-210 nM in cell-free assays. It is less potent to CDK3 and little active to CDK7. Phase 2. |
| 220 | Roscovitine (Seliciclib,CYC202) | CDK | 80 | Roscovitine (Seliciclib, CYC202) is a potent and selective CDK inhibitor for Cdc2, CDK2 and CDK5 with IC50 of 0.65 μM, 0.7 μM and 0.16 μM. It shows little effect on CDK4/6. Phase 2. |
| 221 | IC261 | Casein kinase | 80 | IC261 is a novel inhibitor of CK1. The IC50 of IC261 for CK1 was 16 μM and for Cdk5 is 4.5 mM. |
| 222 | AT9283 | Bcr-Abl, JAK, Aurora Kinase | 80 | AT9283 is a potent JAK2/3 inhibitor with IC50 of 1.2 nM/1.1 nM; also potent to Aurora A/B, Abl(T315I). Phase 1/2. |
| 223 | Barasertib (AZD1152-HQPA) | Aurora Kinase | 80 | AZD1152-HQPA (Barasertib) is a highly selective Aurora B inhibitor with IC50 of 0.37 nM, ~100 fold more selective for Aurora B over Aurora A. |
| 224 | Bisoprolol fumarate | Adrenergic Receptor | 80 | Bisoprolol fumarate is a selective type β1 adrenergic receptor blocker. |
| 225 | CGS 21680 HCl | 5-alpha Reductase | 80 | CGS 21680 HCl is an adenosine A2 receptor agonist with IC50 of 22 nM, exhibits 140-fold over A1 receptor. |
| 226 | SB505124 | TGF-beta/Smad | 75 | SB505124 is a selective inhibitor of TGFβR for ALK4, ALK5 with IC50 of 129 nM and 47 nM, respectively, also inhibits |

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| | | | | ALK7, but does not inhibit ALK1, 2, 3, or 6. |
| 227 | Dasatinib Monohydrate | Src | 75 | Dasatinib Monohydrate is a novel, potent and multi-targeted inhibitor that targets Abl, Src and c-Kit, with IC50 of <1 nM, 0.8 nM and 79 nM, respectively. |
| 228 | SRT1720 | Sirtuin | 75 | SRT1720 is a selective SIRT1 activator with EC50 of 0.16 μM, but is >230-fold less potent for SIRT2 and SIRT3. |
| 229 | RAF265 (CHIR-265) | Raf, VEGFR | 75 | RAF265 (CHIR-265) is a potent selective inhibitor of C-Raf/B-Raf/B-Raf V600E with IC50 of 3-60 nM, and exhibits potent inhibition on VEGFR2 phosphorylation with EC50 of 30 nM. Phase 2. |
| 230 | Imidapril HCl | RAAS | 75 | Imidapril HCl is a angiotensin-converting enzyme (ACE) inhibitor with IC50 of 2.6 nM, used for the treatment of hypertension. |
| 231 | BKM120 (NVP-BKM120, Buparlisib) | PI3K | 75 | BKM120 is a selective PI3K inhibitor of p110α/β/δ/γ with IC50 of 52 nM/166 nM/116 nM/262 nM, respectively. Reduced potency against VPS34, mTOR, DNAPK, with little activity to PI4Kβ. Phase 1/2. |
| 232 | CP-673451 | PDGFR | 75 | CP 673451 is a selective inhibitor of PDGFRα/β with IC50 of 10 nM/1 nM, exhibits >450-fold selectivity over other angiogenic receptors, has antiangiogenic and antitumor activity. |
| 233 | S-(+)-Rolipram | PDE | 75 | S-(+)-Rolipram inhibits human monocyte cyclic AMP-specific PDE4 with IC50 of 0.75 μM, has anti-inflammatory and anti-depressant activity in the central nervous system, less potent than its R enantiomer. |
| 234 | Dextrose | Others | 75 | Dextrose, a simple sugar (monosaccharide), is an important carbohydrate in biology. |
| 235 | Mefloquine HCl | Others | 75 | Mefloquine HCl is a blood schizonticide by inhibiting hemozoin formation, used as an antimalarial drug. |
