



Supplementary Materials: Hidradenitis Suppurativa and Comorbid Disorder Biomarkers, Druggable Genes, New Drugs and Drug Repurposing—A Molecular Meta-Analysis

Viktor A. Zouboulis, Konstantin C. Zouboulis and Christos C. Zouboulis

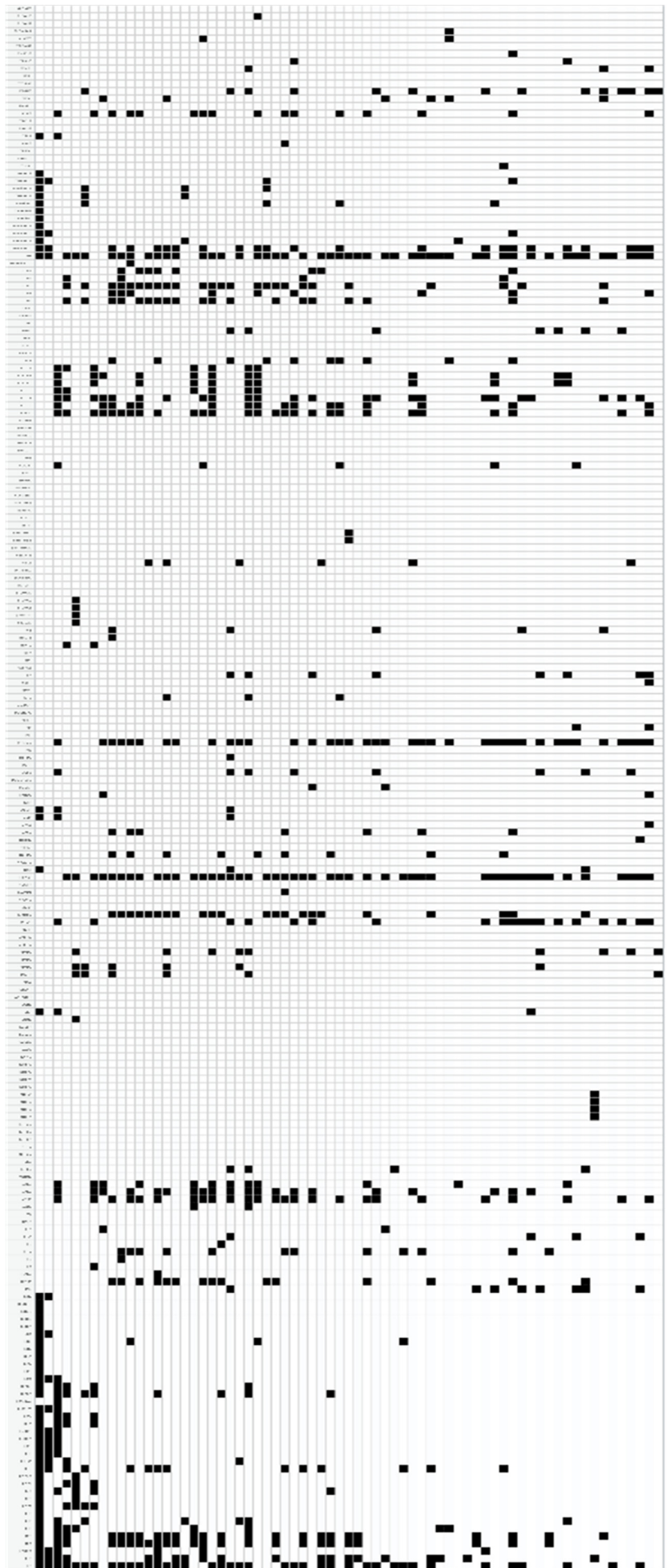




Figure S1. Enrichment of HS-associated DEGs (n = 386) resulting from the comparison of transcriptomic profiles and protein expression studies between lesional HS and non-lesional skin biopsies and blood samples from HS patients and healthy controls, respectively, in signaling pathways.

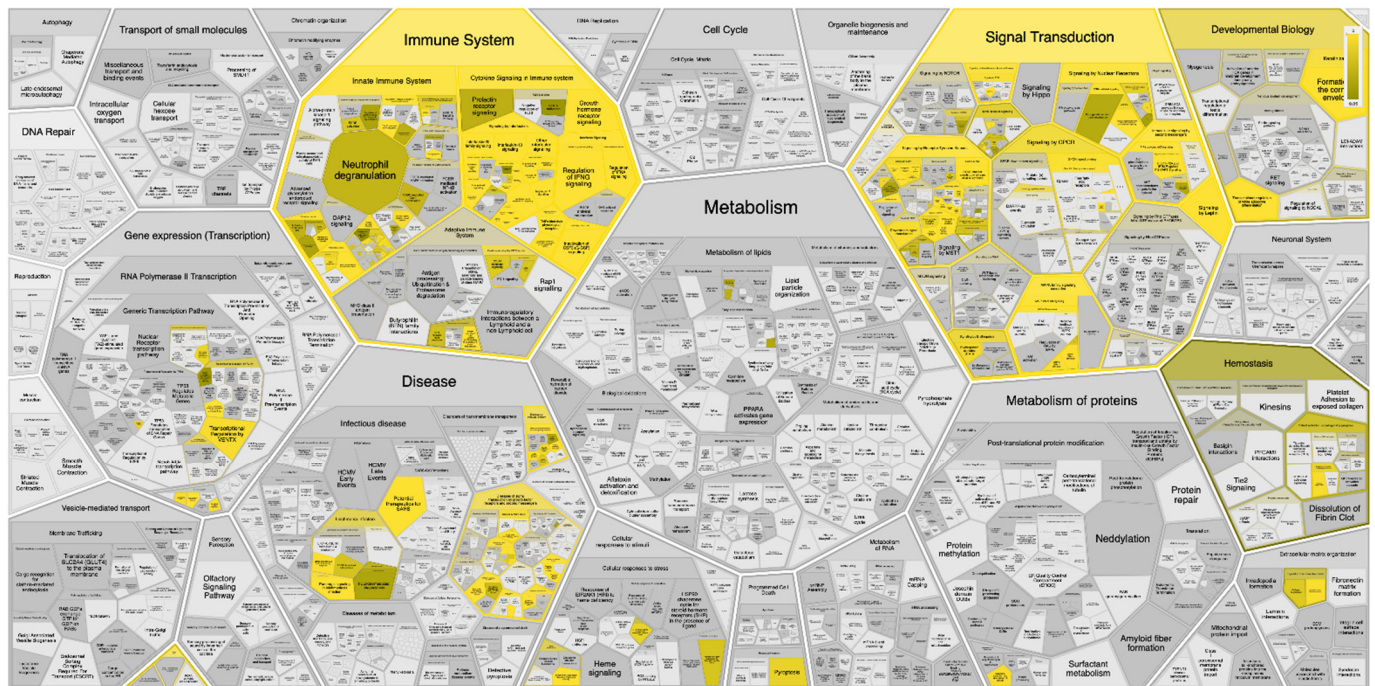


Figure S2: Global REAC evaluation of possibly involved signaling pathways in HS. The intensity of yellow areas and letter size indicate the importance of the specific pathways in HS.



Figure S3. Enrichment of druggable HS-associated genes (n = 116) resulting from the comparison of transcriptomic profiles and protein expression studies between lesional HS and non-lesional skin biopsies and blood samples from HS patients and healthy controls, respectively, in signaling pathways.

Table S1. DEGs resulting from the comparison of transcriptomic profiles and protein expression studies between lesional HS and non-lesional skin biopsies and blood samples from HS patients and healthy controls, respectively. Bold letters indicate druggable genes. Background: white = result reported in a single study; grey = result reported in at least two independent studies in one target (biological material); orange = result reported in two targets; yellow = result reported in three targets. + = upregulation; - = downregulation; +/- = diversified dysregulation in different biological materials; () = lower level of evidence.

Gene	Blood		Skin		Gene/protein regulation
	mRNA	Protein	mRNA	Protein	
ACKR2			[26]		-
ACTN4			[3]		+
ADAM12			[3,27]		+
ADAMDEC1			[27]		+
ADAMTS12			[26]		-
ADH1C			[3]		-
ADIPOQ		[28]	[27]		-
ADIRF			[3]		-
AGO1			[29]		-
AGO2			[29]		-
AHR			[30]		+
AKR1B10			[27]		+
AKT1			[30]		+
AKT1S1			[30]		+
ALOX5			[31]		+
ALOX5AP			[31]		+
ALOX12			[31]		-
ALOX15			[31]		-
ALOXE3			[31]		-
APELA			[27]		+
APOE			[26]		-
APP			[26]		+
AQP5			[32]		-
AR			[3,33,34]	[35]	+
AS3MT			[3]		-
ATP6V0A4			[27]		-
AXIN1				[36]	+
BCL6			[30]		+
BRD4			[30]		+
BTC			[3,27,33,34]		+/(-)
BTK			[30]		+
C10orf99			[3]		+
C1QTNF6			[3]		+
C3		[27]	[30]		-/+
C5		[37]			+
C5AR1			[3,30]		+
C5orf46			[33]		-
C7			[27]		-
CA6			[27]		-
CAMP			[30]		+
CASP1				[38,39]	+
CASP5				[38]	+
CCDC88B			[3]		+
CCDC9			[3]		-
CCL2			[40]		+

