DCP
Donated Chemical Probes
SGC

Chemical probes are validated biologically active small molecules, modulating the properties of their target protein(s).

The probes meet the following criteria:

- ✓ **Potency < 100 nM** (IC_{50} or K_D)
- ✓ **Selectivity within target family >30-fold**
- ✓ **Extensive off-targets profiling outside target family**
- ✓ **Cellular on-target activity < 1 µM** (IC_{50} or EC_{50})
- ✓ **100 x less potent control compound**
- ✓ **No PAINS elements**

Contact:
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www.sgc-frankfurt.de

Probe contribution

abbvie · Takeda · gsk · janssen · Boehringer Ingelheim · MSD INVENTING FOR LIFE · Pfizer · BAYER Science For A Better Life

Donated Chemical Probes

Target	Probe	Target	Probe
ACVR1B, TGFBR1	TP-008	ITGAL	BI-1950
ADRA1D	(R)-9s	KAT6A, KAT6B	WM-1119
ALOX5AP	BI 665915	KISS1R	KISS1-305
BCAT1/2	BAY-069	LHCGR	BAY-899
BCL2	A-1211212	LRRK2	MLi-2
BCL2L1	A-1155463	MALT1	NVS-MALT1
BCL6	TP-021	MAPK1/3	ERKi
BRD2, BRD3, BRD4, BRDT	BD1: GSK778, GSK789 BD2: GSK046, GSK620, GSK973	MAPK7	BAY-885
CCR1	BI 639667, BAY-3153	MAPK14	FS-694, Skepinone-L, SR-318
CFTR	A-1596586	MET	BAY-474
CHRM1	MSD-M1PAM	METAP2	TP-004
CLK1/2/3/4	T3-CLK	MGAT2	TP-020
CNR1	MRL-650	MIF	BTZO-1
Complex I	BAY-179	MMP12	BAY-7598
CYP11B2	MSD-CYP11B2	MMP13	BI-4394, T-26c
DDR1/2, MAPK11/14	SR-302	MRGPRX2	(R)-ZINC-3573
DRD4	ABT-724, UCSF924	NR3C1	BI 653048
DHODH	IPP/CNRS-A017	NUDT1	BAY-707
EDNRA	ABT-546	P2RX4	BAY-1797
EDNRB	A-192621	P2RY14	PPTN
ELANE	BAY-678	PDE10A	THPP-1
ENPP2	BI-2545	PRKAA1, RPS6KA1	BAY-3827
EP300, CREBBP	A-485	PTGDR2	CRTH2 antagonist
EPHX2	BI-1935	PTGER2	PF-04418948
F2R	BAY-386	PTGFR	BAY-6672
FAAH	PF-04457845	PTK2, PTK2B	PF-04554878
FASN	BI 99179	RIPK1	TP-030 -1, TP-030-2
FNTB	ABT-100	ROCK1/2	BAY-549
γ Secretase complex	GSM1, MRK-560	SLC2A1	BAY-876
GNRHR	BAY-784	SLC9A1	BI-9627
GPR52	TP-024	SOS1	BAY-293
GPR68	Ogerin	SYK	MRL-SYKi
HCV NS3	BI-1230	TBK1, IKBKE	BAY-985
HCV NS5B	BI 207127	TIE1, TEK, DDR1/2	BAY-826
HIV NNRT	BI-2540	TRPA1	A-079, BAY-390
IKBKB	BI 605906	TRPM8	PF-05105679

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Donated chemical probe library; Please visit https://www.sgc-ffm.uni-frankfurt.de

