

## Supplementary Material

### **Selected histone deacetylase inhibitors reverse the Frataxin transcriptional defect in a novel Friedreich's ataxia induced pluripotent stem cell-derived neuronal reporter system**

**Anna M. Schreiber<sup>1</sup>, Yanjie Li<sup>1</sup>, Yi-Hsien Chen<sup>2</sup>, Jill S. Napierala<sup>1</sup>, Marek Napierala\*<sup>1</sup>**

<sup>1</sup>Department of Biochemistry and Molecular Genetics, Stem Cell Institute, University of Alabama at Birmingham, Birmingham, AL, USA

<sup>2</sup>Genome Engineering and iPSC Center, Washington University, St Louis, MO, USA

Supplementary Figure 1	page 2
Supplementary Figure 2	page 6
Supplementary Figure 3	page 7
Supplementary Table 1	page 8
Supplementary Table 2	page 9

**Supplementary Figure 1: DNA sequence of a fragment of the *FXN* gene.** A fragment of *FXN* is shown along with the *NLuc* gene and the five amino acids linker between the coding sequences. Exact locations of the gRNA and all primers used in PCR amplifications to validate correct *NLuc* integration are shown. An overview of the strategy is presented in Figure 1.



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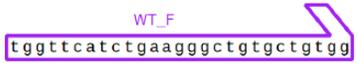
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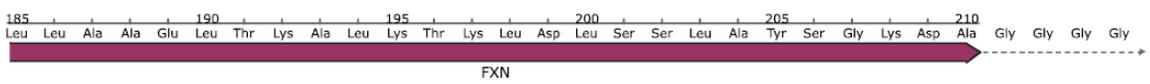
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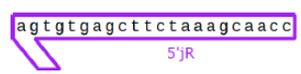
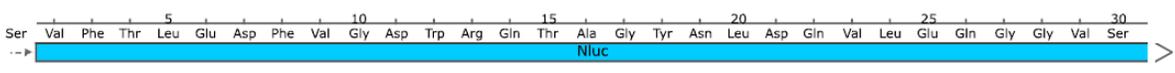
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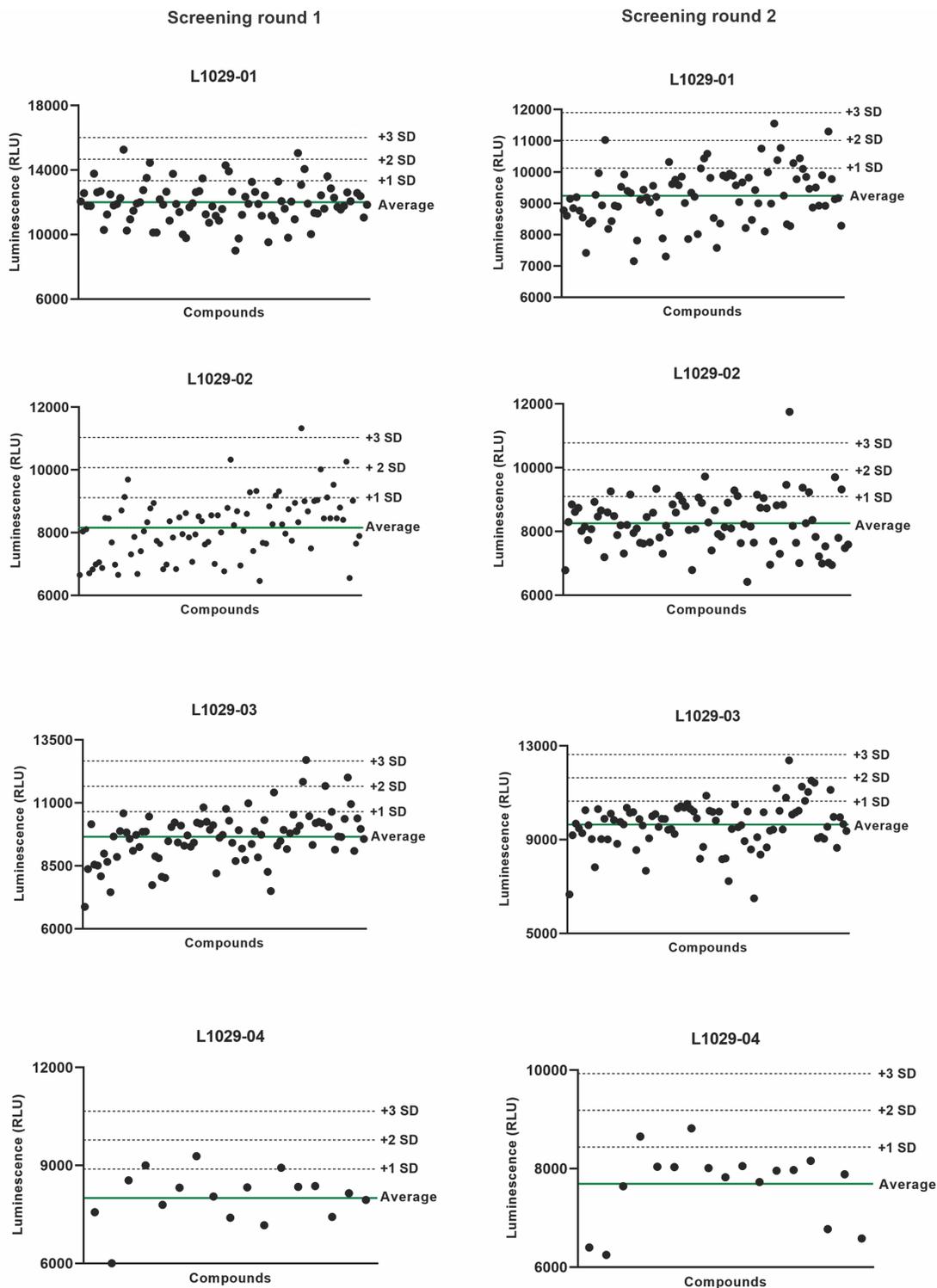
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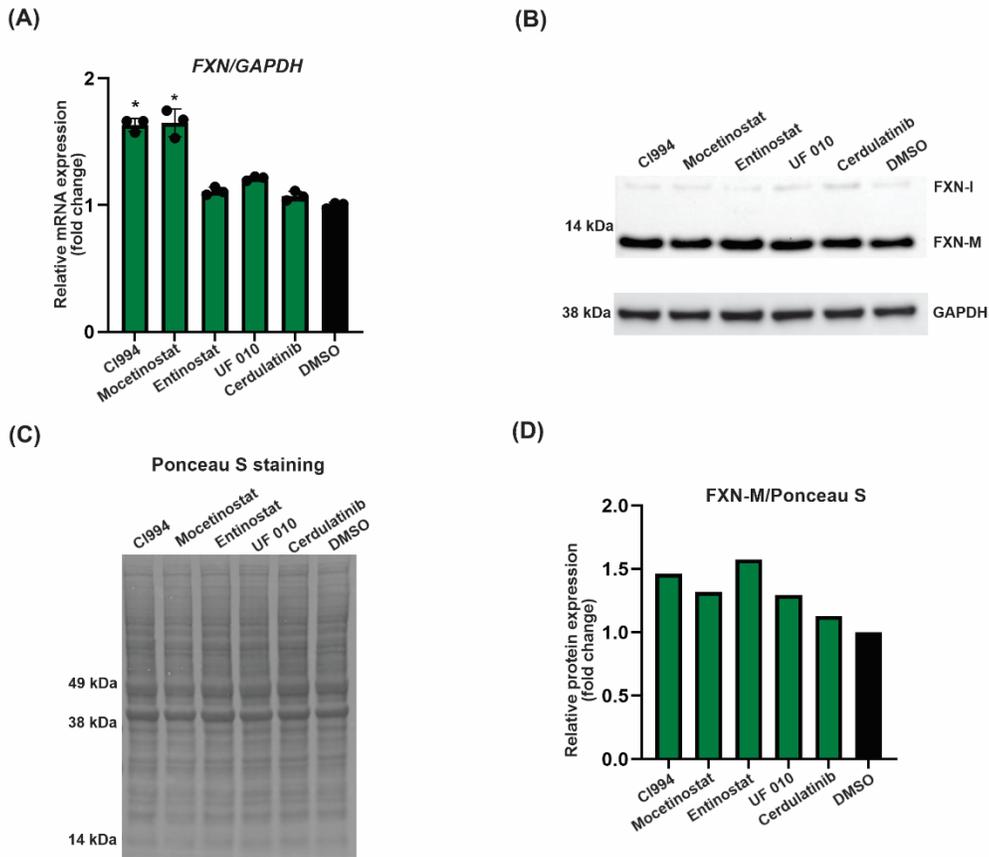
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**Supplementary Figure 2: Screening of an epigenetic compound library to identify novel inducers of *FXN* expression.** Complete datasets from two rounds of screening, four 96-well plates each, are presented. All compounds of the APEX BIO DiscoveryProbe™ Epigenetics Compound Library were tested at 10  $\mu$ M concentration for 24 h. Luminescence signal was plotted independently per each plate. Green line corresponds to plate average signal; dashed lines indicate average signal plus 1, 2 and 3 standard deviations of the mean.



