

The background features a complex network diagram with white and grey nodes connected by thin lines. Several red triangles of various sizes are scattered across the light grey background. The TargetMol logo is positioned in the upper left corner.

**TargetMol**

A Drug Screening Expert

2018-2019

# **INHIBITORS OF SIGNALING PATHWAYS**

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*Inhibitors, Libraries, Natural Compounds*

## About us

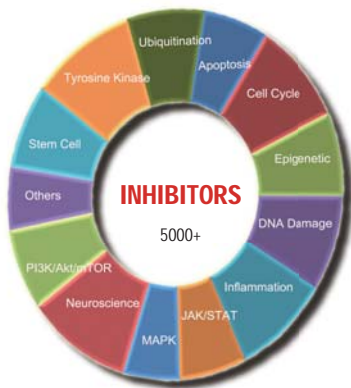
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## Our Product Portfolio

### Inhibitor

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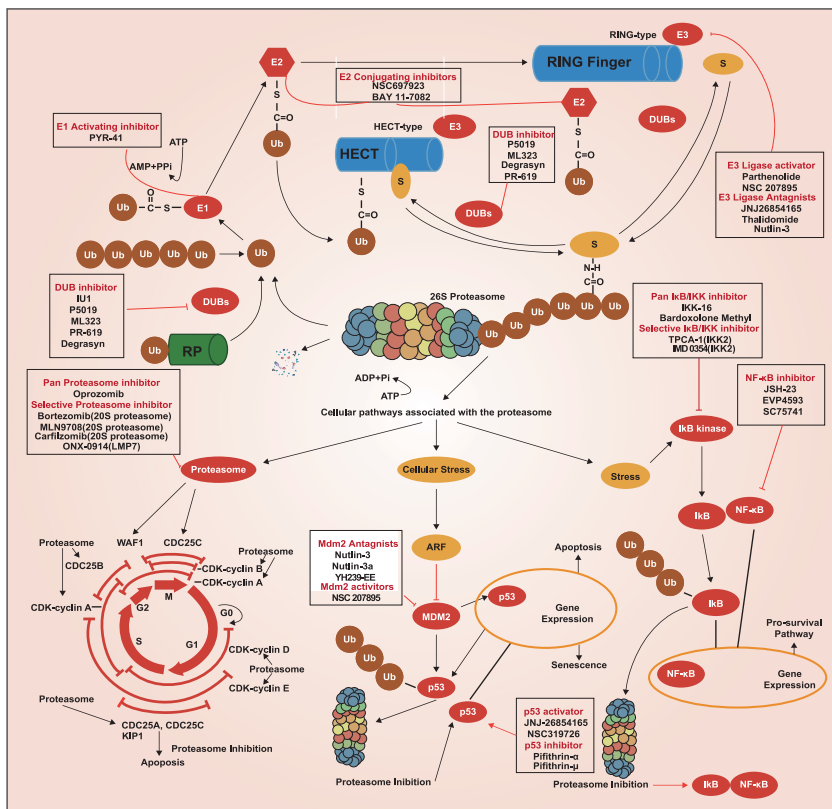
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# Proteases/Proteasome






## Proteasome

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2399	Bortezomib (PS-341)	179324-69-7	Selective	20S proteasome	(Ki) 0.6 nM	FDA Approved	Mantle-cell lymphoma; Multiple myeloma
T2154	MG-132	133407-82-6	Selective	20S proteasome	100 nM		
T1795	Carfilzomib (PR-171)	868540-17-4	Selective	20S proteasome	<5 nM	FDA Approved	Multiple myeloma
T2016	MLN9708	1201902-80-8	Selective	LMP7	10 nM		

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# Chromatin/Epigenetics

	Epigenetic Writer	Epigenetic Reader	Epigenetic Eraser
<p><b>Pan inhibitor</b> I-BET151 I-BET-762 <b>Selective inhibitor</b> RVX-208(BRD2) UNC1215(L3MBTL3)</p>		<p><b>Alteration of DNA-templated Process</b></p> 	
<p><b>Histone Acetylation</b></p> <p><b>Histone Acetyltransferase inhibitor</b> C646 MG149</p>	<p><b>Histone Acetyltransferase (HATs)</b> GCN5/PCAF GNAT Related (e.g., HAT1) Myst Family (e.g. TIP60, HBO1) <b>CBP/p300 Family</b> TAF250 Family <b>Src Family</b> (e.g. Src3, Src1)</p>	<p><b>Bromodomain Proteins</b> e.g. most HATs <b>BET Family</b> (BRD2, BRD, BDF) Brg-1</p>	<p><b>Histone Deacetylases (HDACs)</b> Class I: HDAC1-3 HDAC8 Class IIa: HDAC4-5 HDAC7 HDAC9 Class IIb: HDAC6 HDAC10 Class III: Sirt 1-7 Class IV: HDAC11</p>
<p><b>Histone Methylation</b></p> <p><b>Histone Methyltransferase inhibitor</b> Decitabine Azacitidine SGI-1027 RG108 Zebularine</p>	<p><b>Lysine Methyltransferase (KMTs)</b> KMT1A—1F (e.g. G9a, GLP) MLL Family (e.g. NSD1) DOT1/DOT1L KMT3A-KMT3C KMT5A, KMT5B <b>KMT6/EZH2</b> KMT7/SET7&amp;9 KMT8/RIZ1</p>	<p><b>Royal Family</b> -Chromo-domain Proteins e.g. HP-1 like -Tudor-domain Proteins, e.g. SMN -PHD Proteins, e.g. CBD, ING2, DNMT3L</p>	<p><b>Lysine Demethylases (KDMs)</b> LSD1/KDM JHDM/Jumonji</p>
<p><b>Histone Phosphorylation</b></p> <p><b>DNA Methyltransferase inhibitor</b> Pinomostostat BIX 01294 EP2005687 Lomeguatrab</p>	<p><b>Serine/Threonine Kinases</b> e.g. MST, <b>AMPK</b> Haspin, VRK, <b>Aurora B</b> <b>PKC<math>\alpha</math></b>, <b>PKC<math>\beta</math></b>, <b>MSK1/2</b>, <b>JNK</b></p>	<p><b>14-3-3 Proteins</b>  Seven Isoforms: theta, gamma, zeta, eta, epsilon, beta, mu</p>	<p><b>Protein Phosphatases</b> e.g. Serine/Threonine Phosphatases (PPP2CA, PPP2CB, PPP1CC) Protein Phosphatase 1D Eye-absent Homologues(EYA1-3)</p>
<p><b>DNA Methylation</b></p>	<p><b>DNMT1</b> <b>DNMT3A</b> <b>DNMT3B</b></p>	<p>MeCP2 MBD1-4</p>	<p>Not Clear  —only putative targets so far</p>

## Epigenetic Reader Domain

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2110	(+)-JQ-1	1268524-70-4	Selective	BRD4(1) BRD4(2)	77 nM 33 nM		
T2480 <b>NEW</b>	RVX-208	1044870-39-4	Selective	BD2	0.51 $\mu$ M	Phase 2	Diabetes
T1906 <b>NEW</b>	GSK-525762A (I-BET-762)	1260907-17-2	Pan	BET proteins	~35 nM		
T2442 <b>NEW</b>	CPI-203	202591-23-9	Selective	BRD4	37		
T2379 <b>NEW</b>	UNC1215	1415800-43-9	Selective	L3MBTL3	40		

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## Aurora Kinase

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T3068	AT9283	896466-04-9	Selective	Aurora A	3 nM	Phase 1	Non-Hodgkins Lymphoma; Unspecified Adult Solid Tumor
				Aurora B	3 nM		
T2241	MLN8237 (Alisertib)	1028486-01-2	Selective	<b>Aurora A</b>	<b>1.2 nM</b>	Phase 3	Advanced Solid Tumors; Relapsed Lymphoma
				Aurora B	396.5 nM		
T2509	VX-680 (Tozasertib, MK-0457)	639089-54-6	Pan	Aurora A	Ki (0.6 nM)	Phase 2	Advanced Cancer
				Aurora B	Ki (18 nM)		
				Aurora C	Ki (4.6 nM)		
T2602	Barasertib (AZD1152-HQPA)	722544-51-6	Selective	<b>Aurora B</b>	<b>0.37 nM</b>	Phase 1	Acute Myeloid Leukaemia
				Aurora A	1368 nM		
T2617	SNS-314 Mesylate	1146618-41-8	Pan	Aurora A	9 nM	Phase 1	
				Aurora B	31 nM		
				Aurora C	3 nM		

## HDAC

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T6233	Entinostat (MS-275)	209783-80-2	Pan	HDAC1 HDAC3	0.51 $\mu$ M 1.7 $\mu$ M	Phase 2	Non-Small Cell Lung Cancer
T2383	Panobinostat (LBH589)	404950-80-7	Pan	HDAC	5 nM	Phase 3	
T6270	Trichostatin A	58880-19-6	Pan	<b>HDAC</b>	<b>~1.8 nM</b>		
T1857 <small>NEW</small>	TMP269	1314890-29-3	Pan	HDAC4	157 nM		
				HDAC5	97 nM		
				HDAC7	43 nM		
				HDAC9	23 nM		
T1819 <small>NEW</small>	Nexturastat A	1403783-31-2	Selective	<b>HDAC6</b>	<b>5 nM</b>		
T1762	RGFP 966	1357389-11-7	Selective	HDAC3	0.08 $\mu$ M		