Target	Probe	Cellular Potency (human)	Cellular usage recommendation	Control	Donated by
ACVR1B, TGFBR1	TP-008	IC_{50} = ACVR1B: 526 ± 96 nM IC_{50} = TGFBR1: 245 ± 41 nM	1 -10 µM	AI11	Takeda
ADRA1D	(R)-9s	IC_{30} = 15 nM	< 1 µM	(S)-9s	Takeda
ALOX5AP	BI 665915	IC_{50} = 45 nM	30 – 500 nM	BI-0153	Boehringer Ingelheim
BCAT1/2	BAY-069	IC_{50} = BCAT1: 358 nM BCAT2: 874 nM	Coming soon	BAY-771	Bayer
BCL2	A-1211212	EC_{50} = 6 nM	< 5 µM	A-1210227	Abbvie
BCL2L1	A-1155463	IC_{50} = 0.55 nM	< 5 µM	A-1107969	Abbvie
BCL6	TP-021	IC_{50} = 0.72 µM	1 -10 µM	TP-021n	Takeda
BRD2, BRD3, BRD4, BRDT (BD1)	GSK778	pIC_{50} = 7.3	≤ 1 µM	No	GlaxoSmithKline
BRD2, BRD3, BRD4, BRDT (BD1)	GSK789	IC_{50} = 125 nM (MV-4–11 cells)	≤ 10 µM	GSK791	GlaxoSmithKline
BRD2, BRD3, BRD4, BRDT (BD2)	GSK046	pIC50 = 7.5 (LPS-PBMC assay)	≤ 10 µM	No	GlaxoSmithKline
BRD2, BRD3, BRD4, BRDT (BD2)	GSK620	pIC50 = 7.2 (LPS-PBMC assay)	≤ 10 µM	No	GlaxoSmithKline
BRD2, BRD3, BRD4, BRDT (BD2)	GSK973	pIC50 = 7.3 (MCP-1 whole blood)	≤ 10 µM	GSK943	GlaxoSmithKline
CCR1	BI 639667	IC_{50}= 2.4 nM	100 nM	BI-9307	Boehringer Ingelheim
CCR1	BAY-3153	-	≤ 100 nM	BAY-173	Bayer
CFTR	A-1596586	EC_{50} = 28 nM	< 1 µM	A-1596584	Abbvie
CHRM1	MSD-M1PAM	Inflection point = 136 nM	< 1 µM	MSD-M1PAM-NC	MSD
CLK1/2/3/4	T3-CLK	IC_{50} = CLK1: 3.49 nM ; CLK2: 16.6 nM ; CLK4: 1.98 nM	< 100 nM	T3-CLK-N	Takeda
CNR1	MRL-650	IC_{50} < 10 nM	< 1 µM	MRL-CB1-NC	MSD
Complex I	BAY-179	IC_{50} = 33 nM	Coming soon	BAY-070	Bayer
CYP11B2	MSD-CYP11B2	IC_{50} = 2.3 nM	25 -100 nM	MSD-CYP11B2 Negative control	MSD
DDR1/2, MAPK11, MAPK14	SR-302	IC_{50} = DDR1: 23 nM ; DDR2: 18 nM; MAPK11: 196 nM; MAPK14: 125 nM	100 nM	SR-301	SGC Frankfurt
DHODH	IPP/CNRS-A017	EC_{50}= 2.5 nM	< 100 nM	IPP/CNRS-A019	IPP/CNRS
DRD4	ABT-724	2.2 nM < EC_{50} < 12.4 nM	0.001 – 10 µM	A-769	Abbvie
DRD4	UCSF924	0.2 nM < EC_{50} < 4.2nM	1 µM	UCSF924NC	UCSF, UNC, Stanford University
EDNRA	ABT-546	IC_{50} = 0.59 nM	< 100 nM	A-545	Abbvie
EDNRB	A-192621	IC_{50} = 0.8 nM	< 300 nM	A-1806262	Abbvie
ELANE	BAY-678	-	Not for cell. use	BAY-677	Bayer
ENPP2	BI-2545	IC_{50} = 29 nM	1 µM	BI-3017	Boehringer Ingelheim
EP300, CREBBP	A-485	IC_{50} = 150 nM	0.8 µM	A-486	Abbvie
EPHX2	BI-1935	IC_{50} < 1 nM	< 1 nM	BI-2049	Boehringer Ingelheim
F2R	BAY-386	IC_{50}= 10 nM	Coming soon	BAY-448	Bayer
FAAH	PF-04457845	Complete inhibition	0.2 – 1 µM	PF-04875474	Pfizer
FASN	BI 99179	IC_{50} = 0.18 µM	1 – 10 µM	BI 99990	Boehringer Ingelheim
FNTB	ABT-100	IC_{50} = 0.73 nM	0.01 – 1000 nM	A-108	Abbvie
γ secretase complex	GSM1	IC_{50} < 100 nM	< 1 µM	GSM-NC	MSD
γ secretase complex	MRK-560	pM cellular potency	< 100 nM	GSI-NC	MSD
GNRHR	BAY-784	IC_{50} = 21 nM	< 1 µM	BAY-786	Bayer
GPR52	TP-024	EC_{50} = 93 nM	1 µM	TP-024n	Takeda
GPR58	Ogerin	pEC_{50} 6.83 (FLIPR)	< 1 µM	ZINC32547799	UNC
HCV NS3	BI-1230	EC_{50} = 4.6 nM (Genotype 1a) EC_{50} < 1.8 nM (Genotype 1b)	< 100 nM	BI-1675	Boehringer Ingelheim
HCV NS5B	BI 207127	EC_{50} = 23 nM (Genotype 1a) EC_{50} = 11 nM (Genotype 1b)	Coming soon	BI-7656	Boehringer Ingelheim