| 236 | PTC-209 HBr | Others | 75 | PTC-209 HBr is the hydrobromide salt of PTC-209, which is a potent and selective BMI-1 inhibitor with IC50 of 0.5 μM, and results in irreversible reduction of cancer-initiating cells (CICs). |
| 237 | Ascomycin (FK520) | Others | 75 | Ascomycin (FK520), an FK-506 analog, is a neutral macrolide immunosuppressant, which prevents rejection after an organ transplant. Phase 3. |
| 238 | Bexarotene | Others | 75 | Bexarotene is a retinoid specifically selective for retinoid X receptors, used as an oral antineoplastic agent in the treatment of cutaneous T-cell lymphoma. |
| 239 | Dronedarone HCl | Others | 75 | Dronedarone HCl is a therapy for the treatment of patients with paroxysmal and persistent atrial fibrillation or atrial flutter. |
| 240 | Sulconazole Nitrate | Others | 75 | Sulconazole Nitrate is an imidazole derivative with broad-spectrum antifungal activity. |
| 241 | Arbidol HCl | Others | 75 | Arbidol is an antiviral treatment for influenza infection. |
| 242 | Ciclesonide | others | 75 | Ciclesonide is a glucocorticoid used to treat obstructive airway |

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| | | | | diseases. |
| 243 | PA-824 | Others | 75 | PA-824 is an anti-tuberculosis drug for tuberculosis with MIC less than 2.8 μM. |
| 244 | Naltrexone HCl | Opioid Receptor | 75 | Naltrexone is an opioid receptor antagonist with IC50 of 8 nM used primarily in the management of alcohol dependence and opioid dependence. |
| 245 | PF-04691502 | mTOR, PI3K, Akt | 75 | PF-04691502 is an ATP-competitive PI3K(α/β/δ/γ)/mTOR dual inhibitor with Ki of 1.8 nM/2.1 nM/1.6 nM/1.9 nM and 16 nM, little activity against either Vps34, AKT, PDK1, p70S6K, MEK, ERK, p38, or JNK. Phase 2. |
| 246 | Paclitaxel | Microtubule Associated | 75 | Paclitaxel is a microtubule polymer stabilizer with IC50 of 0.1 pM in human endothelial cells. |
| 247 | PF-06447475 | LRRK2 | 75 | PF-06447475 is a potent, selective, and brain penetrant LRRK2 kinase inhibitor with IC50 of 3 nM. |
| 248 | WS3 | IκB/IKK | 75 | WS3 is a β cell proliferation inducer via modulation of Erb3 binding protein-1 (EBP1) and the IκB kinase pathway. |
| 249 | KW-2478 | HSP | 75 | KW-2478 is a nonansamycin HSP90 inhibitor with IC50 of 3.8 nM. Phase 1/2 |
| 250 | Lovastatin | HMG-CoA Reductase | 75 | Lovastatin is an inhibitor of HMG-CoA reductase with IC50 of 3.4 nM, used for lowering cholesterol (hypolipidemic agent). |
| 251 | Pracinostat (SB939) | HDAC | 75 | SB939 is a potent pan-HDAC inhibitor with IC50 of 40-140 nM with exception for HDAC6. It has no activity against the class III isoenzyme SIRT I. Phase 2. |
| 252 | LAQ824 (Dacinostat) | HDAC | 75 | LAQ824 (Dacinostat) is a novel HDAC inhibitor with IC50 of 32 nM and is known to activate the p21 promoter. |
| 253 | TWS119 | GSK-3 | 75 | TWS119 is a GSK-3β inhibitor with IC50 of 30 nM; capable of inducing neuronal differentiation and may be useful to stem cell biology. |
| 254 | Lapatinib | EGFR, HER2 | 75 | Lapatinib, used in the form of Lapatinib Ditosylate, is a potent EGFR and ErbB2 inhibitor with IC50 of 10.8 and 9.2 nM, respectively. |
| 255 | FT-207 (NSC 148958) | DNA/RNA Synthesis | 75 | FT-207 (NSC 148958) is a substance being used in the treatment of some types of cancer. |
