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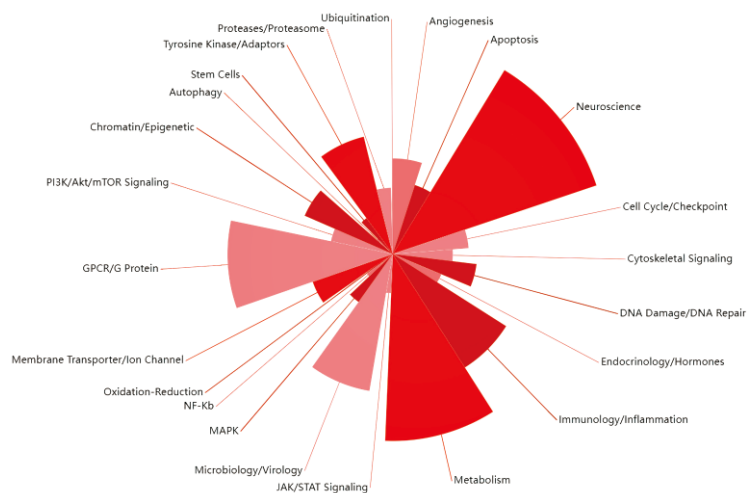
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Science
VOLUME 368|ISSUE 6497|19 JUN 2020



Nature
Volume 582 Issue 7811, 11 June 2020



Nature
2021 592(7854) 469-473



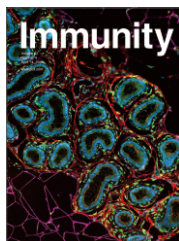
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2020 588(7838) 479-484



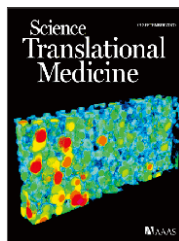
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2021 54(6) 1123-1136.e8.e2-5523



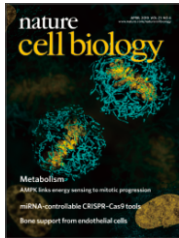
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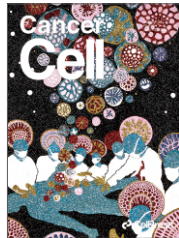
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2020, 38(1)115-128.e9



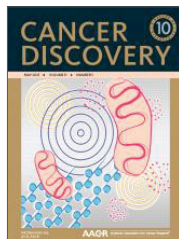
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2020, 30(11)966-979.



Cancer Discovery
2021, 11(3) 638-659.

Article

Feeding induces cholesterol biosynthesis via the mTORC1-USP20-HMGCR axis

Xiao Y¹, Wang J¹, Wang W¹, Li S¹, Wang W¹, He D¹, Wang J¹, Wang S¹, Zhou C¹, He M¹, He Q¹, Liang H¹

Cholesterol is an essential lipid and its synthesis is nutritionally and energetically costly. In mammals, cholesterol synthesis increases after feeding and is inhibited under fasting conditions. However, the regulatory mechanisms of cholesterol biosynthesis at the feeding-fasting transition remain poorly understood. Here we show that the deubiquitinase ubiquitin-specific peptidase 20 (USP20) stabilizes HMG-CoA reductase (HMGCR), the rate-limiting enzyme in cholesterol biosynthesis, in the feeding state. The post-prandial increase in insulin and glucose concentration stimulates USP20 to phosphorylate USP20 at S12 and S124. USP20 is recruited to the HMGCR complex and antagonizes its degradation. The feeding-induced stabilization of HMGCR is abolished in mice with specific Usp20 deletion and USP20S124S124S124 knock-in mice. Genetic deletion or pharmacological inhibition of USP20 markedly decreases endogenous body weight gain, reduces lipogenesis in the subcutaneous fat, impairs insulin sensitivity and increases energy expenditure. These metabolic changes are reversed by co-expression of HMGCR and USP20. Our study identifies USP20 as a novel regulator of cholesterol biosynthesis in mammals. (Usp20^{-/-} mice were fed with high-calorie diet for 14 days, and then fasted for 14 days. The body weight gain, insulin sensitivity, and energy expenditure were significantly reduced in Usp20^{-/-} mice compared to wild-type mice. USP20 knock-in mice (USP20^{S124S124S124}) showed restored metabolic phenotypes. USP20 inhibition with the inhibitor GSK-2606414 (GSK2606414) mimicked the effects of USP20 deletion.)

Letter

Molecular architecture of lineage allocation and tissue organization in early mouse embryo

Guanghui Peng^{1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,195,196,197,198,199,200,201,202,203,204,205,206,207,208,209,210,211,212,213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230,231,232,233,234,235,236,237,238,239,240,241,242,243,244,245,246,247,248,249,250,251,252,253,254,255,256,257,258,259,260,261,262,263,264,265,266,267,268,269,270,271,272,273,274,275,276,277,278,279,280,281,282,283,284,285,286,287,288,289,290,291,292,293,294,295,296,297,298,299,300,301,302,303,304,305,306,307,308,309,310,311,312,313,314,315,316,317,318,319,320,321,322,323,324,325,326,327,328,329,330,331,332,333,334,335,336,337,338,339,340,341,342,343,344,345,346,347,348,349,350,351,352,353,354,355,356,357,358,359,360,361,362,363,364,365,366,367,368,369,370,371,372,373,374,375,376,377,378,379,380,381,382,383,384,385,386,387,388,389,390,391,392,393,394,395,396,397,398,399,400,401,402,403,404,405,406,407,408,409,410,411,412,413,414,415,416,417,418,419,420,421,422,423,424,425,426,427,428,429,430,431,432,433,434,435,436,437,438,439,440,441,442,443,444,445,446,447,448,449,450,451,452,453,454,455,456,457,458,459,460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000}

Article

Structures of full-length glycoprotein hormone receptor signaling complexes

Ji Du¹, Yan Yu¹, Xi Chen¹, Chen Ma¹, Tian-Dan Guo¹, Xiang-Hu He¹, Jing-Hui Du¹, Xue-Li Wang¹, Wen-Hua Yu¹, Di-Yu Qu¹, Qun-Lin Liu¹, Shuang-Dong Wang¹, Hui-Li Wang¹, Yan-Hua Wang¹, Xiang-Hu He¹, Ji Du¹

Leiotropic hormones and chorionic gonadotropin (CG) are glycoprotein hormones that are critical for follicle-stimulating hormone (FSH) and luteinizing hormone (LH) signaling in the mammalian reproductive system. The structures of the human chorionic gonadotropin receptor (CGR) and the human luteinizing hormone receptor (LHR) are essential for understanding their signaling mechanisms. Here we report the cryo-electron microscopy structures of the full-length wild-type human CGR and LHR signaling complexes. The active structures are bound to chorionic gonadotropin and the stimulatory G-protein (G_s), and one of the structures also contains Dept55, an "adhesion" protein. The structure reveals distinct "push" and "pull" mechanisms of receptor activation, in which the extracellular domain is pushed by the bound hormone and the intracellular domain is pulled by the bound G-protein. A highly conserved 10-residue fragment (R10) from the hinge-C is critical for the activation of the receptor. The structure also reveals the mechanism of the receptor activation, in which the extracellular domain is pushed by the bound hormone and the intracellular domain is pulled by the bound G-protein. The structure reveals distinct "push" and "pull" mechanisms of receptor activation, in which the extracellular domain is pushed by the bound hormone and the intracellular domain is pulled by the bound G-protein. The structure reveals distinct "push" and "pull" mechanisms of receptor activation, in which the extracellular domain is pushed by the bound hormone and the intracellular domain is pulled by the bound G-protein.

Article

Cancer Cell

MDMX acts as a pervasive preleukemic-to-acute myeloid leukemia transition mechanism

Koki Ueda, Rami Kumar, Emily Schwinger, ... Jacqueline Buchhold, Amit Verma, Ulrich Steidl

Correspondence: ulrich.steidl@einsteinmed.org

In brief: Using mouse models and data from MDS patients, Ueda et al. identify MDMX as a pervasive preleukemic-to-acute myeloid leukemia transition mechanism across multiple different genetic disease subtypes. MDMX physically interacts with CK1α, inducing accumulation of β-Catenin. Blocking both canonical and non-canonical activity of MDMX enhances therapeutic effects against preleukemic/leukemic.

MDMX overexpression induces preleukemic-to-AML transition in multiple mouse models

Articles

Prediction of drug efficacy from transcriptional profiles with deep learning

Jie Zhu^{1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,195,196,197,198,199,200,201,202,203,204,205,206,207,208,209,210,211,212,213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230,231,232,233,234,235,236,237,238,239,240,241,242,243,244,245,246,247,248,249,250,251,252,253,254,255,256,257,258,259,260,261,262,263,264,265,266,267,268,269,270,271,272,273,274,275,276,277,278,279,280,281,282,283,284,285,286,287,288,289,290,291,292,293,294,295,296,297,298,299,300,301,302,303,304,305,306,307,308,309,310,311,312,313,314,315,316,317,318,319,320,321,322,323,324,325,326,327,328,329,330,331,332,333,334,335,336,337,338,339,340,341,342,343,344,345,346,347,348,349,350,351,352,353,354,355,356,357,358,359,360,361,362,363,364,365,366,367,368,369,370,371,372,373,374,375,376,377,378,379,380,381,382,383,384,385,386,387,388,389,390,391,392,393,394,395,396,397,398,399,400,401,402,403,404,405,406,407,408,409,410,411,412,413,414,415,416,417,418,419,420,421,422,423,424,425,426,427,428,429,430,431,432,433,434,435,436,437,438,439,440,441,442,443,444,445,446,447,448,449,450,451,452,453,454,455,456,457,458,459,460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000}

Article

Time-resolved protein activation by proximal decaying in living systems

Yan He^{1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,195,196,197,198,199,200,201,202,203,204,205,206,207,208,209,210,211,212,213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230,231,232,233,234,235,236,237,238,239,240,241,242,243,244,245,246,247,248,249,250,251,252,253,254,255,256,257,258,259,260,261,262,263,264,265,266,267,268,269,270,271,272,273,274,275,276,277,278,279,280,281,282,283,28}

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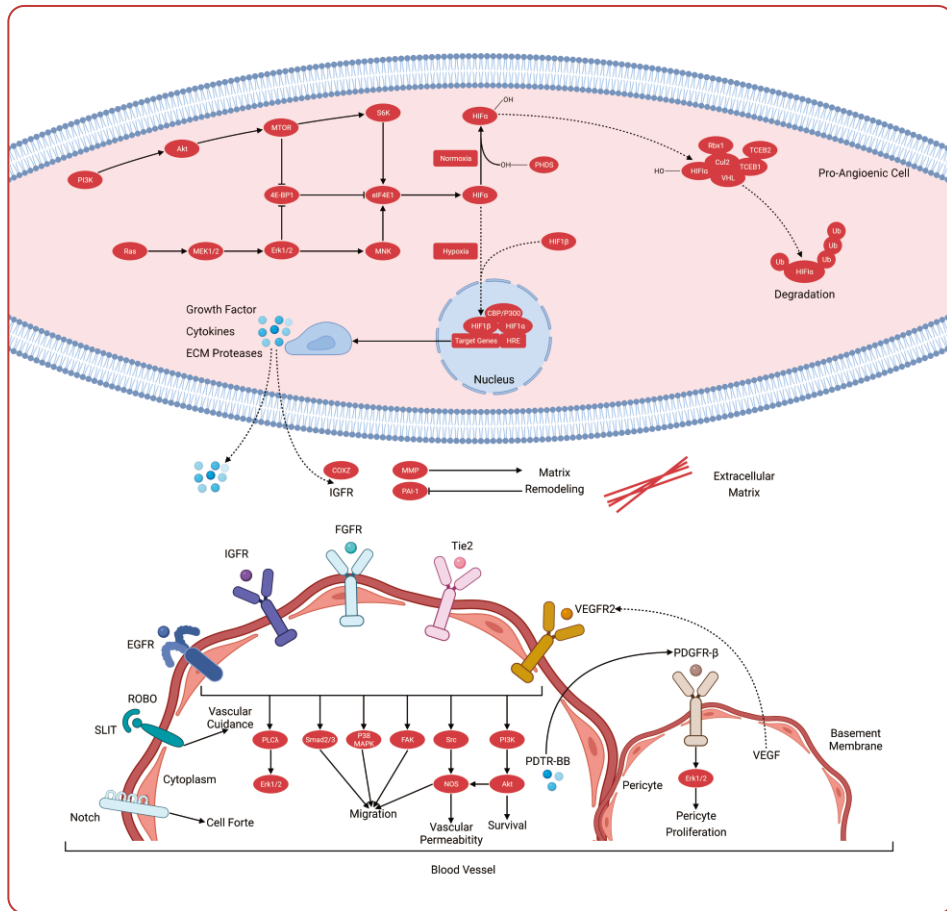
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Angiogenesis



EGFR

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21312	850140-72-6	Afatinib free base	EGFR	0.5 nM	FDA Approved	Locally advanced or metastatic non-small cell lung Cancer (NSCLC)
T19814	179688-29-0	CP-380736	EGFR			
T16369	847949-49-9	O-Desmethyl gefitinib	EGFR			
T11213	2071195-74-7	Epertinib hydrochloride	EGFR;HER 4;HER2	1.48 nM		
T11161	2267329-76-8	EGFR-IN-7	EGFR			
T2116	497839-62-0	AEE788	c-Abi; c-Fms; EGFR; HER2/Erb B2; FLT1	2 nM	Phase 1/2	Glioblastoma; Solid tumours
T2106	1421227-53-3	WS6	ErbB3-Binding Protein-1 (EBP2); IκB kinase	0.28 μM		
T2063	118409-57-7	AG18	EGFR	35 μM	Preclinical	Cancer; Psoriasis
T2055	1421227-52-2	WS3	ErbB3-Binding Protein-1 (EBP1); IκB kinase	28 nM(ec50)		

FGFR

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T22306	T22306	DGY-06-116	Src;FGFR1			
T12401	1513857-77-6	Pemigatinib	FGFR1;FGFR2;FGFR3;FGFR4	0.4 nM	FDA Approved	Cholangiocarcinoma
T4235	1708971-55-4	Roblitinib	FGFR4	1.1 nM	Phase 1/2	Liver Cancer; Solid tumours
T4075	1816307-67-1	Sulfatinib	FGFR1; HERG; KDR		Phase 3	Neuroendocrine tumours
T3726	1346242-81-6	Erdafitinib	FGFR1; FGFR2; FGFR3; FGFR4	1.2 nM	FDA Approved	Urogenital Cancer
T3714	704869-38-5	SUN 11602	ERK1; ERK2; FGFR			
T3492	192705-79-6	PD166866	FGFR1	52.4 nM		
T3456	1707289-21-1	BLU554	FGFR1; FGFR2; FGFR3; FGFR4	5 nM	Phase 1	Cholangiocarcinoma; Liver Cancer