**Supplementary Figure 3: Effect of selected compounds on *FXN* expression in control NPCs.**

(A) Results of qRT-PCR analysis of *FXN* mRNA expression upon 48 h treatment with 10  $\mu$ M CI994, Mocetinostat, Entinostat, UF 010 and Cerdulatinib. Results represent mean  $\pm$  SD from three technical repeats; \* indicates  $p < 0.05$  (one-way ANOVA). DMSO treatment served as a control. (B) *FXN* protein expression determined by western blot after treatment with indicated compounds for 48 h at 10  $\mu$ M. Signals corresponding to mature *FXN* (*FXN*-M) and intermediate *FXN* (*FXN*-I) are indicated. GAPDH and Ponceau S (C) staining served as loading controls. (D) Quantification of *FXN*-M levels shown in panel B relative to Ponceau S staining.



**Supplementary Table 1: Characteristics of induced pluripotent stem cell lines used in the study.**

<b>Type:</b>	<b>Age of disease onset:</b>	<b>Sex:</b>	<b>GAA repeats:</b>
FRDA 4676	10	M	867/867
FRDA 86	18	F	450/450
FRDA 4259	15	M	550/830
Control 7522	-	F	-

**Supplementary Table 2: Complete list of compounds included in APExBIO DiscoveryProbe™ Epigenetics Compound Library.** For each compound the CAS number, molecular weight, formula, targeted pathway and molecular target are presented.

