







Group	drug_name	Target/Pathway	SMILES	Cas-number	Molecular Weight	Part Num	Description
Investigational	MLN8237 (Alistertib)	Aurora Kinase A	C1=CC=C(C=C1)OC2=NC3=C(C4=C2C=C(C=C4)N)C=N(C3)NC5=CC=C(C=C5)C(O)=O)OC	1028486-01-2	518.92	S1133	MLN8237 (Alistertib) is a selective Aurora A inhibitor with IC50 of 1.2 nM.
Investigational	MK-5108 (VX-689)	Aurora Kinase A	c1cc(nc(c1)C[C@H]2(C)[C@H](CC2)OC3C(c(ccc3)F)C(=O)O)N4scn4	1010085-13-8	461.94	S2770	MK-5108 (VX-689) is a highly selective Aurora A inhibitor with IC50 of 0.064 nM in a cell-free assay and is 220- and 190-fold more selective for Aurora A than Aurora B/C, while it inhibits TrkA with less than 100-fold selectivity.
Investigational	AT9283	Aurora Kinase A/B	N(C(=O)N1C(=N)N=C1)C2N3C(N=2)=CC(=O)C3)C4N5C(=O)C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	896466-04-9	381.43	S1134	AT9283 is a potent pan-Aurora inhibitor for Aurora A, Aurora B, JAK3, JAK2 and Abl with IC50 of 3 nM, 3 nM, 1.1 nM, 1.2 nM and 4 nM, respectively.
Investigational	PF-03814735	Aurora Kinase A/B	C12=C(C=C1)C2=C(C=C2)N3C4=NC(=O)C5=C(C=C5)N6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	942487-16-3	474.48	S2725	PF-03814735 is a novel, potent and reversible inhibitor of both Aurora A and Aurora B with IC50 of 0.8 nM and 5 nM, respectively.
Investigational	SNS-314 Mesylate	Aurora Kinase A/B	C12=C(C=C1)C2=C(C=C2)N3C4=NC(=O)C5=C(C=C5)N6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	1146618-41-8	527.04	S1154	SNS-314 Mesylate is a potent and selective inhibitor of Aurora A, Aurora B and Aurora C with IC50 of 9 nM, 31 nM, and 3.4 nM, respectively.
Investigational	Danuserib (PHA-739558)	Aurora Kinase A/B/C	C1=C(C=CC=C1)C2=C(C=C2)N3C4=NC(=O)C5=C(C=C5)N6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	827318-97-8	474.55	S1107	Danuserib (PHA-739558) is an Aurora inhibitor for Aurora A/B/C, Bcr-Abl, c-RET and FGFR with IC50 of 13 nM/79 nM/61 nM, 25 nM, 31 nM and 47 nM, respectively.
Investigational	AMG 900	Aurora Kinase A/B/C	C1=CC=C(C=C1)OC2=CC=C(C=C2)N3C4=C(C=C4)C5=CC=C(C=C5)C6=CC=C(C=C6)N	945595-80-2	503.58	S2719	AMG 900 is a potent and highly selective pan-Aurora inhibitor for Aurora A, Aurora B and Aurora with IC50 of 5 nM, 4 nM and 1 nM, respectively.
Investigational	CYC116	Aurora Kinase A/VEGFR2	C1(=NC=CC(=N1)C2S(C=NC2)N)N3C4=CC(=C(C=C3)N4)C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	693228-63-6	368.46	S1171	CYC116 is a potent inhibitor of Aurora A/B and VEGFR with Ki of 8.0 nM/9.2 nM and 44 nM, respectively.
Investigational	Barasertib (AZD1152-HQPA)	Aurora Kinase B	C1(=CC=C2C(=C1)N=CN=C2N3N=C(C=C3)C4=CC=C(C=C4)F)O)OCCN(CCO)CC	722544-51-6	507.56	S1147	AZD1152-HQPA (Barasertib) is a highly selective Aurora B inhibitor with IC50 of 0.37 nM.
Investigational	VX-680 (MK-0457, Tozasertib)	Aurora Kinases	C1(=CC(=NC(=N1)S)C2=CC=C(C=C2)N3C4=CC(=O)C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	639089-54-6	464.59	S1048	VX-680 (MK-0457, Tozasertib) is a pan-Aurora inhibitor of Aurora A, Aurora B and Aurora C with Kiapp of 0.6 nM, 18 nM and 4.6 nM, respectively.