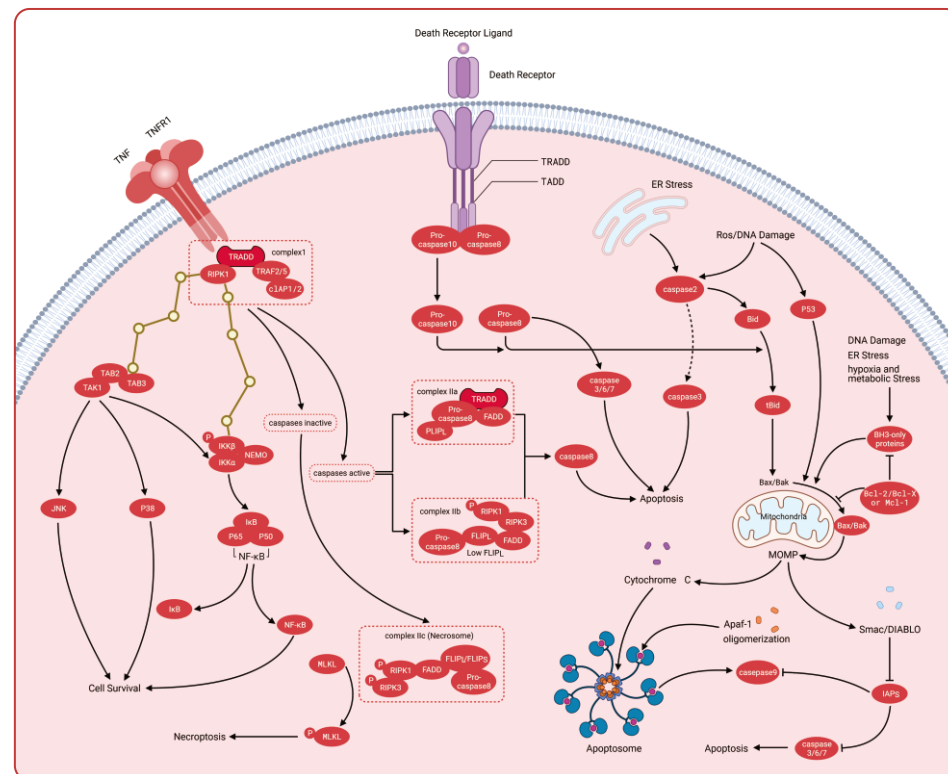
VEGFR

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T22432	62540-08-3	SU5208	VEGFR2			
T22431	186611-11-0	SU5204	VEGFR2;HER2	4 μM		
T17219	212141-54-3	Vatalanib free base	VEGFR2			
T6199	1211441-98-3	Ribociclib	CDK4;VEGFR4;VEGFR6	10nM	FDA Approved	Breast Cancer
T6184	252916-29-3	Orantinib	FGFR1; PDGFRβ; Flk1	8 nM(Ki)	Phase 1	Unspecified Adult Solid Tumor, Protocol Specific
T6166	332012-40-5	Telatinib	c-Kit; PDGFRα; VEGFR2; VEGFR3	1 nM	Phase 2	Gastric Cancer
T6154	658084-23-2	SU11274	CDK2; Met; RON; FGFR1; Flk1	0.01 μM	Preclinical	Cancer
T4554	71308-34-4	AG 1406	VEGFR2			
T4425	942655-44-9	JK-P3	VEGFR2	7.8 μM		

HER

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T22431	186611-11-0	SU5204	VEGFR2;HER2	4 μM		
T11213	2071195-74-7	Epertinib hydrochloride	EGFR;HER4;HER2	1.48 nM		
T7819	2088323-16-2	TAS0728	HER2	8.5 nM	Phase 1/2	Advanced Solid Tumors;HER2 Abnormalities;HER3 Abnormalities
T6712	148741-30-4	Tyrphostin AG 879	EGFR; HER2-Neu; PDGFR; Trk	1 μM		
T6341	908115-27-5	PF04929113	HER2; HSP90	37 nM	Phase 2	Cancer
T5398	T5398	BMS 599626 2HCl (873837-23-1(HCl))	HER1; HER2; HER4	20 nM (cell free)	Phase 1	Breast Cancer; Glioma, Non-small cell lung Cancer; Solid tumours
T4342	1173111-67-5	PF-04929113 Mesylate	HSP90;HER2	37 nM	Phase 2	
T4075	1816307-67-1	Sulfatinib	FGFR1; HERG; KDR		Phase 3	
T3673	55481-88-4	Mollugin	HER2; JAK2			

Apoptosis



TNF-α

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T15437	1622849-43-7	GSK3145095	RIP1		Phase 2	Neoplasms, Pancreatic
T13951	1515888-53-5	UCB-9260	TNF			
T1265	60719-84-8	Amrinone	PDE;TNF-α		FDA Approved	Heart Failure
T0213	50-35-1	Thalidomide	TNF-α		FDA Approved	Leprosy; Multiple myeloma
T0131	481-49-2	Cepharanthine	TNF-α		Approved	promotes leukocytosis
T0122	477-90-7	Bengenin	IL-1β;IL-6; NF-κB; NOD; TNF-α	15 μM	Approved	Chronic Bronchitis

Caspase

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T10990	10605-03-5	Dehydrocoyrdaline chloride	p38 MAPK; Bax;Bcl-2; caspase-7; caspase-8; PARP			
T10580	634911-80-1	BOC-D-FMK	Caspase			
T9113	607-91-0	Myristicin	Antifection; Bcl-2; Caspase; CYP17; GABA Receptor; ILReceptor ; NO;PARP			
T0282	1135695-98-5	Q-VD-OPH	Caspase-1; Caspase-3; Caspase-8; Caspase-9	25 nM-400 nM		
T2503	315183-21-2	PAC1	Procaspase -3	0.22 μM(EC50)	Phase 1	Anaplastic astrocytoma; Glioblastoma
T2122	1072833-77-2	Ixazomib	20S proteasome; 20S proteasome;caspase-like (β1)	0.93 nM(Ki)	FDA Approved	Multiple myeloma
T1772	79183-19-0	Apoptosis Activator 2	Caspase-3			

Mdm2

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21773	1253491-42-7	SP 141	Mdm2			
T11980	2136247-12-4	MD-224	Mdm2;PRO TAC			
T3517	1309684-94-3	RO8994	Mdm2; P53	20 nM		
T3184	66592-89-0	Keveirin hydrochloride	Mdm2; p53		Phase 2	Ovarian Cancer
T2243	881202-45-5	Serdemetan	HDM2; Mdm2; p53	0.24 μM	Phase 1	Non-small cell lung Cancer; Prostate Cancer; Solid tumours
T2179	38748-32-2	Triptolide	heat shock factor (HSF1)(in ALL cell lines); Mdm2		Approved	Psoriasis (psoriasis)

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Bcl-2

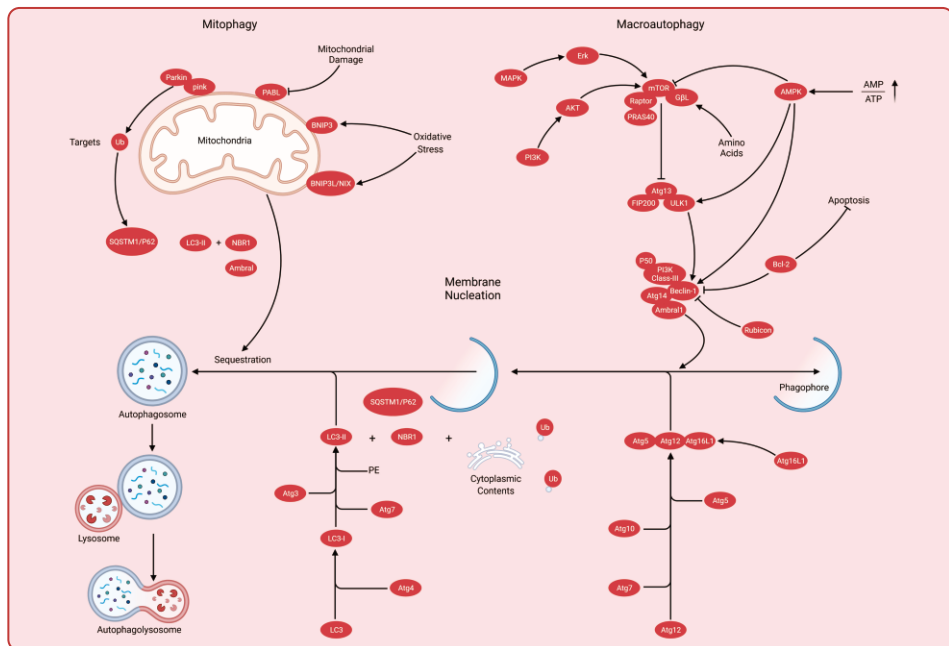
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T14834	34576-94-8	BT2	BDK;Mcl-1			
T14561	2166387-64-8	BI-3812	Bcl-6			
T14376	1357576-48-7	AZD4320	BCL-2; BCL-xL	17 nM(KPUM-UH1 cells)		
T1119	136236-51-6	Rasagiline	Bcl-2; MAO-A; MAO-B	4.43 nM	FDA Approved	Parkinson's disease
T10990	10605-03-5	Dehydrocoyrdaline chloride	p38 MAPK; Bax;Bcl-2; caspase-7; caspase-8; PARP			
T0448	51146-66-6	Dexibuprofen	Bcl-2;COX; Cystic fibrosis transmembrane conductance regulator; PPARγ; thrombomodulin	13 μM	Approved	Back Pain; Dysmenorrhoea; Headache; Inflammation; Musculoskeletal Pain; Osteoarthritis; Pain; Postoperative Pain; Rheumatic Disorders
T0186	148408-66-6	Docetaxel trihydrate	Bcl-2; Tubulin β-1 chain		FDA Approved	Adenocarcinoma; Breast Cancer; Head and neck Cancer; Non-small cell lung Cancer; Prostate Cancer
T2099	852808-04-9	ABT737	Bcl-2; Bcl-B; Bcl-w; Bcl-xL	30.3 nM(EC50, cell free)	Preclinical	Cancer
T1980	65673-63-4	HA14-1	Bcl-2	9 μM	Preclinical	Cancer
T1901	300801-52-9	TG003	mCLK1; mCLK2; mCLK4	15 nM		

P53

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T7703	874146-69-7	PK11007	p53			
T6910	803647-40-7	NSC59984	p53			
T2707	63208-82-2	Pifithrin-α	p53			
T2464	71555-25-4	NSC319726	p53 (R175)	8 nM		
T3637	511296-88-1	Pifithrin-β hydrobromide	p53	23 μM(EC50)	Preclinical	Alopecia

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Autophagy



CXCR

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T17208	1373268-67-7	USL311	CXCR4		Phase 1/2	Solid Tumors (Phase 1)Relapsed/Recurrent GBM (Phase 2)
T14665L	T14665L	Motixafortide TFA(664334-36-5,Free)	CXCR4	~1 nM	Phase 2	Acute myeloid leukaemia; Pancreatic cancer; Precursor cell lymphoblastic leukaemia-lymphoma
T10297L	473719-41-4	AMG 487	CXCR3	8 nM		
T8497	1648843-04-2	SX-682	CXCR1;CXCR2		Phase 1	Melanoma Stage IIIIMelanoma Stage IV
T7681	878385-84-3	AZD-5069	CXCR2	0.79 nM	Phase 2	Bladder Cancer; Coronary disorders; Head and neck Cancer; Non-small cell lung Cancer; Solid tumours
CXCR	T4033	4051-59-6	MSX130		CXCR4	
CXCR	T4032	6616-56-4	MSX127		CXCR4	
CXCR	T5849	1380392-05-1	JMS-17-2		CX3CR1	

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Autophagy

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T20879	109581-93-3	Tacrolimus hydrate	FKBP;Phosphatase; Autophagy;Bacteria L;Antibiotic		FDA Approved	For use after allogenic organ transplant to reduce the activity of the patient's immune system and so the risk of organ rejection
T16791	82-08-6	Rottlerin	PKC δ ; PKC ζ ; PKC η ; PKC θ ; PKC ν ; PKC ξ ; CKII; PKA;CaM kinase III; Apoptosis;Autophagy	3 μ M(Porcine spleen)		
T15024	1309357-15-0	Silmitasertib sodium salt	CK2;Autophagy	1 nM	Phase 1/2	Medulloblastoma; Childhood
T0754	144-82-1	Sulfamethizole	DHPS		FDA Approved	Infections
T0750	127-69-5	Sulfisoxazole	DHPS	0.60 microM	FDA Approved	Antibiotic(Urinary Tract Infections; Meningococcal Meningitis; Acute Otitis Media; Trachoma; Inclusion Conjunctivitis; Nocardiosis; Chancroid; Toxoplasmosis; Malaria And Other Bacterial Infections.)
T0087L	127-56-0	Sulfacetamide sodium	Autophagy		FDA Approved	Seborrhoeic Dermatitis
T1035	520-26-3	Hesperidin	Autophagy	116.68 μ mo/L	Approved	Inflammation; Thrombus; Pain