Item Name	QAS Number	M.w.	Formula	Pathway	Target	Information
Daptomycin	103060-933	1620.67	C72H101N17O26	Cancer Biology	DNA Synthesis	Calcium-dependent antibiotic
Gemcitabine HCl	121111-039	299.66	C8H11F2N3O4.HCl	Cancer Biology	DNA Synthesis	Inhibits DNA synthesis, deoxycytidine analog
XAV-939	294028-993	312.31	C14H11F2N2O6	Cancer Biology	PARP	Tarlatamycin 1/2 inhibitor
Declatone (NIG127716, SAZA-CdR)	2353-314	228.08	C8H11N3O6	Cancer Biology	DNA Methyltransferase	Decoytine analog and cellular differentiation inducer
5-Azacytidine	320-97-2	244.2	C8H12N4O5	Cancer Biology	DNA Methyltransferase	DNA methyltransferase inhibitor
BIX 01294	935693-622	490.65	C28H38N6O2	Cancer Biology	Histone Methyltransferase	G9a and GLP inhibitor
Bromodomain inhibitor, (+)-J1	1268524-704	456.99	C23H25ClN4O2S	Cancer Biology	Bromodomain	BET bromodomain inhibitor
Lonegualar	152441-090	326.17	C10H8N8H5O6	Cancer Biology	DNA Methyltransferase	326.17
RO 105	482028-360	334.33	C18H14N2O4	Cancer Biology	DNA Methyltransferase	DNA methyltransferase inhibitor
UNC0638	1265580-76-7	509.72	C30H47N5O2	Cancer Biology	Histone Methyltransferase	G9a/GLP HMTase inhibitor, potent and selective
Zebularine	3690-104	228.2	C8H12N2O5	Cancer Biology	DNA Methyltransferase	DNA methylation inhibitor
Carbotolant	41575-94-4	371.25	C6H12N2O4P	Cancer Biology	DNA Synthesis	Antitumor agent that forms platinum-DNA adducts.
Elicig, 304	476-664	302.19	C14H8O8	Cancer Biology	Typosomerase	Casein kinase 2 (CK2) inhibitor
(+)-Ergoloidecthin palmitate (EEOG)	989-61-6	458.37	C22H18O11	Cancer Biology	PKC	Antioxidant, antiangiogenic and antitumor agent
ABT-888 (Velpar)	912444-009	244.3	C18H18N4O	Cancer Biology	PARP	Potent PARP inhibitor
Ruxolitinib (INC018424)	941678-93-6	306.37	C17H18N6	Cancer Biology	JAK	JAK inhibitor
AD11152	722543-319	587.54	C35H31F17N10O6P	Cancer Biology	Aurora Kinase	Aurora B kinase inhibitor, highly potent and selective
Baricitinib methyl	218620-274	505.69	C32H43N5O4	Cancer Biology	JAK	ROK inhibitor, potent anti-inflammatory modulator
Curcumin	458-37-7	368.38	C21H20O6	Cancer Biology	KEAP1-Nrf2	Tyrosinase inhibitor
CX-6258	1202916-90-2	461.54	C26H24ClN3O3	Cancer Biology	Pim	Pan-Pim kinases inhibitor
Daminozide	1596-94-6	160.17	C6H12N2O3	Cancer Biology	HDAC	KDM2A inhibitor
OSK126	1346514-97-9	526.67	C13H18N6O2	Cancer Biology	EZH2	EZH2 inhibitor
OSK343	1346704-33-3	541.69	C13H18N7O2	Cancer Biology	EZH2	EZH2 inhibitor, potent, selective and cell permeable
JANEX-1	202475-60-3	297.31	C16H15N3O3	Cancer Biology	JAK	JAK3 inhibitor
M-2	1271738-62-6	375.55	C18H25N5S2	Cancer Biology	Menin-MLL	Menin-MLL inhibitor
MK-827	1038915-60-4	320.39	C18H23N4O	Cancer Biology	PARP	PARP-1/2 inhibitor, potent and selective
NVP-850805	105489-91-9	490.55	C28H32F2N2O6	Cancer Biology	JAK	ATP-competitive JAK2 inhibitor
OTX-015	202590-98-6	491.99	C28H22ClN5O2S	Cancer Biology	Bromodomain	BRD inhibitor
Pyridone 6	457081-03-7	309.34	C18H16N3O	Cancer Biology	JAK	Pan-JAK inhibitor
Reversine	656620-32-6	393.49	C21H27N7O	Chromatin/EpiGenetics	Aurora Kinase	A3 adenosine receptor antagonist, ARK-1/2-3 inhibitor
RO3233	1215493-66-3	338.43	C21H25N5O2	Cancer Biology	HDAC	Smn-activator, HDAC inhibitor
Ruxolitinib phosphate	1052839-17-7	404.36	C17H16N6O4P	Chromatin/EpiGenetics	JAK	JAK1/JAK2 inhibitor
SB1317	937270-47-8	372.46	C23H24N4O	Cancer Biology	JAK	COX, JAK and FLT inhibitor
Tasquinimod	254964-60-8	406.36	C20H17F3N2O4	Cancer Biology	HDAC	Antiangiogenic and antineoplastic agent
UNC11215	1418804-93-9	529.72	C32H43N5O2	Chromatin/EpiGenetics	Bromodomain	Chemical probe for the methyllysine (Kme)
XL015	948755-99-6	444.63	C28H32N6O2	Cancer Biology	JAK	JAK2 inhibitor, potent and selective
XL238	986280-07-4	437.54	C23H31N8O	Cell Cycle/Checkpoint	Aurora Kinase	IGF1R/ALKBH8/ROPR1-3/ABL/SRC family kinases inhibitor
Velpar dihydrochloride	912445-05-7	317.21	C18H18ClN4O	Chromatin/EpiGenetics	PARP-2	PARP-2 inhibitor
AZD1208	1204144-28-4	378.48	C21H21N3O3S	Chromatin/EpiGenetics	Pim	Pim kinase inhibitor
A-753653	844489-71-4	360.39	C21H21N3O3S	Cancer Biology	Others	AMPK activator, potent and reversible
BI 2536	755038-02-9	521.67	C28H38N7O3	Cell Cycle/Checkpoint	PLK	Plk1 inhibitor, potent and ATP-competitive
Radiostab (ACY-1215)	1316214-52-4	433.5	C24H27N5O4	DNA Damage/DNA Repair	HDAC	Selective HDAC6 inhibitor
Vorinostat (SAHA, MK0683)	149647-78-9	264.3	C14H20N2O3	DNA Damage/DNA Repair	HDAC	HDAC inhibitor