CCL4		[41]	+
CCL5		[30]	+
CCL11		[42]	+
CCL17		[30]	+
CCL18		[27,30] [43]	+
CCL19		[26]	+
CCL20		[30,44]	+
CCL21		[26]	+
CCL22		[30]	-
CCL26	[41]	[30]	+
CCL27		[30,33,44]	-/(+)
CCR2		[30]	+
CCR4	[45]	[30,45]	+
CCR5		[30]	+
CCR6		[30]	+
CCR7		[30]	+
CCR9		[30]	+
CCR10		[30]	+
CD3G		[46]	+
CD5		[36]	+
CD6		[36]	+
CD19		[45]	+
CD40		[30]	+
CD40LG		[30]	+
CD79a		[45]	+
CD80		[30,38]	+
CD163		[43]	+
CD177		[45]	+
CD244		[36]	+
CD274		[30]	+
CDH1		[47]	-
CEBPB		[3]	+
CERS2		[48]	-
CFD		[3]	-
CHI3L1	[49]	[50]	+
CLDN8		[27]	-
CLEC3B		[3]	-
COX6B2		[3]	-
CPNE5		[3]	+
CSF1		[3,33,34,40]	+
CSF2		[26]	+
CSF3		[51]	+
CST5		[36]	+
CTLA-4		[30]	+
CTNNA1		[26]	-
CTNND1		[47]	-
CXCL1		[27,40,42,44,45] [40]	+
CXCR4		[3]	+
CXCR5		[30] [26]	+
CXCL6		[42]	+
CXCL8		[30,42,44] [41]	+
CXCL9		[30]	+
CXCL10	[41]	[30] [41]	+/(-)

CXCL13	[30,42,45]	[26]	+
CYP2W1	[3]		-
DCD	[27,32,33]	[32]	-
DEFB1	[44,46]		-
DEFB4A	[3,27,30,32,39,44,45,46]	[3,53]	+ / (-)
DEFB4B	[54]		+
DEFB103B	[46,52]		+
DGCR8	[55]		-
DROSHA	[55]		-
DSC2	[27]		+
EBI3	[40]		+
EGF	[3,33,34]		+
EHF	[3]		+
EPGN	[3,33,34]		+
ERBB4	[27,32]		-
EREG	[3,33,34]		+
FABP4	[27]		-
FABP5	[3]		+
FABP7	[27]		-
FAM118A	[3]		-
FAM74A4	[3]		-
FBN2	[27]		+
FGF1	[11]		+
FGF7	[11]		+
FGFBP2	[27]		-
FLG	[30]		+
FOXA1	[32]		-
FOXQ1	[32]		-
FUT6	[3]		-
GAPDH	[27]		+
GAS6	[3,33,34]		+
GBP6	[3]		-
GDNF	3,33,34]	[36]	+
GFI1	[26]		-
GFOD1	[3]		-
GHRL	[28]		-
GJB2	[3]	[3]	+
GPD1	[3]		-
GPR155	[3]		-
GPR68	[3]		+
GSN	[3]		-
GZMH	[30]		+
HAVCR2	[30]		+
HBEGF	[3,33,34]		+
HGF	[3,33,34]		+
HIF3A	[27]		-
HMGCS2	[27]		-
HRG	[3,33,34]		+
HSCB	[3]		-
HYAL4	[3]		-
ICOS	[30]		+
IDO1	[30]		+
IFNA1	[3,26,30,33, 34]		+

IFNA2	[26]	+		
IFNB1	[30]	+		
IFNG	[3,26,30,33,34,40,44,45,46]	+		
IGF2	[3,33,34]	+		
IGH	[46]	+		
IGHD	[27,30]	+		
IGHG3	[27,30]	+		
IGK	[45]	+		
IGKC	[27]	+		
IGKV1D-13	[27,30]	+		
IGKV1ORY-1	[33]	+		
IGKV3-20	[33]	+		
IGL	[45]	+		
IGLL1	[33]	+		
IGLL3P	[33]	+		
IGLV	[27,30]	+		
IGLV3-27	[45]	+		
IKZF2	[26]	-		
IL1A	[3,26,30,33,34,40]	[39]	+	
IL1B	[26,30,38,40,42,46]	[38,56]	+	
IL1R1	[30]	+		
IL1RN	[26]	-		
IL2	[26,30]	+		
IL2RA	[49,56]	[30]	+	
IL4	[3,30,33,34,40]	+		
IL4R	[30]	+		
IL5	[30]	+		
IL6	[40]	[3,26,30,33,34,40,42]	[40,58]	+
IL10		[30,38,44,46]	[52,56]	+
IL10RA		[26]	-	
IL12A		[59]	[41]	+
IL12B		[30]	[36]	+
IL13		[3,30,45]	+/(-)	
IL15		[30]	+	
IL16		[30]	[41]	+
IL17A	[59]	[3,30,33,34,38,39,40,42,44,46,60]	[4,36,38,39,41]	+
IL17C		[45]	-	
IL17D		[32]	-	
IL17F		[30,39,40,42,45]	+	
IL17R		[3]	[4]	+
IL18		[26,30]	[38]	+/(-)
IL18R1			[36]	+
IL19		[3,30,40]	+	
IL20		[30,46]	[46]	+/(-)
IL20RA			[46]	-
IL20RB		[30]	+	
IL21		[30,39]	+	
IL22		[3,30,40,42,46]	[46]	+
IL22RA1		[30]	[46]	-
IL22RA2			[46]	+
IL23A		[30,40,61]	+	
IL23R		[30]	+	

IL24		[30,42,46]		+
IL26		[42,46]		+
IL27		[40]		+
IL31		[30]		+
IL32		[30,40,61]		+
IL33		[30]		+
IL34		[42]		-
IL36A	[62]	[30,40,42,45,61]	[39,61]	+
IL36B	[62]		[61]	+
IL36G	[62]	[30,40,42,45]	[61]	+
IL36RN			[61]	+
IL37		[32,33,42]		-
INS	[63]			+
IRAK1		[30]		+
IRAK2		[30]		+
IRF4		[30]		+
IRF5		[30]		+
IRF7		[26]		+
IRF8		[30]		+
IRF9		[44]		+
IRS1		[30]		+
ITK		[30]		+
ITPKA		[30]		+
IVL		[30]		+
JAG2		[26]		-
JAK1		[30]		+
JAK2		[30]		-
JAK3		[3,30]		+
KCNN2		[48]		-
KITLG		[11]		+
KLK6		[30]		+
KMT2D		[26]		-
KRT2		[33]		-
KRT6A		[3,32]	[3]	+
KRT6B		[3]		+
KRT6C		[3]		+
KRT14		[3]		+
KRT16		[3,27,30,32]	[3]	+
KRT19		[32]		-
KRT31		[32]		-
KRT73		[32]		-
KRT74		[32]		-
KRT77		[27,32,33]	[32]	-
KRT79		[32]		-
KYNU		[30]		+
LAG3		[30]		+
LCE2B		[33]		-
LCE3D		[32]	[32]	+
LCE5A		[33]		-
LCN2	[64]			+
LEP	[28]			+
LGR5		[27,32]		-
LORICRIN		[30]		+

LTA4H	[27,65]	[31]	-/(+)	
MAZ		[3]	+	
MMP1		[3,40]	[3]	+
MMP3		[40]	[40]	+
MMP8			[66]	+
MMP9		[3,30,40]	[3]	+
MMP10		[40]		+
MMP12		[27,30]		+
MST1		[3]		+
MTOR		[30]		+
MYD88		[26]		+
MZB1		[33]		+
NAA40		[31]		-
NAMPT	[28,63]			+
NCSTN	[67]			-
NFKB1		[26]		+
NGF		[3,33,34]	[36]	+
NKX2-3		[26]		-
NLRP3			[38]	+
NR1D1		[32]		-
NR1H2		[26]		-
OAS2		[32]		+
OASL		[32]		+
OSM		[3,26]	[36]	+
OSMR		[30]		+
PARD3		[30]		+
PDCD1		[30]		+
PDCD1LG2		[30]		+
PDGFB		[11]		+
PER1		[32]		-
PHLPP2		[30]		+
PI3		[3,27,32,33]	[3]	+
PIK3CD		[30]		+
PIP		[27,32]		-
PKM	[27]			+
PLIN1		[27,48]		+/-
POLR2J2		[3]		-
POU2AF1		[3]		+
PPARG		[26]		-
PRDM1		[30]		+
PRKRA		[29]		-
PSEN1	[67]			-
PTEN		[30]		+
RASAL3		[3]		+
RBP4	[28]			+
RETN	[28]			+
RORC		[30]		+
RPL38		[3]		-
RPS6		[30]		+
S100A7		[3,30,33,39,42,44,46]	[32]	+
S100A7A		[3,27,32]	[3,32]	+
S100A8	[57]	[3,33,34,44]	[3,32]	+
S100A9	[57]	[3,27,32,33,42,44,46]	[3,32]	+