Lysosomal Autophagy

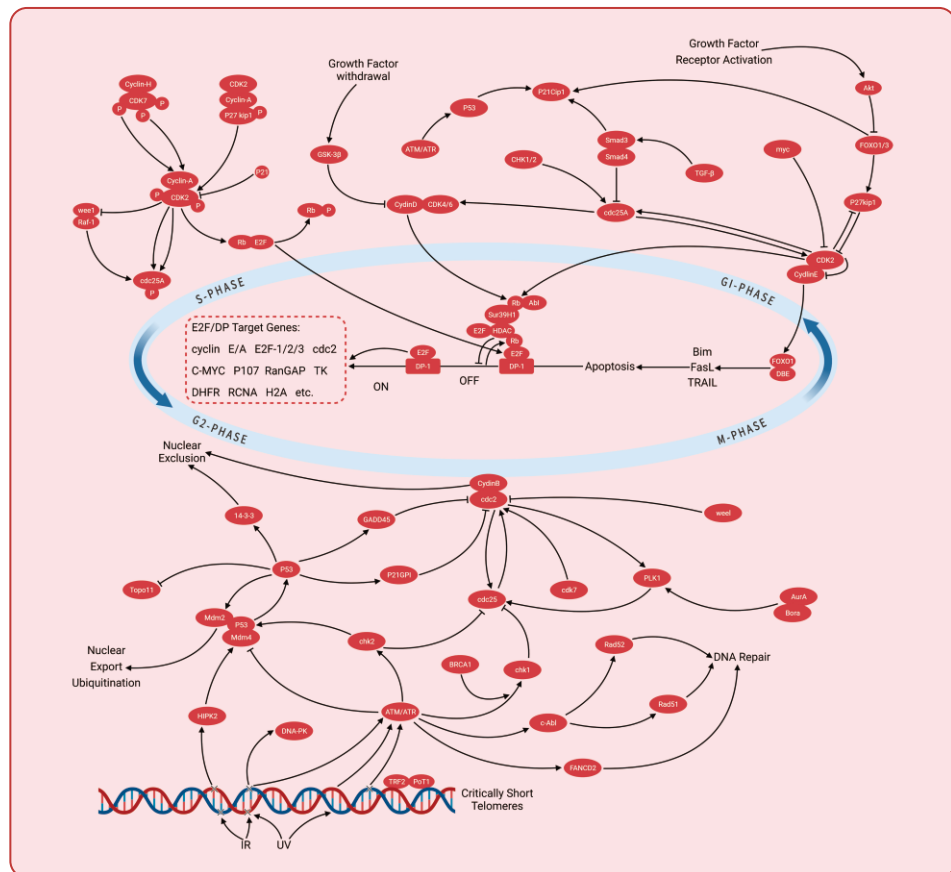
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T3437	1391426-24-6	Lys05	lysosomal autophagy (1205Lu); lysosomal autophagy (c8161); lysosomal autophagy (HT-29); lysosomal autophagy (LN229)	3.6 μ M		
T1885	224177-60-0	Siramesine hydrochloride	lysosome-stabilizing agent; α 2		Preclinical	Anxiety disorders; Cancer; Major depressive disorder

LRRK2

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T7729	1527473-30-8	PF-06454589	LRRK2			
T7196	1351758-81-0	HG-10-102-01	LRRK2			
T7155	1700693-08-8	JH-II-127	LRRK2	6.6 nM		

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Cell Cycle & Checkpoint



Aurora Kinase

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21981	880487-62-7	Phthalazinone pyrazole	Aurora A	31 nM		
T8685	T8685	SP-146	Aurora B	0.316 nM		
T6785	1207293-36-4	BI847325	Aurora A (Human); Aurora B (Xenopus laevis); Aurora C (Human); MEK1; MEK2	4nM	Phase 1	Solid tumours
T6532	422513-13-1	Hesperadin	Aurora B (human); TbAUK1	250 nM		

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CDK

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T17069	2139287-33-3	THAL-SNS-032	CDK9			
T16363	1263373-43-8	NVP-2	CDK9;Apoptosis			
T15732	1374639-75-4	Ribociclib succinate	CDK4;CDK6	10 nM	FDA Approved	help slow the progression of Cancer I inhibiting two proteins called cyclin-dependent kinase 4 and 6 (CDK4/6).
T14919	1421693-22-2	CDKI-73	CDK9	3.27 nM		
T14916	2079895-42-2	CDK2-IN-4	cdk2/cyclinA;Cdk1/cyclinB			
T14778	642008-81-9	BRD6989	CDK8;recombinant CDK8;recombinant CDK19;IL-10			
T13467	1610358-53-6	(±)-BAY-1251152	CDK9			
T10436	2057509-72-3	AZD4573	CDK9		Phase 1	Relapsed or Refractory Haematologic Malignancies Including;Acute Myeloid Leukemia;Acute Lymphocytic Leuker

Chk

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21331	1184843-57-9	SAR-020106	CHK1			
T7300	1196541-47-5	GDC-0575	Chk1	1.2 nM	Phase 1	Lymphoma; Solid tumours
T7080	1489389-18-5	CCT245737	Chk1	1.4 nM (Cell-free)	Phase 2	Solid tumours
T6931	185039-89-8	PD0166285	Wee1; Chk1; Myt1	24 nM	Preclinical	Cancer
T6028	952021-60-2	PF477736	c-Fms; Chk1; Chk2; Yes; VEGFR2	0.49 nM(Ki)	Phase 1	Solid tumours
T4327	1234015-54-3	Prexasertib dihydrochloride	Chk1; Chk2; RSK	0.9 nM	Phase 2	Breast Cancer; Fallopian tube Cancer; Ovarian Cancer; Peritoneal Cancer; Small cell lung Cancer; Solid tumours
T4310	1234015-52-1	Prexasertib	Chk1; Chk2	<1 nM	Phase 2	Breast Cancer; Fallopian tube Cancer; Ovarian Cancer; Peritoneal Cancer; Small cell lung Cancer; Solid tumours

ROCK

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T7301	1817698-21-7	BDP5290	ROCK	5 nM		
T6867	911417-87-3	KD025	ROCK2; ROCK2	41 nM(Ki)	Phase 2	Graft-versus-host disease; Idiopathic pulmonary fibrosis; Plaque psoriasis
T4276	155558-32-0	Hydroxyfasudil Hydrochloride	ROCK	0.73 μM		
T4095	557782-81-7	ZINC00881524	ROCK			
TQ0319	887375-67-9	Ripasudil hydrochloride dihydrate	ROCK1; ROCK2	51 nM	Approved	Glaucoma; Ocular hypertension
T6321	477600-75-2	Tofacitinib	JAK1; JAK2; JAK3 ROCK2; Lck	1 nM	FDA Approved	Rheumatoid arthritis; Ulcerative colitis
T3518	850664-21-0	GSK269962A	MSK1; ROCK1; ROCK2; RSK1	1.6 nM		
T3513	817194-38-0	GSK180736A	GRK1; GRK2; GRK5; PKA; ROCK	0.77 μM		

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HDAC

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T19687	2257-09-2	Phenylethyl isothiocyanate	HDAC			
T16962	2126744-35-0	SW-100	HDAC1;HDAC2;HDAC3;HDAC4;HDAC5;HDAC6;HDAC7;HDAC8;HDAC9;HDAC10;HDAC11	5.23 μM		
T13996	6953-61-3	1-Naphthohydroxamic acid	HDAC8;HDAC1;HDAC6	14 μM		
T6055	875320-29-9	Quisinostat	HDAC1; HDAC10; HDAC11; HDAC2; HDAC3; HDAC4; HDAC5; HDAC8	0.11 nM	Phase 2	Lung Cancer; Ovarian Cancer
T6006	128517-07-7	Romidepsin	HDAC1; HDAC2	36 nM	FDA Approved	Cutaneous T-cell lymphoma; Peripheral T-cell lymphoma
T5886	1821-12-1	Benzenebutyric acid	HDAC		Approved	antibiosis
T5830	1815580-06-3	SKLB-23bb	HDAC6	17 nM		
T5631	2374313-54-7	SIS17	HDAC11			

Histone Demethylase

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T13748	63512-50-5	L-2-Hydroxyglutaric acid disodium	Histone Demethylase; Mitochondrial Metabolism			
T13055	1422535-52-1	T-3775440 hydrochloride	LSD1	2.1 nM		
T7942	13492-01-8	Tranylcypromine (hemisulfate)	MAO; LSD1		FDA Approved	major depressive episode without melancholia.
T6922	1431326-61-2	ORY1001	LSD1/KDM1A	20 nM	Phase 2	Acute myeloid leukaemia; Small cell lung Cancer
T6847	1373422-53-7	GSK J1	JMJD3 (KDM6B); UTX (KDM6A)	28 nM		
T6593	1222800-79-4	ML324	JMJD2	920 nM		
T6073	1357302-64-7	OG-L002	LSD1	20 nM		
T5825	1431303-72-8	ORY-1001(trans)	LSD1/KDM1A		Phase 2	Acute myeloid leukaemia; Small cell lung Cancer
T5484	1628332-52-4	GSK467	JARID1A	10 nM(Ki)		

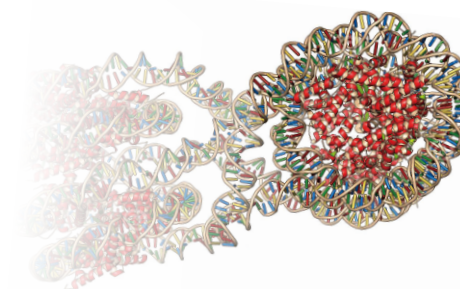
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Histone Acetyltransferase

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T14073	1889279-16-6	A-485	CBP/p300; histone acetyltransferase	9.8 nM		
T12345	2299226-01-8	P300/CBP-IN-3	histone acetyltransferase			
T12098	2055397-88-9	MOZ-IN-2	MOZ			
T8344	357649-93-5	CPTH2	Histone Acetyltransferase inhibitor			
T5468	1311423-89-8	YF-2	CBP;PCAF;GCN5	2.75 μM		
T4679	2055397-28-7	WM1119	KAT6A	0.25 μM		
T4362	2055397-18-5	MOZ-IN-3	MOZ	55 nM		
T3499	949912-58-7	Remodelin	NAT10			

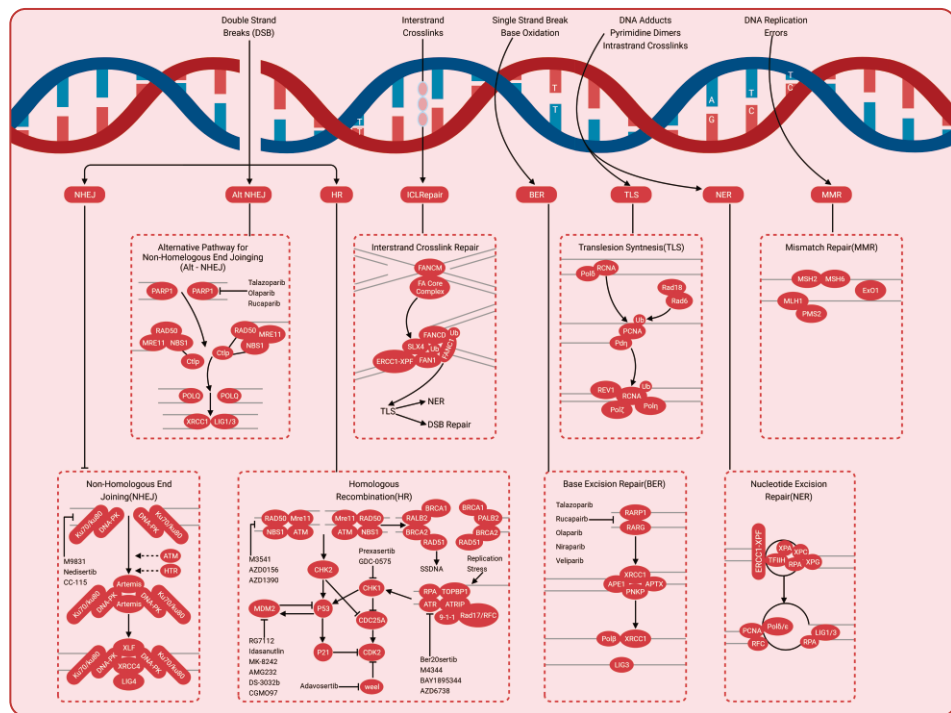
Histone Methyltransferase

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T16435	2514-30-9	PBIT	JARID1B;JARID1A;JARID1C	3 μM		
T16072	1857417-10-7	MI-538	Menin-MLL	21 nM		
T15080	890643-16-0	DC-05	DNMT1;PRMT1	1.09 μM (kd)		
T12428L	1616287-82-1	PF-06726304	EZH2 WT;EZH2 Y641N	0.7 nM (ki)		
T11486	2245255-66-5	GSK2807 Trifluoroacetate	SMYD3	14 nM (ki)		
T3624	1527503-11-2	A366	G9a/GLP	3.3 nM		
T3458	2083627-02-3	EED226	EED; PRC2	22 nM		
T3257	1255580-76-7	UNC0638	G9a/GLP	<15 nM		
T3099	1380288-87-8	Pinometostat	DOT1L	80 pM(Ki)	Phase 1	Acute biphenotypic leukaemia
T3084	1687736-54-4	SGC707	PRMT3; PRMT3	31 nM		



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DNA Damage & DNA Repair



DNA-PK

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T15789	1879887-96-3	LTURM34	DNA-PK; PI3Kβ; PI4Kδ	34 nM		
T7122	2230820-11-6	AZD-7648	DNA-PK	0.63 nM	Phase 2	Solid tumours
T7014	934493-76-2	Voxtalisisb	DNA-PK; PI3Kα; PI3Kβ; PI3Kγ; PI3Kδ	9 nM	Phase 1/2	Chronic lymphocytic leukaemia; Glioblastoma; Mantle-cell lymphoma; Non-Hodgkin's lymphoma; Solid tumours
T6883	1386874-06-1	LY3023414	DNA-PK; mTOR kinase; class I PI3K isoforms	6.07 nM	Phase 2	Endometrial Cancer; Non-small cell lung Cancer; Pancreatic Cancer; Prostate Cancer
T6319	936890-98-1	OSI027	DNA-PK; mTOR; PI3Kγ; mTORC1; mTORC2;	22 nM	Phase 1	Lymphoma; Solid tumours
T6283	19545-26-7	Wortmannin	PI3K; DNA-PK; ATM; MLC0K; ATR	3 nM	Preclinical	Cancer; Graft-versus-host disease
T6276	503468-95-9	NU7441	DNA-PK	13 nM (cell free)		