| 256 | Ifosfamide | DNA/RNA Synthesis | 75 | Ifosfamide is a nitrogen mustard alkylating agent used in the treatment of cancer. |
| 257 | Gossypol | Dehydrogenase | 75 | Gossypol is a polyphenolic aldehyde that permeates cells and acts as an inhibitor for several dehydrogenase enzymes. |
| 258 | Tivantinib (ARQ 197) | c-Met | 75 | Tivantinib (ARQ 197) is the first non-ATP-competitive c-Met inhibitor with K<sub>i</sub> of 0.355 μM in a cell-free assay, little activity to Ron, and no inhibition to EGFR, InsR, PDGFRα or FGFR1/4. Phase 3. |
| 259 | SU9516 | CDK | 75 | SU 9516 is a 3-substituted indolinone CDK inhibitor |

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| | | | | with IC50 of 22 nM, 40 nM, and 200 nM for CDK2, CDK1, and CDK4, respectively. |
| 260 | Flubendazole | Autophagy | 75 | Flubendazole is an autophagy inducer by targeting Atg4B, used to treat internal parasite and worm infection. |
| 261 | Danusertib (PHA-739358) | Aurora Kinase, FGFR, Bcr-Abl, c-RET, Src | 75 | Danusertib (PHA-739358) is an Aurora kinase inhibitor for Aurora A/B/C with IC50 of 13 nM/79 nM/61 nM, modestly potent to Abl, TrkA, c-RET and FGFR1, and less potent to Lck, VEGFR2/3, c-Kit, CDK2, etc. Phase 2. |
| 262 | PF-3716556 | ATPase,Proton Pump | 75 | PF 3716556 is a potent and selective P-CAB (potassium-competitive acid blocker), with pIC50 of 6.026 and 7.095 for the inhibition of porcine H+,K+-ATPase activity in ion-leaky and ion-tight assay, respectively, inhibits gastric acid secretion, displays no activity at Na+,K+-ATPase, used for the treatment of gastroesophageal reflux disease. |
| 263 | Spironolactone | Androgen Receptor | 75 | Spironolactone is a potent antagonist of the androgen receptor with IC50 of 77 nM. |
| 264 | A-674563 | Akt, CDK, PKA | 75 | A-674563 is an Akt1 inhibitor with Ki of 11 nM, modest potent to PKA and >30-fold selective for Akt1 over PKC. |
| 265 | LY3023414 | Akt | 75 | LY3023414 is an oral ATP competitive inhibitor of the class I PI3K isoforms, mTOR and DNA-PK. |
| 266 | Naftopidil | Adrenergic Receptor | 75 | Naftopidil (Flivas) is a selective α1-adrenergic receptor antagonist or alpha blocker with a Ki of 58.3 nM. |
| 267 | Cisatracurium Besylate | Adrenergic Receptor | 75 | Cisatracurium Besylate is a nondepolarizing neuromuscular blocking agent, antagonizing the action of acetylcholine by inhibiting neuromuscular transmission. |
| 268 | Bortezomib (PS-341) | 20S proteasome | 75 | Bortezomib (PS-341) is a potent 20S proteasome inhibitor with Ki of 0.6 favorable selectivity towards tumor cells over normal cells. |
| 269 | Gemcitabine HCl | DNA/RNA Synthesis | 75 | Mizoribine is an imidazole nucleoside, selectively inhibits inosine monophosphate synthetase and guanosine monophosphate synthetase. |
| 270 | SN-38 | Topoisomerase | 70 | SN-38 is an active metabolite of CPT-11, inhibits DNA topoisomerase I, DNA synthesis and causes frequent DNA single-strand breaks. |
| 271 | Tie2 kinase inhibitor | Tie-2 | 70 | Tie2 kinase inhibitor is an optimized compound of SB-203580, selective to Tie2 with IC50 of 0.25 μM, 200-fold more potent than p38. |