## PARP

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T6224	Iniparibnbn(BSI-201)	160003-66-7	Selective	PARP1	N/A	Phase 2	Breast Cancer
T3015	Olaparib (AZD2281, Ku-0059436)	763113-22-0	Pan	PARP1	5 nM	Phase 2	Cancer
				<b>PARP2</b>	<b>1nM</b>		
T2591	Veliparib(ABT-888)	912444-00-9	Pan	PARP1	Ki(5.2 nM)	Phase 3	
				PARP2	Ki(2.9 nM)		

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## Histone Methyltransferase

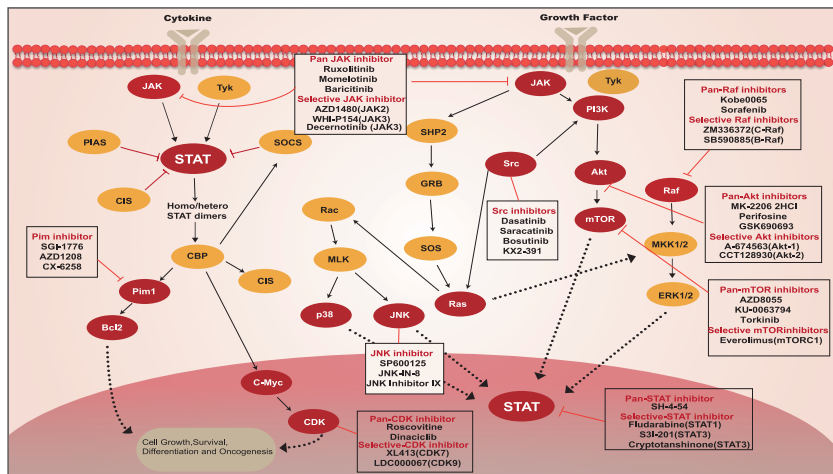
ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T3099	EPZ5676	1380288-87-8	Selective	DOT1L	Ki(80 pM)	Phase 1	
T1905	EPZ005687	1396772-26-1	Selective	EZH2	Ki(24 nM)		
T1959	BIX 01294	1392399-03-9	Selective	G9a	2.7 $\mu$ M		
T3082	SGC0946	1561178-17-3	Selective	DOT1L	0.3 nM		
T3057 <small>NEW</small>	UNC1999	1431612-23-5	Selective	EZH2	2 nM		
				EZH1	45 nM		
T3081 <small>NEW</small>	EPZ004777	1338466-77-5	Selective	DOT1L	0.3 nM		

## Sirtuin

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T6111	EX 527 (Selsistat)	49843-98-3	Selective	SIRT1	38 nM		
T6671	Sirtinol	410536-97-9	Pan	SIRT1	131 $\mu$ M		
				SIRT2	38 $\mu$ M		
T2412	SRT1720	1001645-58-4	Selective	SIRT1 (activator)	EC <sub>50</sub> (0.16 $\mu$ M)		
T2174	Quercetin	117-39-5	Selective	SIRT1 (activator)		Phase 3	Thromboembolism

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# JAK/STAT Signaling



## JAK

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T3043	Ruxolitinib (INCB-18424) phosphate	1092939-17-7	Pan	JAK1 JAK2	3.3 nM 2.8 nM	FDA Approved	Oxidative Stress
T3066	S-Ruxolitinib	1160597-27-2	Selective	JAK1 JAK2 JAK3	3.2 nM 2.8 nM 428 nM	Phase 4	Myelofibrosis (PMF); Splenomegaly
T2398	Tofacitinib Citrate (CP-690550)	540737-29-9	Selective	JAK3 JAK1 JAK2	1 nM 112 nM 20 nM	FDA Approved	
T3069	AZD1480	935666-88-9	Selective	JAK2	0.26nM	Phase 1	Myelopro liferative Diseases
T1995	Fedratinib (SAR302503, TG101348)	936091-26-8	Selective	JAK2 JAK2 (V617F)	3 nM 3 nM	Phase 2	

## STAT

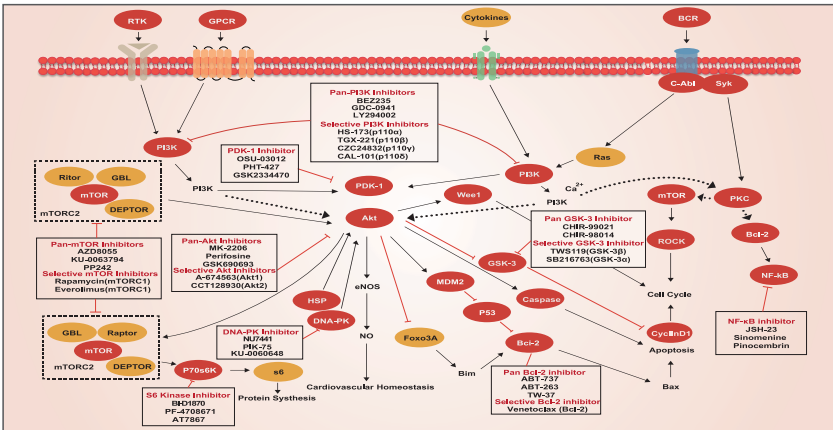
ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2505	SJI-201; NSC 74859	501919-59-1	Selective	STAT3	86 μ M		
T1038	Fludarabine	21679-14-1	Selective	STAT1	N/A	FDA Approved	
T6308	Stattic	19983-44-9	Selective	STAT1	5.1 μ M		
T0711	Niclosamide	50-65-7	Selective	STAT	0.7 μ M	FDA Approved	
T2814	Cryptotanshinone	35825-57-1	Selective	STAT3	4.6 μ M		



EGFR

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T0373L	Erlotinib hydrochloride	183319-69-9	Selective	EGFR/ErbB1	2 nM	FDA Approved	Breast Cancer
T1181	Gefitinib (ZD1839)	184475-35-2	Selective	Tyr1173 (NR62 cells)	26 nM	FDA Approved	Cancer
				Tyr1173 (NR6wtEGFR cells)	37 nM		
				Tyr992 (NR6wtEGFR cells)	37 nM		
				Tyr992 (NR6W cells)	57 nM		
T2303	Afatinib (BIBW2992)	439081-18-2	Pan	EGFR(L858R)	0.4 nM	FDA Approved	Renal Insufficiency
				EGFR(wt)	0.5 nM		
				EGFR(L858R/T790M)	10 nM		
				HER2/ErbB2	14 nM		
T0078	Lapatinib	231277-92-2	Pan	EGFR/ ErbB1	10.8 nM	FDA Approved	Colorectal Cancer; Lung Cancer; Head and Neck Cancer
				EGFR/ ErbB2	9.2 nM		

PI3K/Akt/mTOR Signaling



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## PI3K Inhibitor

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2235	BEZ235 (Dactolisib)	915019-65-7	Pan	p110 $\alpha$	4 nM	Phase2	Pancreatic Neuroendocrine Tumors
				p110 $\gamma$	5 nM		
				p110 $\delta$	7 nM		
T1994	GDC-0941	957054-30-7	Selective	p110 $\alpha$	3 nM	Phase2	Breast Cancer; Non-Squamous Non-Small Cell Lung Cancer
				p110 $\beta$	33 nM		
				p110 $\delta$	3 nM		
T2008	LY294002	154447-36-6	Pan	p110 $\alpha$	0.5 $\mu$ M		
				p110 $\beta$	0.97 $\mu$ M		
				p110 $\delta$	0.57 $\mu$ M		
T1827	BKM120 (NVP-BKM120, Buparlisib)	944396-07-0	Pan	p110 $\alpha$	52 nM	Phase2	Breast Cancer
				p110 $\beta$	166 nM		
				p110 $\delta$	116 nM		
T1879	3-Methyladenine (3-MA)	5142-23-4	Pan	Vps34	25 $\mu$ M		
				p110 $\gamma$	60 $\mu$ M		
T2308	HS-173	1276110-06-5	Selective	p110 $\alpha$	0.8 nM		
T2661	TGX-221	663619-89-4	Selective	p110 $\beta$	5 nM		
T1949	CZC24832	1159824-67-5	Selective	p110 $\gamma$	27 nM		
T1894	CAL-101 (Idelalisib, GS-1101)	870281-82-6	Selective	p110 $\delta$	2.5 nM	FDA Approved	

## Akt Inhibitor

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1952	MK-2206 2HCl	1032350-13-2	Pan	Akt1	8 nM	Phase2	
				Akt2	12 nM		
				Akt3	65 nM		
T1920	AZD-5363	1143532-39-1	Pan	Akt1	3 nM	Phase2	
				Akt2	8 nM		
				Akt3	8 nM		
T2492	Perifosine (KRX-0401)	157716-52-4	Pan	Akt	4.7 $\mu$ M	Phase3	

## ATM/ATR

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T3032	VE-821	1232410-49-9	Selective	ATM	12.9 nM		
T2685	KU55933	587871-26-9	Selective	ATM	6.3 nM		
T2474	KU-60019	925701-49-1	Selective	ATR	26 nM		
T2669	VE822	1232416-25-9	Selective	ATR	19 nM		
T1958	AZ20	1233339-22-4	Selective	ATR	5 nM		