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CDK

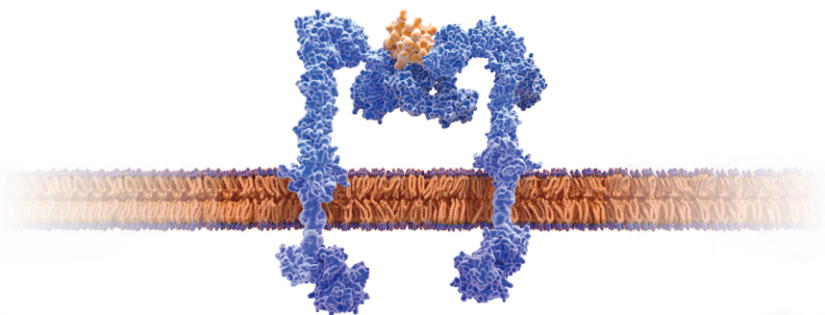
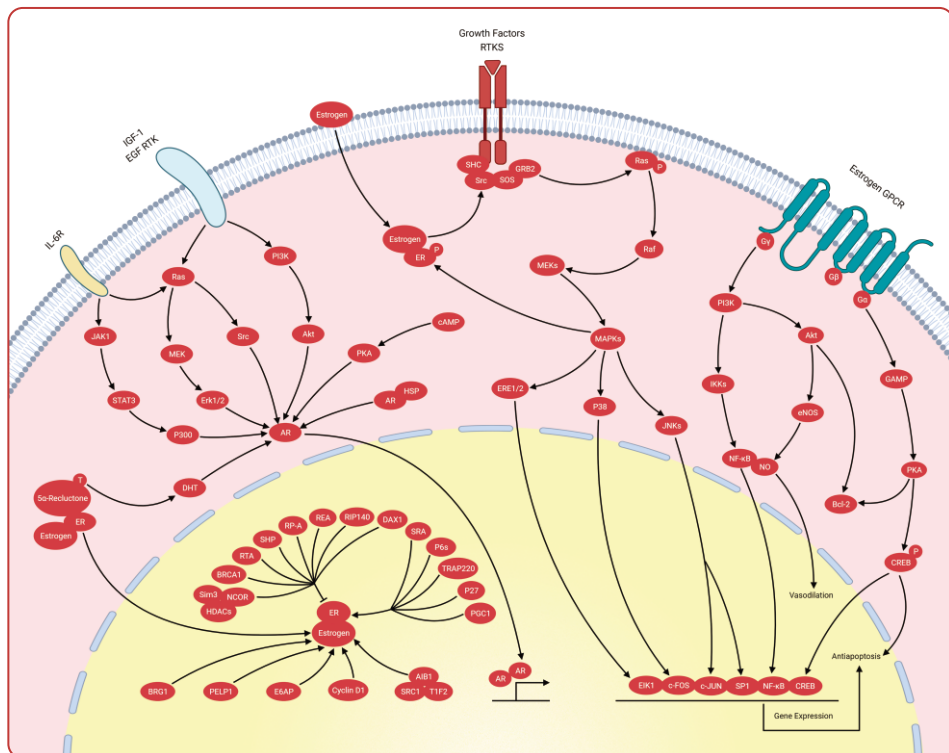
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T13584	1301708-12-2	BMVC-BC30	G-quadruplexe			
T20945	94-75-7	2,4-D	DNA synthesis			
T19833	703-95-7	5-Fluorourotic acid	thymidylate synthase			
T8886	1197896-79-9	NITD-2	RNA Synthesis			
T8800	1099592-35-4	NSAH	RR			
T8785	82186-71-8	HALOFUGINONE LACTATE	prolyl-tRNA synthetase; TGF-β		Phase 2	Duchenne muscular dystrophy
T7747	157000-76-5	Datelliptium chloride hydrochloride	DNA synthesis			
T7655	69123-98-4	Fialuridine	DNA polymerase			
T6501	75607-67-9	Fludarabine Phosphate	DNA polymerase α; DNA polymerase δ	1.1 μM(ki)	FDA Approved	Chronic lymphocytic leukaemia; Mantle-cell lymphoma; Non-Hodgkin's lymphoma
T6456	6960-45-8	CRT0044876	APE1	3 μM		

Other

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T7539	19916-73-5	O6-Benzylguanine	O6-alkylguanine-DNA-alkyltransferas			
T7221	129580-63-8	Satraplatin	DNA Alkylating		Phase 1/2	Squamous cell Cancer
T6798	21919-05-1	Tretazicar	DNA alkylator		Phase 2	Liver Cancer
T5846	70-25-7	Methylnitronitroso guanidine	DNA alkylator			
T4368	141977-79-9	Miriplatin	DNA Alkylator/Crosslinker		Approved	Hepatocellular carcinoma
T4350	31645-39-3	Palifosfamide	DNA alkylator	31.5 μM	Phase 3	Small cell lung Cancer
T13231	147059-72-1	Trovafloxacin	DNA gyrase; Topoisomerase; bacterial		FDA Approved	infections caused by susceptible strains of the designated microorganisms in uncomplicated urethral gonorrhoea in males and endocervical and rectal gonorrhoea in females caused by Neisseria gonorrhoeae as well as non gonococcal urethritis and cervicitis due to Chlamydia trachomatis.
T15611	1361227-90-8	JH-RE-06	REV1-REV7			
T15789	1879887-96-3	LTURM34	DNA-PK; PI3Kβ; PI4Kδ	34 nM		

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Endocrinology & Hormones



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Glucocorticoid Receptor

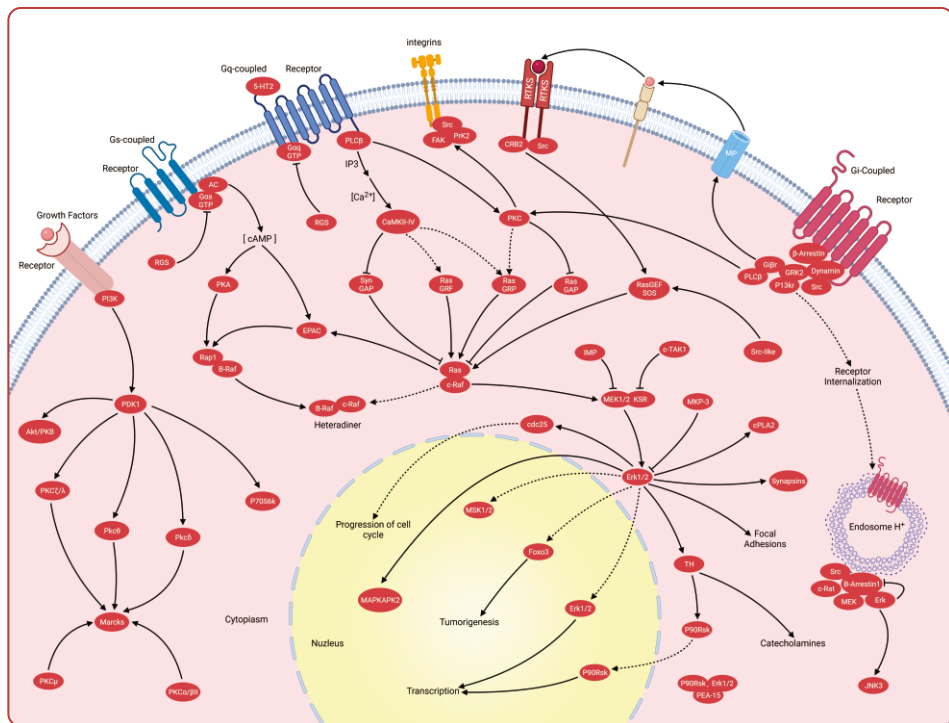
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T15451	827319-43-7	GW-870086	glucocorticoid receptor			
T8777	4419-39-0	Beclomethasone	glucocorticoid receptor		FDA Approved	asthma
T8396	125-10-0	Prednisone acetate	Glucocorticoid Receptor		FDA Approved	anti-inflammatory or immunosuppressive drug for allergic; dermatologic; gastrointestinal; hematologic; ophthalmologic; Nervous system; renal; respiratory; rheumatologic; infectious; endocrine; or neoplastic conditions as well as in organ transplant
T6580	1247-42-3	Meprednisone	Glucocorticoid Receptor		FDA Approved	Systemic lupus erythematosus; rheumatoid arthritis; nephrotic syndrome; ulcerative colitis; autoimmune hepatitis
T3962	79756-69-7	TPI1	recombinant SHP-1	40 nM.		
T3316	426-13-1	Fluoromethalone	Glucocorticoid Receptor		FDA Approved	Skin diseases; Allergic and inflammatory eye disease
T3096	2181-04-6	Potassium canrenoate	Mineralocorticoid Receptor		Approved	Heart Failure
T1559	5593-20-4	Betamethasone dipropionate	Glucocorticoid Receptor		FDA Approved	Psoriasis
T15451	827319-43-7	GW-870086	glucocorticoid receptor			

Other

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T11560	1314796-00-3	hGPR91 antagonist 1	HGPR91	7 μM		
T13414	115730-24-0	ZT 52656A hydrochloride	kappa opioid receptor			
T11857	2245072-21-1	LIT-001	oxytocin receptor			
T13865	41307-63-5	Resorcinolnaphthal ein	ACE2	(EC50) 19.5 μM		
T22355	55-03-8	Levothyroxine sodium	Thyroid Hormone		FDA Approved	hypothyroidism.

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GPCR & G Protein



Hedgehog Smoothened

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T14188	1357350-60-7	ALLO-2	Smoothened			
T2450	304909-07-7	SANT1	Smoothened	1.2 Nm		
T2299	1059734-66-5	BMS833923	Smoothened	21 nM	Phase 2	Chronic myeloid leukaemia
T2825	4449-51-8	Cyclopamine	Smoothened	46 nM (TM3H-1 2 cells)	Preclinical	Breast Cancer; Cancer
T2666	1258861-20-9	Taladegib	Smoothened		Phase 1/2	Oesophageal Cancer; Small cell lung Cancer

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Adrenergic Receptor

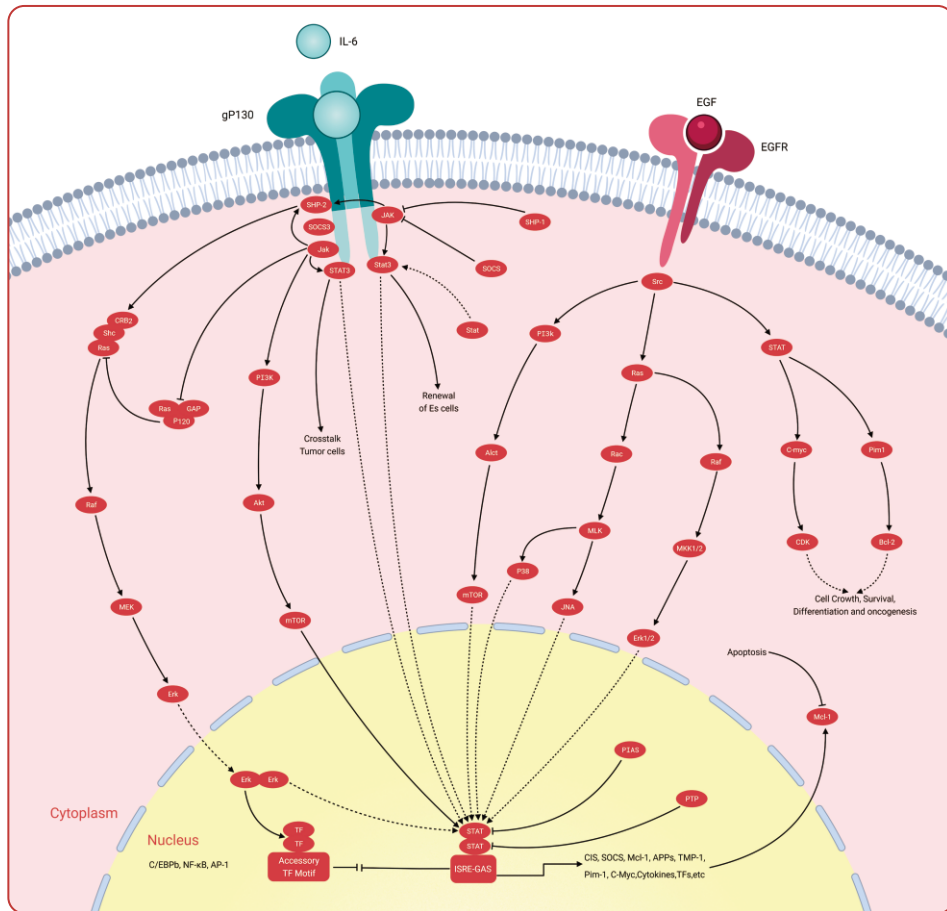
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21066	3414-63-9	Norepinephrine bitartrate salt	Adrenergic Receptor		FDA Approved	vasodilatory shock states such as septic shock and neurogenic shock and has shown a survival benefit over dopamine. Also used as a vasopressor medication for patients with critical hypotension.
T13016	174689-39-5	SR59230A	β3-adrenoceptor	40 nM		
T12643	109351-34-0	(R)-Terazosin	α1a-adrenoceptor; α1b-adrenoceptor; α1d-adrenoceptor		FDA Approved	symptomatic benign prostatic hyperplasia and hypertension
T11318	86484-91-5	Dopexamine hydrochloride	β2-adrenergic receptor		Phase 4	Oral Cancer; Head and Neck Cancer; Free Flap; Hypotension
T10952	219311-44-1	Dabuzalgron	α1A-adrenergic receptor			
T0948	62-13-5	Adrenalone hydrochloride	α1-adrenergic receptor		Approved	Hemorrhage
T0970	17659-49-3	Anisodamine	Adrenergic Receptor		Approved	Acute Circulatory Shock
T0852	51460-26-5	Carbazochrome sodium sulfonate	Adrenergic Receptor		Approved	Capillary And Parenchymal Hemorrhage
T0970	17659-49-3	Anisodamine	Adrenergic Receptor		Approved	Acute Circulatory Shock

Other

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T8497	1648843-04-2	SX-682	CXCR1, CXCR2		Phase 1	Melanoma Stage III; Melanoma Stage IV
T7681	878385-84-3	AZD-5069	CXCR2	0.79 nM	Phase 2	Bladder Cancer; Coronary disorders; Head and neck Cancer; Non-small cell lung Cancer; Solid tumours
T8702	99295-33-7	SKF-83566	D1; D5; 5-HT2			
T8633	1689-64-1	9-FLUORENOL	dopamine reuptake			
T8876	2230198-03-3	PF-06882961 Tris	GLP-1		Phase 1	OBESITY
T8748	914454-01-6	Exendin-4 acetate	GLP-1	3.22 nM	Phase 4	Polycystic Ovary Syndrome
T8901	423145-35-1	YUM70	GRP78	1.5 μM		
T8353	130-85-8	Pamoic acid	GPR35			

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JAK & STAT Signaling



JAK

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T17019	1260181-14-3	TCS 21311	JAK3; JAK2; JAK1 PKCα; PKCβ; GSK-3β	8 nM		
T14687	1609392-27-9	BMS-986165	Tyk2 JH2; JAK1 JH2	0.2 nM	Phase 3	Psoriasis
T14331	1425381-60-7	Gusacitinib	SYK; JAK	5-46 nM	Phase 2	Atopic Dermatitis
T12427	2140301-96-6	PF-06700841 (P-Tosylate)	JAK1; JAK2; JAK3		Phase 2	Chronic Plaque Psoriasis
T8742	939681-36-4	JAK2 inhibitor G5-7	JAK2			
T8719	882290-02-0	SC99	STAT3; JAK2			
T8546	892686-59-8	BD750	JAK3; STAT5			
T7503	1310726-60-3	Upadacitinib	JAK1; JAK2	43 nM	FDA Approved	Rheumatoid arthritis