| 272 | Daunorubicin HCl | Telomerase | 70 | Daunorubicin HCl inhibits both DNA and RNA synthesis and inhibits DNA synthesis with Ki of 0.02 μM. |
| 273 | LDE225 (NVP-LDE225 ,Erismodegib) | Smoothened | 70 | LDE225 (NVP-LDE225) is a Smoothened (Smo) antagonist, inhibiting Hedgehog (Hh) signaling with IC50 of 1.3 nM (mouse) and 2.5 nM (human), respectively. Phase 3. |
| 274 | RKI-1447 | ROCK | 70 | RKI-1447 is a potent inhibitor of ROCK1 and ROCK2, with IC50 of 14.5 nM and 6.2 nM, respectively, has anti-invasive |

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| | | | | and antitumor activities. |
| 275 | Temocapril HCl | RAAS | 70 | Temocapril HCl is the hydrochloride of Temocapril, which is a long-acting angiotensin-converting enzyme (ACE) inhibitor, used for the treatment of hypertension. |
| 276 | PF-4989216 | PI3K | 70 | PF-4989216 is a potent and selective PI3K inhibitor with IC50 of 2 nM, 142 nM, 65 nM, 1 nM, and 110 nM for p110α, p110β, p110γ, p110δ, and VPS34, respectively. |
| 277 | Crenolanib (CP-868596) | PDGFR | 70 | Crenolanib (CP-868596) is a potent and selective inhibitor of PDGFRα/β with Kd of 2.1 nM/3.2 nM, also potently inhibits FLT3, sensitive to D842V mutation not V561D mutation, >100-fold more selective for PDGFR than c-Kit, VEGFR-2, TIE-2, FGFR-2, EGFR, erbB2, and Src. |
| 278 | Cilostazol | PDE | 70 | Cilostazol is a potent cyclic nucleotide phosphodiesterase type 3 (PDE3) inhibitor with IC50 of 0.2 μM and inhibitor of adenosine uptake. |
| 279 | AG-14361 | PARP | 70 | AG14361 is a potent inhibitor of PARP1 with Ki of <5 nM. It is at least 1000-fold more potent than the benzamides. |
| 280 | RITA (NSC 652287) | p53 | 70 | RITA (NSC 652287) induces both DNA-protein and DNA-DNA cross-links with no detectable DNA single-strand breaks, and also inhibits MDM2-p53 interaction by targeting p53. |
| 281 | Atropine sulfate monohydrate | Others | 70 | Atropine sulfate monohydrate is a competitive muscarinic acetylcholine receptor antagonist with an IC50 of 2.5 nM. |
| 282 | Artemisinin | Others | 70 | Artemisinin is a drug used to treat multi-drug resistant strains of falciparum malaria. |
| 283 | Conivaptan HCl | Others | 70 | Conivaptan is a non-peptide inhibitor of antidiuretic hormone (vasopressin receptor antagonist). |
| 284 | Fenbendazole | Others | 70 | Fenbendazole is a broad spectrum benzimidazole anthelmintic used against gastrointestinal parasites with an IC50 of about 0.01 μg/mL. |
| 285 | Tanshinone IIA | Others | 70 | Tanshinone IIA(Tanshinone B) is the most abundant diterpene quinone in Danshen, Salviae miltiorrhizae Radix, a widely prescribed traditional herbal medicine that is used to treat cardiovascular and inflammatory diseases. |
| 286 | Nitazoxanide | Others | 70 | Nitazoxanide is a synthetic nitrothiazolyl-salicylamide derivative and an antiprotozoal agent. (IC50 for canine influenza virus ranges from 0.17 to 0.21 μM) |
| 287 | Bendamustine HCl | Others | 70 | Bendamustine HCL is a DNA-damaging agent with IC50 of 50 μM. |
| 288 | LY2608204 | Others | 70 | LY2608204 activates glucokinase (GK) with EC50 of 42 nM. Phase 2. |