S100A12	[3,30,32,42]	[3,41]	+
SAPCD1	[27]		-
SCGB1D2	[27,32]		-
SCGB2A2	[27,32,33]		-
SELE	[54]		+
SEMA3E	[27]		-
SERPINA12	[33]		-
SERPINB3	[3,27,30]	[3]	+
SERPINB4	[3,27,30]	[3]	+
SIRT1	[26]		-
SIRT2		[36]	+
SLAMF7	[3,27]		+
SLC16A3	[3]		+
SLC35E4	[3]		-
SLC66A1	[3]		-
SMPD2	[48]		+
SND1	[29]		-
SOCS1	[26]		-
SP8	[68]		-
SPPL2A	[30]		+
SPRR2B	[32]	[32]	+
SPRR2C	[32]	[32]	+
SPRR2F	[45]		+
SPRR3	[3]	[3]	+
STAT1	[3,26,30,44]	[36]	+
STAT2	[30]		+
STAT3	[30]		+
STAT4	[30]		+
STAT5A	[30]		+
STAT5B	[30]		+
STAT6	[30]		+
SYK	[30]		+
TBXA2R	[3]		-
TCN1	[3,27,45]	[3]	+
TDO2	[27]		+
TENT5C	[33]		+
TGFA	[11]		+
TGM2	[26]		+
THRSP	[27]		-
THY1	[3]		+
TLR2	[3,68]		+
TLR3	[26]		+
TLR4	[26]	[53]	+ / -
TLR5	[3]		+
TLR9	[26]		+
TMPRSS11D	[3]	[3]	+
TNF	[3,26,30,32,33,38,40]	[56]	+
TNFRSF1A	[3]		+
TNFRSF13B	[30]		+
TNFRSF14	[30]		+
TNFRSF18	[30]		+
TNFRSF4	[45]	[45]	+
TNFRSF9		[36]	+

TNFSF11	[30]	[36]	+
TNFSF13 (APRIL)	[30]	[26]	+
TNFSF13B (BAFF)	[30]	[26]	+
TNFSF14	[30]	[36]	+
TNFSF18	[30]		+
TNIP1	[26,30]		+ / -
TRIM24	[26]		-
TRPV1	[30]		+
TRPV2	[30]		+
TSLP	[30]		+
TSPAN8	[27]		-
TTC28	[3]		-
TYK2	[30]		+
UCHL1		[69]	-
VAV1	[30]		+
VEGFA	[54]		+
WDR97	[3]		-
WIF1	[27,32]		-
WNT1	[30]		+
ZFP36	[26]		-
ZNF713	[3]		-
ZSCAN2	[3]		-
ZNF713	[3]		-
ZSCAN2	[3]		-

Table S2. HS-associated DEGs.

Compound	Function	Gene regulation	Development phase
1,2,3,4,5,6-Hexabromocyclohexane	JAK inhibitor	JAK2	preclinical
1-EBIO	potassium channel activator	KCNN1, KCNN2 , KCNN3, KCNN4	preclinical
1-Octanol	Aliphatisches alcohol	GJA1, GJA10, GJA3, GJA4, GJA5, GJA8, GJA9, GJB1, GJB2 , GJB3, GJB4, GJB5, GJB6, GJB7, GJC1, GJC2, GJC3, GJD2, GJD3, GJD4, GJE1	2
2-Aminobenzenesulfonamide	carbonic anhydrase inhibitor	CA12, CA14, CA2, CA6 , CA9	preclinical
2-APB	1,4,5-trisphosphate inhibitor	TRPC1, TRPC3, TRPC4, TRPC5, TRPC6, TRPC7, TRPM2, TRPM3, TRPM6, TRPV1 , TRPV6	preclinical
2,4-Dinitrophenol	ATP synthase inhibitor	APP	preclinical
2-Hydroxyflutamide	AR antagonist	AR	2
3-Methyladenine	PI3K inhibitor	PI3	preclinical
3,3'-Diindolylmethane	CHK inhibitor, cytochrome P450 activator, indoleamine 2,3-dioxygenase inhibitor	AR , HIF1A, IFNG , PI3	3
3,4-Methylenedioxy- β -nitrostyrene	SRC inhibitor, SYK inhibitor	SRC, SYK	preclinical
4,5,6,7-Tetrabromobenzotriazole	casein kinase inhibitor	AKT1 , CHEK1, CSNK2A1, GSK3B, LCK, MAP2K1, MAPK1, MAPK11, MAPK12, MAPK14, MAPK8, PRKCA, ROCK1, RPS6KB1, SGK1	preclinical
6-Iodo-nordihydrocapsaicin	TRPV antagonist	TRPV1	preclinical
α -Linolenic acid	ω 3 fatty acid stimulant	ELOVL4, FADS1, FADS2, FFAR1, FFAR4, PTGS2 , SLC8A1, TRPV1	3
A-1120	retinoid receptor ligand	RBP4	preclinical
A205804	ICAM1 expression inhibitor	ICAM1, SELE	preclinical
A-674563	AKT inhibitor	AKT1 , PKIA, PRKACA	preclinical
A-784168	transient receptor potential channel antagonist	TRPV1	preclinical
Abametapir	metalloproteinase inhibitor	MMP9	3
Acalabrutinib	Bruton's tyrosine kinase (BTK) inhibitor	BTK	launched
Acalisib	PI3K inhibitor	PIK3CB, PIK3CD	1
Aceneuramic acid	sialic acid	CES1, SELE , SELP	3
Acetohydroxamic acid	urease inhibitor	MMP12	launched
Acetyl-farnesyl-cysteine	methyltransferase inhibitor	PPARG	launched
Acitretin	retinoid receptor agonist	KRT16 , PI3 , RARA, RARB, RARG, RBP1, RXRA, RXRB, RXRG, STAT3	launched
Adalimumab	TNF inhibitor	TNFA	launched
Adaptavir	CC chemokine receptor antagonist	CCR5	2
Adiporon	adiponectin receptor agonist	ADIPOR1 , ADIPOR2	preclinical
AG-490	EGFR inhibitor, JAK inhibitor	EGFR , JAK2 , JAK3	preclinical
AK-7	SIRT inhibitor	SIRT2	preclinical
AKBA	Lipoxygenase inhibitor	ALOX5	3
Alantolactone	apoptosis stimulant, STAT inhibitor	STAT3	preclinical
Allicin	cytokine production inhibitor	TRPA1, TRPV1	2
Alpelisib	PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD , PIK3CG	launched
AMD11070	CC chemokine receptor antagonist	CCR5 , CXCR4	3

AM-24	lipoxygenase inhibitor	ALOX5	2
AM679	cannabinoid receptor agonist, lipoxygenase inhibitor	ALOX5AP , CNR1, CNR2	preclinical
AMG-319	PI3K inhibitor	PIK3CD	2
Amiloride	sodium channel blocker	AOC1, ASIC1, ASIC2, ASIC3, PKD2, PKD2L1, PLA2, SCNN1A, SCNN1B, SCNN1D, SCNN1G, SLC9A1, TRPC7, TRPV2	launched
Aminosalicylate	cyclooxygenase inhibitor	ALOX5 , CHUK, PLA2G2E, PTGS1, PTGS2	launched
Amlexanox	histamine receptor modulator	FGF1 , IL3, PDE4A, PDE4B, PDE4C, PDE4D, S100A12 , S100A13	launched
Amrinone	phosphodiesterase inhibitor	PDE3A, PDE3B, PDE4B, TNFA	launched
Anandamide	cannabinoid receptor agonist	CACNA1G, CACNA1H, CACNA1I, CNR1, CNR2, GLRA1, GPR18, GPR55, KCNA2, KCNK3, KCNK9, TRPM8, TRPV1	2
Andrographolide	tumor necrosis factor production inhibitor	IL1B , IL6 , NFKB1 , NFKB2 , TNFA	2
APcK-110	KIT inhibitor	KIT , STAT3	preclinical
API1903	mTOR inhibitor	MTOR	1 / 2
API-1	AKT inhibitor	AKT1 , AKT2, AKT3	preclinical
Apratastat	matrix metalloprotease inhibitor, tumor necrosis factor production inhibitor	ADAM17, MMP1 , MMP13 , MMP9	2
Apremilast	phosphodiesterase inhibitor	IFNG , PDE4A, PDE4B, PDE4C, PDE4D	launched
APY0201	phosphoinositide dependent kinase inhibitor	IL12A , IL12B , PIKFYVE	preclinical
Arglabin	farnesyltransferase inhibitor	FNTA, NFKB1	launched
ARV-825	bromodomain inhibitor	BRD4	preclinical
Aspartame	non-saccharide sweetener	TAS1R2, TRPV1	launched
Aspirin	cyclooxygenase inhibitor	AKR1C1, ASIC3, EDNRA, HSPA5, IKBKB, NFKB1 , NFKB2, NFKBIA, PRKAA1, PRKAA2, PRKAB1 , PRKAB2, PRKAG1, PRKAG2, PRKAG3, PTGS1 , PTGS2 , RPS6KA3, TP53	launched
AT13148	Protein kinase inhibitor	AKT1 , AKT2, AKT3, ROCK1, ROCK2, SGK3	1
AT-9283	Aurora kinase inhibitor, JAK inhibitor	AURKA, AURKB, JAK2 , JAK3 , RPS6KA6, STK17A	2
Atiprimod	JAK inhibitor, STAT inhibitor	JAK2 , STAT3	2
Atorvastatin	HMGCR inhibitor	AHR	launched
Atractylenolide-i	JAK inhibitor	JAK1 , JAK2 , JAK3	preclinical
AVL-292	Bruton's tyrosine kinase (BTK) inhibitor	BTK , YES1	2
Axitinib	PDGFR tyrosine kinase receptor inhibitor, VEGFR inhibitor	CSF1 , FLT1, FLT4, KDR, PLK4	launched
AZ20	ATR kinase inhibitor	ATR, MTOR	preclinical
AZ876	PPAR γ agonist	PPARG	preclinical
AZ960	JAK inhibitor	JAK2	preclinical
AZD1480	JAK inhibitor	JAK1 , JAK2 , JAK3	1
AZD2014	mTOR inhibitor	MTOR	2
AZD5363	AKT inhibitor	AKT1 , AKT2, AKT3	3
AZD6482	PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD , PIK3CG	1
AZD8055	mTOR inhibitor	MTOR	1
AZD8186	PI3K inhibitor	PIK3CB, PIK3CD	1