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## mTOR Inhibitor

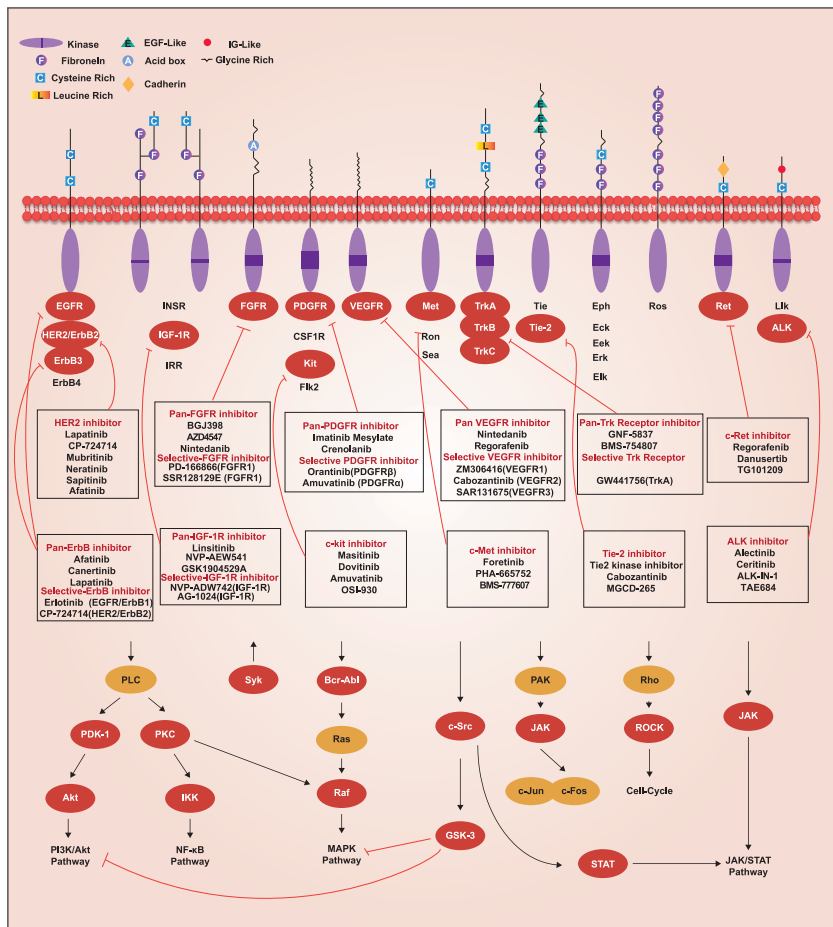
ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1784	Everolimus (RAD001)	159351-69-6	Pan	mTOR	1.6-2.4 nM	FDA approved	
T1859	AZD8055	1009298-09-2	Pan	mTOR	0.8 nM	Phase1	Solid Tumors; Glioblastoma Multiforme
T1537	Rapamycin (Sirolimus)	53123-88-9	Pan	mTOR	0.1 nM	FDA approved	
T2145	Temsirolimus (CCI-779, NSC 683864)	162635-04-3	mTORC1 Selective	mTOR	1.76 $\mu$ M	FDA approved	
T1838	INK 128 (MLN0128)	1224844-38-5	Pan	mTOR	1 nM	Phase2	Thyroid Cancer; Prostate Cancer; Breast Cancer

## GSK-3 inhibitor

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2310	CHIR-99021 HCL	252917-06-9	Pan	GSK-3 $\alpha$	10 nM		
				GSK-3 $\beta$	6.7 nM		
T3077	SB216763	280744-09-4	Pan	GSK-3 $\alpha$	34.3 nM		
				GSK-3 $\beta$	~34.3 nM		
T2166	TWS119	601514-19-6	Selective	GSK-3 $\beta$	30 nM		
T1917	6-BIO	667463-62-9	Pan	GSK-3 $\alpha$	5 nM		
				GSK-3 $\beta$	5 nM		
T2608	CHIR-98014	252935-94-7	Pan	GSK-3 $\alpha$	0.65 nM		
				GSK-3 $\beta$	0.58 nM		
T1957	AZD2858	486424-20-8	Pan	GSK-3	68 nM		
T1881	AR-A014418	487021-52-3	Selective	GSK-3 $\beta$	104 nM		
T3067	Tideglusib	865854-05-3	Selective	GSK-3 $\beta$	60 nM	Phase2	

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# Tyrosine Kinase/Adaptors



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## VEGFR

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1797	XL184 (Cabozantinib malate)	1140909-48-3	Selective	VEGFR2	0.035 nM	FDA Approved	Renal cancer; Thyroid cancer
T1656	Vandetanib (ZD6474)	443913-73-3	Selective	VEGFR2	40 nM	FDA Approved	Thyroid cancer
T1452	Axitinib	319460-85-0	Pan	VEGFR1	0.1 nM	FDA Approved	Renal cancer
				VEGFR2	0.2 nM		
				VEGFR3	0.1-0.3 nM		
T1777	Nintedanib (BIBF 1120)	656247-17-5	Pan	VEGFR1	34 nM	Phase 3	Idiopathic pulmonary fibrosis; Non-small cell lung cancer
				VEGFR2	13 nM		
				VEGFR3	13 nM		
T2421 <small>NEW</small>	SKLB1002	1225451-84-2	Selective	VEGFR2	32 nm		

## c-MET

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1661	Crizotinib	877399-52-5	Non-specific	c-MET ALK	11 nM 24 nM	FDA Approved	Non-small cell lung cancer
T3113	Foretinib (GSK1363089)	849217-64-7	Non-specific	Met KDR	0.4 nM 0.9 nM	Phase 2	Cancer
T2293	SGX-523	1022150-57-7	Selective	Met	4 nM	Phase 1	Solid tumours
T1963	INCB28060 (Capmatinib)	1029712-80-8	Selective	c-Met	0.13 nM	Phase 2	Glioblastoma; Hepatocellular carcinoma; Non-small cell lung cancer

## Bcr-Abl

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1621	Imatinib Mesylate (STI571)	220127-57-1	Non-specific	v-Abl	600 nM	FDA Approved	Acute lymphoblastic leukaemia; Chronic myeloid leukaemia
				c-Kit	100 nM		
				PDGFR	100 nM		
T1448L	Dasatinib monohydrate	863127-77-9	Non-specific	Abl Src	<1 nM 0.8 nM	FDA Approved	
T1524	Nilotinib (AMN-107)	641571-10-0	Selective	Bcr-Abl	<30 nM	FDA Approved	Chronic myeloid leukaemia
T1803 <small>NEW</small>	GNF-5	778277-15-9	Selective	Bcr-Abl	220 nM		

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## PDGFR

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T6230	Imatinib (STI571)	152459-95-5	Pan	PDGFR	100 nM	FDA Approved	
				c-Kit	100 nM		
T0374	Sunitinib Malate	341031-54-7	Selective	PDGFR $\beta$	2 nM	FDA Approved	Gastrointestinal stromal tumours; Pancreatic cancer; Renal cancer
T2677	Crenolanib (CP-868596)	670220-88-9	Pan	PDGFR $\alpha$	2.1 nM	Phase 3	Acute myeloid leukaemia; Gastrointestinal stromal tumours
				PDGFR $\beta$	3.2 nM		
T6184	TSU-68 (SU6668, Orantinib)	252916-29-3	Selective	PDGFR $\beta$	8 nM	Phase 3	Solid tumours
T1452	Axitinib	319460-85-0	Pan	PDGFR $\beta$	1.6 nM	FDA Approved	Renal cancer
				c-Kit	1.7 nM		

## FGFR


ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1975	BGJ398 (NVP-BGJ398)	872511-34-7	Pan	FGFR1	0.9 nM	Phase 2	Bladder cancer; Cholangiocarcinoma; Glioblastoma; Haematological malignancies
				FGFR2	1.4 nM		
				FGFR3	1.0 nM		
				FGFR3 (K650E)	4.9 nM		
T2642	PD173074	219580-11-7	Selective	FGFR1	0.37 nM		
T1948	AZD4547	1035270-39-3	Pan	FGFR1	0.2 nM	Phase 2/3	Non-small cell lung cancer
				FGFR2	1.5 nM		
				FGFR3	2.8 nM		
				FGFR4	165 nM		
T6082 <small>NEW</small>	SSR128129E	848318-25-2	Selective	FGFR1	1.9 $\mu$ M		

## HER2

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T0078L	Lapatinib ditosylate	388082-78-8	Pan	EGFR/ErbB2	10.8 nM	FDA Approved	Breast cancer
				HER2/ErbB2	9.8 nM		
T2325	Neratinib(HKI-272)	698387-09-6	Pan	EGFR/ErbB2	92 nM	Phase 2	
				HER2/ErbB2	59 nM		