Mocetinostat (MK000103, MK0103)	726169-73-9	396.44	C22H29N5O	DNA Damage/DNA Repair	HDAC	HDAC inhibitor, isotype-selective and potent
JNJ-25481565	975320-22-6	394.48	C21H25N5O2	DNA Damage/DNA Repair	HDAC	Potent HDAC inhibitor
ICI-34051	990762-95-6	296.32	C17H19N3O3	DNA Damage/DNA Repair	HDAC	HDAC inhibitor, potent and selective
CUDC-101	1012054-59-9	434.49	C24H28N4O4	DNA Damage/DNA Repair	HDAC	Multitargeted HDAC inhibitor
ITP257 (Givinostat)	732302-99-7	475.97	C24H27N5O4.HCl.H2O	DNA Damage/DNA Repair	HDAC	HDAC inhibitor
MC1569	652475-26-4	314.31	C17H15FN2O2	DNA Damage/DNA Repair	HDAC	Class I HDAC inhibitor, potent and selective
Pracinostat (IB939)	529016-96-6	358.48	C20H28N4O2	DNA Damage/DNA Repair	HDAC	Pan-HDAC inhibitor
Belinostat (PXD101)	414864-00-9	318.35	C15H14N2O4S	DNA Damage/DNA Repair	HDAC	Hydroxamate-type HDAC inhibitor
CUDC-907	1339928-25-4	508.55	C23H24N6O4S	DNA Damage/DNA Repair	HDAC	Potent P300/HDAC inhibitor
ICI-24781 (CRA-024781)	783389-60-2	397.42	C21H23N5O6	Cancer Biology	HDAC	Pan-HDAC inhibitor
Elicig and sodium salt (Sodium valproate)	105649-6	168.19	C8H16N2O4	DNA Damage/DNA Repair	HDAC	HDAC inhibitor
Drocinostat	99873-43-5	243.69	C11H14ClN3O3	DNA Damage/DNA Repair	HDAC	Selective HDAC inhibitor
Tubastatin A	1252003-15-8	335.4	C20H21N3O2	DNA Damage/DNA Repair	HDAC	HDAC6 inhibitor, potent and selective
CI994 (Tacedinaline)	112523-64-2	269.3	C15H15N3O2	Cancer Biology	HDAC	HDAC inhibitor
LAQ824 (NVP-LAQ824, Dacinostat)	404861-63-7	379.46	C22H25N3O3	DNA Damage/DNA Repair	HDAC	HDAC inhibitor, potent and novel
AR-42 (OSU-HDAC2)	935881-37-1	319.36	C18H23N3O3	DNA Damage/DNA Repair	HDAC	DNA Damage/DNA Repair
MB44	251456-60-7	307.39	C16H23N3O3	DNA Damage/DNA Repair	HDAC	HDAC inhibitor, potent and cell-permeable
Scriptaid	287383-93-9	326.36	C18H18N2O4	Cancer Biology	HDAC	HDAC inhibitor, novel and cell-permeable
Sodium Phenybutyrate	1716-12-7	186.19	C11H13ClN2	DNA Damage/DNA Repair	HDAC	Histone deacetylase inhibitor
MLN2237 (Aisenb)	1028484-01-2	510.82	C27H32N6O4	Chromatin/EpiGenetics	Aurora Kinase	Aurora Kinase inhibitor, Potent and selective
VX-680 (MK-0457, Tozasertib)	639089-64-6	464.59	C28H32N8O6	Cancer Biology	Aurora Kinase	Aurora Kinase inhibitor
Banzarotib (AZD1152+H2O)	722544-51-6	507.56	C28H30FN7O3	Chromatin/EpiGenetics	Aurora Kinase	Aurora Kinase B inhibitor, Potent and selective
MLN4439	331771-20-1	513.59	C28H31N5O4	Chromatin/EpiGenetics	Aurora Kinase	Aurora Kinase inhibitor, potent and selective
MLN8254	669363-13-3	476.86	C25H15ClF2N4O2	Chromatin/EpiGenetics	Aurora Kinase	Aurora A inhibitor
JNJ1705621	443791-96-2	394.36	C15H13F2N3O3S	Chromatin/EpiGenetics	Aurora Kinase	Aurora Kinase inhibitor
Danusertib (PHA-739358)	827318-97-8	474.55	C28H30N6O3	Tyrosine Kinase	c-RET	Pan-vanura kinase inhibitor
AT5283	896466-04-9	381.43	C18H23N7O2	Chromatin/EpiGenetics	Aurora Kinase	Aurora Kinase/JAK inhibitor
Hesperadin	422513-13-1	516.65	C22H29N4O3S	Chromatin/EpiGenetics	Aurora Kinase	Aurora B kinase inhibitor
AKI5-900	948596-90-2	503.68	C28H31N7O2	Cancer Biology	Aurora Kinase	Aurora kinase inhibitor
MK-5108 (VX-689)	1010085-13-8	461.94	C22H21ClFN3O3S	Chromatin/EpiGenetics	Aurora Kinase	Aurora-A kinase inhibitor, highly selective
SN6-314 Mesylate	1146618-41-8	527.04	C18H15ClN6O6.C4H8O3S	Chromatin/EpiGenetics	Aurora Kinase	Aurora A/B/C kinases inhibitor, potent and selective
PHA-80532	398493-79-3	501.62	C28H35N7O2	Chromatin/EpiGenetics	Aurora Kinase	Aurora Kinase inhibitor, novel and potent
KU-2499	1002669-72-6	332.4	C22H29N4O2	Cancer Biology	FLT3	Multikinase inhibitor
TAK-901	934541-31-4	504.64	C28H32N4O3S	Chromatin/EpiGenetics	Aurora Kinase	Novel Aurora A/B inhibitor
CYC 116	693228-63-6	368.46	C18H20N6O6	Chromatin/EpiGenetics	Aurora Kinase	Potent Aurora A/B inhibitor
Aurora A inhibitor 1	1158838-45-9	588.07	C31H31ClFN7O2	Cell Cycle/Checkpoint	Aurora Kinase	Aurora A inhibitor
EMD-2076 L-(+)-Tartaric acid	1291074-87-7	525.56	C28H31N7O6	Chromatin/EpiGenetics	Aurora Kinase	Aurora kinases inhibitor
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CCT129202	942947-93-6	497.02	C23H25ClN8O6	Cancer Biology	Aurora Kinase	Aurora Kinase inhibitor, ATP-competitive and potent
CCT137690	1095382-05-0	551.48	C26H31BrN8O6	Chromatin/EpiGenetics	Aurora Kinase	Aurora A/B/C inhibitor
Tofacitinib (CP-690550) Citrate	540737-29-9	504.49	C16H20N6O.C6H8O7	Chromatin/EpiGenetics	JAK	Potent JAK inhibitor