AZD8835	PI3K inhibitor	PIK3CA, PIK3CD	1
Baicalein	lipoxygenase inhibitor	ALOX5 , GLO1, PREP, SELL, SELP, TNFA , XDH	preclinical
Balsalazide	cyclooxygenase inhibitor	ALOX5 , PPARG , PTGS1 , PTGS2	launched
Bardoxolone	nuclear factor erythroid derived/like (NRF2) activator	NOS2, PPARG	1
Bardoxolone-methyl	nuclear factor erythroid derived/like (NRF2) activator	PPARG , STAT3	3
Baricitinib	JAK inhibitor	JAK1 , JAK2	launched
Batimastat	matrix metalloprotease inhibitor	ADAM28, ADAMTS5, MMP12 , MMP16, MMP2, MMP8	3
BAY-61-3606	SYK inhibitor	SYK	preclinical
BCTC	TRPV antagonist	TRPV1	preclinical
Bergenin	interleukin inhibitor	IL1B , TNFA	preclinical
β -Amyloid-synthesis-inhibitor	β -amyloid synthesis inhibitor	APP	preclinical
β -Elemene	apoptosis stimulant	MMP2, MMP9	launched
β -hydroxy-beta-Methylbutyrate	protein synthesis stimulant	MTOR	launched
Bezafibrate	PPAR agonist	PPARA, PPARD, PPARG	launched
BGT226	PI3K inhibitor	MTOR , PIK3CA, PIK3CB, PIK3CG	1 / 2
Bicalutamide	AR antagonist	AR	launched
BI-2536	PLK inhibitor	BRD4 , PLK1, PLK2, PLK3	2
Bindarit	NF κ B pathway inhibitor	CCL2 , CCL7, CCL8	2
Bisindolylmaleimide-IX	PKC inhibitor	AKT1 , GSK3B, LCK, MAPK1, MAPK11, MAPK12, MAPK14, MAPK8, PRKCA, ROCK1, RPS6KB1, SIRT1	preclinical
Bisphenol-A	synthetic estrogen	AR , ESR1, ESR2, ESRRG, PPARG	1
Bleomycin	EGFR expression inhibitor	EGFR	launched
BMS-536924	IGF-1 inhibitor	AKT1 , CCNE1, CDK2, CYP3A4 , ERBB2, IGF1R, KDR, LCK, MAPK1, MET, PDGFRA, PDGFRB	preclinical
BMS-754807	IGF-1 inhibitor	AKT1 , IGF1R	2
BMS-777607	AXL kinase inhibitor, c-Met inhibitor, FLT3 inhibitor, hepatocyte growth factor receptor inhibitor, macrophage migration inhibiting factor inhibitor, tyrosine kinase inhibitor	AXL, MERTK, MET, MST1R , TYRO3	1 / 2
BMS-779788	Liver X receptor agonist	LXR	1
BMS-911543	JAK inhibitor	JAK1 , JAK2 , JAK3	1 / 2
BMS-935177	Bruton's tyrosine kinase (BTK) inhibitor	BTK	preclinical
BMS-986142	Bruton's tyrosine kinase (BTK) inhibitor	BTK	2
BMS-986158	bromodomain inhibitor	BRD4	1 / 2
BMS-986195	Bruton's tyrosine kinase (BTK) inhibitor	BTK	1
BMS-CCR2-22	CC chemokine receptor antagonist	CCR2	preclinical
Brodalumab	IL-17 receptor inhibitor	IL17R , KRT6A , S100A7A , S100A8 , S100A9	launched
BTK-IN-1	Bruton's tyrosine kinase (BTK) inhibitor	BTK	preclinical
BW-A4C	lipoxygenase inhibitor	ALOX5	1
BW-B70C	lipoxygenase inhibitor	ALOX5	preclinical

C-021	CC chemokine receptor antagonist	CCR4	preclinical
C34	toll-like receptor inhibitor	TLR4	preclinical
Caffeic acid	lipoxygenase inhibitor, tumor necrosis factor production inhibitor	ALOX5 , MIF	preclinical
Caffeine	adenosine receptor antagonist, phosphodiesterase inhibitor	ADORA1, ADORA2A, ADORA2B, ADORA3, ATM, ITPR1, ITPR2, ITPR3, PDE10A, PDE11A, PDE1A, PDE1B, PDE1C, PDE2A, PDE3A, PDE3B, PDE4A, PDE4B, PDE4C, PDE4D, PDE5A, PDE6A, PDE6B, PDE6C, PDE7A, PDE7B, PDE8A, PDE8B, PDE9A, PIK3CA, PIK3CB, PIK3CD , PRKDC, RYR1, RYR2, RYR3	launched
CaMKII-IN-1	calcium/calmodulin dependent protein kinase inhibitor	AKT1 , CAMK2A, CAMK4, MYLK	preclinical
Canertinib	EGFR inhibitor	AKT1 , EGFR, ERBB2, ERBB4	3
Captopril	angiotensin converting enzyme inhibitor	ACE, LTA4H , MMP2, MMP9	launched
Carbenoxolone	11-beta hydroxysteroid dehydrogenase inhibitor	GJA1, GJA10, GJA3, GJA4, GJA5, GJA8, GJA9, GJB1, GJB2 , GJB3, GJB4, GJB5, GJB6, GJB7, GJC1, GJC2, GJC3, GJD2, GJD3, GJD4, GJE1, HSD11B1, PANX1, PANX2, PANX3	launched
Carboxyamidotriazole	calcium channel blocker	CXCL8	3
Carzenide	Carbonic anhydrase IX inhibitor	CA1, CA12, CA14, CA2, CA6 , CA9	preclinical
CB-03-01	AR antagonist	AR	3
CBS-1114	lipoxygenase inhibitor	ALOX5	1
CC-115	DNA protein kinase inhibitor, mTOR inhibitor	MTOR	2
CC-223	mTOR inhibitor	MTOR	2
CH223191	Aryl hydrocarbon receptor antagonist	AHR	preclinical
CHF5074	γ -secretase modulator	PSEN1	2
Chrysophanic acid	EGFR inhibitor	EGFR , MTOR	preclinical
CEP-33779	JAK inhibitor	JAK2	preclinical
Certolizumab pegol	TNF inhibitor	TNFA	launched
CH5132799	PI3K inhibitor	MTOR , PIK3CA, PIK3CB, PIK3CD , PIK3CG	1
Cholic acid	bile acid synthesis disorders, peroxisomal disorders	ADH1C	launched
Ciglitazone	PPAR γ agonist	GPD1 , PPARG , TBXA2R	2
CINPA-1	CAR antagonist	NR1H4 , NR1I3, PPARG	preclinical
Cipemastat	metalloproteinase inhibitor	ADAM17, MMP1 , MMP13, MMP2, MMP3 , MMP8 , MMP9	3
Citric acid	coagulation factor inhibitor	AKR1B1, ANG, APRT, BHMT, C8G, CA4, CPB1, CS, CTDSP1, GNMT, HGS, HS3ST3A1, IL4I1, ITPA, LSM6, MDH2, MIF, PDE5A, PKD2L1, PLEKHA1, RNASE1, RNASE3, SRC, TNFSF13B , UCK2	preclinical
CKD-712	NF κ B pathway inhibitor	JAK2 , STAT1	1
Cloprostenol-(+/-)	prostaglandin receptor agonist	PTGDR, PTGER1, PTGER3, PTGFR, TBXA2R	launched
CNX-774	Bruton's tyrosine kinase (BTK) inhibitor	BTK	preclinical