| 289 | WYE-125132 (WYE-132) | mTOR | 70 | WYE-125132 is a highly potent, ATP-competitive mTOR inhibitor with IC50 of 0.19 nM; highly selective for mTOR versus PI3Ks or PI3K-related kinases hSMG1 and ATR. |

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| 290 | Batimastat (BB-94) | MMP | 70 | Batimastat (BB-94) is a potent, broad spectrum matrix metalloprotease (MMP) inhibitor for MMP-1, MMP-2, MMP-9, MMP-7 and MMP-3 with IC50 of 3 nM, 4 nM, 4 nM, 6 nM and 20 nM, respectively. |
| 291 | NSC 405020 | MMP | 70 | NSC 405020 is a noncatalytic inhibitor of MT1-MMP, directly interacts with PEX domain of MT1-MMP, affects PEX homodimerization but not catalytic activity of MT1-MMP. |
| 292 | PD98059 | MEK | 70 | PD98059 is a non-ATP competitive MEK inhibitor with IC50 of 2 μM, specifically inhibits MEK-1-mediated activation of MAPK; does not directly inhibit ERK1 or ERK2. |
| 293 | MEK162 (ARRY-162, ARRY-438162) | MEK | 70 | ARRY-438162 is a potent inhibitor of MEK1/2 with IC50 of 12 nM. |
| 294 | Rasagiline Mesylate | MAO | 70 | Rasagiline Mesylate is a new MAO-B inhibitor for the treatment of idiopathic Parkinson's disease. |
| 295 | CH5138303 | HSP (e.g. HSP90) | 70 | CH5138303 is an orally available Hsp90 inhibitor with Kd of 0.48 nM. |
| 296 | PF-04929113 (SNX-5422) | HSP | 70 | PF-04929113 (SNX-5422) is a potent and selective HSP90 inhibitor with Kd of 41 nM and induces Her-2 degradation with IC50 of 37 nM. Phase 1/2. |
| 297 | 2-Methoxyestradiol (2-MeOE2) | HIF | 70 | 2-Methoxyestradiol depolymerizes microtubules and blocks HIF-1α nuclear accumulation and HIF-transcriptional activity. Phase 2. |
| 298 | GW9508 | GPR | 70 | GW9508 is a potent and selective agonist for FFA1 (GPR40) with pEC50 of 7.32, 100-fold selective against GPR120, stimulates insulin secretion in a glucose-sensitive manner. |
| 299 | Dacarbazine | DNA/RNA Synthesis | 70 | Dacarbazine is an antineoplastic chemotherapy drug used in the treatment of various cancers. |
| 300 | Aloxistatin | Cysteine Protease | 70 | Aloxistatin is an irreversible and membrane-permeable cysteine protease inhibitor. |
| 301 | ON123300 | CDK | 70 | ON123300 is a potent and multi-targeted kinase inhibitor with IC50 of 3.9 nM, 5 nM, 26 nM, 26 nM, 9.2 nM and 11nM for CDK4, Ark5, PDGFRβ, FGFR1, RET, and Fyn, respectively. |
| 302 | Odanacatib (MK-0822) | Cathepsin K | 70 | Odanacatib (MK 0822) is a potent, selective, and neutral inhibitor of cathepsin K (human/rabbit) with IC50 of 0.2 nM/1 nM, and demonstrated high selectivity versus off-target cathepsin B, L, S. Phase 3. |
| 303 | Azelnidipine | Calcium Channel | 70 | Azelnidipine is a dihydropyridine calcium channel blocker. |
| 304 | TAK-901 | Aurora Kinase | 70 | TAK-901 is a novel inhibitor of Aurora A/B with IC50 of 21 nM/15 nM. It is not a potent inhibitor of cellular JAK2, c-Src or Abl. Phase 1. |

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| 305 | Formestane | Aromatase | 70 | Formestane(Lentaron(R)) is a second generation selective aromatase inhibitor with an IC50 of 80 nM. |
| 306 | Silodosin | Adrenergic Recepto | 70 | Silodosin(Rapaflo) is an α1-adrenoceptor antagonist with high uroselectivity. |