TO-101348 (SAR302503)	936291-25-8	524.68	C27H36N6O3S	Chromatin/EpiGenetics	JAK	JAK-2 inhibitor, potent and selective
AZD1480	636666-89-4	348.77	C18H14ClFN8	Cancer Biology	JAK	JAK2 inhibitor, ATP-competitive and novel
Tofacitinib (CP-690550, Tascotinib)	477600-75-2	312.37	C16H20N6O	Chromatin/EpiGenetics	JAK	Janus kinase inhibitor
Ac-490	133550-30-8	294.3	C17H14N2O3	JAK/STAT Signaling	EGFR	JAK2/EGFR inhibitor
WP 1066	897064-38-1	396.22	C17H14BrN3O	Chromatin/EpiGenetics	JAK	JAK2/STAT3 inhibitor, cell-permeable
Saritinib (LY3009104, INC023050)	1181594-05-7	371.42	C17H14BrN3O	Cancer Biology	JAK	JAK1/JAK2 inhibitor, selective, orally bioavailable
CYT387	1056634-68-4	414.46	C23H22N6O2	Chromatin/EpiGenetics	JAK	JAK-1/2 inhibitor, ATP-competitive
TO101209	936091-14-4	509.67	C26H35N7O2S	Tyrosine Kinase	c-RET	JAK2/3 inhibitor
CFP-33779	125700-57-6	462.67	C24H28N6O2S	Cancer Biology	JAK	JAK2 inhibitor, highly selective
MLN8254	1252326-66-6	469.34	C27H25N5FN7O	Chromatin/EpiGenetics	JAK	JAK2 inhibitor, highly potent and selective
WHP-154	211655-04-3	376.2	C16H14BrN3O3	Cancer Biology	JAK3	JAK3 inhibitor
ZM 39923 HCl	1021868-92-7	367.91	C23H28N6O4.HCl	JAK/STAT Signaling	JAK	JAK3 inhibitor, potent and selective
BM5-911543	1271022-90-2	432.52	C23H28N8O	JAK/STAT Signaling	JAK	JAK2 inhibitor, selective, small molecule
BMN 873	1207456-01-6	380.35	C19H14F2N6O	DNA Damage/DNA Repair	PARP	Potent PARP inhibitor
Osiparib (AZD2281, KU-0059436)	753113-22-0	434.46	C24H23F4N4O2	Cancer Biology	PARP	Potent PARP1/PARP2 inhibitor
Rucaparib (ACQ14699, PF-01367338)	458668-92-9	421.36	C18H18FN3O3.H3PO4	Chromatin/EpiGenetics	PARP	Potent PARP inhibitor
Iniparib (BI-1201)	160003-66-7	282.03	C7H8N2O3	Chromatin/EpiGenetics	PARP	PARP1 inhibitor, intravenously administered
AC-14361	328543-09-6	320.39	C19H20N4O	DNA Damage/DNA Repair	PARP	Potent PARP1 inhibitor
FL34 hydrochloride	344449-15-7	331.8	C17H17N3O3.HCl	Cancer Biology	PARP	PARP inhibitor, potent and cell-permeable
A-66642	934162-61-6	324.35	C18H17FN4O	Chromatin/EpiGenetics	PARP	PARP-1/2 inhibitor, highly potent
INC-1001	3544-34-9	136.15	C7H8N2O	Chromatin/EpiGenetics	PARP	Potent PARP inhibitor
UPF 1069	1048371-03-4	279.29	C17H13N3O3	Chromatin/EpiGenetics	PARP	Selective PARP2 inhibitor
AZD2461	1174043-19-3	395.43	C22H22F3N3O3	Cancer Biology	PARP	Novel PARP inhibitor
EPZ5676	1386289-87-8	562.71	C20H24N6O3	Chromatin/EpiGenetics	HDAC	DOT1L inhibitor, potent and SAM competitive
SOX 0846	1581178-17-3	618.57	C28H40BrN7O4	Chromatin/EpiGenetics	Histone Methyltransferase	DOT1L inhibitor, highly potent and selective
Ertacizine	130529-57-6	305.29	C14H15N3O5	Chromatin/EpiGenetics	Histone Methyltransferase	COMT inhibitor
EPZ004777	1338466-77-5	539.67	C28H41N7O4	Cancer Biology	Histone Methyltransferase	DOT1L inhibitor
EPZ005687	1396772-26-1	539.67	C23H27N5O3	Chromatin/EpiGenetics	Histone Methyltransferase	EZH2 inhibitor, potent and selective
Tioguanine	154-42-7	167.19	C4H5H6N5	DNA Damage/DNA Repair	Purine antimetabolite	Purine antimetabolite
SRT1720 HCl	1001645-58-4	506.02	C25H23N7O6.HCl	Chromatin/EpiGenetics	Sirtuin	Sirtuin activator
EX 527 (S6N0214196)	49843-98-3	248.71	C13H13ClN2O	Cancer Biology	Sirtuin	Sirtuin activator
Resveratrol	501-36-0	228.24	C14H12O3	Chromatin/EpiGenetics	Sirtuin	Sirtuin activator
Sirtuin	4105369-97-9	364.47	C22H22N2O2	Chromatin/EpiGenetics	Sirtuin	Sirtuin activator
PPF-1 (PP-6405761)	1403764-72-6	347.39	C16H17N3O4S	Chromatin/EpiGenetics	Bromodomain	BET inhibitor
Bronisoprine	1619994-69-2	404.44	C17H20N6O4S	Cancer Biology	Bromodomain	Bromodomain inhibitor, non-selective
FO-452 (A6P1517)	808118-40-3	352.34	C18H18N2O6	Angiogenesis	HIF	HIF prolyl-hydroxylase inhibitor
2-Methoxyestradiol (2-MeOE2)	362407-2	302.41	C18H26O3	Apoptosis	Apoptosis Inducers	Apoptotic, antiangiogenic and antiangiogenic agent
INC010396	931398-73-0	352.34	C18H18N2O6	Angiogenesis	HIF	HIF prolyl-hydroxylase-2 (PHD2) inhibitor
OSK J4 HCl	1373423-53-0	453.96	C28H27N5O2.HCl	Cancer Biology	Histone Demethylase	Inhibitor of H3K27 demethylase, JMJD3, potent and cell-permeable
OSK J1	1373422-53-7	389.45	C22H23N5O2	Chromatin/EpiGenetics	Histone Demethylase	H3K27 demethylase, JMJD3, potent and cell-permeable
SOI-1775 free base	1025056-69-3	405.42	C22H22F3N5O	Chromatin/EpiGenetics	Pim	Pim kinase inhibitor, ATP-competitive
OSK J4	438190-29-5	371.25	C14H8F3N3O3S	JAK/STAT Signaling	JAK	Potent Pim inhibitor
Tenovin-1	380315-80-0					