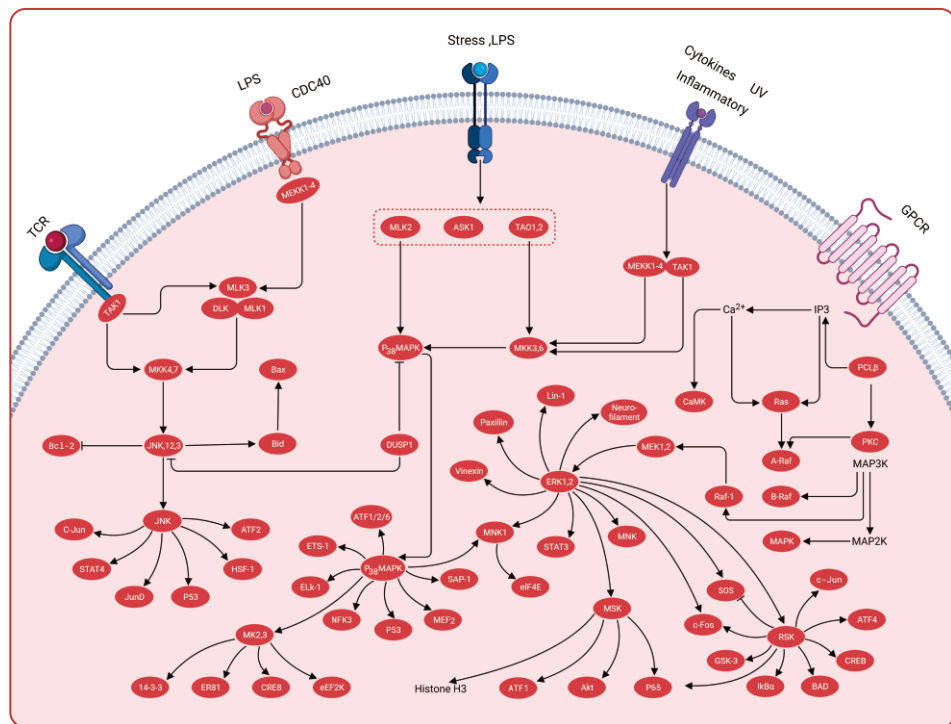
STAT

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21267	28230-32-2	HODHBT	STAT5			
T13009	2059952-75-7	STAT3-IN-1	STAT3	1.82 μM (in HT29 cells)		
T8719	882290-02-0	SC99	STAT3; JAK2			
T8597	744270-00-6	ML116	STAT3			
T8546	892686-59-8	BD750	JAK3; STAT5			
T8478	1400989-25-4	SC-43	SHP-1; STAT3; apoptosis			

Others

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T22431	186611-11-0	SU5204	VEGFR2; HER2	4 μM		
T11213	2071195-74-7	Epertinib hydrochloride	EGFR; HER4; HER2	1.48 nM		
T8742	939681-36-4	JAK2 inhibitor G5-7	JAK2			
T8719	882290-02-0	SC99	STAT3; JAK2			

MAPK



ERK

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T13265	1139-83-9	Urolithin B	NF-kB; JNK; ERK; Akt; AMPK; Human Endogenous Metabolite			
T21295	1265916-41-3	BIX 02189	ERK; MEK	1.5 nM		
T6948	839707-37-8	Pluripotin	ERK1; RasGAP	98 nM(Kd)	Phase 1/2	Gastric Cancer
T6818	181223-80-3	DEL22379	ERK	0.5 μM		
T2356	872573-93-8	Ro 3306	CDK1; ERK; PKA; PKCδ; SGK	20 nM(Ki)		
T21295	1265916-41-3	BIX 02189	ERK; MEK	1.5 nM		
T2027	548470-11-7	ISRIB	PERK			
T1956	865362-74-9	FR180204	ERK1; ERK2	0.14 μM(Ki)		
T1933	362003-83-6	NVP 231	CERK	12±2 nM		

MEK

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21295	1265916-41-3	BIX 02189	ERK; MEK	1.5 nM		
T7742	179246-08-3	GW 284543 hydrochloride	MEK5			
T6971	946128-88-7	RO5126766	MEK1; B-Raf; B-Raf (V600E); C-Raf	8.2 nM	Phase 1	Multiple myeloma; Non-small cell lung Cancer; Solid tumour
T6843	1168091-68-6	GDC0623	MEK1	0.13 nM(ki)	Phase 1	Solid tumours
T6189	391210-10-9	PD0325901	MEK	0.33 nM (cell free)	Phase 2	Neurofibromatosis
T2508	606143-89-9	Binimetinib	MEK	12 nM	FDA Approved	Malignant melanoma
T2443	212631-79-3	CI1040	MEK1; MEK2	17 nM (cell free)	Phase 2	Cancer
T2416	1094614-85-3	BIX02189	ERK5; MEK1; MEK2; MEK5; TGF βR1	1.5 nM		
T2327	257933-82-7	Pelitinib	EGFR; HER2/ErbB2; MEK Raf; Src	38.5 nM	Phase 2	Colorectal Cancer; Non-small cell lung Cancer

p38 MAPK

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T10990	10605-03-5	Dehydrocorydaline chloride	p38 MAPK; Bax; Bcl-2; caspase-7; caspase-8; PARP			
T7667	449811-92-1	R1487	p38α			
T7661	1670-87-7	SD 169	p38			
T7367	836683-15-9	Acumapimod	p38	<1 μM		
T7276	271576-80-8	SD 0006	p38 MAPK			
T7030	139051-27-7	anemarsaponin B	p38			
T2277	585543-15-3	Losmapimod	p38α; p38β	8.1(pKi)	Phase 3	Acute coronary syndromes
T2118	354812-17-2	SC514	Aurora B; CDK2/CyclinA; IKK2; p38α; PRAK	11.2±4.7 μM		
T1974	586379-66-0	PH797804	p38α; p38β	26 nM	Phase 2	Chronic obstructive pulmonary disease; Musculoskeletal pain; Neuropathic pain; Rheumatoid arthritis
T1922	82508-31-4	Pseudolaric Acid B	p38		Preclinical	Mycoses
T1764	152121-47-6	SB203580	p38 MAPK	0.3-0.5 μM (THP-1 cells)	Preclinical	Cancer; Postmenopausal osteoporosis; Rheumatoid arthritis; Septic shock

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Calcium Channel

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T11102	T11102	DS16570511	mitochondrial calcium uniporter			
T12032	116666-63-8	Mibefradil dihydrochloride	T-type calcium channel; L-type calcium channel		Phase 1	Brain and Central Nervous System Tumors
T16339	67812-42-4	Norverapamil hydrochloride	Calcium channel blocker; P-gp (P-glycoprotein)			
T21454	55985-32-5	Nicardipine	calcium channel		FDA Approved	chronic stable angina/hypertension.
T19765	66774-02-5	MDK-4025	Calcium Channel			
T8867	1219927-22-6	RO2959 Hydrochloride	CRAC channel; IL-2	402 nM		
T8815	64748-79-4	Azumolene	Calcium Channel			
T8681	92564-34-6	HA-1004 dihydrochloride	PKA; PKC; calcium channel			
T6777	71145-03-4	Bay K 8644	L-type calcium channel	17.3nM(IE C50)		
T6633	95635-55-5	Ranolazine	Calcium Channel		FDA Approved	Angina pectoris
T6577	89226-50-6	Manidipine	Calcium Channel	2.6 nM	Approved	Hypertension

Potassium Channel

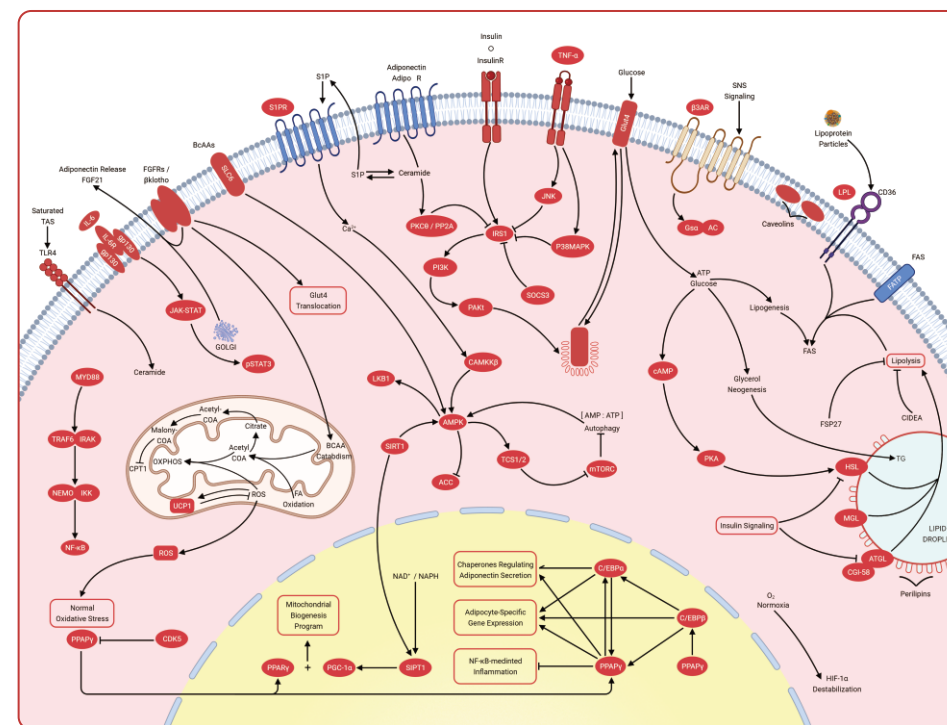
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21487	150812-13-8	Retigabine dihydrochloride	KCNQ3/5; KCNQ2/Q3; KCQN4			
T17262	122955-13-9	XE 991 dihydrochloride	Kv7.1 channel; Kv7.2 channel; Kv7.2 + Kv7.3 channel; M-current	0.75 μM		
T16110	1928763-08-9	ML418	Kir7.1			
T15758	105431-72-9	Linopirdine	TRPV1; M-type K+ current	2.4 μM		
T15555	500715-03-7	IK1 inhibitor PA-6	KIR2.x currents	12-15 nM		
T15545	325457-89-4	ICA-27243	KCNQ2/Q3 potassium channel			
T13320	1315380-70-1	VU591 hydrochloride	Kir1.1	0.24 μM		
T13316	1052515-91-9	VU0134992 hydrochloride	Kir4.1			
T12478	85371-64-8	Pinacidil monohydrate	Potassium Channel		FDA Approved	hypertension
T10979	82749-70-0	DCPIB	VRAC; TRESK; TASK-1; TASK-3	0.14 μM		
T0916	94-25-7	Butyl 4-aminobenzoate	Potassium Channel inhibitor		Approved	chronic pain

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Sodium Channel

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T19644	104-31-4	Benzonatate	sodium channel		FDA Approved	antitussive
T8711	1235406-03-7	PF-05186462	Nav1.7 channel			
T8444	1356834-62-2	N-Me-aminopyrimidinone9	Sodium Channel			
T8299	875313-64-7	Dimethyl lithospermate B	Sodium Channel			
T7811	88069-49-2	Pilsicainide HCl	Sodium Channel		Approved	cardiac arrhythmia
T7547	202825-45-4	Ralfinamide mesylate	Sodium Channel			
T7349	133865-88-0	Ralfinamide	Na-channel		Phase 3	Neuropathic pain
T7336	313254-51-2	ICA-121431	Nav1.7 channel	19 nM		
T2342	934240-30-9	CNV1014802	Sodium Channel		Phase 3	Trigeminal neuralgia
T2192	271-44-3	Indazole	Sodium Channel			

Metabolism



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D Dehydrogenase

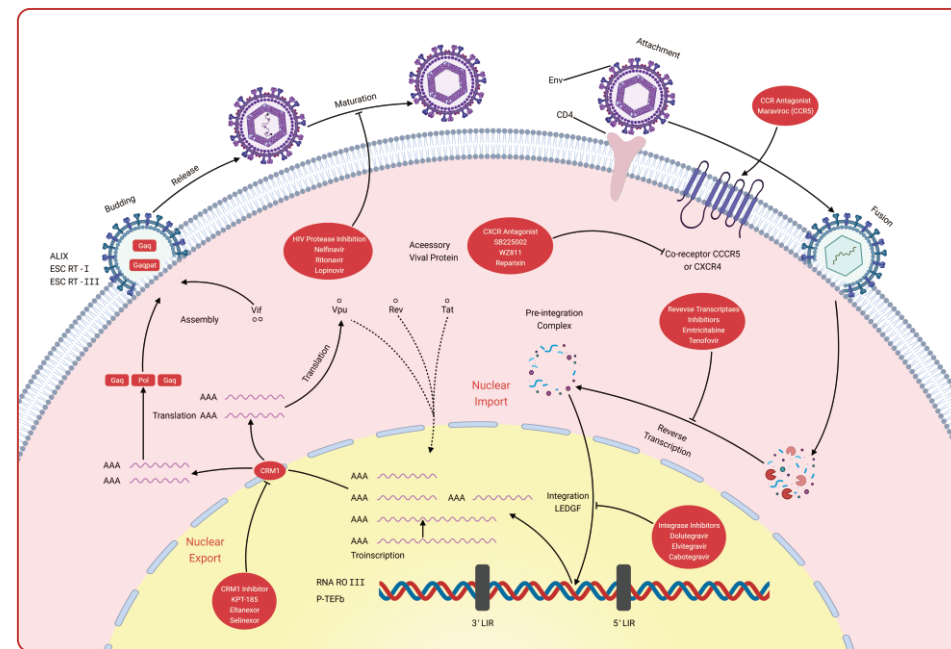
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T23533	1477-57-2	WIN 18446	ALDH1a2			
T22253	1448346-63-1	AG-120 (racemic)	IDH1		FDA Approved	acute myeloid leukemia (AML)
T19831	565-73-1	Sodium Oxamate	LDH; CDK; Apoptosis			
T16384	1887014-12-1	Olutasidenib	R132C-IDH1; R132H-IDH1		Phase 1/2	Acute Myeloid Leukemia; Acute Myelogenous Leukemia; Myelodysplastic Syndrome
T16068	921605-87-0	MF-438	SCD			
T15435	1445879-21-9	GSK2837808A	LDH; LDHB	1.9 nM		
T15022	1005334-57-5	CVT-10216	ALDH2	29 nM		
T14884	681159-27-3	CBR-5884	PHGDH; serine synthesis			
T14878	944808-88-2	CAY10566	SCD1			
T14501	2225819-06-5	BAY-2402234	DHODH		Phase 1	Leukemia
T11829	1964515-43-2	LDH-IN-1	LDHA; LDHB			
T11020	1263303-95-2	DHODH-IN-11	DHODH	5.03(pKa)		
T10384	1035688-66-4	ASLAN003	DHODH		Phase 2	Acute Myeloid Leukemia

D Other

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21629	1977-10-2	Loxapine	5-HT2 (bovine); 5-HT2 (bovine); 5-HT2 (human); D2; D4		FDA Approved	Schizophrenia
T20446	93-51-6	Creosol	Human Endogenous Metabolite			
T20257	121-98-2	Methyl 4-anisate	Endogenous Metabolite			
T19418	62697-73-8	Methionine sulfoxide	Human Endogenous Metabolite		Approved	Adjuvant therapy, such as cirrhosis and fatty liver, can also be used for acetaminophen poisoning and liver damage caused by drugs such as alcohol and sulfa.
T11557	2097262-60-5	FASN-IN-3	FASN			
T13092	863239-61-6	Tauro-Obeticholic acid	FXR			
T21344	73285-50-4	Duvoglustat hydrochloride	α -glucosidase			
T13130	52452-60-5	Terphenyllin	α -glucosidase			
T16994	1260533-36-5	TAS-116	HSP90 α ; HSP90 β		Phase 1	Advanced Solid Tumors
T13554	289893-26-1	Arimoclomol maleate	HSP			
T11897	1033805-22-9	Telotristat ethyl	tryptophan hydroxylase		Approved	reduce serotonin levels, carcinoid syndrome.