**Table S2.** Preliminary screening bioactive compounds that facilitate ZIKV infection in SNB-19 cells

| No. | Name | Target | Fold change | Brief introduction |
|---|---|---|---|---|
| 1 | URMC-099 | MLK3 | 2.9 | URMC-099 is an orally bioavailable, brain penetrant mixed lineage kinase (MLK) inhibitor with IC50 of 19 nM, 42 nM, 14 nM, and 150 nM, for MLK1, MLK2, MLK3, and DLK, respectively, and also inhibits LRRK2 activity with IC50 of 11 nM. |
| 2 | BV-6 | PLK | 2.8 | BV-6 is a SMAC mimetic, dual cIAP and XIAP inhibitor. |
| 3 | LDK378 | IAP | 2.8 | LDK378 is potent inhibitor against ALK with IC50 of 0.2 nM, shows 40- and 35-fold selectivity against IGF-1R and InsR, respectively. Phase 2. |
| 4 | BI2536 | ALK | 2.8 | BI2536 is a potent Plk1 inhibitor with IC50 of 0.83 nM. It shows 4- and 11-fold greater selectivity against Plk2 and Plk3. Phase 2. |
| 5 | BMS-833923 | Hedgehog/Smoothened | 2.3 | BMS-833923 is an orally bioavailable Smoothened antagonist. Phase 2. |
| 6 | GSK503 | Histone Methyltransferase | 2.3 | GSK503 is a potent and specific EZH2 methyltransferase inhibitor. |
| 7 | LDN-214117 | TGF-beta/Smad | 2.1 | LDN-214117 is a potent and selective BMP type I receptor kinase ALK2 inhibitor with IC50 of 24 nM. |
| 8 | DDR1-IN-1 | DDR(receptor tyrosine kinase) | 2.1 | DDR1-IN-1 is a potent and selective discoidin domain receptor 1 (DDR1) receptor tyrosine kinase inhibitor with IC50 of 105 nM, about 3-fold selectivity over DDR2. |
| 9 | KC7F2 | HIF | 2.0 | KC7F2 is a selective HIF-1α transcription inhibitor with IC50 of 20 μM in a cell-based assay. |
| 10 | Ruxolitinib (INCB018424) | JAK | 2.0 | INCB018424 is the first potent, selective, JAK1/2 inhibitor to enter the clinic with IC50 of 3.3 nM/2.8 nM, >130-fold selectivity for JAK1/2 versus JAK3. Phase 3. |
| 11 | Radotinib | Bcr-Abl | 2.0 | Radotinib is a selective BCR-ABL1 tyrosine kinase inhibitor with IC50 of 34 nM, used to treat Chronic Myeloid Leukemia. |
| 12 | EUK 134 | Beta Amyloid | 2.0 | EUK 134, a synthetic superoxide dismutase (SOD)/catalase mimetic, exhibits potent antioxidant activities, and inhibits the formation of β-amyloid and related amyloid fibril. |
| 13 | WZ4003 | AMPK | 1.9 | WZ4003 is a highly specific NUAK kinase inhibitor with IC50 of 20 nM and 100 nM for NUAK1 and NUAK2, respectively, without significant inhibition on 139 other kinases. |
| 14 | LY2119620 | AChR | 1.9 | LY2119620 is a specific, and allosteric agonist of human M2 and M4 muscarinic acetylcholine receptors. |
| 15 | Belinostat (PXD101) | HDAC | 1.9 | Belinostat (PXD101) is a novel HDAC inhibitor with IC50 of 27 nM, with activity demonstrated in cisplatin-resistant tumors. Phase 1/2. |

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| 16 | Fatostatin | Estrogen/progestogen Receptor | 1.9 | 17-Hydroxyprogesterone (17-OHP) is an endogenous progestogen as well as chemical intermediate in the biosynthesis of other steroid hormones, including the corticosteroids and the androgens and the estrogens. |
| 17 | PD 151746 | Cysteine Protease | 1.9 | PD 151746 is a selective, cell-permeable calpain inhibitor with Ki of 0.26 μM for μ-Calpain, about 20-fold selectivity over m-calpain. |