Investigational	BMS 777607	Axl/c-Met	C1(=C(N=CC=C1)OC2=CC=C(C=C2)N3C4=CC(=O)C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	1025720-94-8	512.89	S1561	BMS-777607 is a Met-related inhibitor for c-Met, Axl, Ron and Tyro3 with IC50 of 3.9 nM, 1.1 nM, 1.8 nM and 4.3 nM, respectively.
Investigational	ABT-263 (Navitoclax)	Bcl-2	C1=CC(=CC=C1)C2=C(C=C2)N3C4=CC(=O)C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	923564-51-6	974.61	S1001	ABT-263 (Navitoclax) is a potent inhibitor of Bcl-xL, Bcl-2 and Bcl-w with Ki of 0.5 nM, <1 nM and <1 nM, respectively.
Investigational	DCC-2036 (Rebastinib)	Bcr-Abl/Tie2	C1(=CC(=CC=C1)OC2=CC=C(C=C2)N3C4=CC(=O)C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	1020172-07-9	553.59	S2634	DCC-2036 is a conformational control inhibitor of Abl1 and Abl1(T315I) with IC50 of 0.8 nM and 4 nM, respectively.
Investigational	Cyclosporin A (Cyclosporine A)	Calcineurin	N1(C=O)[C@@H](N(C(=O)C)C)C2(C)C3(C)C4(C)C5(C)C6(C)C7(C)C8(C)C9(C)C10(C)C11(C)C12(C)C13(C)C14(C)C15(C)C16(C)C17(C)C18(C)C19(C)C20(C)C21(C)C22(C)C23(C)C24(C)C25(C)C26(C)C27(C)C28(C)C29(C)C30(C)C31(C)C32(C)C33(C)C34(C)C35(C)C36(C)C37(C)C38(C)C39(C)C40(C)C41(C)C42(C)C43(C)C44(C)C45(C)C46(C)C47(C)C48(C)C49(C)C50(C)C51(C)C52(C)C53(C)C54(C)C55(C)C56(C)C57(C)C58(C)C59(C)C60(C)C61(C)C62(C)C63(C)C64(C)C65(C)C66(C)C67(C)C68(C)C69(C)C70(C)C71(C)C72(C)C73(C)C74(C)C75(C)C76(C)C77(C)C78(C)C79(C)C80(C)C81(C)C82(C)C83(C)C84(C)C85(C)C86(C)C87(C)C88(C)C89(C)C90(C)C91(C)C92(C)C93(C)C94(C)C95(C)C96(C)C97(C)C98(C)C99(C)C100(C)	59865-13-3	1202.61	S2286	Cyclosporin A (Cyclosporine A) is an immunosuppressant agent widely used in post-allogeneic organ transplant to reduce the activity of the immune system.
Investigational	Doxercalciferol (Hectorol)	Calcium-Bone metabolism	C1(=CC(=CC=C1)OC2=CC=C(C=C2)N3C4=CC(=O)C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	54573-75-0	412.65	S1467	Doxercalciferol (Hectorol) is a synthetic analog of vitamin D.
Investigational	AT7519	CDK1 and -2	C1=C(C(=C(C=C1)C)C)N2=C(NN=C2)C3=CC(=O)N3C4C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100	844442-38-2	382.24	S1524	AT7519 is a novel multi-CDK inhibitor for CDK1/cyclin B, CDK2/cyclin A, CDK3/cyclin E, CDK4/cyclin D1, CDK5/p35 and CDK6/cyclin D3 with IC50 of 210 nM, 47 nM, 360 nM, 100 nM, 13 nM and 170 nM, respectively.