Coenzyme-I	AASS, ACADS, ADH1A, ADH1B, ADH1C , ADH4, ADH5, ADH7, AKR1B1, AKR1C1, AKR1C2, AKR1C3, AKR1C4, ALDH1A1, ALDH1A2, ALDH1A3, ALDH1B1, ALDH2, ALDH3A1, ALDH3A2, ALDH3B1, ALDH3B2, ALDH4A1, ALDH5A1, ALDH6A1, ALDH7A1, ALDH9A1, AMT, BDH1, BLVRA, BLVRB, CDO1, CYB5R3, CYP17A1, CYP4A11, DHCR7, DHFR, DLAT, DLD, EHHADH, GAPDH , GAPDHS, GLUD1, GLUD2, GPD1 , GSR, H6PD, HADH, HADHA, HIBADH, HMGCR, HMOX1, HMOX2, HPGD, HSD11B1, HSD11B2, HSD17B1, HSD17B10, HSD17B2, HSD17B3, HSD17B4, HSD17B7, HSD17B8, HSD3B1, HSD3B2, IDH3A, IDH3B, IDH3G, IMPDH1, IMPDH2, LDHA, LDHAL6A, LDHAL6B, LDHB, LDHC, MDH1, MDH2, ME1, ME2, ME3, MSMO1, MT-ND1, MT-ND2, MT-ND3, MT-ND4, MT-ND4L, MT-ND5, MT-ND6, MTHFD1, MTHFD2, NDUFA1, NDUFA10, NDUFA11, NDUFA12, NDUFA13, NDUFA2, NDUFA3, NDUFA4, NDUFA4L2, NDUFA5, NDUFA6, NDUFA7, NDUFA8, NDUFA9, NDUFAB1, NDUFB1, NDUFB10, NDUFB2, NDUFB3, NDUFB4, NDUFB5, NDUFB6, NDUFB7, NDUFB8, NDUFB9, NDUFC1, NDUFC2, NDUFS1, NDUFS2, NDUFS3, NDUFS4, NDUFS5, NDUFS6, NDUFS7, NDUFS8, NDUFV1, NDUFV2, NDUFV3, NNT, NQO2, NSDHL, OGDH, PDHA1, PDHA2, PDHB, PHGDH, PYCR1, PYCR2, QDPR, RDH5, SORD, TSTA3, TYR, UGDH			2
Compound-401	DNA dependent protein kinase inhibitor	MTOR , PRKDC	preclinical	
Copanlisib	PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD , PIK3CG	launched	
CP-471474	matrix metalloprotease inhibitor	MMP1 , MMP13, MMP2, MMP3 , MMP9	preclinical	
CPI-1189	tumor necrosis factor release inhibitor	TNFA	2	
Cortodoxone	AR antagonist	AR	3	
Coumarin	vitamin K antagonist	CA1, CA12, CA14, CA2, CA4, CA6 , CA9, CYP2A6	launched	
CPI-0610	bromodomain inhibitor	BRD4	2	
CPI-203	bromodomain inhibitor	BRD4	preclinical	
Cryptotanshinone	acetylcholinesterase inhibitor, STAT inhibitor	STAT3	preclinical	
CTS-1027	metalloproteinase inhibitor	MMP1 , MMP13, MMP2, MMP3 , MMP9	2	
CU-CPT-4a	toll-like receptor inhibitor	TLR3	preclinical	
Curcumin	cyclooxygenase inhibitor, histone acetyltransferase inhibitor, lipoxygenase inhibitor, NFκB pathway inhibitor	APP , CA1, CA12, CA14, CA2, CA4, CA6 , CA9, CHRM3, CYP3A4 , DNMT3B, EP300, MMP13, MMP9 , NOS2, PTGS1 , PTGS2 , XDH	launched	

Curcumol	JAK inhibitor	JAK1, JAK2, JAK3	1
Cyproterone acetate	AR antagonist	ADORA1, AR	launched
Cyt387	JAK inhibitor	JAK1, JAK2, JAK3	3
Danazol	estrogen receptor antagonist, progesterone receptor agonist	AR, CCL2, ESR1, GNRHR, GNRHR2, PGR	launched
Darglitazone	PPAR γ agonist	PPARG	2
Darolutamide	AR antagonist	AR	launched
Dasatinib	Bcr-Abl kinase inhibitor, ephrin inhibitor, KIT inhibitor, PDGFR tyrosine kinase receptor inhibitor, SRC inhibitor, tyrosine kinase inhibitor	ABL1, ABL2, BLK, EPHA2, FGR, FRK, FYN, HCK, KIT, LCK, LYN, PDGFRB, SRC, SRMS, STAT5B, YES1	launched
DCEBIO	potassium channel activator	KCNN2, KCNN3, KCNN4	preclinical
D-serine	glutamate receptor agonist	GLRA1, GRIN1, GRIN2A, GRIN2B, GRIN2C, GRIN2D, SERPINB3	launched
Decernotinib	JAK inhibitor	JAK3	2 / 3
Deforolimus	mTOR inhibitor	MTOR	3
Delgocitinib	JAK inhibitor	JAK1, JAK2, JAK3	2
Dexfosfoserine	membrane integrity inhibitor	CFTR, GRM4, GRM6, GRM7, GRM8, KCNC4, PDPK1, PIM1, PRKACA, PRKCQ, PYGL, PYGM, REG1A, RHO, SERPINB3, SMAD2, TAOK2	preclinical
Diacerein	interleukin inhibitor	IL1B	launched
Diclofenac	cyclooxygenase inhibitor	AKR1C3, ALOX5, ASIC1, ASIC3, KCNQ2, KCNQ3, PLA2G2A, PPARG, PTGS1, PTGS2, SCN4A	launched
Diethylcarbamazine	lipoxygenase inhibitor	ALOX5, PTGS1	launched
Dinoprost	prostacyclin analog	PTGDR, PTGDR2, PTGER1, PTGER2, PTGER3, PTGER4, PTGFR, TBXA2R	launched
Docebenone	lipoxygenase inhibitor	ALOX5	2
Doxycycline	bacterial 30S ribosomal subunit inhibitor, metalloproteinase inhibitor	MMP1, MMP8, PI3	launched
Dupilumab	interleukin receptor antagonist	IL4R	launched
Duvelisib	PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD, PIK3CG	launched
Edaglitazone	PPAR γ agonist	PPARG	2
Efatutazone	PPAR γ agonist	PPARG	2
Elafibranor	PPAR agonist	PPARA, PPARD, PPARG	3
Ellagic acid	glutathione transferase inhibitor, non-nucleoside reverse transcriptase inhibitor	CA1, CA12, CA14, CA2, CA3, CA4, CA5A, CA5B, CA6, CA7, CA9, CSNK2A1, GSK3B, PRKACA, PRKCA, PRKCB, SQLE, SYK	2
Emricasan	caspase inhibitor	CASP1, CASP3, CASP7	2
Enzalutamide	AR antagonist	AR	launched
Enzastaurin	PKC inhibitor	AKT1, GSK3B, PRKCA, PRKCB, PRKCD, PRKCG	3
Epinephrine	adrenergic receptor agonist, carbonic anhydrase activator, neurotransmitter	ADRA1A, ADRA1B, ADRA1D, ADRA2A, ADRA2B, ADRA2C, ADRB1, ADRB2, ADRB3, PAH, TNFA	launched
Ephedrine (racemic)	adrenergic receptor agonist	ADRA1A, ADRA2A, ADRB1, ADRB2, ATF1, ATF2, ATF3, ATF4, ATF5, ATF6, ATF7, FOS, IL2, JDP2, JUN, NFATC1, SLC6A2, SLC6A3, SLC6A4, TNFA	launched
ER-27319	mediator release inhibitor, SYK inhibitor	SYK	preclinical
Erlotinib	EGFR inhibitor	EGFR, NR1I2	launched

Etanercept	TNF- α receptor antagonist	TNFR	launched
Ethanolamine-oleate	immunostimulant	F12, FABP4, FFAR1, FFAR4, PLD2	launched
Ethoxzolamide	carbonic anhydrase inhibitor	CA1, CA12, CA13, CA14, CA2, CA3, CA4, CA5A, CA5B, CA6, CA7, CA9	launched
ETP-45658	PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD, PIK3CG	preclinical
Eugenol	AR antagonist	AR	launched
Everolimus	mTOR inhibitor	MTOR	launched
Evobrutinib	Bruton's tyrosine kinase (BTK) inhibitor	BTK	2
Fedratinib	FLT3 inhibitor, JAK inhibitor	BRD4, JAK1, JAK2, JAK3, TYK2	launched
Fenebrutinib	Bruton's tyrosine kinase (BTK) inhibitor	BTK	2
Ferulic acid	Antioxidant	CA1, CA12, CA14, CA2, CA4, CA6, CA9	2
Filgotinib	JAK inhibitor	JAK1, JAK2, JAK3, TYK2	3
Flufenamic acid	chloride channel blocker	AKR1C3, ANO1, AR, GJA1, GJA10, GJA3, GJA4, GJA5, GJA8, GJA9, GJB1, GJB2, GJB3, GJB4, GJB5, GJB6, GJB7, GJC1, GJC2, GJC3, GJD2, GJD3, GJD4, GJE1, PANX1, PANX2, PANX3, PKD2L1, PTGS1, PTGS2, TRPC5, TRPM2, TRPM5	preclinical
Flutamide	Androgen receptor antagonist	AR, AHR	launched
Fostamatinib	SYK inhibitor	SYK	launched
Gallic acid	beta-amyloid protein neurotoxicity inhibitor, PPAR agonist	CA1, CA12, CA14, CA2, CA4, CA6, CA9, SELP	preclinical
Ganoderic-acid-a	JAK inhibitor	JAK1, JAK2, JAK3	preclinical
GDC-0068	AKT inhibitor	AKT1, AKT2, AKT3, PRKG1	3
GDC-0834	Bruton's tyrosine kinase (BTK) inhibitor	BTK	1
GDC-0941	PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD, PIK3CG	2
GDC-0980	mTOR inhibitor, PI3K inhibitor	FGR, MAP3K9, MTOR, PIK3CA, PIK3CB, PIK3CD, PIK3CG, SYK	2
Gefitinib	EGFR inhibitor	EGFR	launched
Genistein	tyrosine kinase inhibitor	CFD, CFT, DEFB4B, ESR1, ESR2, ESRRA, ESRRB, ESRRG, GJB2, MMP1, NCOA1, NCOA2, PI3, PPARG, PTK2B, TOP2A, TRPC5	3
GK921	transglutaminase inhibitor	TGM2	preclinical
Glipizide	sulfonylurea	ABCC8, KCNJ10, KCNJ11, PPARG	launched
Glycitein	tumor necrosis factor release inhibitor	TNFA	3
Glucosamine	glycosylated protein precursor	IL1B	launched
Golimumab	TNF inhibitor	TNFA	launched
GS-9973	SYK inhibitor	SYK	2
GSK2110183	AKT inhibitor	AKT1, AKT2, AKT3	2
GSK2126458	mTOR inhibitor, PI3K inhibitor	MTOR, PIK3CA, PIK3CB, PIK3CD, PIK3CG	1
GSK2190915	lipoxygenase inhibitor	ALOX5AP	2
GSK690693	AKT inhibitor	AKT1, AKT2, AKT3, PAK4P, PAK6, PAK7, PRKCQ, PRKG1, PRKX	1
GW-1929	PPAR γ agonist	PPARG	preclinical
GW-3965	Liver X receptor agonist	NR1H2, NR1H3	preclinical
Halofuginone	collagenase inhibitor	COL1A1, MMP2	launched
Hemomex-s	PPAR γ agonist	PPARG	launched