| 18 | MS436 | Epigenetic Reader Domain | 1.9 | MS436 is a selective BET bromodomain inhibitor with K<sub>i</sub> of <0.085 μM and 0.34 μM for BRD4 (1) and BRD4 (2), respectively. |
| 19 | Palbociclib (PD0332991) Isethionate | CDK | 1.9 | Palbociclib (PD0332991) Isethionate is a highly selective inhibitor of CDK4/6 with IC50 of 11 nM/16 nM in cell-free assays. It shows no activity against CDK1/2/5, EGFR, FGFR, PDGFR, InsR, etc. Phase 3. |
| 20 | Deltarasin | PDE | 1.9 | Deltarasin is a small molecular inhibitor of KRAS-PDEδ interaction with Kd of 38 nM for binding to purified PDEδ. |
| 21 | Olmutinib (HM61713, BI 1482694) | EGFR | 1.9 | Olmutinib is a novel third-generation epidermal growth factor receptor (EGFR) mutation-specific tyrosine kinase inhibitor (TKI). Also a potent inhibitor of Bruton's tyrosine kinase. |
| 22 | NQDI-1 | Gamma-secretase | 1.9 | MK-0752 is a moderately potent γ-secretase inhibitor, which reduces Aβ40 production with IC50 of 5 nM. Phase 1/2. |
| 23 | Entrectinib (RXDX-101) | Trk receptor | 1.8 | Entrectinib (RXDX-101) is an orally bioavailable pan-TrkA/B/C, ROS1 and ALK inhibitor with IC50 ranging between 0.1 and 1.7 nM. Phase 2. |
| 24 | Erlotinib | EGFR | 1.8 | Erlotinib is an EGFR inhibitor with IC50 of 2 nM, >1000-fold more sensitive for EGFR than human c-Src or v-Abl. |
| 25 | LTX-315 | Others | 1.8 | LTX-315 is the oncolytic peptide that kills cancer cells through Bax/Bak-regulated mitochondrial membrane permeabilization. |
| 26 | (+)-JQ1 | BET | 1.8 | (+)-JQ1 is a BET bromodomain inhibitor, with IC50 of 77 nM/33 nM for BRD4(1/2), binding to all bromodomains of the BET family, but not to bromodomains outside the BET family. |
| 27 | 4-Hydroxytamoxifen | Estrogen/progestogen Receptor | 1.7 | 4-Hydroxytamoxifen is the active metabolite of tamoxifen and a selective estrogen receptor (ER) modulator that is widely used in the therapeutic and chemopreventive treatment of breast cancer. |
| 28 | Ponesimod | S1P Receptor | 1.7 | Ponesimod(ACT-128800) is an orally active, selective sphingosine-1-phosphate receptor 1 (S1P1) immunomodulator with EC50 of 5.7 nM. |
| 29 | Elesclomol (STA-4783) | HSP | 1.7 | Elesclomol (STA-4783) is a novel potent oxidative stress inducer that elicits pro-apoptosis events among tumor cells. |
| 30 | Pimavanserin | 5-HT Receptor | 1.7 | Pimavanserin is a potent and selective serotonin 5-HT2A inverse agonist with pIC50 of 8.73, used to treat psychosis |

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| | | | | associated with Parkinson’s disease. |
| 31 | Ozanimod (RPC1063) | S1P Receptor | 1.7 | Ozanimod (RPC1063) is a selective oral S1P Receptor 1 modulator. Phase 3. |
| 32 | ZSTK474 | PI3K | 1.7 | ZSTK474 inhibits class I PI3Kisoforms with IC50 of 37 nM, mostly PI3Kδ. |
| 33 | Citric acid trilithium salt tetrahydrate | others | 1.6 | Citric acid trilithium salt tetrahydrate is a pharmaceutical and construction material. It is commonly used in HPLC gradient elution for quantification of amino acids. |