Investigational	Flavopiridol (Alvocidib) HCl	CDK1, -2, -4, -5, -6, -7, -8 and -9	C1(=C(C=C2C(=C1)O)C3=C(C=C2)C4=C(C=C3)C5=C(C=C4)C6=C(C=C5)C7=C(C=C6)C8=C(C=C7)C9=C(C=C8)C10=C(C=C9)C11=C(C=C10)C12=C(C=C11)C13=C(C=C12)C14=C(C=C13)C15=C(C=C14)C16=C(C=C15)C17=C(C=C16)C18=C(C=C17)C19=C(C=C18)C20=C(C=C19)C21=C(C=C20)C22=C(C=C21)C23=C(C=C22)C24=C(C=C23)C25=C(C=C24)C26=C(C=C25)C27=C(C=C26)C28=C(C=C27)C29=C(C=C28)C30=C(C=C29)C31=C(C=C30)C32=C(C=C31)C33=C(C=C32)C34=C(C=C33)C35=C(C=C34)C36=C(C=C35)C37=C(C=C36)C38=C(C=C37)C39=C(C=C38)C40=C(C=C39)C41=C(C=C40)C42=C(C=C41)C43=C(C=C42)C44=C(C=C43)C45=C(C=C44)C46=C(C=C45)C47=C(C=C46)C48=C(C=C47)C49=C(C=C48)C50=C(C=C49)C51=C(C=C50)C52=C(C=C51)C53=C(C=C52)C54=C(C=C53)C55=C(C=C54)C56=C(C=C55)C57=C(C=C56)C58=C(C=C57)C59=C(C=C58)C60=C(C=C59)C61=C(C=C60)C62=C(C=C61)C63=C(C=C62)C64=C(C=C63)C65=C(C=C64)C66=C(C=C65)C67=C(C=C66)C68=C(C=C67)C69=C(C=C68)C70=C(C=C69)C71=C(C=C70)C72=C(C=C71)C73=C(C=C72)C74=C(C=C73)C75=C(C=C74)C76=C(C=C75)C77=C(C=C76)C78=C(C=C77)C79=C(C=C78)C80=C(C=C79)C81=C(C=C80)C82=C(C=C81)C83=C(C=C82)C84=C(C=C83)C85=C(C=C84)C86=C(C=C85)C87=C(C=C86)C88=C(C=C87)C89=C(C=C88)C90=C(C=C89)C91=C(C=C90)C92=C(C=C91)C93=C(C=C92)C94=C(C=C93)C95=C(C=C94)C96=C(C=C95)C97=C(C=C96)C98=C(C=C97)C99=C(C=C98)C100=C(C=C99)C101=C(C=C100)C102=C(C=C101)C103=C(C=C102)C104=C(C=C103)C105=C(C=C104)C106=C(C=C105)C107=C(C=C106)C108=C(C=C107)C109=C(C=C108)C110=C(C=C109)C111=C(C=C110)C112=C(C=C111)C113=C(C=C112)C114=C(C=C113)C115=C(C=C114)C116=C(C=C115)C117=C(C=C116)C118=C(C=C117)C119=C(C=C118)C120=C(C=C119)C121=C(C=C120)C122=C(C=C121)C123=C(C=C122)C124=C(C=C123)C125=C(C=C124)C126=C(C=C125)C127=C(C=C126)C128=C(C=C127)C129=C(C=C128)C130=C(C=C129)C131=C(C=C130)C132=C(C=C131)C133=C(C=C132)C134=C(C=C133)C135=C(C=C134)C136=C(C=C135)C137=C(C=C136)C138=C(C=C137)C139=C(C=C138)C140=C(C=C139)C141=C(C=C140)C142=C(C=C141)C143=C(C=C142)C144=C(C=C143)C145=C(C=C144)C146=C(C=C145)C147=C(C=C146)C148=C(C=C147)C149=C(C=C148)C150=C(C=C149)C151=C(C=C150)C152=C(C=C151)C153=C(C=C152)C154=C(C=C153)C155=C(C=C154)C156=C(C=C155)C157=C(C=C156)C158=C(C=C157)C159=C(C=C158)C160=C(C=C159)C161=C(C=C160)C162=C(C=C161)C163=C(C=C162)C164=C(C=C163)C165=C(C=C164)C166=C(C=C165)C167=C(C=C166)C168=C(C=C167)C169=C(C=C168)C170=C(C=C169)C171=C(C=C170)C172=C(C=C171)C173=C(C=C172)C174=C(C=C173)C175=C(C=C174)C176=C(C=C175)C177=C(C=C176)C178=C(C=C177)C179=C(C=C178)C180=C(C=C179)C181=C(C=C180)C182=C(C=C181)C183=C(C=C182)C184=C(C=C183)C185=C(C=C184)C186=C(C=C185)C187=C(C=C186)C188=C(C=C187)C189=C(C=C188)C190=C(C=C189)C191=C(C=C190)C192=C(C=C191)C193=C(C=C192)C194