DMOG	89484-03-1	175.14	C8H9NO5	Chromatin/EpiGenetics	HIF	Competitive HIF-PH inhibitor, cell-permeable
KC7F2	927822-89-4	570.38	C18H16O4N2O4S4	Cancer Biology	HIF-1 $\alpha$ inhibitor	HIF-1 $\alpha$ inhibitor
FX112	141400-59-0	169.31	C7H12N2S2	Chromatin/EpiGenetics	HIF	HIF-1 inhibitor
1,2,3,4,5,6-Hexabromocyclohexane	1837-91-8	557.54	C6H8Br6	Chromatin/EpiGenetics	JAK	JAK2 tyrosine kinase inhibitor
ZM 448229	4452-6-6	182.22	C13H10O	Chromatin/EpiGenetics	JAK	JAK3 inhibitor
TCS PIM-1 1	491871-58-0	367.2	C18H11BN2O2	Chromatin/EpiGenetics	Pim	Pim-1 kinase inhibitor,ATP-competitive
4-H2N	461-36-1	146.15	C8H8N2O	Chromatin/EpiGenetics	PARP	PARP inhibitor
JW 55	694993-53-7	434.48	C28H29NO5	Cancer Biology	PARP	PARP domain inhibitor
WK14	838818-26-1	521.59	C20H23N5O3S	Chromatin/EpiGenetics	PARP	Inhibitor of Wnt/PC-Catenin signaling and tankyase
Sal 003	1104470-53-4	463.21	C18H15O4N3O5	Cancer Biology	Protein Ser/Thr Phosphatases	Cellular phosphatase complex inhibitor
NSC 87877	56960-57-9	459.45	C18H13N3O7S2	Chromatin/EpiGenetics	Protein Ser/Thr Phosphatases	Shp2 /shp1 PTP inhibitor
Oflonox	82419-36-1	351.37	C18H20FN3O4	DNA Damage/DNA Repair	Topoisomerase	Fluoroquinolones,antibiotics
Fasudil (HA-1077) HCl	105628-07-7	327.83	C14H17N3O2S.HCl	Chromatin/EpiGenetics	TGF- $\beta$ / Smad Signaling	Protein kinase inhibitor
Entinostat (MS-275,SNDX-275)	209783-80-2	376.4	C21H22NO4	DNA Damage/DNA Repair	HDAC	HDAC1 and HDAC3 inhibitor
Romidepsin (FK228, depsipeptide)	128517-07-7	540.7	C24H36NO4O6S2	DNA Damage/DNA Repair	HDAC	HDAC1/HDAC2 inhibitor,potent and selective
Panobinostat (LBH589)	404950-89-7	349.43	C21H23NO2	DNA Damage/DNA Repair	HDAC	HDAC inhibitor
(+)-JQ1	1285524-71-5	456.99	C23H25ClN4O2S	Chromatin/EpiGenetics	HDAC	BET bromodomain inhibitor
3-Deazaneplanocin A (DZNep) hydrochloride	120094-45-6	298.73	C12H14N4O3.HCl	Stem Cell	EZH2	SAH and ENZ2 inhibitor
Trichostatin A (TSA)	58880-19-6	302.37	C17H22NO2	DNA Damage/DNA Repair	HDAC	HDAC inhibitor
Nanaomyonin A	52934-83-5	302.28	C18H14O6	Chromatin/EpiGenetics	DNA Methyltransferase	DNMT3B inhibitor
EPZ-5439	1403254-09-8	572.74	C34H44N4O4	Chromatin/EpiGenetics	Histone Methyltransferase	EDH2 inhibitor,potent and selective
CID 2011756	838195-11-3	396.87	C22H12ClN2O3	Chromatin/EpiGenetics	Protein Ser/Thr Phosphatases	PKD inhibitor
TAK-632	1228591-30-7	554.52	C27H18F4N4O3S	MAPK Signaling	Raf	Pan-RAF inhibitor,potent and selective
Spilitomycin	5690-3-9	198.22	C13H10O2	Chromatin/EpiGenetics	Sirtuin	inhibitor of Sir2p and RMLP-induced free radicals
Tenovin-6	1011567-82-0	454.6	C26H34N4O2S	Chromatin/EpiGenetics	Sirtuin	SIRT inhibitor,potent and p53 activator
CG 6933	130503-29-0	442.51	C28H28N4O3	TGF- $\beta$ / Smad Signaling	PKC	pan-PKC inhibitor
Cytarabine	147-94-4	243.2	C8H9N3O5	DNA Damage/DNA Repair	DNA Synthesis	cytotoxic agent, blocks DNA synthesis
Sostrastaurin (AEB071)	425637-18-9	438.48	C26H22N8O2	TGF- $\beta$ / Smad Signaling	PKC	PKC inhibitor
Tubastatin A HCl	1310693-02-5	371.88	C20H21N3O2.HCl	DNA Damage/DNA Repair	HDAC	HDAC6 inhibitor,potent and selective
Tankyrase inhibitors (TNKS) 49		448.54	C24H24N4O3S	Chromatin/EpiGenetics	PARP	Tankyrase inhibitor
Septin1	13098-73-2	168.54	C9H9ClN4	Chromatin/EpiGenetics	Protein Ser/Thr Phosphatases	Selective FPP1R15A inhibitor
MCB-613	1162656-22-5	305.37	C10H19NO3	Chromatin/EpiGenetics	Histone Acetyltransferases	stimulator of steroid receptor coactivator (SRC)
RGFP966	1357380-11-7	362.4	C21H19FN4O	DNA Damage/DNA Repair	HDAC	Specific HDAC3 inhibitor
TMP269	1314890-29-3	514.52	C25H21F3N4O3S	DNA Damage/DNA Repair	HDAC	HDAC 4/5/7/9 inhibitor
MR-3745	885325-71-3	431.91	C20H16ClFN6O5	Cell Cycle/Checkpoint	Aurora Kinase	Aurora A inhibitor,potent and selective
UNC999	1314241-44-5	339.24	C18H20N4O	Chromatin/EpiGenetics	MLL1 antagonist	MLL1 antagonist,bipolar disorder medicine
HTH-01-015	1613724-42-7	468.55	C28H28N8O	PI3K/Akt/mTOR Signaling	AMPK	NUAK1 inhibitor,highly specific and selective
Rucaparib (free base)	283173-50-2	323.36	C16H18FN3O	Chromatin/EpiGenetics	PARP	Potent PARP inhibitor
MS436	1360684-25-9	383.42	C18H17N5O3S	Chromatin/EpiGenetics	Bromodomain	BRD4 inhibitor
GSK1324726A	1300031-42-2	434.61	C24H22ClN2O3	Chromatin/EpiGenetics	Bromodomain	BET proteins inhibitor
Eli1	1418308-27-9	390.48	C23H26N4O2	Stem Cell	EZH2	EZH2 inhibitor
CPI-203	1446144-04-2	399.9	C19H18ClN5O5	Chromatin/EpiGenetics	Bromodomain	BET bromodomain inhibitor
UNC0631	1320288-19-4	635.03	C37H61N7O2	Chromatin/EpiGenetics	Histone Methyltransferase	G9a inhibitor
GLP50634	1206161-67-8	425.5	C21H23N5O3S	JAK/STAT Signaling	JAK	JAK1 inhibitor
ABC24640	915385-61-8	360.91	C26H28N2O2	Chromatin/EpiGenetics	Springinase Kinase-2	Springinase kinase 2 inhibitor,selective and competitive
Valproic acid	99-06-1	144.21	C8H16O2	DNA Damage/DNA Repair	HDAC	HDAC1 inhibitor
Dorsomorphin 2HCl	1219168-18-9	472.41	C24H25N5O2.HCl	PI3K/Akt/mTOR Signaling	AMPK	AMPK inhibitor
Phenformin HCl	834-28-6	241.72	C10H16ClN2	Others	Others	biguanidine drug with anti-diabetic activity
WZ4003	1214265-59-3	466.99	C25H26ClN6O3	Ubiquitination/ Proteasome	Autophagy	NUAK1/2 inhibitor, potent and selective