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## ALK

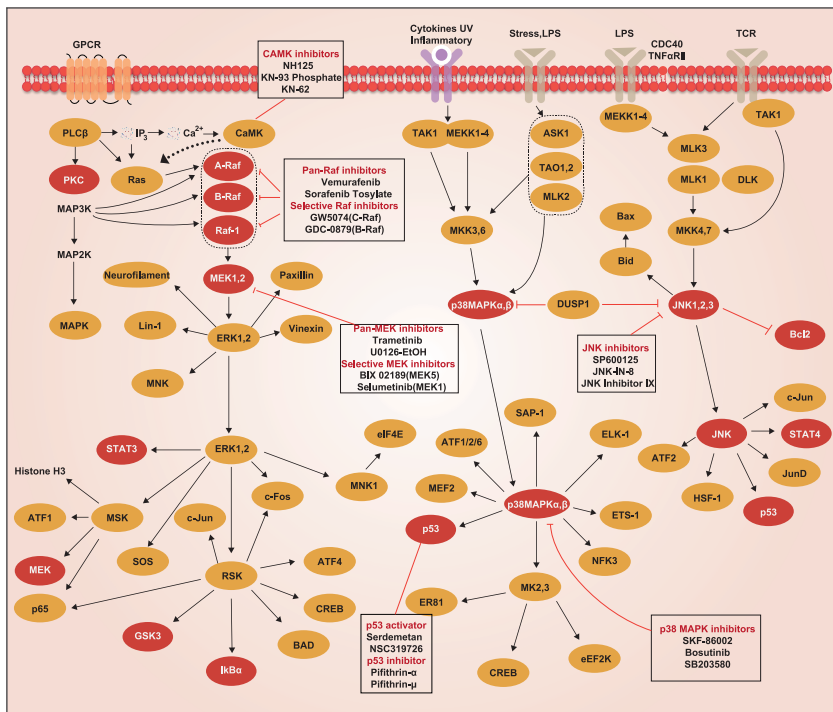
ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2251	TAE684 (NVP-TAE684)	761439-42-3	Selective	ALK	3 nM		
T1936	Alectinib (CH5424802)	1256580-46-7	Mutant-targeted	ALK	1.9 nM	FDA Approved	Non-small cell lung cancer
				ALK(F1174L)	1 nM		
				ALK(3.5)	3.5 nM		
T1791	LDK378(Ceritinib)	1032900-25-6	Selective	ALK	0.2 nM	Phase 3	
				InsR	7 nM		
				IGF-1R	8 nM		
T1962 	ASP 3026	1097917-15-1	Non-specific	ALK	3.5 nM		

## FLT3

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2066	Quizartinib (AC220)	950769-58-1	Mutant-targeted	FLT3(WT)	4.2 nM	Phase 3	Acute myeloid leukaemia
				FLT3(ITD)	1.1 nM		
T2341	KW2449	1000669-72-6	Mutant-targeted	FLT3	6.6 nM	Phase 1	
				FLT3(D835Y)	1 nM		
				Abi	14 nM		
				Abi(t315i)	4 nM		

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# MAPK Signaling



## MEK

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T6218	Selumetinib (AZD6244)	606143-52-6	Selective	MEK1	14 nM	Phase 1	Solid Tumours
T6189	PD0325901	391210-10-9	Pan	MEK	0.33 nM	Phase 2	
T2125	Trametinib (GSK1120212)	871700-17-3	Pan	MEK1	0.92 nM	FDA Approved	Malignant melanoma
				MEK2	1.8 nM		
T2443	PD184352(CI-1040)	212631-79-3	Pan	MEK1	17 nM	Phase 2	
				MEK2	17 nM		
T2623	PD 98059	167869-21-8	Selective	MEK1	1 μM		
T6636	Refametinib (RDEA119, Bay 86-9766)	923032-37-5	Pan	MEK2	19 nM	FDA Approved	Neoplasms
				MEK1	47 nM		

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## Raf

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1903	Dabrafenib (GSK2118436)	1195765-45-7	Mutant-targeted	B-Raf(V600E)	0.8 nM	FDA Approved	Neoplasms, Brain
				B-Raf	3.2 nM		
				C-Raf	5 nM		
T0093L	Sorafenib	284461-73-0	Pan	Raf-1	6 nM	FDA Approved	Hepatocellular Carcinoma
				B-Raf	22 nM		
				B-Raf(V599E)	38 nM		
				VEGFR2/Flk1	15 nM		
T0093	Sorafenib tosylate	475207-59-1	Pan	Raf-1	6 nM	FDA Approved	
				B-Raf	22 nM		
				B-Raf(V599E)	38 nM		
				VEGFR2/Flk1	15 nM		
T2382	Vemurafenib (PLX4032, RG7204)	918504-65-1	Mutant-targeted	B-Raf(V600E)	31 nM	FDA Approved	
				B-Raf	100 nM		
				C-Raf	48 nM		
T2473	PLX4720	918505-84-7	Mutant-targeted	C-Raf-1 (Y340D/Y341D)	6.7 nM		
				B-Raf(V600E)	13 nM		
				B-Raf	160 nM		

## p38 MAPK

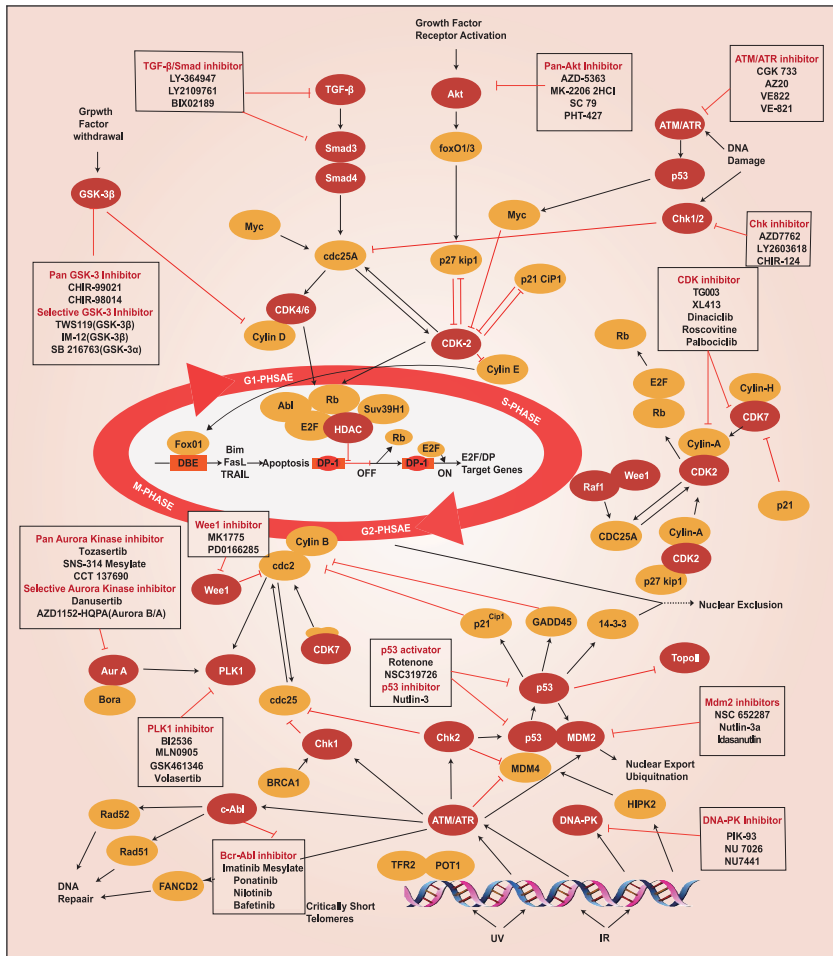
ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2301	SB202190 (FHPI)	152121-30-7	Pan	p38 $\alpha$ MAPK	50 nM		
				p38 $\beta$ MAPK	100 nM		
T6277	BIRB 796 (Doramapimod)	285983-48-4	Selective	p38 $\alpha$ MAPK	0.1 nM		
T1764	SB203580	152121-47-6	Pan	p38 MAPK	0.3-0.5 $\mu$ M		
				PKB	3-5 $\mu$ M		
T6047	LY2228820	862507-23-1	Selective	p38 $\alpha$ MAPK	7 nM	Phase 1/2	
T1974	PH797804	586379-66-0	Pan	p38 $\alpha$ MAPK	26 nM	phase 2	
				p38 $\beta$ MAPK	102 nM		

## ERK

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1956	FR180204	865362-74-9	Selective	ERK1	Ki(0.31 $\mu$ M)		
				ERK2	Ki(0.14 $\mu$ M)		
T6066 <small>NEW</small>	SCH772984	942183-80-4	Selective	ERK1	4 nM		
				ERK2	1 nM		
T6511	GDC-0994	1453848-26-4	Selective	ERK1	1.1 nM	Phase 1	
				ERK2	0.3 nM		

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# Cell Cycle/Checkpoint



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## CDK

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1785	Palbociclib	571190-30-2	Pan	CDK4/ CyclinD3	9 nM	FDA Approved	Breast cancer
				CDK4/ CyclinD1	11 nM		
				CDK6/ CyclinD2	15 nM		
T2095	Roscovitine (CYC202, Seliciclib)	186692-46-6	Pan	CDK5/p35	0.16 $\mu$ M	Phase 2	Non-small Cell Lung Cancer
				Cdc2/ CyclinB	0.65 mm		
				CDK2/ CyclinA	0.7 $\mu$ M		
				CDK2/ CyclinE	0.7 $\mu$ M		
T1912	Dinaciclib (SCH727965)	779353-01-4	Pan	CDK1	3 nM	Phase 3	Chronic lymphocytic leukaemia
				CDK2	1 nM		
				CDK5	1 nM		
				CDK9	4 nM		
T1901 <small>NEW</small>	TG003	300801-52-9	Pan	Clk1	20 nM		
				Clk2	200 nM		
				Clk4	15 nM		
T6563	LDC000067	1073485-20-7	Selective	CDC7	3.4 nM		
T6735	XL413 (BMS-863233)	1169562-71-3	Selective	CDK9	44 nM		