Hexamethylenebisacetamide	AKT inhibitor, differentiation inducer, NFκB pathway inhibitor	AKT1	2
Honokiol	AKT inhibitor	ALOX5 , PTGS1, PTGS2	3
Hydroxychloroquine	antimalarial agent	TLR7, TLR9	launched
Hypoestoxide	IKK inhibitor	IKKBK, IL1B , TNFA	1
I-BET151	bromodomain inhibitor	BRD2, BRD3, BRD4	preclinical
I-BET-762	bromodomain inhibitor	BRD2, BRD3, BRD4	2
Ibrutinib	Bruton's tyrosine kinase (BTK) inhibitor	BLK, BMX, BTK	launched
Ibudilast	leukotriene receptor antagonist, phosphodiesterase inhibitor	IL1B , IL6 , PDE3A, PDE4A, PDE4B, PDE4C, PDE4D, PDE5A	launched
Ibuproxam	cyclooxygenase inhibitor, prostaglandin inhibitor	ALOX5	launched
Icosapent	platelet aggregation inhibitor	ACSL3, ACSL4, FADS1, FFAR1, PPARG, PPARG , PTGS1 , PTGS2 , SLC8A1, TRPV1	launched
Icotinib	EGFR inhibitor	EGFR	launched
ID-1101	insulin sensitizer	INS	1
Idelalisib	PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD , PIK3CG	launched
Ilomastat	matrix metalloprotease inhibitor	CAN, ADAM28, MMP1 , MMP12 , MMP13, MMP14, MMP2, MMP3 , MMP8 , MMP9	3
Iloprost	platelet aggregation inhibitor, prostanoid receptor agonist	PTGDR, PTGER1, PTGER2, PTGER3, PTGER4, PTGFR, PTGIR, TBXA2R	launched
INCB-3284	CC chemokine receptor antagonist	CCR2	2
Indeglitazar	PPAR agonist	NCOA1, PPARA, PPARG, PPARG	2
Indisulam	CDK inhibitor	CA1, CA12, CA14, CA2, CA6 , CA7, CA9	2
Indomethacin	cyclooxygenase inhibitor	GLO1, PLA2G2A, PPARA, PPARG , PTGDR2, PTGR2, PTGS1 , PTGS2 , SLC46A1	launched
Infliximab	TNF inhibitor	IL6 , TNFA	launched
Itacitinib	JAK inhibitor	JAK1	3
JAK3-inhibitor-V	JAK inhibitor	JAK3	preclinical
JNJ-17203212	TRPV antagonist	TRPV1	preclinical
JNJ-27141491	CC chemokine receptor antagonist	CCR2	preclinical
JQ1-(+)	bromodomain inhibitor	BRD4 , BRDT	preclinical
JTE-607	cytokine production inhibitor	IL10 , IL1B , IL6 , TNFA	2
JW-67	WNT pathway inhibitor	APC, AXIN1 , GSK3B	preclinical
KN-62	calcium/calmodulin dependent protein kinase inhibitor, purinergic receptor antagonist	AKT1 , CAMK2A, CHEK1, LCK, MAPK1, MAPK11, MAPK12, MAPK14, MAPK8, P2RX7, PRKCA, ROCK1, RPS6KB1, SGK1	preclinical
KU-0063794	mTOR inhibitor	MTOR	preclinical
L-alanine	Non-essential aminoacid	AARS, AARS2, ABAT , AGXT, AGXT2, GPRC6A, GPT, GPT2, KYNU , NFS1, PHYKPL, SLC1A4, SLC36A1, SLC7A8	launched
Laropiprant	prostanoid receptor antagonist	PTGDR, PTGDR2, PTGER1, PTGER2, PTGER3, PTGFR, PTGIR, TBXA2R	launched
Latamoxef	cephalosporine	DACB , MRCA, MRCA, PBPC	launched
Lauric acid	bacterial permeability inducer	GPR84, HNF4A, LTF, LY96, PLA2G2A, TLR4	3

L-cysteinesulfinic acid	glutamate receptor agonist	GRM1, GRM5, GSR, HMGCS2 , PAPOLA, PRDX2	preclinical
LDN-27219	transglutaminase inhibitor	TGM2	preclinical
Leflunomide	dihydroorotate dehydrogenase inhibitor, PDGFR tyrosine kinase receptor inhibitor	AHR , DHODH, PTK2B	launched
Lenalidomide	tumor necrosis factor production inhibitor	TNFA	launched
LFM-A13	Bruton's tyrosine kinase (BTK) inhibitor	BTK	preclinical
Licofelone	cyclooxygenase inhibitor, lipoxigenase inhibitor	ALOX5 , PLA2G2E, PTGS2	3
Ligustilide	tumor necrosis factor production inhibitor	TNFA	preclinical
Linifanib	PDGFR tyrosine kinase receptor inhibitor, VEGFR inhibitor	CSF1 , CSF1R, FLT1, FLT3, FLT4, KDR, KIT, PDGFRB, RET, TEK	3
Linoleic acid	oxidative stress inducer	FABP4 , FFAR, FFAR4, HNF4A, KCNB1, PPARG , TRPM8	3
Lupanine	sodium channel blocker	INS	1
LXR-623	Liver X receptor agonist	AR , NR1H2 , NR1H3 , NR1I2, NR3C1	1
LY2784544	JAK inhibitor	JAK2 , JAK3	2
LY294002	DNA dependent protein kinase inhibitor, mTOR inhibitor, phosphodiesterase inhibitor, PI3K inhibitor, PLK inhibitor	AKT1 , CHEK1, GSK3B, LCK, MAPK1, MAPK11, MAPK12, MAPK14, MAPK8, MTOR , PIK3CA, PIK3CB, PIK3CD , PIK3CG, PIM1, PLK1, PRKCA, PRKDC, ROCK1, RPS6KB1, SGK1	preclinical
LY3023414	mTOR inhibitor, PI3K inhibitor	MTOR	2
LY303511	casein kinase inhibitor, mTOR inhibitor, PI3K inhibitor	BRD2, BRD3, BRD4	preclinical
Mafenide	carbonic anhydrase inhibitor	CA12, CA14, CA2, CA4, CA6 , CA9	launched
Magnolol	PPAR γ agonist	GABRA1, PPARG	preclinical
Maraviroc	CC chemokine receptor antagonist	CCR5	launched
Marimastat	matrix metalloprotease inhibitor	MMP1 , MMP10 , MMP11, MMP12 , MMP13, MMP14, MMP15, MMP16, MMP17, MMP19, MMP2, MMP20, MMP21, MMP23A, MMP24, MMP25, MMP26, MMP27, MMP28, MMP3 , MMP7, MMP8 , MMP9	3
MC-1	purinergic receptor inhibitor, intracellular Ca ²⁺ influx inhibitor	AADAT, ABAT, AGXT, AGXT2, ALAS1, AZIN2, BCAT1, BCAT2, CBS, CCBL1, CCBL2, CSAD, CTH, DDC, FTCD, GAD1, GAD2, GADL1, GCAT, GLDC, GOT1, GOT2, GPT, GPT2, HDC, IGSF10, KYNU , MOCOS, NFS1, OAT, ODC1, PDXDC1, PDXP, PHYKPL, PNPO, PROSC, PSAT1, PYGB, PYGL, PYGM, SCLY, SDS, SDSL, SEPSECS, SGPL1, SHMT1, SHMT2, SPTLC1, SPTLC2, SPTLC3, SRR, TAT, THNSL1	3
Masoprocol	lipoxigenase inhibitor	ALOX5	launched
MCC950	NOD like receptor inhibitor	NLRP3	preclinical
Meclofenamic acid	cyclooxygenase inhibitor, prostanoid receptor antagonist	ALOX5 , CNR1, KCNQ2, KCNQ3, PTGS1, PTGS2	launched
Meglitinide	potassium channel blocker	CCR2	2
Meisoindigo	STAT inhibitor	STAT3	3