DINC16 Sodium	78564-70-9	310.41	C18H19ClN5O2	Ubiquitination/ Proteasome	Autophagy	Epigenetic drug
Procabazine HCl	366-70-1	257.76	C12H19N3O.HCl	DNA Damage/DNA Repair	DNA Synthesis	Antineoplastic chemotherapy drug
Mizoribine	50024-40-7	259.22	C9H13N3O6	Others	IMPDH	DNA/RNA synthesis inhibitor
I-BET-762	1280607-17-2	423.9	C22H22ClN5O2	Chromatin/EpiGenetics	Bromodomain	BET inhibitor,highly potent
RVX-209	1044870-39-4	370.4	C20H22ClN5O	Chromatin/EpiGenetics	Bromodomain	Potent bromodomain inhibitor
I-BET151 (GSK1210151A)	1300031-40-5	415.44	C23H21N5O3	Chromatin/EpiGenetics	Bromodomain	Selective BET inhibitor
C646	329898-36-1	445.42	C24H19N3O6	Chromatin/EpiGenetics	Histone Acetyltransferases	HAT p300-CBP inhibitor,cell-permeable
JIB-04	199598-05-9	308.78	C17H13ClN4	Chromatin/EpiGenetics	Histone Demethylases	Jumonji histone demethylase inhibitor
OG-L002	1367302-64-7	225.29	C16H15NO	Chromatin/EpiGenetics	Histone Demethylases	LSD1 inhibitor,potent and specific
MM-102	1417329-24-9	669.8	C35H46F2N10O4	Chromatin/EpiGenetics	Histone Methyltransferase	MLL1 inhibitor,high-affinity peptidomimetic
UNC1999	1431612-23-5	590.74	C33H43N7O2	Chromatin/EpiGenetics	Histone Methyltransferase	EZH2 inhibitor
Donepezil HCl	120011-70-3	415.85	C24H30ClN3O3	Chromatin/EpiGenetics	Histone Acetyltransferases	ACHE inhibitor
SGI-1027	1020149-73-8	461.52	C27H23N7O	Chromatin/EpiGenetics	Histone Methyltransferase	DNMT inhibitor
Sodium butyrate	156-54-7	110.09	C4H7NaO2	Others	Others	Histone deacetylase inhibitor
Mefenformin HCl	1115-70-4	265.62	C14H13ClN3	Others	Others	DNA synthesis inhibitor
Nedaplatin	95734-82-0	303.17	C22H22Cl2O3P	GPCR/G protein	Adrenergic Receptor	DNA synthesis inhibitor
Mitoxantrone HCl	70476-82-3	517.4	C22H20ClNO4.HCl	Others	Topoisomerase II inhibitor,anti-neoplastic drug	Topoisomerase II inhibitor,anti-neoplastic drug
Ro 31-8220 Mesylate	138486-18-6	553.85	C25H23N5O2S.H4O3O3S	Others	Pan-PKC inhibitor	Pan-PKC inhibitor
Flarubizol	72496-41-4	627.64	C32H37NO12	DNA Damage/DNA Repair	Topoisomerase	Topoisomerase II inhibitor,anthracycline antibiotic
Iauzinol	309271-04-1	469.58	C26H19N5O5S2	DNA Damage/DNA Repair	Topoisomerase	SIRT1 inhibitor
MG 149	1243583-85-8	340.46	C22H28O3	Chromatin/EpiGenetics	HDAC	HAT inhibitor
Nexrutastat A	1403783-31-2	341.4	C19 H23 N3 O3	Chromatin/EpiGenetics	HDAC	HDAC6 inhibitor,highly potent and selective
BMS-345541 (free base)	445430-59-0	255.32	C14H17N5	Chromatin/EpiGenetics	HDAC	IKK-1/IKK-2 inhibitor,potent and selective
CPI-109	1450855-78-1	529.66	C28H28N4O5	Stem Cell	EZH2	EZH2 inhibitor
Santacuzumate A (CAY10883)	1477940-42-0	278.55	C16H22N2O3	DNA Damage/DNA Repair	HDAC	HDAC inhibitor, potent and selective
Procainamide HCl	614-39-1	271.79	C13H22ClN3O	Membrane Transporter/Channel	Sodium Channel	sodium channel blocker
CAY10803	1045762-66-2	446.5	C22H30N4O6	DNA Damage/DNA Repair	HDAC	potent and selective inhibitor of HDAC6
PF-1	1627676-59-8	469.52	C23H25F4N3O3S	Chromatin/EpiGenetics	Histone Methyltransferase	SETD7 methyltransferase inhibitor
RJ3061in	1622921-15-4	363.38	C15H15Br4N4S	Chromatin/EpiGenetics	Histone Acetyltransferases	BTK
ML324	1222800-79-4	349.43	C21H23N3O2	Chromatin/EpiGenetics	Histone Demethylases	JMJD2 demethylase inhibitor, potent and cell-permeable
SP2509	1423715-00-0	437.9	C19H20ClN3O6S	Chromatin/EpiGenetics	Histone Demethylases	Demethylase 1 (LSD1) antagonist, novel Lysine-specific
OF-1	191973-83-4	440.31	C17H18BrN3O4S	Chromatin/EpiGenetics	Bromodomain	BRPF1 and BRPF2 bromodomain inhibitor
GSK 5659	901245-06-6	364.47	C22H26N4O3	Chromatin/EpiGenetics	Bromodomain	BRPF1 bromodomain inhibitor
A366	1527503-11-2	329.44	C16H27N3O2	Chromatin/EpiGenetics	Histone Methyltransferase	Chromatin demethylase inhibitor
WDR5 0103	890190-22-4	383.44	C21H25N3O4	Chromatin/EpiGenetics	Histone Methyltransferase	WD repeat-containing protein 5 (WDR5) antagonist
GSK-LSD1 2HCl	1431388-48-7	289.24	C14H22Cl2N2	Chromatin/EpiGenetics	Histone Demethylases	irreversible, and selective LSD1 inhibitor
EPZ015668	1618391-05-1	383.44	C20H25N5O3	Chromatin/EpiGenetics	Histone Methyltransferase	PRMT5 inhibitor
Mirin	1169097-97-0	220.25	C14H19N3O5	Cell Cycle/Checkpoint	ATM/ATR	line1-1-Rad50-Nbs1 (MRE11A-ATR) pathway inhibitor
IOX 1	6852-78-8	189.17	C10H7NO3	Chromatin/EpiGenetics	Histone Demethylases	histone demethylase JMJD inhibitor
GSK J2	1394854-52-4	389.45	C22H23N5O2	Chromatin/EpiGenetics	Histone Demethylases	inactive control of GSK J1, JMJD3 (KDM6B) and UTX (KDM8A) inhibitor
GO7-LK	1380672-07-0	529.96	C25H16ClN7O3S	DNA Damage/DNA Repair	tankyrase	tankyrase 1/2 inhibitor
GSK503	1346572-63-1	526.67	C31H38N6O2	Stem Cell	EZH2	EZH2 inhibitor
FX2118	223387-71-5	280.69	C12H19ClN2O4	Angiogenesis	HIF	Novel HIF hydrolyase inhibitor
Molidustat (BAY85-3934)	1154028-82-6	314.3	C13H14N8O2	Chromatin/EpiGenetics	HIF	Novel HIF-PH inhibitor
GSK2879552	1401666-06-5	364.48	C23H28N2O2	Chromatin/EpiGenetics	Histone Demethylases	Novel and irreversible LSD1 inhibitor
ORY-1001	1431328-61-2	303.27	C15H24Cl2N2	DNA Damage/DNA Repair	HDAC	Selective inhibitor of KDM1A