## Chk

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T6093	AZD7762	860352-01-8	Pan	Chk1	5 nM	Phase 1	
				Chk2	<10 nM		
T6084	LY2603618	911222-45-2	Selective	Chk1	N/A	Phase 2	
T6350	CHIR-124	405168-58-3	Selective	Chk1	0.3 nM		
				Chk2	697.4 nM		
T6028	PF-477736	952021-60-2	Selective	Chk1	Ki(0.49 nM)	Phase 1	
				Chk2	Ki(47 nM)		

## PLK

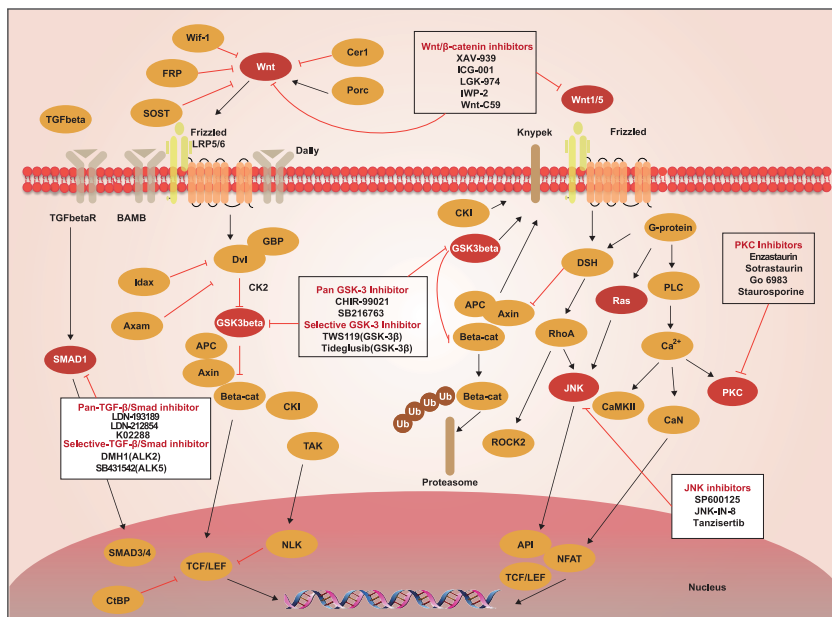
ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T6173	BI 2536	755038-02-9	Pan	Plk1	0.83 nM	Phase 2	
				Plk2	3.5 nM		
				Plk3	9 nM		
T2704	MLN0905	1228960-69-7	Selective	Plk1	2 nM		
T2634	Ro3280	1062243-51-9	Selective	Plk1	3 nM		
T6019	Volasertib (BI 6727)	755038-65-4	Selective	Plk1	0.87 nM	Phase 3	Acute myeloid leukaemia
T6070	Rigosertib (ON-01910)	1225497-78-8	Selective	Plk1	9 nM	Phase 3	
T6282	GSK461364	929095-18-1	Selective	Plk1	Ki(2.2 nM)	Phase 1	

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Rock

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1725	Y-27632 2HCl	129830-38-2	Pan	ROCK1	140 nM		
				ROCK2	300 nM		
T3060	Fasudil (HA-1077) HCl	105628-07-7	Non-specific	ROCK2	0.33 $\mu$ M	FDA Approved	Cerebral ischaemia; Cerebral vasospasm
				PKA	1.6 $\mu$ M		
				PKG	1.6 $\mu$ M		
				PKC	3.3 $\mu$ M		
T2155	Thiazovivin	1226056-71-8	Pan	ROCK	$\sim$ 0.5 $\mu$ M		
T1898	RKI-1447	1342278-01-6	Pan	ROCK1	14.5 nM		
				ROCK2	6.2 nM		
T2633	GSK429286A	864082-47-3	Pan	ROCK1	14 nM		
				ROCK2	63 nM		

Stem Cell



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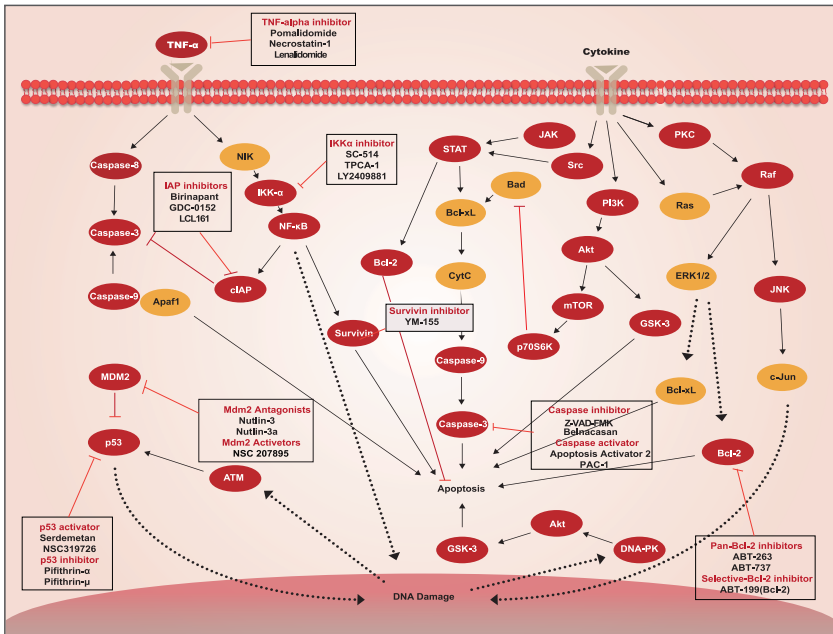
## TGF-beta/ Smad

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1726	SB 431542	301836-41-9	Selective	ALK5	94 nM		
T1935	LDN-193189	1062368-24-4	Pan	ALK2	20 nM		
				ALK3	30 nM		
T1763	SB525334	356559-20-1	Selective	TGF $\beta$ R1/ALK5	14.3 nM		
T1900	LDN212854	1432597-26-6	Pan	ALK1	2.4 nM		
				ALK2	1.3 nM		
				ALK3	85.8 nM		
				ALK4	2133 nM		

## Wnt beta-catenin

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1878	XAV939	284028-89-3	Selective	TNKS1	11 nM		
				TNKS2	4 nM		
T2242	Wnt-C59	1243243-89-1	Selective	Porcn	74 Pm		
T2618	LGK-974	1243244-14-5	Pan	Porcn	0.4 nM	Phase 2	Colorectal cancer

## Apoptosis



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## Bcl-2

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2101	ABT-263 (Navitoclax)	923564-51-6	Pan	Bcl-XI	(Ki) ≤ 0.5 nM	Phase 2	
				Bcl-2	(Ki) ≤ 1 nM		
				Bcl-W	(Ki) ≤ 1 nM		
T6275	Obatoclax Mesylate (GX15-070)	803712-79-0	Selective	Bcl-2	220 nM		
T2099	ABT-737	852808-04-9	Pan	Bcl-XI	78.7 nM	Phase 2	
				Bcl-2	30.3 nM		
				Bcl-W	197.8 nM		
T2119	ABT-199 (GDC-0199)	1257044-40-8	Selective	Bcl-XI	(Ki)<0.01nM	FDA Approved	Chronic lymphocytic leukaemia
				Bcl-2	(Ki)<48 nM		
				Bcl-W	(Ki)<246 nM		
				Mcl-1	(Ki)>444 nM		
T1980	HA14-1	65673-63-4	Selective	Bcl-2	~9 μ M		

## p53

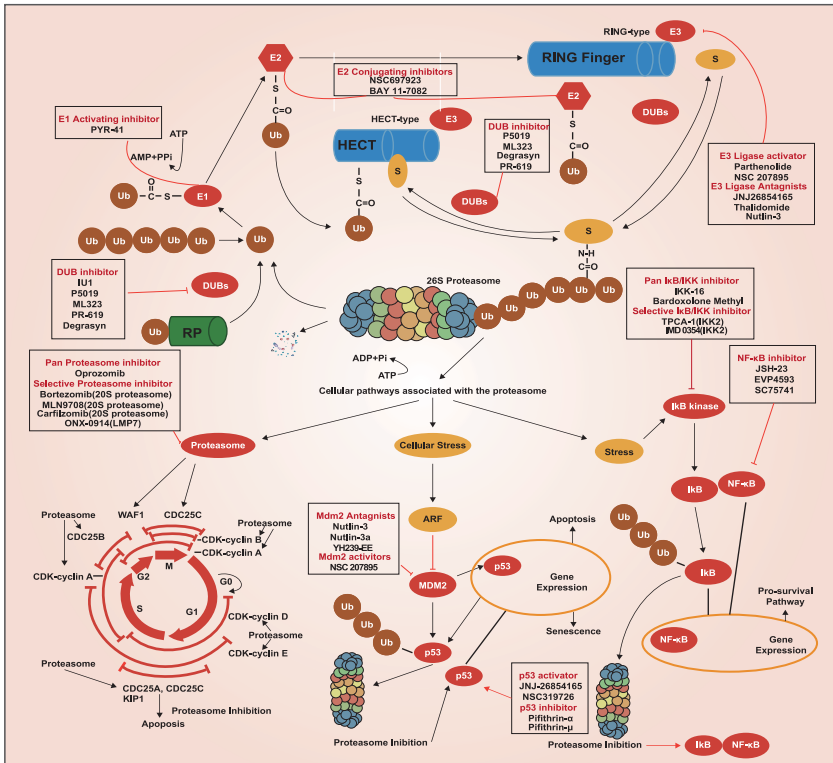
ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2707	Pifithrin-α	63208-82-2	Pan	p53	N/A		
T1919	Tenovin-1	380315-80-0	Pan	p53	Activator		
T1798	RITA (NSC 652287)	213261-59-7		MDM2			
				p53			

