SGC

The SGC conducts pre-competitive, open access research to facilitate new drug discovery programs. The consortium generates knowledge and reagents that can be used to validate therapeutic targets.

Since 2008, the SGC has led the development of chemical probes which inhibit or antagonize proteins involved in epigenetic signaling. These chemical probes are made available to the research community with no restriction on use: innovation for everyone.

SGC Chemical Probes are small, drug-like molecules which meet these criteria:

- ✓ *in vitro* IC_{50} or Kd < 100 nM
- ✓ > 30-fold selectivity over proteins in the same family
- ✓ significant on-target cellular activity at 1 μM
- ✓ negative control

The SGC also characterizes reagents that may be used in downstream assays:

- a control compound for probes
- biotin-labelled probes
- antibodies to epigenetic proteins

This initiative is sustained by a team of cross-disciplinary scientists from industry and academia specializing in Research Informatics, Biotechnology, Biophysics, and Structural and Chemical Biology.

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www.thesgc.org/chemcal-probes

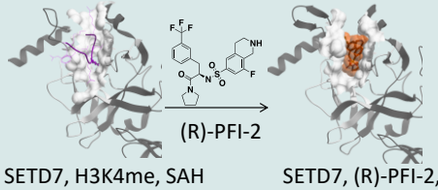
SGC Epigenetic Chemical Probes

Protein	Probe
ATAD2	BAY-850, GSK8814
BET family	(+)-JQ1, PFI-1
BAZ2A/2B	GSK2801, BAZ2-ICR
BPTF	NVS-BPTF-1
BRD9/7	LP99; BI-9564; TP-472
BRD9	I-BRD9
BRPF1/2/3; BRPF1B	OF-1, NI-57; PFI-4, GSK6853
BRPF2/TAF1	BAY-299
CECR2	NVS-CECR2-1
CECR2/BPTF	TP-238
CREBBP, EP300	(BRD) SGC-CBP30, I-CBP112
SMARCA2/4, PB1	PFI-3
PCAF/GCN5	L-Moses, GSK4027
MLLT1/3	NVS-MLLT-1
IDH1 mutant	GSK864
JMJD3/UTX	GSK-J4*
LSD1	GSK-LSD1
L3MBTL3	UNC1215
DOT1L	SGC0946
EED	A-395
EZH2/H1	GSK343, UNC1999
G9a/GLP	UNC0638, A-366, UNC0642
PRDM9	MRK-740
PRMT Type I	MS023
PRMT3	SGC707
PRMT4/6	MS049
PRMT4	TP-064, SKI-73*
PRMT5	GSK591, LLY-283
PRMT6	SGC6870
PRMT7	SGC3027*
SETD7	(R)-PFI-2
SPIN1	VinSpinIn
SMYD2	BAY-598; PFI-5; LLY-507
SMYD3	BAY-6035
SUV420H1/H2	A-196
PAD4	GSK484
NSD2 (PWWP1)	UNC6934
NSD3 (PWWP1)	BI-9321
WDR5	OICR-9429
CREBBP, EP300	(AT) A-485

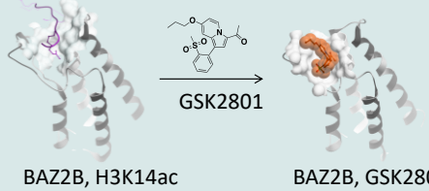
*pro-drug

SGC

Structural Genomics Consortium is a public-private partnership focusing on pre-competitive protein-based research in emerging and under-studied diseases.