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Microbiology & Virology



D HIV

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T16764	431980-38-0	RN-18	HIV-1			
T15436	1443460-91-0	GSK2838232	HIV			
T13647	9011-18-1	Dextran sulfate sodium salt (MW 16000-24000)	HIV; Apoptosis		FDA Approved	restoration of blood mass during surgical interventions
T11451	186452-09-5	GPI-1046	HIV			
T10570	864953-39-9	Fostemsavir Tris	HIV-1		FDA Approved	HIV Infections
T10111	86583-19-9	3-Deazaadenosine hydrochloride	HIV-1; A012 isolate; HIV-1; A018 isolate; S-adenosylhomocysteine hydrolase			

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HBV

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T5832	441785-25-7	Besifovir	HBV		Approved	Hepatitis B
T4475	1572510-42-9	JNJ-632	HBV			
T4121	118159-48-1	Bicyclol	HBV		Approved	Fatty liver; Viral hepatitis

HCV

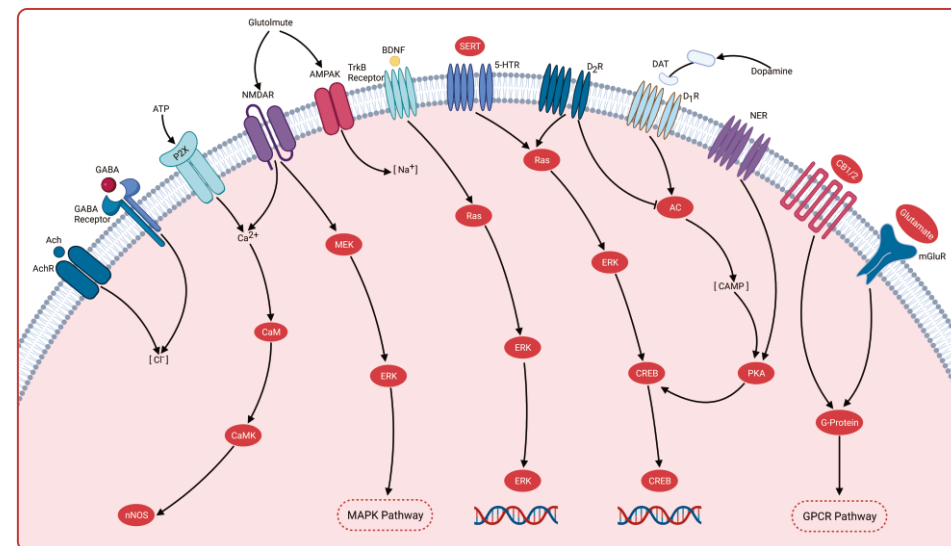
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T17029	1000787-75-6	Tegobuvir	HCV NSSB polymerase		Phase 2	Hepatitis C; Chronic
T19862	1535212-07-7	Voxilaprevir	HCV		FDA Approved	chronic Hepatitis C
T16088	443642-29-3	MK-0608	HCV replicon	(EC50)0.3 μM		
T15573	942123-43-5	Inarigvir soproxil	HCV	(EC50)2.2 /1.0 μM	Phase 2	HBV; Hepatitis B; Hepatitis B; Chronic
T14667	321673-30-7	BLT-1	HCV; SR-BI			
T8689	54-05-7	CHLOROQUINE	HIV-1; autophagy; TLR; SARS-COV-2		FDA Approved	infections of P. vivax, P. malariae, P. ovale, and susceptible strains of P. falciparum, extraintestinal amebiasis
T8311	1258453-75-6	ABX-464	HIV	0.1 μM - 0.5 μM	Phase 2	Rheumatoid Arthritis
T7903	127779-20-8	Saquinavir	HIV Protease		FDA Approved	HIV-1 with advanced immunodeficiency
T7212	147221-93-0	Delavirdine (mesylate)	HIV-1		FDA Approved	HIV-1 infection
T7111	201341-05-1	Tenofovir Disoproxil	HIV		FDA Approved	HIV-1 infection
T6653	94749-08-3	Salmeterol Xinafoate	β2-adrenergic receptor; WT β2AR		FDA Approved	asthma and chronic obstructive pulmonary disease COPD

Others

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T13041	24730-31-2	Surfactin	HSV-1			
T14495	1985605-59-1	Baloxavir	Influenza virus		Approved	anti-influenza virus
T13229	11089-65-9	Tunicamycin	Bacterial; antiFungal; Influenza virus; Antibiotic			

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Neuroscience



Dopamine Receptor

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T8702	99295-33-7	SKF-83566	D1; D5; 5-HT2			
T8633	1689-64-1	9-FLUORENOL	dopamine reuptake			
T8423	1386162-69-1	ML417	D3	38 nM (EC50)		
T8389	117-89-5	Trifluoperazine	D2	1.2 nM	FDA Approved	anxiety disorders, depressive symptoms secondary to anxiety and agitation
T8385	54143-57-6	Metoclopramide hydrochloride hydrate	D2		FDA Approved	gastroesophageal reflux disease (GERD)
T5954	41372-08-1	Alpha-Methyldopa Sesquihydrate	DOPA decarboxylase			
T5858	106516-24-9	Sertindole	D2; 5-HT		Approved	Chronic obstructive pulmonary disease
T4576	150915-41-6	Perospirone	5-HT2A; D2; 5-HT1A	2.9 nM (Ki)	Approved	Schizophrenia
T4369	125941-87-9	SCH 23390 hydrochloride	D1; D5	0.2 nM		
T2592	91374-20-8	Ropinirole hydrochloride	D2	29 nM (Ki)	FDA Approved	Parkinson's disease; Restless legs syndrome
T2574	59338-87-3	Alizapride hydrochloride	Dopamine		Approved	Nausea And Vomiting

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5-HT Receptor

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21337	367514-87-2	Lurasidone	5-HT7; 5-HT1A; D2		FDA Approved	schizophrenia.
T21231	154323-57-6	Almotriptan	5-HT1B/1D		FDA Approved	acute migraine headache
T21013	303-49-1	Clomipramine	5-HT		FDA Approved	obsessive-compulsive disorder and disorders with an obsessive-compulsive component (e.g. depression, schizophrenia, Tourette's disorder)
T16421	220643-77-6	p-MPPI hydrochloride	5-HT1A			
T8757	856681-05-5	R-Lorcaserin hydrochloride hemihydrate	5-HT2C			
T8737	148547-33-5	GR 125743	5-HT1B/1D			
T8720	903580-39-2	PRX-07034	5-HT6			
T8702	99295-33-7	SKF-83566	D1; D5; 5-HT2			
T8666	121679-13-8	Naratriptan	5-HT1		FDA Approved	Naratriptan
T0031	138982-67-9	Ziprasidone hydrochloride monohydrate	5-HT transporter; 5-HT1A; 5-HT1B; 5-HT1D; 5-HT2A; 5-HT2C; 5-HT6; 5-HT7; α 1A-adrenergic receptor; α 2A-adrenergic receptor; D1; D2; D3; H1 receptor; norepinephrine transporter (NET)		FDA Approved	Bipolar disorders; Schizophrenia
T0025	52-86-8	Haloperidol	5-HT; Dopamine		FDA Approved	Schizophrenia

AChR

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T19084	830-81-9	1-Naphthyl acetate	AChE			
T14140	666-99-9	Agaric acid	adenine nucleotide translocase			
T14094	135410-20-7	Acetamiprid	nAChR			
T8868	360791-49-7	4BP-TQS	α 7 nAChRs			
T8770	525-57-5	Harmalol	AChR			
T8725	T8725	A 582941 HCl (848591-90-2 (free base))	α 7 nAChR			
T8585	5778-80-3	TA-03	AChE			
T6575	886047-22-9	LY2119620	M2 mAChR; M4 mAChR			

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Adrenergic Receptor

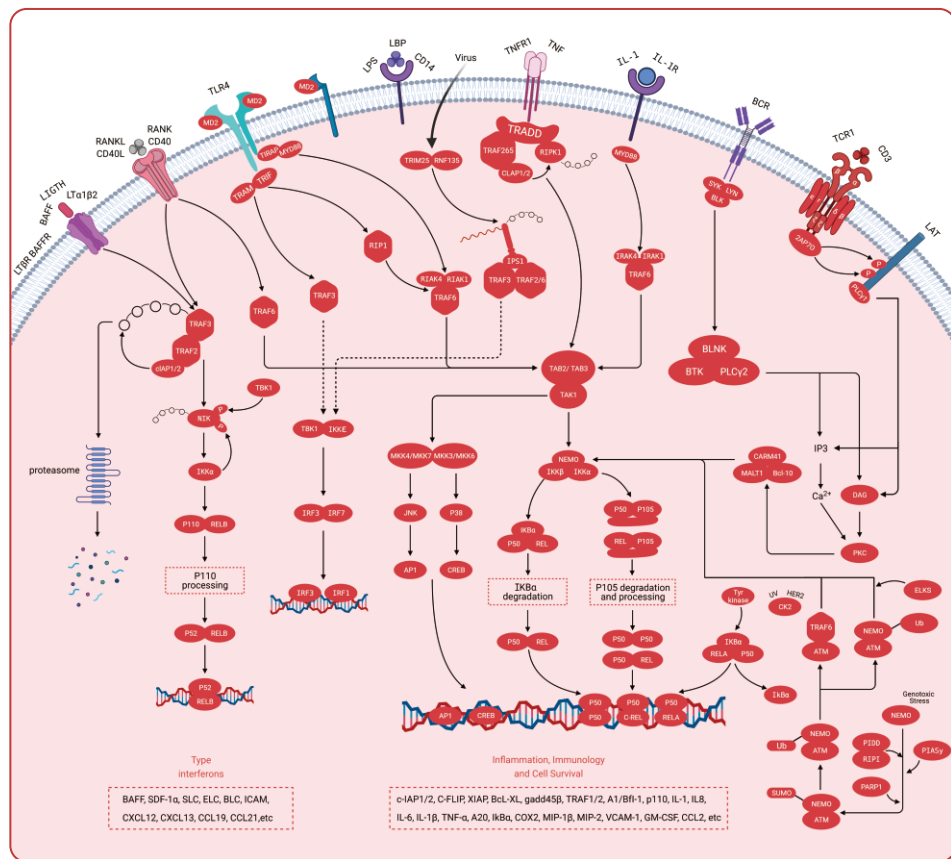
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T23283	109544-45-8	RX 821002 hydrochloride	α 2-adrenoceptor			
T21066	3414-63-9	Norepinephrine bitartrate salt	Adrenergic Receptor		FDA Approved	vasodilatory shock states such as septic shock and neurogenic shock and has shown a survival benefit over dopamine. Also used as a vasopressor medication for patients with critical hypotension.
T13016	174689-39-5	SR59230A	β 3-adrenoceptor	40 nM		
T12643	109351-34-0	(R)-Terazosin	α 1a-adrenoceptor; α 1b-adrenoceptor; α 1d-adrenoceptor		FDA Approved	symptomatic benign prostatic hyperplasia and hypertension
T11318	86484-91-5	Dopexamine hydrochloride	β 2-adrenergic receptor		Phase 4	Oral Cancer/Head and Neck Cancer; Free Flap; Hypotension
T10952	219311-44-1	Dabuzalgron	α 1A-adrenergic receptor			
T8810	23031-25-6	Terbutaline	β 2-adrenergic receptor		FDA Approved	reversible, obstructive airway disease
T8738	T8738	LUN42518 HCl 47142-51-8 (free base)	α -adrenergic receptor			
T8696	3506-09-0	Propranolol hydrochloride	β 1-adrenergic receptor; β 2-adrenergic receptor		FDA Approved	hypertension; angina pectoris due to coronary atherosclerosis; atrial fibrillation; myocardial infarction; migraine; essential tremor; hypertrophic subaortic stenosis; pheochromocytoma; and proliferating infantile hemangioma

Others

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T19624	110958-19-5	Fasoracetam	GABA			
T12568	55476-47-6	PSB-12062	P2X4	1.38 μ M		
T21422	73232-52-7	Methylnaltrexone bromide	μ -opioid receptor		FDA Approved	constipation
T17222	342577-38-2	Velneperit	neuropeptide Y (NPY) Y5 receptor		Phase 2	Obesity
T8907	25953-17-7	Minaprine dihydrochloride	MAO-A		Approved	antidepressant
T12717	802906-73-6	Basimglurant	mGlu5		Phase 1	Major Depressive Disorder

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NF - κB



NOD

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T15052	54863-37-5	Dapansutril	NLRP3		Phase 2	Schnitzler Syndrome
T7682	30315-93-6	Asymmetric dimethylarginine	NO synthesis; Human Endogenous Metabolite			
T7597	22150-76-1	6-Biopterin	NO synthesis			
T0122	477-90-7	Bengenin	IL-1β; IL-6; NF-κB; NOD; TNF-α	15 μM	Approved	Chronic Bronchitis
T0109	25717-80-0	Molsidomine	NOD		Approved	Angina Pectoris

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NF - κB

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T16974	1450833-55-2	TAK-243	UBA1; NF-κB; Apoptosis	1 nM	Phase 1	Advanced Malignant Solid Tumors
T16706	2797-51-5	Quinoclimine	NF-κB			
T16290	1660114-31-7	NIK SMI1	NIK			
T13265	1139-83-9	Urolithin B	NF-κB; JNK; ERK; Akt; AMPK Human Endogenous Metabolite			
T0907	599-79-1	Sulfasalazine	COX-1; COX-2; NF-κB		FDA Approved	Rheumatoid Arthritis
T0694	103177-37-3	Pranlukast	IL-5; CysLTR; NF-κB; Eosinophil cationic protein; Mucin-2; TNF-α		Approved	Allergic rhinitis; Asthma
T0646	89-57-6	Mesalamine	COX; ALOX5; MPO; NF-κB; PPARγ		FDA Approved	Ulcerative colitis
T0607	71939-50-9	Dihydroartemisinin	Autophagy; NF-κB		Approved	malaria
T0429	3416-24-8	Glucosamine	Chitosanase; MMP-9; NF-κB IFγ; TNF-α		Approved	Osteoarthritis
T0335	54-21-7	Sodium salicylate	COX-1; COX-3; NF-κB		Approved	rheumatism
T0307	25301-02-4	Tyloxapol	NF-κB; LPL		FDA Approved	inhaled surfactant that assists in removing and liquefying and removing bronchopulmonary secretions with mucus and pus