## TNF-α

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1642	Lenalidomide (CC-5013)	191732-72-6		Lenalidomide is a TNF-α secretion inhibitor with IC50 of 13 nM		FDA Approved	Cancer
T2384	Pomalidomide	19171-19-8		Pomalidomide inhibits TNF-α release that induced by LPS with IC50 of 13 nM		FDA Approved	
T1847	Necrostatin-1	4311-88-0		Necrostatin-1 is a specific RIP1 inhibitor and inhibits the necroptosis that induced by TNF-α with EC50 of 490 nM			

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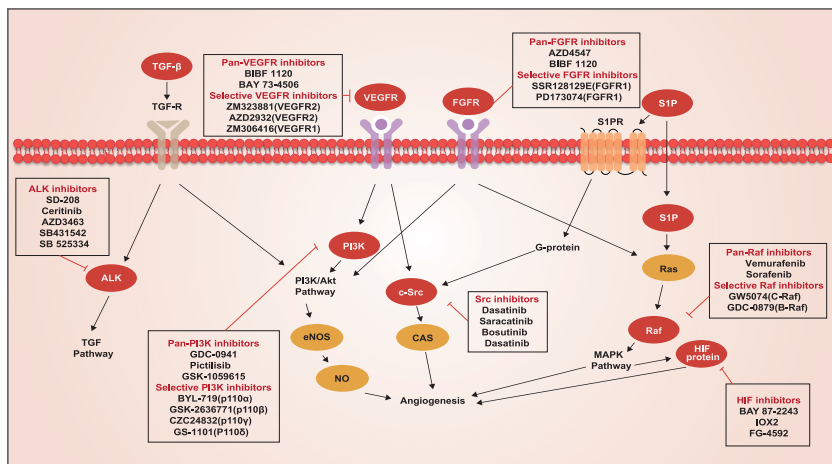
# Ubiquitination



ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1924	LDN-57444	668467-91-2	Pan	UCH-L1	0.88 $\mu$ M		
				UCH-L3	25 $\mu$ M		
T1932	B-AP15	1009817-63-3	Pan	USP14	N/A		
				UCH-L5	2.1 $\mu$ M		
T1757	ML323	1572414-83-5	Selective	USP1-UAF1	76 nM		

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# Angiogenesis



## BTK

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1835	Ibrutinib (PCI-32765)	936563-96-1	Non-specific	BTK	0.5 nM	FDA Approved	Chronic lymphocytic leukaemia; Mantle-cell lymphoma; Waldenstrom's macroglobulinaemia
				BLK	0.5 nM		
				Bmx	0.8 nM		
				CSK	2.3 nM		
T2302 <small>NEW</small>	CNX-774	1202759-32-7	BTK	<1 nM			
T2472 <small>NEW</small>	CGI1746	910232-84-7	BTK	1.9 nM			
T2603 <small>NEW</small>	CC-292 (AVL-292)	1202757-89-8	BTK	<0.5nM		Phase 1	Rheumatoid arthritis

## Syk

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2467	R406	841290-80-0	Selective	Syk	41 nM	Phase 3	Immune thrombocytopenic purpura
T2605	R788(Fostamatinib) Disodium	1025687-58-4	Selective	Syk	42 nM	Phase 3	Immune thrombocytopenic purpura
T2696	PRT062607 (P505-15, BIIB057) HCl	1370261-97-4	Selective	Syk	1 nM	Phase 1	
				FGFR	81 nM		
				MLK1	88 nM		
				YES	123 nM		

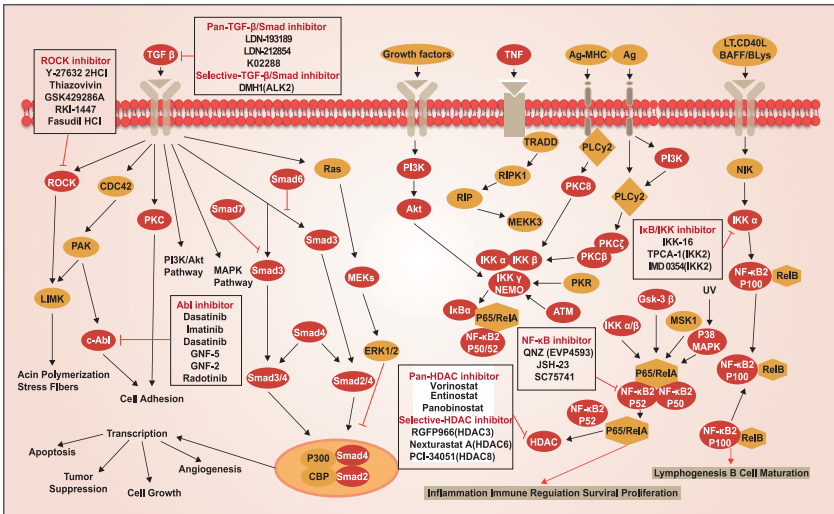
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Src

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1448	Dasatinib	302962-49-8	Non-specific	Src	0.8 nM	FDA Approved	Acute lymphoblastic leukaemia; Chronic myeloid leukaemia
				Abl	0.6 nM		
				c-Kit	79 nM		
T6078	Saracatinib (AZD0530)	379231-04-6	Non-specific	c-Src	2.7 nM	Phase 2	Alzheimer's disease; Breast cancer; Cancer pain; lymphangioleiomyomatosis
				Lck	<4 nM		
				c-Yes	<4 nM		
T0152	Bosutinib	380843-75-4	Non-specific	Src	1.2 nM	FDA Approved	Chronic myeloid leukaemia
				Abl	1 nM		

## Immunology/Inflammation

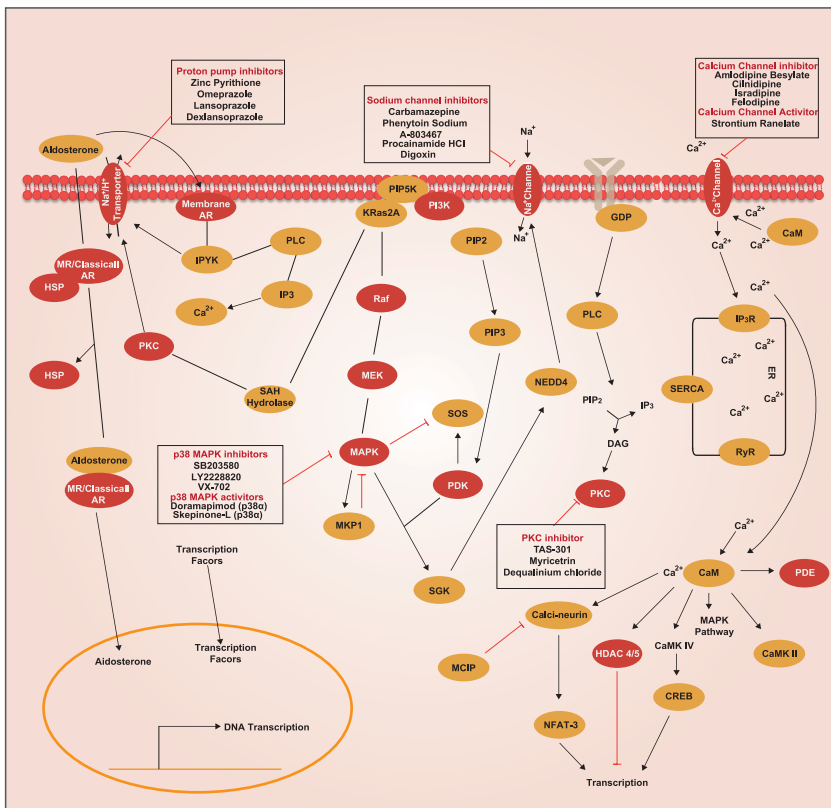


NF-κ b

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1930	JSH-23	749886-87-1	Selective	NF-κ b	7.1 μ M		
T0020	Sodium 4-Aminosalicylate	6018-19-5		Sodium 4-Aminosalicylate is an antibiotic used to treat tuberculosis via NF-κ B inhibition and free radical scavenging.			