Mesalazine	cyclooxygenase inhibitor, lipoxygenase inhibitor, prostanoid receptor antagonist	ALOX5 , CHUK , IKBKB , MPO , PPARG , PTGS1 , PTGS2	launched
Metacresol	phenol derivative	INS	launched
Metformin	insulin sensitizer	ACACB , PRKAB1	launched
Mimosine	DNA replication inhibitor	CCL2 , SHMT1 , SHMT2 , TYR	preclinical
Mitiglinide	insulin secretagogue	ABCC8 , KCNJ10 , PPARG	launched
MK-0812	CC chemokine receptor antagonist	CCR2	2
MK-2206	AKT inhibitor	AKT1 , AKT2 , AKT3	2
MK-2295	TRPV antagonist	TRPV1	2
MK-2461	FGFR inhibitor, VEGFR inhibitor	FGFR1 , FGFR2 , FGFR3 , FLT1 , FLT3 , FLT4 , KDR , MERTK , MET , MST1R , NTRK1 , NTRK2 , PDGFRB	1 / 2
MLN0128	mTOR inhibitor	MTOR , PIK3CA , PIK3CD , PIK3CG	2
Monepantel	mTOR inhibitor	MTOR	preclinical
Montelukast	leukotriene receptor antagonist	ALOX5 , CYSLTR1	launched
MRK-560	γ -secretase inhibitor	APP	preclinical
Naloxone	opioid receptor antagonist	CREB1 , ESR1 , OPRD1 , OPRK1 , OPRM , TLR4	launched
Napabucasin	STAT inhibitor	STAT3	3
Nateglinide	insulin secretagogue	ABCC8 , KCNJ10 , KCNJ11 , PPARG	launched
Niclosamide	DNA replication inhibitor, STAT inhibitor	STAT3	launched
Nilutamide	AR antagonist	AR	launched
NLG919	indoleamine 2,3-dioxygenase inhibitor IDO1	IDO1	1
NDT-9513727	complement antagonist	C5AR1	preclinical
NS-018	JAK inhibitor	JAK1 , JAK2 , JAK3 , TYK2	1 / 2
NS-309	calcium-activated potassium channel activator	KCNN1 , KCNN2 , KCNN3 , KCNN4	preclinical
NS-8593	calcium-activated potassium channel modulator	KCNN1 , KCNN2 , KCNN3	preclinical
NSC-405020	matrix metalloprotease inhibitor	MMP1	preclinical
nTZDpa	PPAR γ agonist	PPARG	preclinical
NVP-BEZ235	mTOR inhibitor, PI3K inhibitor	ATR , MTOR , PIK3CA , PIK3CD , PIK3CG	3
NVP-BSK805	JAK inhibitor	JAK2	preclinical
Ochromycinone	STAT inhibitor	STAT3	2
Olmudinib	Bruton's tyrosine kinase (BTK) inhibitor, EGFR inhibitor	BTK , EGFR	launched
Olopatadine	histamine receptor antagonist	HRH1 , S100A1 , S100A12 , S100A13 , S100A2 , S100B	launched
Olsalazine	cyclooxygenase inhibitor	IFNG , TPMT	launched
ONO-4059	Bruton's tyrosine kinase (BTK) inhibitor	BTK	1
ONO-4817	matrix metalloprotease inhibitor	MMP8	1
OSI-027	mTOR inhibitor	MTOR	1
Osimertinib	EGFR inhibitor	EGFR	launched
OTX015	bromodomain inhibitor	BRD2 , BRD3 , BRD4	1 / 2
OXF-BD-02	bromodomain inhibitor	BRD4	preclinical
Pacritinib	FLT3 inhibitor, JAK inhibitor	FLT3 , JAK1 , JAK2 , JAK3	3
Palomid-529	AKT inhibitor, mTOR inhibitor	MTOR	1
Paquinimod	S100A9 inhibitor	S100A9	2
Para-toluenesulfonamide	G1 cell cycle arrest inducer	CA12 , CA2 , CA6 , CA9	3

Paclitaxel	tubulin polymerization inhibitor	BCL2, MAP2, MAP4, MAPT, NR1I2, TLR4 , TUBA1A, TUBA1B, TUBA1C, TUBA3C, TUBA3D, TUBA3E, TUBA4A, TUBB, TUBB1, TUBB2A, TUBB2B, TUBB3, TUBB4A, TUBB4B, TUBB6, TUBB8	launched
Paracetamol	cyclooxygenase inhibitor	FAAH, PTGS1 , PTGS2 , TRPV1	launched
Pazopanib	KIT inhibitor, PDGFR tyrosine kinase receptor inhibitor, VEGFR inhibitor	CSF1R, FGF1 , FGFR1, FGFR3, FLT1, FLT4, ITK , KDR, KIT, PDGFRA, PDGFRB, SH2B3	launched
PCI-29732	Bruton's tyrosine kinase (BTK) inhibitor	BTK	preclinical
PD1-PDL-inhibitor-1	programmed death ligand inhibitor	CD274	preclinical
PD-166793	collagenase inhibitor, metalloproteinase inhibitor	MMP13, MMP2, MMP3	preclinical
PD-98059	MEK inhibitor	AKT1 , CHEK1, GSK3B, LCK, MAP2K1, MAPK1, MAPK11, MAPK12, MAPK14, MAPK8, PRKCA, RAF1, ROCK1, RPS6KB1, SGK1	preclinical
Peficitinib	JAK inhibitor	JAK1 , JAK2 , JAK3	launched
Pentoxifylline	phosphodiesterase inhibitor	ADORA, ADORA2A, ADORA2B, ADORA2B, NT5E, PDE10A, PDE1A, PDE1B, PDE1C, PDE2A, PDE3A, PDE3B, PDE4A, PDE4B, PDE4C, PDE4D, PDE5A, PDE6A, PDE6B, PDE6C, PDE6D, PDE6G, PDE6H, PDE7A, PDE7B, PDE8A, PDE8B, PDE9A, TNFA	launched
Perifosine	AKT inhibitor	AKT1	3
PF-04691502	mTOR inhibitor, PI3K inhibitor	MTOR , PIK3CA	2
PF-05212384	mTOR inhibitor, PI3K inhibitor	MTOR , PIK3CA	2
PF-06651600	JAK inhibitor	JAK1 , JAK2 , JAK3	2 / 3
PFI-1	bromodomain inhibitor	BRD4	preclinical
PI-103	mTOR inhibitor, PI3K inhibitor	MTOR , PIK3CA, PIK3CB, PIK3CD , PIK3CG, PRKDC	preclinical
PIK-293	PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD , PIK3CG	preclinical
PIK-294	PI3K inhibitor	PIK3CB, PIK3CD , PIK3CG	preclinical
PIK-75	DNA protein kinase inhibitor, PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD , PIK3CG, PRKDC	preclinical
Pioglitazone	insulin sensitizer, PPAR γ agonist	PPARG , ADIPOQ , TRPM3	launched
Pirfenidone	TGF beta receptor inhibitor	FURIN , TNFA	launched
PKI-179	mTOR inhibitor, PI3K inhibitor	MTOR	1
Plerixafor	CC chemokine receptor antagonist	ACKR3, CCR4 , CXCR4, MMP1 , PI3	launched
PP-121	protein tyrosine kinase inhibitor	ABL1, EGFR , HCK, KDR, MTOR , PDGFRA, PIK3CA, PIK3CB, PIK3CD , PIK3CG, PRKDC, SRC	preclinical
PP242	mTOR inhibitor	MTOR , PASK	preclinical
Pranlukast	leukotriene receptor antagonist	CYSLTR1, CYSLTR2, IL5 , MUC2, NFKB1 , RNASE3, TNFA	launched
PRN1008	Bruton's tyrosine kinase (BTK) inhibitor	BTK	preclinical
PRT062070	JAK inhibitor, SYK inhibitor	FGR, MAP3K9, SYK	2 / 3
PRT062607	SYK inhibitor	SYK	2
Pyrvinium pamoate	AR antagonist	AR	launched

Quilflapon	leukotriene synthesis inhibitor	ALOX5, ALOX5AP	2
R112	SYK inhibitor	SYK	1
R406	SYK inhibitor	RET, SYK	1
Repaglinide	insulin secretagogue	ABCC8, KCNJ11, PPARG	launched
Resatorvid	toll-like receptor inhibitor	TLR4	3
REV-5901	leukotriene receptor antagonist, lipoxygenase inhibitor	ALOX5	2
RGB-286638	CDK inhibitor	CDK1, CDK2, CDK3, CDK4, CDK5, CDK6, CDK7, CDK9, FLT3, GSK3B, JAK2, MAP3K7, MAPK9	1
RGX-104	Liver X receptor agonist	LXR	1
Ro-90-7501	β -amyloid protein neurotoxicity inhibitor	APP	preclinical
Rovazolac	liver X receptor agonist	LXR	preclinical
RS-102895	CCR antagonist	CCR2	preclinical
RS-504393	CC chemokine receptor antagonist	CCL2, CCR2	preclinical
RU-58841	AR inhibitor	AR	2
Ruxolitinib	JAK inhibitor	JAK1, JAK2, JAK3, TYK2	launched
Ruxolitinib-(S)	JAK inhibitor	JAK1, JAK2	preclinical
S26948	PPAR γ agonist	PPARG	preclinical
Saroglitazar	PPAR agonist	PPARA, PPARG	launched
Salvianolic acid-B	EGFR inhibitor, metalloproteinase inhibitor	MMP9	2
SAR-245409	PI3K inhibitor	MTOR, PIK3CG	1 / 2
SB-202190	p38 MAPK inhibitor	AKT1, ALOX5, CHEK1, GSK3B, LCK, MAPK1, MAPK11, MAPK12, MAPK14, MAPK8, PRKCA, ROCK1, RPS6KB1, SGK1	preclinical
SB-203580	p38 MAPK inhibitor	AKT1, ALOX5, CHEK1, CYP2D6, CYP3A4, GAK, GSK3B, LCK, MAPK1, MAPK10, MAPK11, MAPK12, MAPK14, MAPK8, MAPK9, PRKCA, RAF1, RIPK2, ROCK1, RPS6KB1, SGK1, SRC, TNFA	preclinical
SB-2343	mTOR inhibitor, PI3K inhibitor	MTOR, PIK3CA, PIK3CB, PIK3CD, PIK3CG	1
SB-366791	TRPV antagonist	TRPV1	preclinical
SB-452533	TRPV antagonist	TRPV1	preclinical
SB-705498	TRPV antagonist	TRPV1	preclinical
SB-747651A	kinase inhibitor	AKT1, AKT3, ROCK1, RPS6KA5, RPS6KB1	preclinical
SC-12267	dihydroorotate dehydrogenase inhibitor	IL17A	2
SD-2590	matrix metalloprotease inhibitor	MMP1, MMP13, MMP2	preclinical
SEN-1269	β -amyloid inhibitor	APP	preclinical
Silibinin	cytochrome P450 inhibitor	ALOX5	launched
Sirolimus	mTOR inhibitor	CFD1, FKBP1A, GPD1, MMP1, MTOR, PI3, RPL38	launched
SirReal-2	SIRT inhibitor	SIRT2	preclinical
SKF-86002	p38 MAPK inhibitor	ALOX5, MAPK14	preclinical
SKF-96365	calcium channel blocker	CYP3A4, PKD2, TRPC1, TRPC3, TRPC4, TRPC5, TRPV2	preclinical
Solcitinib	JAK inhibitor	JAK1	1
SP-100030	NFkB pathway inhibitor	JUN, NFKB1	preclinical