HIV NNRT	BI-2540	EC50 = 2.6 nM	Coming soon	BI-2439	Boehringer Ingelheim
IKBKB	BI 605906	EC_{50} = 0.7 – 0.9 µM	≤ 5 µM	BI-5026	Boehringer Ingelheim
ITGAL	BI-1950	3 nM < IC_{50} < 120 nM	100 nM	BI-9446	Boehringer Ingelheim
KAT6A, KAT6B	WM-1119	IC_{50} = 250 nM (EMRK1184 cell growth inhibition)	1 -10 µM	WM-2474	Monash University, SGC Toronto
KISS1R	KISS1-305	IC_{50} = 8.94 nM	1 nM -1 µM	KISS1-543	Takeda
LHCGR	BAY-899	IC_{50} = 185 nM	Coming soon	BAY-897	Bayer
LRRK2	MLi-2	IC_{50} = 3.5 nM; EC_{50} = 1.22 nM	< 1 µM	MLi-2-NC	MSD
MALT1	NVS-MALT1	IC_{50} = 3.4 nM (Jurkat IL-2 (IL2-RGA PMA + anti-CD28)	1 µM	NVS-MALT1-C	Novartis
MAPK1/3	ERKi	IC_{50} = 280 nM to 0 .85 µM (MAPK1); 6.69 µM (MAPK3) (NanoBRET)	1 µM	ERKi-NC	MSD
MAPK7	BAY-885	IC_{50} = 115 nM	1 µM	BAY-693	Bayer
MAPK14	FS-694	IC_{50} = 14.9 nM	100 nM (< 1 µM)	FM-743	Tübingen Uni/ SGC FFM
MAPK14	Skepinone-L	IC_{50} = 13.6 nM	1 µM	FM-743	Tübingen Uni/ SGC FFM
MAPK14	SR-318	IC_{50} = 3.7nM (p38α); IC_{50} = 10nM (p38β)	< 100 nM	SR-321	SGC FFM
MET	BAY-474	IC_{50} = 2.9 nM	0.001 -1 µM	BAY-827	Bayer
METAP2	TP-004	Accumulation of NMet14-3-3γ = 15 nM	0.2 – 1 µM	TPn-004	Takeda
MGAT2	TP-020	IC_{50} = 160 nM	1 – 10 µM	TP-020n	Takeda
MIF	BTZO-1	MEC2.0 = 820 nM; MEC1.5= 16 nM	0.8 -1 µM	BTZO-4	Takeda
MMP12	BAY-7598	-	< 10 nM	BAY-694	Bayer
MMP13	T-26c	IC_{50} < 100 nM	0.1 µM	T-26f	Takeda
MMP13	BI-4394	IC_{50} = 31 nM	0.1 µM	BI-4395	Boehringer Ingelheim
MRGPRX2	(R)-ZINC-3573	EC_{50} = 740 nM	< 1µM	(S)-ZINC-3573	UNC
NR3C1	BI 653048	IC_{50} = 23 nM	1 µM	BI-3047	Boehringer Ingelheim
NUDT1	BAY-707	EC_{50} = 7.6 nM	0.001 – 1 µM	BAY-604	Bayer
P2RX4	BAY-1797	IC_{50} = 274 nM	0.1 – 1 µM	BAY-207	Bayer
P2RY14	PPTN	-	~ 100 nM	PPTN-NC	MSD
PDE10A	THPP-1	IC_{50} = 49 nM	~ 100 nM	THPP-1-NC	MSD
PRKAA1, RPS6KA1	BAY-3827	IC_{50} = 1.4 nM (PRKAA1); IC_{50} = 9.1 nM (RPS6KA1)	150 nM	BAY-974	Bayer
PTGDR2	CRTH2 antagonist	IC_{50} = 3 nM	0.1 – 1 µM	CRTH2 negative control	MSD
PTGER2	PF-04418948	Kg = 5.4 nM	< 300 nM	PF-04475866	Pfizer
PTGFR	BAY-6672	IC_{50} = 11 nM	≤ 500 nM	BAY-403	Bayer
PTK2, PTK2B	PF-04554878	IC_{50} = 3 nM	Coming soon	PF-00911705	Pfizer
RIPK1	TP-030-1	IC_{50} = 18 nM	100 nM	TP-030n	Takeda
RIPK1	TP-030-2	IC_{50} = 1.3 nM	100 nM	TP-030n	Takeda
ROCK1/2	BAY-549	IC_{50} = 65 nM	< 100 nM	BAY-4900	Bayer
SLC2A1	BAY-876	IC_{50} = 3.2 nM	0.1 – 75 nM	BAY-588	Bayer
SLC9A1	BI-9627	IC_{50} = 31 nM	< 5 µM	BI-0054	Boehringer Ingelheim
SOS1	BAY-293	IC_{50} < 1 µM	0.02 – 1.1 µM	BAY-294	Bayer
SYK	MRL-SYKi	IC_{50} < 100 nM (cell. assay); IC_{50} < 300 nM (whole blood)	100 nM	MRL-SYKi-NC	MSD
TBK1, IKBKE	BAY-985	TBK1: IC_{50}= 312 nM; IKBKE IC_{50}= 1725 nM (NanoBRET)	< 1 µM	BAY-440	Bayer
TIE1, TEK, DDR1/2	BAY-826	IC_{50} = TIE1: 2.7 nM, TEK: 0.7 nM, DDR1: 3 nM, DDR2: 4.5 nM	< 500 nM	BAY-309	Bayer
TRPA1	A-079	IC_{50} = 51 nM	1 µM	A-226	Abbvie
TRPA1	BAY-390	IC_{50} = 82 nM	100 nM	BAY-9897	Bayer
TRPM8	PF-05105679	IC_{50} = 103 (± 29.4) nM	Coming soon	PF-05257137	Pfizer