=C(C=C193)C195=C(C=C194)C196=C(C=C195)C197=C(C=C196)C198=C(C=C197)C199=C(C=C198)C200=C(C=C199)C201=C(C=C200)C202=C(C=C201)C203=C(C=C202)C204=C(C=C203)C205=C(C=C204)C206=C(C=C205)C207=C(C=C206)C208=C(C=C207)C209=C(C=C208)C210=C(C=C209)C211=C(C=C210)C212=C(C=C211)C213=C(C=C212)C214=C(C=C213)C215=C(C=C214)C216=C(C=C215)C217=C(C=C216)C218=C(C=C217)C219=C(C=C218)C220=C(C=C219)C221=C(C=C220)C222=C(C=C221)C223=C(C=C222)C224=C(C=C223)C225=C(C=C224)C226=C(C=C225)C227=C(C=C226)C228=C(C=C227)C229=C(C=C228)C230=C(C=C229)C231=C(C=C230)C232=C(C=C231)C233=C(C=C232)C234=C(C=C233)C235=C(C=C234)C236=C(C=C235)C237=C(C=C236)C238=C(C=C237)C239=C(C=C238)C240=C(C=C239)C241=C(C=C240)C242=C(C=C241)C243=C(C=C242)C244=C(C=C243)C245=C(C=C244)C246=C(C=C245)C247=C(C=C246)C248=C(C=C247)C249=C(C=C248)C250=C(C=C249)C251=C(C=C250)C252=C(C=C251)C253=C(C=C252)C254=C(C=C253)C255=C(C=C254)C256=C(C=C255)C257=C(C=C256)C258=C(C=C257)C259=C(C=C258)C260=C(C=C259)C261=C(C=C260)C262=C(C=C261)C263=C(C=C262)C264=C(C=C263)C265=C(C=C264)C266=C(C=C265)C267=C(C=C266)C268=C(C=C267)C269=C(C=C268)C270=C(C=C269)C271=C(C=C270)C272=C(C=C271)C273=C(C=C272)C274=C(C=C273)C275=C(C=C274)C276=C(C=C275)C277=C(C=C276)C278=C(C=C277)C279=C(C=C278)C280=C(C=C279)C281=C(C=C280)C282=C(C=C281)C283=C(C=C282)C284=C(C=C283)C285=C(C=C284)C286=C(C=C285)C287=C(C=C286)C288=C(C=C287)C289=C(C=C288)C290=C(C=C289)C291=C(C=C290)C292=C(C=C291)C293=C(C=C292)C294=C(C=C293)C295=C(C=C294)C296=C(C=C295)C297=C(C=C296)C298=C(C=C297)C299=C(C=C298)C300=C(C=C299)C301=C(C=C300)C302=C(C=C301)C303=C(C=C302)C304=C(C=C303)C305=C(C=C304)C306=C(C=C305)C307=C(C=C306)C308=C(C=C307)C309=C(C=C308)C310=C(C=C309)C311=C(C=C310)C312=C(C=C311)C313=C(C=C312)C314=C(C=C313)C315=C(C=C314)C316=C(C=C315)C317=C(C=C316)C318=C(C=C317)C319=C(C=C318)C320=C(C=C319)C321=C(C=C320)C322=C(C=C321)C323=C(C=C322)C324=C(C=C323)C325=C(C=C324)C326=C(C=C325)C327=C(C=C326)C328=C(C=C327)C329=C(C=C328)C330=C(C=C329)C331=C(C=C330)C332=C(C=C331)C333=C(C=C332)C334=C(C=C333)C335=C(C=C334)C336=C(C=C335)C337=C(C=C336)C338=C(C=C337)C339=C(C=C338)C340=C(C=C339)C341=C(C=C340)C342=C(C=C341)C343=C(C=C342)C344=C(C=C343)C345=C(C=C344)C346=C(C=C345)C347=C(C=C346)C348=C(C=C347)C349=C(C=C348)C350=C(C=C349)C351=C(C=C350)C352=C(C=C351)C353=C(C=C352)C354=C(C=C353)C355=C(C=C354)C356=C(C=C355)C357=C(C=C356)C358=C(C=C357)C359=C(C=C358)C360=C(C=C359)C361=C(C=C360)C362=C(C=C361)C363=C(C=C362)C364=C(C=C363)C365=C(C=C364)C366=C(C=C365)C367=C(C=C366)C368=C(C=C367)C369=C(C=C368)C370=C(C=C369)C371=C(C=C370)C372=C(C=C371)C373=C(C=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