SETD7, H3K4me, SAH — SETD7, (R)-PFI-2, SAM



BAZ2B, H3K14ac — BAZ2B, GSK2801

SGC's scientific contributions include chemical probe development, novel crystal structures of human proteins, and target-enabling packages.

www.thesgc.org/chemcal-probes

SGC Epigenetic Chemical Probe Library

#	Domain: Target	Probe	*in vitro* IC_{50} or Kd (nM)	Cell line/Assay, Target/Biomarker: IC_{50}/EC_{50} (nM)	Control	PubMed ID	Supplier
1	BRD: ATAD2A/B	GSK8814	50	nanoBRET ATAD2 (BD): **2700**	GSK8815	27530368	New
2	BRD: ATAD2A	BAY-850	85‡; 753#; 166/H4K12Kac^{T}	FRAP/ATAD2: **1000**	BAY-460	29043777	Y
3	BRD: BET family	(+)-JQ1	BRD4 1st/2nd BRD: 50/90	NMC 797, BRD4: **500**	(-)-JQ1	20871596	Y
4	BRD: BAZ2A/2B	BAZ2-ICR	130/180	FRAP, BAZ2A: **1000**	-	25719566	Y
5		GSK2801	257/136	FRAP, BAZ2B: **1000**	GSK8573	25799074	Y
6	BRD: BRD9/7	BI-9564	14/239	FRAP, BRD9/7: **100/1000**	-	26914985	Y
7		TP-472	33/340	nanoBRET, BRD9: **323** (EC_{50})	TP-472N		Y
8	BRD: BRD9	I-BRD9	50 ± 17	nanoBRET, BRD9: **159**	-	25856009	Y
9	BRD: BRPF1/2/3	OF-1	100/500/2400	nanoBRET, BRPF1B: **80**	-		Y
10		NI-57	31/108/408	FRAP, BRD1: **1000**	-	28714688	Y
11	BRD: BRPF1B	GSK6853	8	nanoBRET BRPF1B (BD): **20**	GSK9311	27326325	Y
12	BRD: BRPF2/TAF1	BAY-299	BRPF2: 67; TAF1 (2nd): 14	nanoBRET, BRPF2: **970**; TAF1 2nd BRD: **575**	BAY-364	28402630	Y
13	BRD: CECR2/BPTF	TP-238	CECR2/BPTF: 20/200	nanoBRET, CECR2 (BD)/BPTF (BD): **289/228**	TP-422		Y
14	BRD: BPTF	NVS-BPTF-1	71	nanoBRET, BPTF (BD): **16**	NVS-BPTF-C		New
15	BRD: CREBBP/EP300	SGC-CBP30	21/38	FRAP, CREBBP: **1000**	BDOIA513	24946055	Y
16		I-CBP112	151/625	FRAP, CREBBP: **1000**	-	26552700	Y
17	BRD: PCAF/GCN5	GSK4027	PCAF/GCN5: 1.2 (BROMOscan)	nanoBRET PCAF (full length)/H3.3: **60**	GSK4028	28002667	Y
18		L-Moses	PCAF/GCN5: 126/600#	nanoBRET PCAF (BD)/H3.3: **260**	D-Moses	27966810	Y
19	BRD: SMARCA2/4	PFI-3	SMARCA4:89; PB1 (5th):48	FRAP, SMARCA2: **1000**	BDF25488524	26139243	Y
20	YEATS: MLLT1/3	NVS-MLLT-1	MLLT1/3: 150/250^{T}	nanoBRET MLLT3/H3.3Kcr: **0.5**	NVS-MLLT-C		New
21	AT: CREBBP, EP300	A-485	EP300: 10^{T}	PC-3 cells, ↓ H3K27ac: **800**	A-486	28953875	Y
22	DEHYDR: IDH1 mutant	GSK864	R132C: 9; R132H: 15; R132G:17	HT-1080, IDH1 (R132C mutation): **320**	-	26436839	Y
23	KDM: JMJD3/UTX	GSK-J4*/J1	GSK-J1: 60	(GSK-J4) PBMC, TNF-alpha: **9000**	GSK-J5	22842901	Y