BET bromodomain inhibitor	1380087-99-7	365.51	C20H16ClN5O2	Chromatin/EpiGenetics	Bromodomain	Potent and selective inhibitor for BRD4
C172046	887865-67-7	378.95	C14H16ClN2O2S	Chromatin/EpiGenetics	Histone Methyltransferase	Novel PRMT1 inhibitor
Chidamide	743420-02-2	390.41	C22H19FN4O2	Chromatin/EpiGenetics	HDAC	Novel HDAC inhibitor
Decomethyl(VX-509)	944842-54-0	362.38	C18H19F3N8O	Chromatin/EpiGenetics	JAK	Selective and orally active JAK3 inhibitor
ACY-241	1318215-12-9	467.85	C24H26ClN5O3S	Chromatin/EpiGenetics	HDAC	Selective and orally active HDAC6 inhibitor
LFMA-113	244240-24-2	300	C11H8Br2N2O2	Angiogenesis	BTK	BTK-specific tyrosine kinase inhibitor
UF 010	537672-41-8	271.15	C11H15BrN2O	Chromatin/EpiGenetics	HDAC	Novel and selective class I HDAC inhibitor
BML-210(CAY10433)	537034-17-6	339.43	C20H25N3O2	Chromatin/EpiGenetics	HDAC	Novel HDAC inhibitor
2-hexyl-4-pentynoic Acid	96017-59-3	182.26	C11H18O2	Chromatin/EpiGenetics	HDAC	Potent and robust HDACs inhibitor
Thioacetyl Resveratrol	42206-94-0	354.35	C20H18O6	Chromatin/EpiGenetics	Sirtuin	Cell-permeable resveratrol produg
2,4-Pyridinedicarboxylic Acid	469-80-9	107.12	C7H5NO4	Chromatin/EpiGenetics	Histone Demethylases	Histone LSD inhibitor
PF14	900305-37-5	380.44	C21H24N4O3	Chromatin/EpiGenetics	Bromodomain	Potent and selective BRPF1 Bromodomain inhibitor
Suberoylanoylamic Acid	38937-86-5	204.22	C18H16N2O4	Chromatin/EpiGenetics	HDAC	HDAC inhibitor
MN 64	92831-11-3	264.32	C18H18O2	DNA Damage/DNA Repair	tankyrase	tankyrase inhibitor
GSK2801	1616964-08-1	371.45	C20H16ClN5O2	Chromatin/EpiGenetics	Bromodomain	inhibitor of BAZ2A and BAZ2B bromodomains
PI-478 2HCl	866585-44-0	394.12	C13H20Cl2N4O3	Chromatin/EpiGenetics	HIF	HIF-1 $\alpha$ inhibitor
SirReal2	709002-48-0	420.55	C22H20N4O5S2	Chromatin/EpiGenetics	Histone Methyltransferase	Sirt2 inhibitor
SGC707	1687736-54-4	268.34	C16H18N4O2	Chromatin/EpiGenetics	Histone Methyltransferase	PRMT3 inhibitor
AS8351	796-42-9	261.3	C17H13N3O2	Chromatin/EpiGenetics	Histone Demethylases	histone demethylase inhibitor
Dicoumatin(GSK1278893)	960530-70-2	363.43	C19H21N3O2	Chromatin/EpiGenetics	Histone Methyltransferase	HIF-prolyl hydroxylase inhibitor
LLY507	1793053-37-8	574.76	C36H42N8O	Chromatin/EpiGenetics	Histone Methyltransferase	SMYD2 inhibitor
Picolinamide	1452-77-3	122.12	C8H8N2O	DNA Damage/DNA Repair	PARP	poly (ADP-ribose) synthetase inhibitor
Benzamide	55-21-0	121.14	C7H7NO	DNA Damage/DNA Repair	PARP	poly (ADP-ribose) synthetase inhibitor
GSK591	1618361-87-7	380.48	C22H28N4O2	Chromatin/EpiGenetics	Histone Methyltransferase	PRMT5 inhibitor
MS023	1831110-54-3	387.4	C17H23ClN3O	Chromatin/EpiGenetics	Bromodomain	Class I PRMT1 inhibitor
BI-7273	1883420-21-7	353.41	C20H23N3O3	Chromatin/EpiGenetics	Bromodomain	BRD9 bromodomain inhibitor
AGK 2	304866-28-4	434.27	C23H13Cl2N3O2	Chromatin/EpiGenetics	Sirtuin	SIRT2 inhibitor, potent and selective
Tranylcypromine hydrochloride	1988-47-6	169.85	C9H11N.HCl	Chromatin/EpiGenetics	Histone Demethylases	LSD1/BHC110 and monoamine oxidase (MAO) inhibitor
(R)-(+)-Etomoxif sodium salt	826934-44-14	320.74	C14H16ClN2O4	Chromatin/EpiGenetics	Histone Acetyltransferases	camptin, pantoic/transferase I (CPT1) inhibitor
PI3	1818983-80-8	351.37	C16H19N3O2	Chromatin/EpiGenetics	Bromodomain	inhibitor of poly(ubiquitin) 1 and SMARCA4
UNC 0642	1481877-78-4	548.7	C20H44F2N6O2	Chromatin/EpiGenetics	Histone Methyltransferase	G9a and GLP histone lysine methyltransferase inhibitor
CPI-837	1884712-47-3	386.45	C22H22N6O	Chromatin/EpiGenetics	Bromodomain	CBPF300 bromodomain inhibitor
ITSA-1 (ITSA1)	200626-81-5	292.12	C13H7Cl2N3O	Chromatin/EpiGenetics	HDAC	HDAC activator via Trichostatin A (TSA) suppression
Thiomristinol	1429749-41-6	551.37	C24H15N3O5S	Chromatin/EpiGenetics	Others	Others
Cerdulatinib (FRT082070)	1168300-79-6	445.54	C20H27N7O3S	Chromatin/EpiGenetics	JAK	Syk/JAK inhibitor
PTP Inhibitor II	2632-13-6	229.1	C9H9BrO2	Chromatin/EpiGenetics	Protein Ser/Thr Phosphatases	protein tyrosine phosphatase (PTP) inhibitor
PTP Inhibitor I	2491-38-5	215	C8H7BrO2	Chromatin/EpiGenetics	Protein Ser/Thr Phosphatases	tyrosine phosphatase (PTP) inhibitor
4-iodo-SAHA	1219807-87-0	360.2	C14H16BrN2O3	Chromatin/EpiGenetics	HDAC	class I and class II histone deacetylase (HDAC) inhibitor
$\beta$ -Glycerol phosphate (sodium salt hydrate)	13408-09-9	308.1	C3H7O6P $\cdot$ 2Na [5H2O]	Chromatin/EpiGenetics	Protein Ser/Thr Phosphatases	protein phosphatase inhibitor
Parthenolide	20554-84-1	248.32	C15H20O3	Immunology/Inflammation	NF- $\kappa$ B	PARP-1 inhibitor
6-gingerol	23513-14-6	294.39	C17H26O4	Nature Products	Nature Products	Precurser in chemical reaction
Nicotinamide	98-92-0	122.13	C6H8N2O	Nature Products	Nature Products	PARP-1 inhibitor
Coumarin	81-84-5	146.14	C9H6O2	Nature Products	Nature Products	Precurser in chemical reaction
Diosgenin	512-04-9	414.61				

Curcumin	4871-97-0	236.35	C15H24O2	Nature Products		
Quercetin	117-39-5	302.24	C15H10O7	PI3K/Akt/mTOR Signaling	PI3K	Antitumor agent
Ginkgolide C	15291-76-6	440.4	C20H24O11	Nature Products		
Fisetin	528-48-3	286.05	C15H10O6	Nature Products		