IκB / IKK

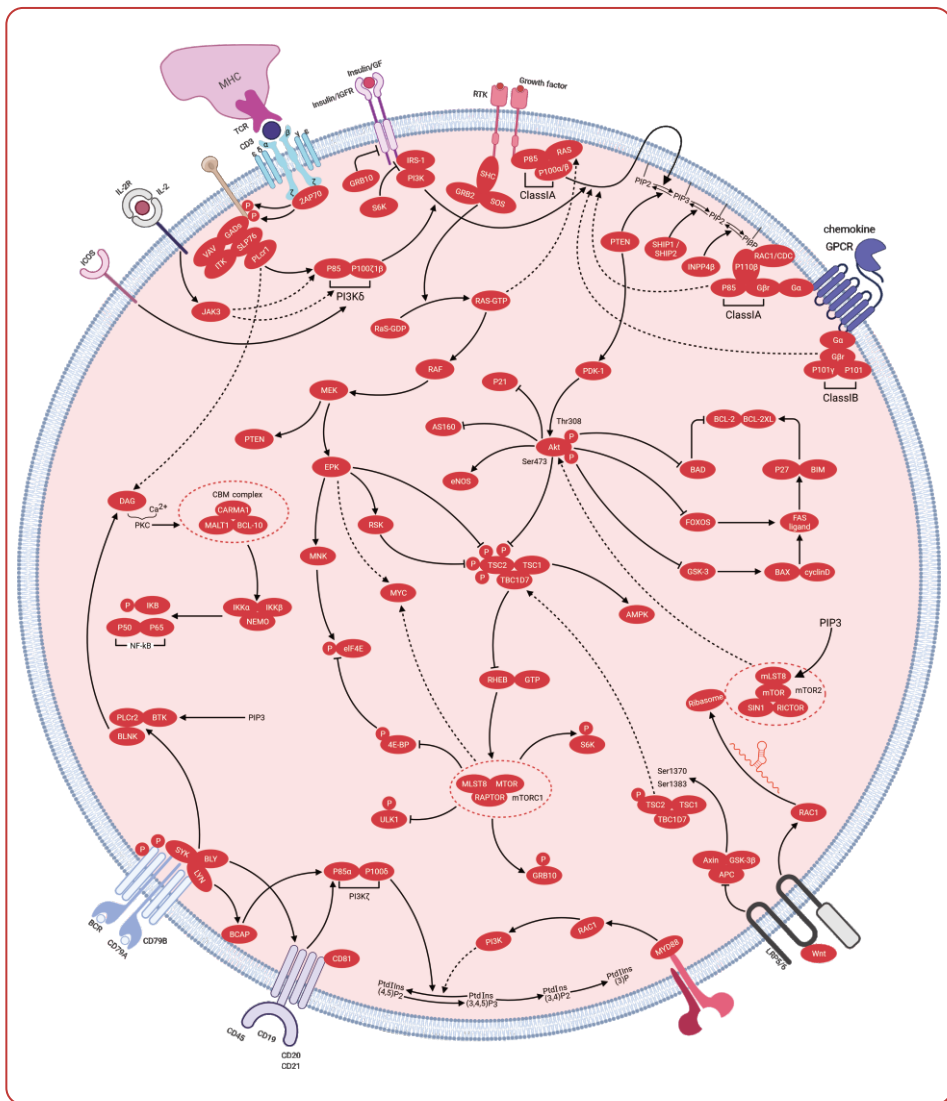
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T15559	1292310-49-6	TBK1 /IKKε-IN-2	TBK1; IKKε	0.6 nM (IC50, at 5 μM ATP)		
T10477	2409479-29-2	BAY-985	TBK1; TBK1; IKKε	2 nM (low ATP)		
T8705	113760-29-5	BOT-64	IKK2			
T8542	547757-23-3	BMS-345541 hydrochloride	IKK1; IKK2	0.3 μM		
T7951	1893397-65-3	TBK1 /IKKε-IN-5	TBK1; IKKε	1 nM		
T1558	501-36-0	Resveratrol	COX-1; COX-2; DNA polymerase α; IKKβ; LOX; Quinone reductase 2; SIRT1; SIRT2	1.1 μM (cell free)	Approved	Herpes labialis infections
T1934	196309-76-9	Bay 11-7085	IκBα phosphorylation	10 μM		
T1902	19542-67-7	Bay 11-7082	E2-conjugating enzymes; IκB α phosphorylation	10 μM		
T2118	354812-17-2	SC514	Aurora B; CDK2/CyclinA; IKK2; p38α; PRAK	11.2±4.7 μM		
T2106	1421227-53-3	WS6	ErbB3-Binding Protein-1 (EBP2); IκB kinase	0.28 μM		

Rip Kinase

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T7504	852391-15-2	Necrostatin 2 racemate	RIPK1			
T5401	1423186-80-4	GSK2983559	RIP2		Phase 1	Inflammatory bowel diseases

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PI3K & Akt & mTOR Signaling



mTOR

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T16567	1927857-61-1	PQR-530	PI3K; mTORC1; mTORC2			
T16156	1179347-65-9	MT 63-78	AMPK; mTORC1	25 µM (EC50)		
T11728	329182-61-8	JR-AB2-011	mTORC2			
T7343	1220699-06-8	PF-04979064	PI3K; mTOR	0.13 nM (Ki)		
T7166	1033735-94-2	GNE-493	mTOR; PI3K	3.4 nM		
T1861	1086062-66-9	Ompalisib	mTORC1; p110α; p110β; p110γ; p110δ	0.019 nM(Ki)	Phase 1	Idiopathic pulmonary fibrosis; Lymphoma; Solid tumours
T1859	1009298-09-2	AZD8055	mTOR	0.8 nM(MDA-MB-468 cells)	Phase 1	Solid tumours
T1537	53123-88-9	Rapamycin	mTOR; Autophagy	0.1 nM (HEK293 cells)	FDA Approved	Coronary artery restenosis; Lymphangioliomyomatosis; Renal transplant rejection
T1784	159351-69-6	Everolimus	mTOR (FKBP12)	1.6-2.4 nM (cell free)	FDA Approved	Angiomyolipoma; Astrocytoma; Breast Cancer; Coronary artery restenosis; Heart transplant rejection; Kidney disorders; Liver transplant rejection; Neuroendocrine tumours; Partial epilepsies; Renal cell carcinoma; Renal transplant rejection

GSK-3

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T14066	1034895-42-5	9-ING-41	GSK-3β		Phase 2	Myelofibrosis
T11467	187325-53-7	GSK-3β inhibitor 1	GSK-3β	4.9 nM		
T8908	536-38-9	4-Chloro-2'-bromoacetophenone	GSK-3β			
T8605	919936-70-2	GS87	GSK-3			
T7473	10075-50-0	5-Bromaindole	GSK-3			
T1755	603288-22-8	LY2090314	GSK-3α; GSK-3β	0.9 nM	Phase 2	Acute myeloid leukaemia; Acute promyelocytic leukaemia; Pancreatic Cancer
T1741	612487-72-6	AZD1080	GSK-3α; GSK-3β	6.9 nM	Phase 1	Alzheimer's disease

AMPK

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T16156	1179347-65-9	MT 63-78	AMPK; mTORC1	25 µM (EC50)		
T16099	1394371-71-1	MK8722	AMPK			
T8526	657-24-9	Metformin	AMPK; Autophagy		FDA Approved	diabetes mellitus
T8476	140405-36-3	RSVA 405	STAT3; AMPK	1 µM(EC50)		
T0740	1115-70-4	Metformin hydrochloride	AMPK		FDA Approved	Type 2 Diabetes Mellitus

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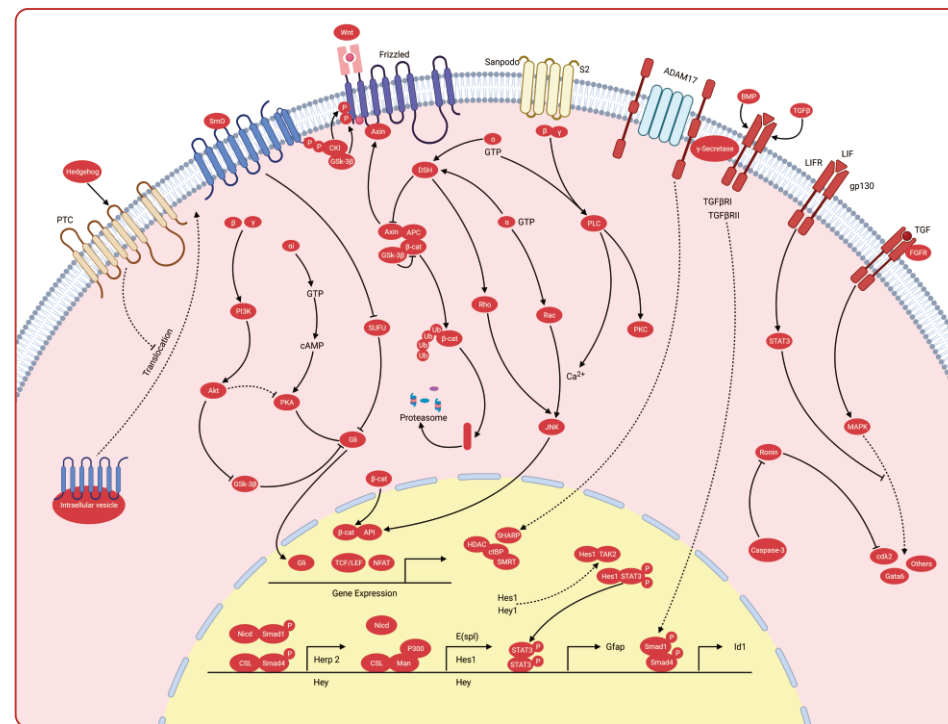
PI3K

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21992	351986-85-1	Vacuolin-1	PIKfyve			
T16567	1927857-61-1	PQR-530	PI3K; mTORC1; mTORC2			
T15789	1879887-96-3	LTURM34	DNA-PK; PI3Kβ; PI4K δ	34 nM		
T14998	1402152-13-9	Copanlisib dihydrochloride	PI3Kα; PI3Kδ; PI3Kβ; PI3Kγ; mTOR	0.5 nM	FDA Approved	relapsed follicular lymphoma
T14511	1375469-38-7	BAY1082439	PI3Kα; PI3Kβ; PI3Kδ		Phase 1	Neoplasms
T4079	934389-88-5	LY-294002 hydrochloride	p110α; p110β; p110 δ	0.5 μM	Preclinical	Cancer
T4976	1532533-67-7	TGR1202	PI3Kδ	22.2 nM	Phase 3	Chronic lymphocytic leukaemia
T4958	517-88-4	Alkannin	PI3Kα			

AKT

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T16104	105637-50-1	ML-9	AKT			
T13265	1139-83-9	Urolithin B	NF-κB; JNK; ERK; Akt; AMPK; Human Endogenous Metabolite			
T6285	937174-76-0	GSK690693	Akt1; Akt3; PKCη; PKCθ; PrkX	2 nM	Phase 1	Lymphoma; Solid tumours
T6252	1001264-89-6	Ipatasertib	Akt1; Akt2; Akt3	5 nM	Phase 3	Breast Cancer; Prostate Cancer
T3132	871361-88-5	SC66	Akt	0.75 μg/ml		
T2274	305834-79-1	SC 79	Akt			
T2176	57-71-6	2,3-Butanedione 2-Monoxime	Akt			
T1961	1009298-59-2	Vistusertib	P-Akt (S473); mTOR; PI3Kα; pS6 (S235/236)	2.8 nM	Phase 1/2	Breast Cancer; Colorectal Cancer; Diffuse large B cell lymphoma; Fallopian tube Cancer; Gastric Cancer; Glioblastoma; Meningioma; Non-small cell lung Cancer; Ovarian Cancer; Peritoneal Cancer; Prostate Cancer; Renal Cancer; Small cell lung Cancer; Solid t
T0033	58066-85-6	Miltefosine	PKC; Akt	7 μM	FDA Approved	Cancer metastases; Cutaneous leishmaniasis; Leishmaniasis; Visceral leishmaniasis

Stem Cell



Hedgehog / Smoothened

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T14188	1357350-60-7	ALLO-2	Smoothened			
T6891	935273-79-3	MK4101	Smoothened		Phase 1	Cancer
T6514	1095173-27-5	Glasdegib	Smoothened	5 nM	FDA Approved	Pani
T4211	T4211	SAG hydrochloride (912545-86-9)(free base))	Hedgehog/Smoothened			
T3588	315703-52-7	JK184	Hedgehog	30 nM		
T3460	496794-70-8	HhAntag	Gli		Preclinical	Brain Cancer; Pancreatic Cancer; Solid tumours
T3363	469-59-0	Jervine	Hedgehog; Smoothened			

TGF-beta / Smad

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T8785	82186-71-8	HALOFUGINONE LACTATE	prolyl-tRNA synthetase; TGF-β		Phase 2	Duchenne muscular dystrophy
T8730	2001559-19-7	BMS986260	TGFβR1			
T8330	746667-48-1	BIO-013077-01	TGFβ			
T7799	100874-08-6	SB 4	bone morphogenetic protein (BMP)	74 nM(EC50)		
T7676	T7676	LSKL, Inhibitor of Thrombospondin TSP-1	TGFβ			
T6337	446859-33-2	RepSox	ALK5; TGFβR1	4 nM		
T2048	396129-53-6	LY364947	CK1δ; MLK-7K; TGFβRI; TGFβRII; RIPK2	59 nM		
T1763	356559-20-1	SB525334	TβR1; ALK5; ALK4	14.3 nM (cell free)		
T1748	4727-31-5	Kartogenin	Smad4; Smad5			