| 34 | Dovitinib (TKI258) Lactate | FLT3 | 1.6 | Dovitinib (TKI258) Lactate is the Lactate of Dovitinib, which is a multitargeted RTK inhibitor, mostly for class III (FLT3/c-Kit) with IC50 of 1 nM/2 nM, also potent to class IV (FGFR1/3) and class V (VEGFR1-4) RTKs with IC50 of 8-13 nM, less potent to InsR, EGFR, c-Met, EphA2, Tie2, IGFR1 and HER2. Phase 4. |
| 35 | NSC59984 | p53 | 1.6 | NSC59984 is a p53 pathway activator via induction of mutant p53 protein degradation and p73 activation. |
| 36 | SL-327 | MEK | 1.6 | SL327 is a selective inhibitor for MEK1/2 with IC50 of 0.18 μM/ 0.22 μM, no activity towards Erk1, MKK3, MKK4, c-JUN, PKC, PKA, or CamKII;capable of transport through the blood-brain barrier. |
| 37 | SB216763 | GSK-3 | 1.6 | SB216763 is a potent and selective GSK-3 inhibitor with IC50 of 34.3 nM for GSK-3α and equally effective at inhibiting human GSK-3β. |
| 38 | Dasatinib | Src, Bcr-Abl, c-Kit | 1.6 | Dasatinib is a novel, potent and multi-targeted inhibitor that targets Abl, Src and c-Kit, with IC50 of ＜1 nM, 0.8 nM and 79 nM, respectively. |
| 39 | SB203580 | p38 MAPK | 1.6 | SB203580 is a p38 MAPK inhibitor with IC50 of 0.3-0.5 μM, 10-fold less sensitive to SAPK3(106T) and SAPK4(106T) and blocks PKB phosphorylation with IC50 of 3-5 μM. |
| 40 | Quizartinib (AC220) | Flt | 1.6 | Quizartinib (AC220) is a second-generation FLT3 inhibitor for Flt3(ITD/WT) with IC50 of 1.1 nM/4.2 nM, 10-fold more selective for Flt3 than KIT, PDGFRα, PDGFRβ, RET, and CSF-1R. Phase 1/2. |
| 41 | Filgotinib (GLPG0634) | JAK | 1.5 | Filgotinib (GLPG0634) is a selective JAK1 inhibitor with IC50 of 10 nM, 28 nM, 810 nM, and 116 nM for JAK1, JAK2, JAK3, and TYK2, respectively. Phase 2. |
| 42 | Cobimetinib (GDC-0973, RG7420) | MEK | 1.5 | Cobimetinib (GDC-0973, RG7420) is a potent and highly selective MEK1 inhibitor with IC50 of 4.2 nM. Phase 3. |
| 43 | Tranexamic Acid | Others | 1.5 | Tranexamic Acid is an antifibrinolytic for blocking lysine-binding sites of plasmin and elastase-derived plasminogen fragments with IC50 of 5 mM. |
| 44 | WZB117 | Others | 1.5 | WZB117 is an inhibitor of Glucose Transporter 1 (GLUT1). It |

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| | | | | inhibited cell proliferation in lung cancer A549 cells and breast cancer MCF7 cells with an IC50 of approximately 10 μM. |
| 45 | Iniparib (BSI-201) | PARP | 1.5 | BSI-201 (Iniparib, SAR240550) is a PARP1 inhibitor with demonstrated effectiveness in triple-negative breast cancer (TNBC). Phase 3. |
| 46 | Lomitapide | others | 1.5 | Lomitapide is a potent microsomal triglyceride transfer protein (MTP) inhibitor, used in the treatment of familial hypercholesterolemia. |
| 47 | Toremifene Citrate | Others | 1.5 | Toremifene Citrate is an oral selective estrogen receptor modulator (SERM) which helps oppose the actions of estrogen in the body. |
| 48 | BS-181 HCl | CDK | 1.5 | BS-181 is a highly selective CDK7 inhibitor with IC50 of 21 nM. It is more than 40-fold selective for CDK7 than CDK1, 2, 4, 5, 6, or 9. |
| 49 | L-Ornithine | others | 1.5 | L-ornithine has an antifatigue effect in increasing the efficiency of energy consumption and promoting the excretion of ammonia. It is one of the key reactants in the urea cycle. |