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# Membrane Transporter/Ion Channel

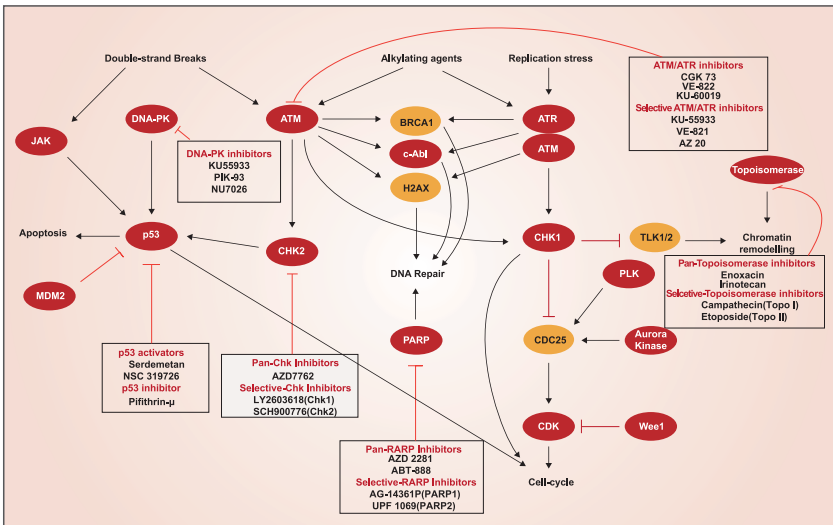


## CFTR

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1805	Ataluren (PTC124)	775304-57-9		PTC124 (Ataluren) selectively induces ribosomal read-through of premature but not normal termination codons, with EC50 of 0.1 μ M, may provide treatment for genetic disorders caused by nonsense mutations (e.g. CF caused by CFTR nonsense mutation).		FDA Approved	Duchenne muscular dystrophy
T2355	CFTRinh-172	307510-92-5	Selective	CFTR	(Ki)300 nm		

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## DNA Damage/DNA Repair

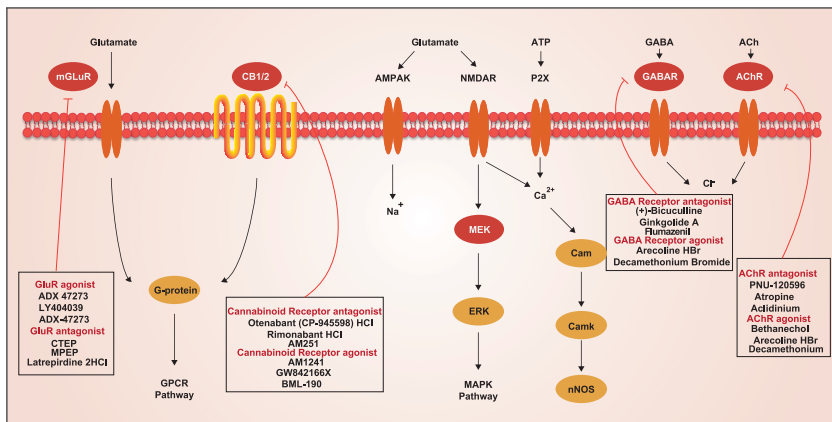


## DNA/ RNA Synthesis

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1564	Cisplatin	15663-27-1		Cisplatin is able to inhibit DNA synthesis by conforming DNA adducts		Phase 1	Solid tumours
T0251	Gemcitabine	95058-81-4	Pan	PANC1	50 nM	FDA Approved	Biliary cancer; Bladder cancer; Breast cancer; Non-small cell lung cancer; Ovarian cancer; Pancreatic cancer
				MIAPaCa2	40 nM		
				BxPC3	18 nM		
				Capan2	12 nM		
T6116	Bleomycin Sulfate	9041-93-4		Bleomycin Sulfate is a glycopeptide antibiotic and an anticancer agent for SCC with IC50 of 4 nM		Phase 3	Hodgkin's disease
T0164	Oxaliplatin	61825-94-3		Cisplatin is able to inhibit DNA synthesis by conforming DNA adducts		FDA Approved	Colorectal cancer

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## Neuroscience

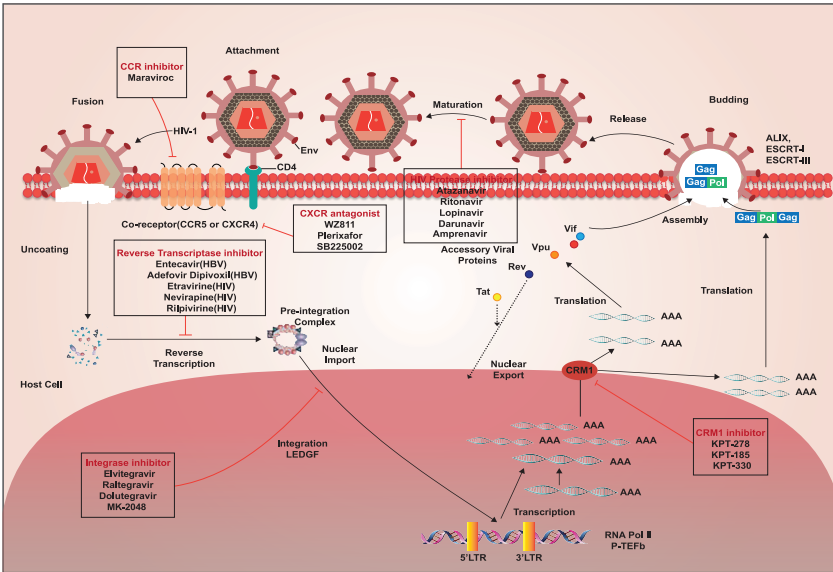


## Gamma-Secretase

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T6202	DAPT (GSI-HX)	208255-80-5	Selective	$\gamma$ -secretase [ $\alpha$ $\beta$ ]	20 nM		
T2625	MK0752	471905-41-6	Selective	$\alpha$ $\beta$ 40	5 nM	Phase 1	Breast cancer; CNS cancer; Pancreatic cancer; Solid tumours
T3075 <b>NEW</b>	FLI-06	313967-18-9	Selective	Notch	2.9 $\mu$ M		

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# Microbiology & Virology



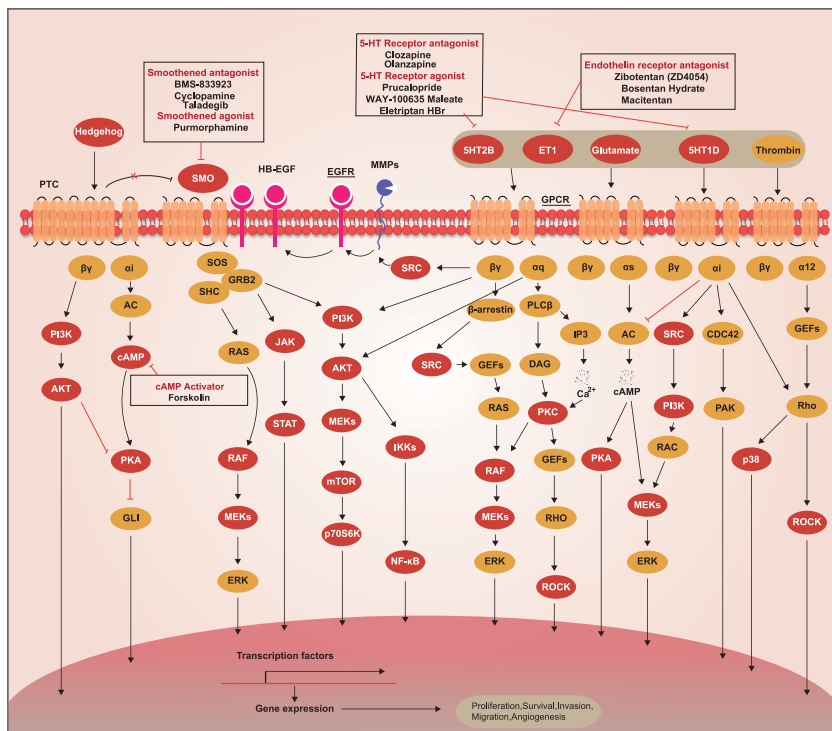
ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T0100L	Atazanavir	198904-31-3	Protease Inhibitor (PI)	HIV protease	~100 nM	FDA Approved	HIV infection
T1525	Ritonavir	155213-67-5	Protease Inhibitor (PI)	HIV protease	~100 nM	FDA Approved	HIV infection
T1623	Lopinavir	192725-17-0	Protease Inhibitor (PI)	HIV protease	~100 nM	FDA Approved	HIV infection
T2162	Maribavir	176161-24-3	Protein Kinase Inhibitor	UL97	~100 nM	Phase 2	CMV infections
T1786	Daclatasvir, BMS 790052	1009119-65-6	NS5A Inhibitor	HCV NS5A	9-50 pM	FDA Approved	HCV infection

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### DNA/ RNA Synthesis

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1564	Cisplatin	15663-27-1		Cisplatin is able to inhibit DNA synthesis by conforming DNA adducts		Phase 1	Solid tumours
T0251	Gemcitabine	95058-81-4	Pan	PANC1	50 nM	FDA Approved	Biliary cancer; Bladder cancer; Breast cancer; Non-small cell lung cancer; Ovarian cancer; Pancreatic cancer
				MIAPaCa2	40 nM		
				BxPC3	18 nM		
				Capan2	12 nM		
T6116	Bleomycin Sulfate	9041-93-4		Bleomycin Sulfate is a glycopeptide antibiotic and an anticancer agent for SCC with IC50 of 4 nM		Phase 3	Hodgkin's disease
T0164	Oxaliplatin	61825-94-3		Cisplatin is able to inhibit DNA synthesis by conforming DNA adducts		FDA Approved	Colorectal cancer