24	KDM: LSD1	GSK-LSD1	16	EC_{50} < **5**	-	26175415	Y
25	Kme: L3MBTL3	UNC1215	40	Inhibit foci formation HEK293, L3MBTL3: **500**	UNC1079	23292653	Y
26	Kme, Rme: SPIN family	VinSpinIn	ITC SPIN1/2/3/4: 10/46/131/18	nanoBRET SPIN1/H3: **270**	VinSpinIC		New
27	MT: DOT1L	SGC0946	0.3 ± 0.1	MCF10A, ↓ H3K79me: **10**	SGC0649	23250418	Y
28	Kme: EED	A-395	34	RD rhabdoid cells, ⊥ H3K27me3: **90**	A-395N	28135237	Y
29	MT: EZH2	GSK343	4	HCC1806, ↓ H3K27me3: **174**	-	24900432	Y
30	MT: EZH2/H1	UNC1999	10/45 ± 3	MCF10A, ↓ H3K27me3: **124 ± 11**	UNC2400	23614352	Y
31	MT: G9a/GLP	A-366	3.3/38	PC3, ↓ H3K9me2: **300**	-	24900801	Y
32		UNC0642	< 2.5	MDA-MB231, ↓ H3K9me2: **110** ; PC3: **130**	-	24102134	Y
33	MT: PRDM9	MRK-740	85	HEK293T, ↓ H3K4me3: **800**	MRK-740-NC	31848333	Y
34	MT: PRMT type 1	MS023	PRMT1/3/4/6/8: 39/135/93/4/5	HEK293T PRMT1/6, ↓ H4R3me2a/H3R2me2a: **9/56**	MS094	26598975	Y
35	MT: PRMT3	SGC707	31 ± 2	HEK293T flag-PRMT3, ↓ H4R3me2a: **91**	XY-1	25728001	Y
36	MT: PRMT4	SKI-73*/SKI-72	SKI-72: 13	(SKI-73) HEK293, ↓ med12-Rme2a: **540**	SKI-73N	31657716	New
37		TP-064	< 10	HEK293T, ↓ med12-Rme2a: **43**	TP-064N	29719619	Y
38	MT: PRMT5	GSK591	11	Z138, ↓ SmD3-Rme2s: **56** (EC_{50})	SGC2096	26985292	Y
39		LLY-283	22	MCF7, ↓ SmBB'-Rme2s: **30**	LLY-284	30034588	Y
40	MT: PRMT6	SGC6870	77	HEK293T, ↓ H4R3me2a: 800	SGC6870N		New
41	MT: PRMT7	SGC3027*/8158	< 2.5	C2C12, ↓ HSP70-Rme: **2400**	SGS3027N		Y
42	MT: SETD7	(R)-PFI-2	2.0 ± 0.2	MCF7, induces nuclear YAP: **100**	(S)-PFI-2	25136132	Y
43	MT: SMYD2	BAY-598	27	KYSE-150, ↓ p53K370me: **58**	BAY-369	27075367	Y
44		PFI-5	7	MCF7/HEK293T, ↓ p53K370me: **1000/3000**	PFI-5N	31415173	New
45	MT: SMYD3	BAY-6035	88 ± 16	HeLa, ↓ MEKK2K260me ~ **70**	BAY-444		Y
46	MT: SUV420H1/H2	A-196	21 ± 3	U2OS, ↓ H4K20me2/3: **500**	SGC2043	28114273	Y
47	PAD: PADI4	GSK484	50	NB4, ↓ H3 citrullination: **71**	GSK106	25622091	Y
48	PWWP (1st): NSD2	UNC6934	80	nanoBRET NSD2-PWWP1/H3.3 (in U2OS cells): **1090**	UNC7145		New
49	PWWP (1st): NSD3	BI-9321	166	nanoBRET NSD3-PWWP1/H3.3 (in U2OS cells): **1200**	BI-9466	31285596	Y
50	WD40: WDR5	OICR-9429	64	HEK293T Flag-WDR5, disrupt Wdr5-MLL: **223**	OICR-0547	26167872	Y

*pro-drug ; †alphascreen; ‡microscale thermophoresis, #ITC, ^{T}TR-FRET