Wnt / beta-catenin

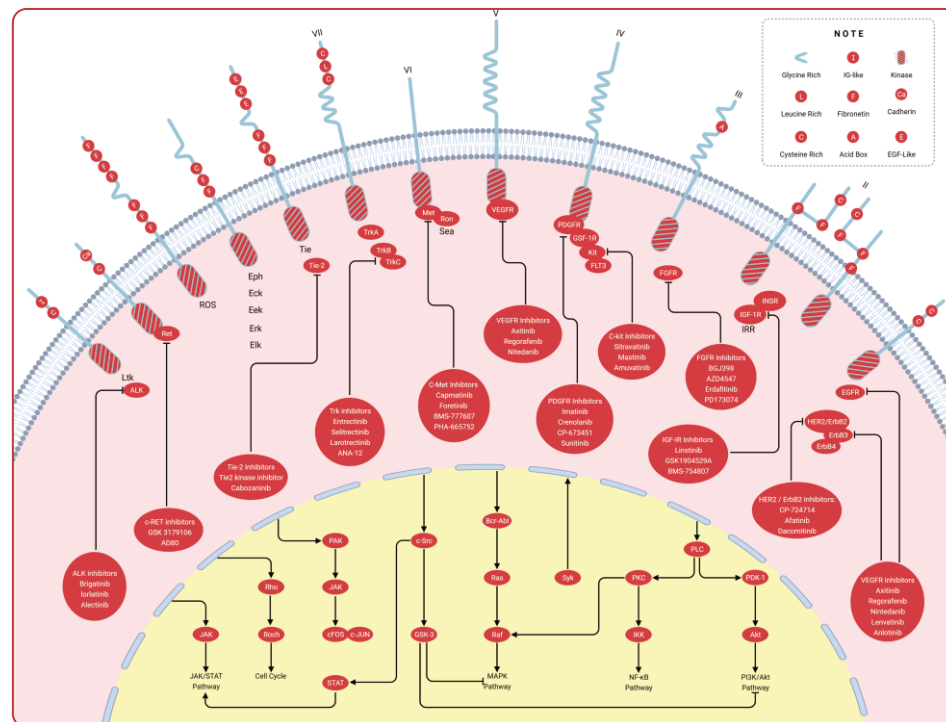
ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T22775	1127442-87-8	exo-IWR-1	wnt			
T17142	84-82-2	Toxoflavin	TCF4/β-catenin			
T14907	1661839-45-7	CCT251545	Wnt	5 nM		
T8820	2095432-75-8	BML-284 HCL	Wnt			
T8710	173436-66-3	MSAB	Wnt/β-catenin			
T8400	40391-99-9	Pamidronic acid	β-catenin; Wnt		Phase 4	Ankylosing Spondylitis
T8005	1049741-55-0	Cardiogenol C hydrochloride	Wnt			

STAT

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T21267	28230-32-2	HODHBt	STAT5			
T3218	83280-65-3	Napabucasin	STAT3		Phase 3	Colorectal Cancer; Gastric Cancer; Non-small cell lung Cancer; Oesophageal Cancer; Pancreatic Cancer
T2896	546-43-0	Helenine	STAT			
T2867	512-04-9	Diosgenin	STAT3			
T2814	35825-57-1	Cryptotanshinone	STAT3	4.6 μM		
T2789	27740-01-8	Scutellarin	Akt; STAT			
T2505	501919-59-1	S3I201	STAT3	86 nM (cell free)		
T2168	65182-56-1	2-NP	STAT1			
T0711	50-65-7	Niclosamide	STAT3	0.7 μM	FDA Approved	tapeworm infections
T0433	88495-63-0	Artesunate	STAT		Approved	malaria

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Tyrosine Kinase & Adaptors



FLT

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T16144	1429882-07-4	MRX-2843	FLT3; MERTK	1.3 nM	Phase 1	Advanced Cancer; Metastatic Cancer; Neoplasms; Neoplasm Metastasis; Neoplastic Processes; Pathologic Processes
T15199	1142363-52-7	Edicotinib	FLT3; CSF-1R; kit	3.2 nM	Phase 2	Recurrent Acute Myeloid Leukemia; Refractory Acute Myeloid Leukemia
T0374L	557795-19-4	Sunitinib	c-Kit; FLT3; PDGFRβ; VEGFR2	2 nM	FDA Approved	Gastrointestinal stromal tumours; Pancreatic Cancer; Renal cell carcinoma
T0093L	284461-73-0	Sorafenib	c-Kit; FLT3; mPDGFRβ; PDGFR β; B-Raf; B-Raf (V599E); Raf-1; VEGFR2/Fk2	6 nM (cell free)	FDA Approved	Liver Cancer; Renal cell carcinoma; Thyroid Cancer

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ALK

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T16708	879487-87-3	R-268712	ALK5			
T8399	1415560-69-8	Crizotinib hydrochloride	ALK; c-Met	20 nM	FDA Approved	locally advanced or metastatic non-small cell lung Cancer (NSCLC)
T8387	1256589-74-8	Alectinib hydrochloride	ALK	1.9 nM	FDA Approved	anaplastic lymphoma kinase (ALK)-positive, metastatic non-small cell lung Cancer (NSCLC) who have progressed on or are intolerant to crizotinib.
T8152	6601-66-7	6-Demethoxy tangeretin	ALK; MAPK			
T8108	2141955-96-4	Blu-782	ALK2	<10 nM	Phase 1	Fibrodysplasia ossificans progressiva
T6496	1352608-82-2	Vactosertib	ALK1; ALK2; ALK3; ALK4; ALK5	11 nM	Phase 1/2	Myelodysplastic syndromes
T6337	446859-33-2	RepSox	ALK5; TGFβR1	4 nM		
T6158	1062368-62-0	LDN-193189 HCl	ALK2; ALK3	0.8 nM		

c-Kit

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T15199	1142363-52-7	Edicotinib	FLT3; CSF-1R; kit	3.2 nM	Phase 2	Recurrent Acute Myeloid Leukemia; Refractory Acute Myeloid Leukemia
T8544	1048007-93-7	Masitinib mesylate	Kit; PDGFRα; PDGFRβ; Lyn; LCK; FGFR3; FAK	200 nM	Approved	mast cell tumors in dogs.
T8541	857890-39-2	Lenvatinib mesylate	VEGFR; VEGFR3; VEGFR1; FGFR1; PDGFRα; PDGFRβ; c-Kit	4 nM	FDA Approved	Treatment of locally recurrent or metastatic, progressive, radioactive iodine-refractory differentiated thyroid Cancer. Treatment of advanced renal cell carcinoma (RCC) in combination with everolimus following one prior antiangiogenic therapy.
T8482	1442472-39-0	Ripretinib	Kit; PDGFR		FDA Approved	Gastrointestinal Stromal Tumors
T7945	627908-92-3	SU14813	VEGFR; Kit	2 nM		
T7861	895519-91-2	Flumatinib mesylate	PDGFRβ; c-Kit; c-Abl		Phase 3	chronic phase chronic myelogenous leukemia

c-RET

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T10157	835621-11-9	Regorafenib N-oxide (M2)	VEGFR1; VEGFR2; VEGFR3; PDGFRβ; RET; Kit; Raf-1	13nM		
T8541	857890-39-2	Lenvatinib mesylate	VEGFR; VEGFR3; VEGFR1; FGFR1; PDGFRα; PDGFRβ; c-Kit	4 nM	FDA Approved	Treatment of locally recurrent or metastatic, progressive, radioactive iodine-refractory differentiated thyroid Cancer. Treatment of advanced renal cell carcinoma (RCC) in combination with everolimus following one prior antiangiogenic therapy.
T8467	2414909-94-5	RET V604M-IN-1	RET V804M	20 nM		
T8402	835621-07-3	Regorafenib Hydrochloride	VEGFR; PDGFR; RET; Raf-1	13 nM	FDA Approved	metastatic colorectal Cancer (CRC)
T8222	2152628-33-4	Selpercatinib	RET	14.0 nM	FDA Approved	Medullary Thyroid Cancer; Infantile Myofibromatosis; Infantile Fibrosarcoma; Papillary Thyroid Cancer; Soft Tissue Sarcoma
T7418	882405-89-2	BBT594	RET			

Tie-2

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T6934	945614-12-0	Pexmetinib	p38 MAPK; Tie-2	4 nM	Phase 1	Myelodysplastic syndromes
T6335	948557-43-5	Tie2 kinase inhibitor	Tie-2	0.25 μM		
T3113	849217-64-7	Foretinib	Met; RON; Tie-2; VEGFR2 (KDR); VEGFR3/FLT4	0.4 nM (cell free)	Phase 1	Breast Cancer; Gastric Cancer; Head and neck Cancer; Liver Cancer; Non-small cell lung Cancer; Renal Cancer
T2054	1345847-93-9	Altiratinib	c-Met; Tie-2; VEGFR; TrkA; TrkC	0.37 nM	Phase 1	Solid tumours

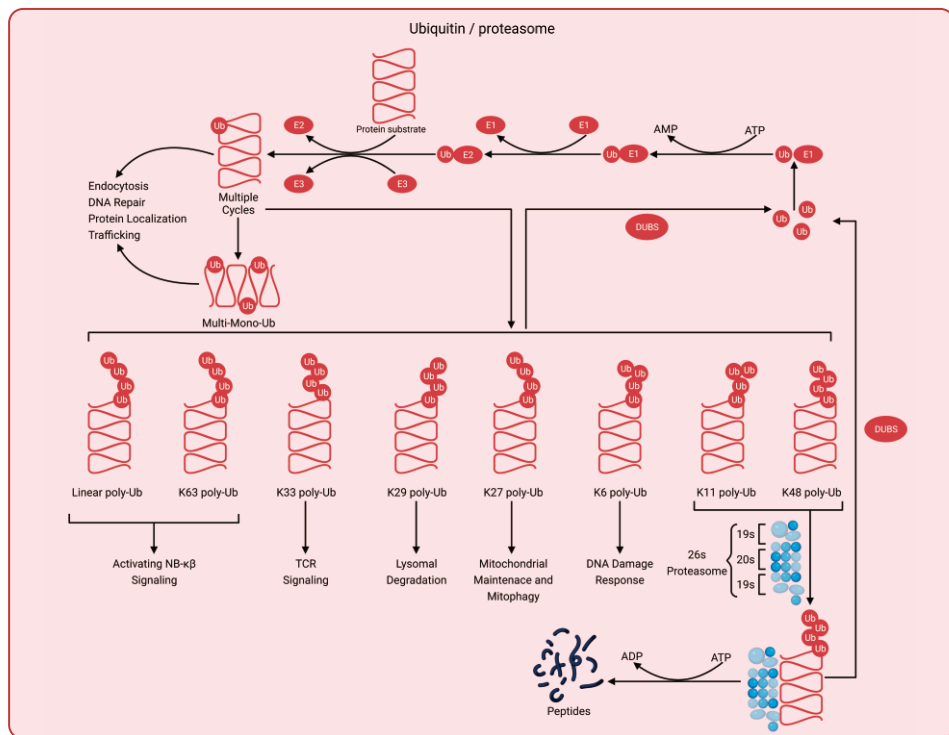
c-Met / HGFR

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T10655	1357072-61-7	c-Met inhibitor 1	c-Met			
T8825	1865733-40-9	Capmatinib hydrochloride	c-Met		FDA Approved	Non-small cell lung Cancer
T8416	1029714-89-3	Capmatinib hydrochloride (free base)	c-Met		FDA Approved	metastatic non-small cell lung Cancer (NSCLC) whose tumors have a mutation
T8399	1415560-69-8	Crizotinib hydrochloride	ALK; c-Met	20 nM	FDA Approved	locally advanced or metastatic non-small cell lung Cancer (NSCLC)
T8326	888719-03-7	BMS-2	Met; FLT3; VEGFR2			
T7900	1033767-86-0	BAY-474	c-Met			
T7787	1174161-69-3	BMS817378	Met	1.7 nM		

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Ubiquitination



E1 / E2 / E3 Enzyme

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T16974	1450833-55-2	TAK-243	UBA1; NF-κB; Apoptosis	1 nM	Phase 1	Advanced Malignant Solid Tumors
T13349	2247544-02-9	WS-383	DCN1-UBC12	11 nM		
T8816	864420-54-2	NAE-IN-M22	NAE			
T7415	65836-72-8	DKM 2-93	UBA5	430 μM		
T7379	144707-18-6	2-D08	sumoylation; AXL	0.49 nM		
T6629	418805-02-4	PYR41	Ubiquitin-activating Enzyme E1	< 10 μM		
T6332	905579-51-3	Pevonedistat	NAE	4.7 nM	Phase 3	Acute myeloid leukaemia; Chronic myelomonocytic leukaemia; Myelodysplastic syndromes

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Proteasome

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T17011	1446350-60-2	TCH-165	Proteasome			
T16684	58-60-6	Puromycin aminonucleoside	apoptosis; dipeptidyl peptidase II; antibiotic			
T13858	1617495-03-0	RA190	Proteasome	0.15 μM		
T12628	1211877-36-9	(R)-MG-132	Proteasome			
T12579	145888-79-5	PTP1B-IN-9	Proteasome			
T1176	81110-73-8	Racecadotril	Endopeptidase	4.5 μM	Approved	Diarrhoea
T8397	1239908-20-3	Ixazomib citrate	Proteasome	3.4 nM	FDA Approved	multiple myeloma who have received at least one prior therapy
T7854	205393-22-2	Bortezomib-pinanediol	Proteasome			
T7814	2244-11-3	Alloxan Monohydrate	Proteasome			
T6830	134381-21-8	Epoxomicin	20S proteasome			
T6041	935888-69-0	Oprozomib	20S proteasome; 20S proteasome	36 nM	Phase 1/2	Haematological malignancies; Multiple myeloma
T6029	960374-59-8	ONX0914	immunoproteasome	10 nM	Preclinical	Autoimmune disorders; Haematological malignancies
T6027	847499-27-8	Delanzomib	Chymotrypsin-like proteasome	3.8 nM	Phase 1	Non-Hodgkin's lymphoma; Solid tumours; Systemic lupus erythematosus

DUB

ID	CAS Number	Product Name	Target	IC50	Condition	Indication
T7678	63388-44-3	SJB2-043	USP1-UAF1	544 nM		
T6925	882257-11-6	P005091	USP7	4.2 μM	Preclinical	Cancer
T6697	30675-13-9	TOID	UCH-L1; UCH-L3	0.6 μM		
T6107	314245-33-5	IU1	USP14	4.7 μM		
T5461	2009273-67-8	GENE-6640	USP7	0.75 μM		
T4634	2009273-71-4	GEN6776	USP7			
T4338	1247825-37-1	USP7/USP47 inhibitor	USP7; USP47	0.42 M m(EC50)		
T4067	1431280-51-1	VLX1570	DUB	4.2-8.6 μM	Phase 1/2	Multiple myeloma
T3951	157654-67-6	NSC632839	SENP2; USP2; USP7	45±4 μM (EC50)		
T3555	1991986-30-1	ML364	USP2			

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