## GPCR/G Protein



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## Hedgehog Smoothened

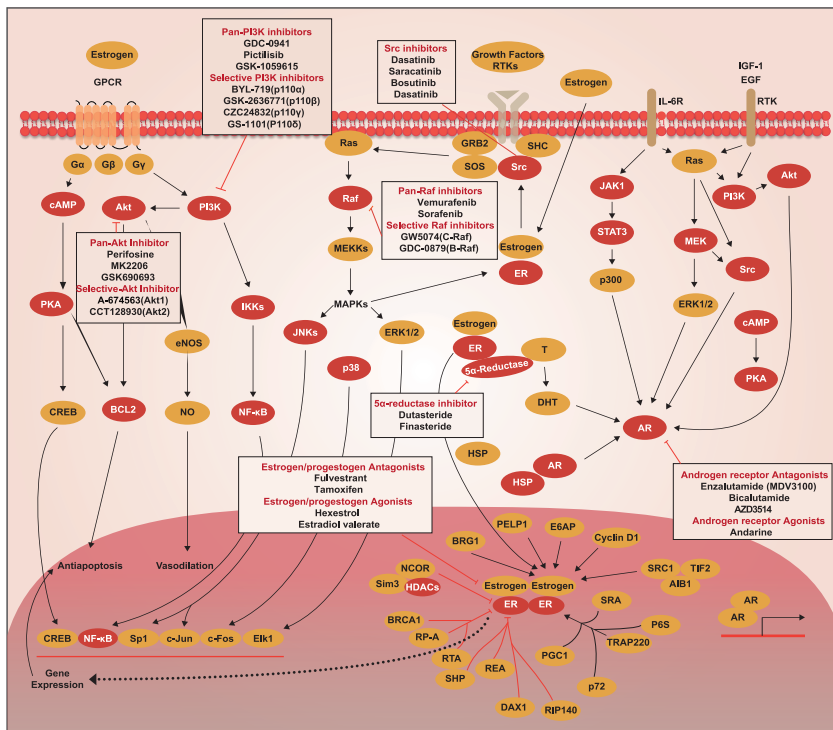
ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T2299	BMS-833923	1059734-66-5	Selective	Smoothened (antagonist)		Phase 2	
T2666	Taladegib (LY2940680)	1258861-20-9	Selective	Smoothened		Phase 1/2	
T2590	Vismodegib (GDC-0449)	879085-55-9	Selective	Hedgehog	3 nM		
T1926	LDE225 (NVP-LDE225, Erismodegib)	956697-53-3	Selective	Smoothened (Mouse)	1.3 nM	Phase 3	
				Smoothened (Human)	2.5 nM		

## Adrenergic

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T0101	Doxazosin mesylate	77883-43-3	Selective	$\alpha$ 1-adrenergic		FDA Approved	Cocaine Dependence; Prostatic Hyperplasia
T1056	Isoprenaline HCl	51-30-9	Pan	$\beta$ -adrenergic agonist		FDA Approved	
T0487	Metoprolol tartrate	56392-17-7	Selective	$\beta$ -adrenergic	42 ng/ml	FDA Approved	Hypertension

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# Endocrinology/ Hormones



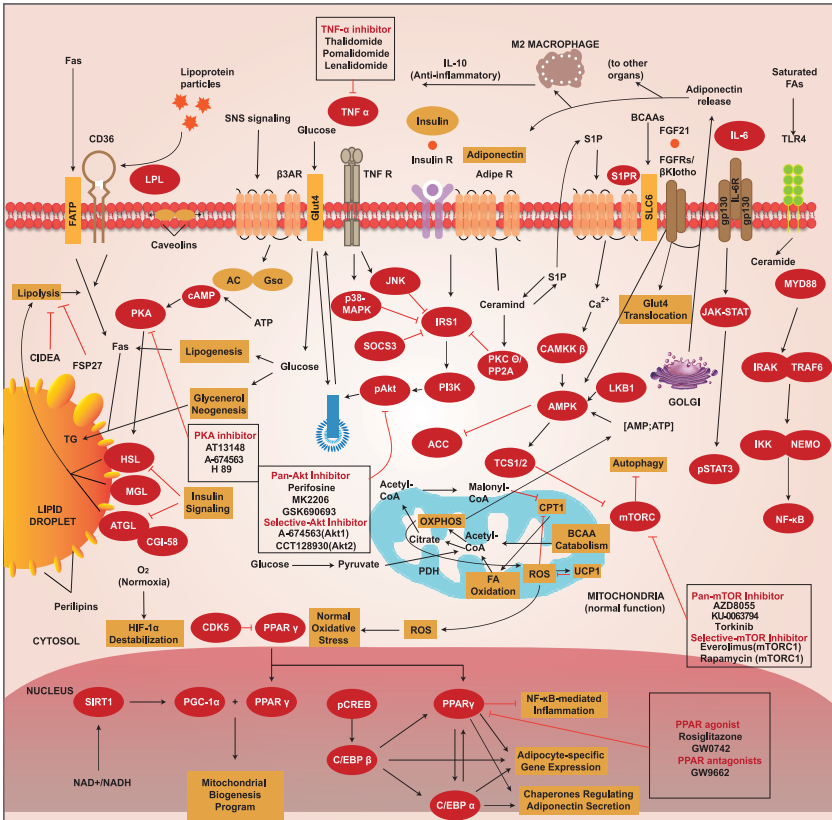
## Androgen Receptor

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T6002	Enzalutamide (MDV3100)	915087-33-1	Selective	Abdrigebe Receptor	36 nM	FDA Approved	Prostate cancer
T0380	Bicalutamide	90357-06-5	Selective	Abdrigebe Receptor	0.16 μM	FDA Approved	Prostate cancer
T2339	ARN-509	956104-40-8	Selective	Abdrigebe Receptor GAPAA Receptor	16 nM 3000 nM	Phase 3	Prostate cancer
T1167	Cyproterone acetate	427-51-0	Selective	Abdrigebe Receptor	7.1 nM		

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# Metabolism



## PDE

ID	Product Name	Cas Number	Type	Target	IC50	Clinical Trail	Condition
T1024	Roflumilast	162401-32-3	Selective	PDE4	0.2-4.3 nM	FDA Approved	Chronic obstructive pulmonary disease
T1708	Pimobendan	74150-27-9	Selective	PDE3	110 nM	FDA Approved	Heart failure
T6042	PF-2545920	1292799-56-4	Selective	PDE10A	0.37 nM	Phase 2	Huntington's disease; Schizophrenia
T0462	Cilostazol	73963-72-1	Selective	PDE3	0.2 μM	Phase 2	Arterial occlusive disorders; Intermittent claudication; Stroke

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## Enzyme

Carbonic anhydrase	Hydrogenase	PP2A
Cathepsin K	Hydrolase	Reductase
LXR	Hydroxylase	Squalene epoxidase
CzcO-like	sGC	Tyrosinase
DHPS	Oxidosqualene cyclase	VKOR
Endopeptidase	Peroxiredoxin-5	
Hexokinase	Phosphorylase	

## Others

ACCase	MCT	RAGE
Adrenodoxin	MELK	Ryanodine receptor
AGE	mTOT	SAA
APN	Oct3/4	SGK1;SGK2
ATX	PCSK9	SRPK1
BMI-1	Pepsin	TTR
Calcineurin phosphatase	PFKFB3	Xylose isomerase
CART	p-HBH	$\alpha$ -glucosidase
DYRK	Phytoestrogen	Others
Lysozyme	PPM1D	
MALT1	Purine nucleoside phosphorylase	

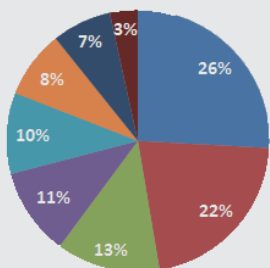
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### Research fields:



- |                   |                      |
|-------------------|----------------------|
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| ■ Neuropsychiatry | ■ Oncology           |
| ■ Metabolism      | ■ Endocrinology      |
| ■ Cardiology      | ■ Respiratory system |

### Database Contains:

- CAS, Chemical name, 3D structure, Formula, Solubility;
- Bioactivity, Targets, IC50 Value, References, Clinical Data;
- COA, MSDS, Datasheet, NMR, LCMS, HPLC, etc.

# Headquarters

## North America



### United States

#### Order & Inquiry

Tel: 857-239-0968

Fax: 857-239-8801

Email: [info@targetmol.com](mailto:info@targetmol.com)

Add: One Boston Place Suite 2600 Boston, MA 02108

#### Technical Support

E-mail: [tech@targetmol.com](mailto:tech@targetmol.com)

## Europe



### Germany

#### Order & Inquiry

Tel: +0049-0163-1922118

E-mail: [eu.order@targetmol.com](mailto:eu.order@targetmol.com)

Add: Willi-Graf-Str.25/384 80805/Munich

## Asia Pacific region



### China

#### Order & Inquiry

E-mail: [sales@targetmol.com](mailto:sales@targetmol.com)

Tel: 400-821-2233

Fax: 021-34692979

Add: NO 228 Jiangchang San Road ,Shanghai,China

#### Technical Support

E-mail: [tech@targetmol.com](mailto:tech@targetmol.com)

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