Spermine	Cellular metabolism	CA14, CA4, CA6 , CA9, CASR, GRIN1, GRIN2A, KCNJ4, ODC1, SMOX, SMS, TRPM4, TRPM5	preclinical
SR-1664	PPAR ligand	PPARG	preclinical
SR-2211	retinoid receptor inverse agonist	RORC	preclinical
SRT1720	SIRT activator	SIRT1	preclinical
SRT2104	SIRT activator	SIRT1	2
ST-2825	myeloid differentiation primary response inhibitor	MYD88	preclinical
STA-5326	interleukin synthesis inhibitor	IL12A	2
STAT3 inhibitor-VI	STAT inhibitor	STAT3	preclinical
Stemregenin-1	Aryl hydrocarbon receptor antagonist	AHR	preclinical
Sulfasalazine	cyclooxygenase inhibitor	ACAT1, ALOX5 , CHUK, IKBKB, PLA2G1B, PPARG , PTGS1 , PTGS2 , SLC46A1, SLC7A11, TBXAS1	launched
T-0901317	Liver X receptor agonist	NCOA1, NCOA2, NR1H2 , NR1H3 , NR1I2, RXRB	preclinical
TAK-220	CC chemokine receptor antagonist	CCR5	1
Talmapimod	p38 MAPK inhibitor	IL1B , MAPK11, MAPK14, MT-CO2, TNFA	2
Tanshinone-I	AP inhibitor	IFNG	2
Tanshinone-IIA	anti-inflammatory agent, interleukin inhibitor	IL1B , NR1I2, TNFA	2 / 3
Tapinarof	aryl hydrocarbon receptor agonist	AHR	3
Taxifolin	opioid receptor antagonist	ADIPOR2	2
TCS-21311	JAK inhibitor	JAK3	preclinical
Teijin compound-1	CC chemokine receptor antagonist	CCR2	preclinical
Telmisartan	angiotensin receptor antagonist	AGTR1, PPARG	launched
Temsirolimus	mTOR inhibitor	MTOR	launched
Tepoxalin	cyclooxygenase inhibito, lipoxygenase inhibitor	ALOX5	launched
Terreic-acid(-)	Bruton's tyrosine kinase (BTK) inhibitor	BTK	preclinical
Tesaglitazar	insulin sensitizer, PPAR agonist	PPARA, PPARG	3
Thalidomide	tumor necrosis factor production inhibitor	HGF , TNFA	launched
Thiram	JAK inhibitor	JAK2	launched
TG-02	CDK inhibitor, FLT3 inhibitor, JAK inhibitor	CDK1, CDK2, CDK7, CDK9, FLT3, JAK2	1 / 2
TG100-115	PI3K inhibitor	PIK3CA, PIK3CB, PIK3CD , PIK3CG	1 / 2
TG-101209	JAK inhibitor	JAK2 , JAK3	preclinical
TGX-221	PI3K inhibitor	PIK3CB, PIK3CD	preclinical
TIC10	AKT inhibitor, TRIL modulator	AKT1 , MAPK1	2
Tofacitinib	JAK inhibitor	JAK1 , JAK2 , JAK3	launched
Topilutamide	AR antagonist	AR	preclinical
Torin-1	mTOR inhibitor	MTOR	preclinical
Torin-2	mTOR inhibitor	MTOR	preclinical
Tramiprosate	β -amyloid protein neurotoxicity inhibitor	APP	3
Triciribine	AKT inhibitor	AKT1 , AKT2, AKT3	1 / 2

Triflusal	cyclooxygenase inhibitor, platelet aggregation inhibitor, thromboxane synthase inhibitor	NFKB1, NOS2, PDE10A, PTGS1	launched
Trofinetide	cytokine production inhibitor	IFNG, IL6, TNFA	2
Trometamol	organic amine proton acceptor	AMD1, CANT1, DCN, NEIL1, VEGFA	launched
U-0126	MEK inhibitor	AKT1, CHEK1, GSK3B, LCK, MAP2K1, MAP2K2, MAP2K7, MAPK1, MAPK11, MAPK12, MAPK14, MAPK8, PRKCA, RAF1, ROCK1, RPS6KB1, SGK1	preclinical
UK-356618	metalloproteinase inhibitor	MMP13, MMP14, MMP2, MMP3, MMP9	preclinical
Upadacitinib	JAK inhibitor	JAK1, JAK2, JAK3	launched
Uprosertib	AKT inhibitor	AKT1, AKT2, AKT3	2
Ustekinumab	IL12/IL23 inhibitor	FSH, HCG, LH, LTA4H	launched
Vandetanib	EGFR inhibitor, RET tyrosine kinase inhibitor, VEGFR inhibitor	EGFR, EPHA1, EPHA10, EPHA2, EPHA3, EPHA4, EPHA5, EPHA6, EPHA7, EPHA8, EPHB1, EPHB2, EPHB3, EPHB4, EPHB6, ERBB2, ERBB3, ERBB4, FLT1, FLT4, KDR, PTK6, RET, SRC, TEK, VEGFA	launched
VE-822	ATR kinase inhibitor	ATM, ATR, MTOR, PIK3CG	2
Vecabrutinib	Bruton's tyrosine kinase (BTK) inhibitor	BTK	1 / 2
Veliflapon	leukotriene synthesis inhibitor	ALOX5AP	3
VGX-1027	tumor necrosis factor receptor antagonist	TLR4	1
Vercirmon	CC chemokine receptor antagonist	CCR9	3
Vicriviroc	CC chemokine receptor antagonist	CCR5	3
Voxtalisib	mTOR inhibitor, PI3K inhibitor	MTOR, PIK3CA	2
VX-702	p38 MAPK inhibitor	IL1B, IL6, MAPK11, MAPK12, MAPK14, TNFA	2
VX-765	caspase inhibitor	CASP1	2
W-54011	anaphylatoxin chemotactic receptor antagonist	C5AR1	preclinical
WAY-200070	estrogen receptor agonist	ERBB2, ERBB3, ERBB4, ESR2	preclinical
WAY-600	mTOR inhibitor	MTOR	preclinical
WHI-P154	JAK inhibitor	EGFR, JAK1, JAK2, JAK3	preclinical
Wortmannin	PI3K inhibitor	PI4KA, PI4KB, PIK3CA, PIK3CD, PIK3CG, PIK3R1, PLK1, PRKDC	preclinical
WP1066	STAT inhibitor	STAT3	1
WP1130	deubiquitinase inhibitor	JAK2, UCHL5, USP14, USP9X	preclinical
WYE-125132	mTOR inhibitor	MTOR	preclinical
WYE-354	mTOR inhibitor	MTOR	preclinical
WYE-687	mTOR inhibitor	MTOR	preclinical
XD-14	bromodomain inhibitor	BRD2, BRD3, BRD4, BRDT	preclinical
XL019	JAK inhibitor	JAK1, JAK2, JAK3	1
XL041	liver X receptor agonist	LXR	preclinical
XL147	PI3K inhibitor	PIK3CA, PIK3CD, PIK3CG	2
XL388	mTOR inhibitor	MTOR	preclinical
Y-320	interleukin inhibitor	IL17A	preclinical
YM-90709	IL5 inhibitor	CSF2RB, IL5RA	preclinical
Zileuton	leukotriene synthesis inhibitor, lipoxygenase inhibitor	ALOX5	launched
ZM-39923	JAK inhibitor	JAK1, JAK3	preclinical

Zonisamide	sodium channel blocker, T-type calcium channel blocker	CA1, CA10, CA11, CA12, CA13, CA1, CA2, CA3, CA4, CA5A, CA5B, CA6 , CA7, CA8, CA9, CACNA1G, CACNA1H, CACNA1I, MAOA, MAOB, SCN10A, SCN11A, SCN1A, SCN1B, SCN2A, SCN2B, SCN3A, SCN3B, SCN4A, SCN4B, SCN5A, SCN7A, SCN8A, SCN9A	launched
Zopolrestat	GLO1 inhibitor	AKR1B1, AKR1B10	2
ZSTK-474	PI3K inhibitor	PIK3CB, PIK3CD , PIK3CG	1 / 2