Supporting Information

Identification of N-(4-((1R,3S,5S)-3-amino-5-methylcyclohexyl)pyridin-3-yl)-6-(2,6-difluorophenyl)-5-fluoropicolinamide (PIM447), a Potent and Selective Proviral Insertion Site of Moloney Murine Leukemia (PIM) 1,2 and 3 Kinase Inhibitor in Clinical Trials for Hematological Malignancies

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Contents

1. Kinome Scan Data for compound 8 (PIM447)

Ambit Gene Symbol	Entrez Gene Symbol	Percent Control	Compound Concentration (nM)
AAK1	AAK1	81	1000
ABL1(E255K)-phosphorylated	ABL1	88	1000
ABL1(F317I)-nonphosphorylated	ABL1	100	1000
ABL1(F317I)-phosphorylated	ABL1	100	1000

ABL1(F317L)-nonphosphorylated	ABL1	100	1000
ABL1(F317L)-phosphorylated	ABL1	100	1000
ABL1(H396P)-nonphosphorylated	ABL1	99	1000
ABL1(H396P)-phosphorylated	ABL1	100	1000
ABL1(M351T)-phosphorylated	ABL1	100	1000
ABL1(Q252H)-nonphosphorylated	ABL1	91	1000
ABL1(Q252H)-phosphorylated	ABL1	92	1000
ABL1(T315I)-nonphosphorylated	ABL1	100	1000
ABL1(T315I)-phosphorylated	ABL1	80	1000
ABL1(Y253F)-phosphorylated	ABL1	91	1000
ABL1-nonphosphorylated	ABL1	100	1000
ABL1-phosphorylated	ABL1	100	1000
ABL2	ABL2	100	1000
ACVR1	ACVR1	87	1000
ACVR1B	ACVR1B	88	1000
ACVR2A	ACVR2A	100	1000
ACVR2B	ACVR2B	90	1000
ACVRL1	ACVRL1	77	1000
ADCK3	CABC1	83	1000
ADCK4	ADCK4	100	1000
AKT1	AKT1	100	1000
AKT2	AKT2	100	1000
AKT3	AKT3	94	1000
ALK	ALK	96	1000
AMPK-alpha1	PRKAA1	93	1000
AMPK-alpha2	PRKAA2	85	1000
ANKK1	ANKK1	100	1000
ARK5	NUAK1	81	1000
ASK1	MAP3K5	100	1000
ASK2	MAP3K6	100	1000
AURKA	AURKA	93	1000
AURKB	AURKB	98	1000
AURKC	AURKC	100	1000
AXL	AXL	97	1000
BIKE	BMP2K	96	1000
BLK	BLK	89	1000
BMPR1A	BMPR1A	84	1000
BMPR1B	BMPR1B	100	1000
BMPR2	BMPR2	100	1000
BMX	BMX	100	1000
BRAF	BRAF	90	1000
BRAF(V600E)	BRAF	99	1000
BRK	PTK6	100	1000

BRSK1	BRSK1	100	1000
BRSK2	BRSK2	100	1000
BTK	BTK	98	1000
CAMK1	CAMK1	100	1000
CAMK1D	CAMK1D	100	1000
CAMK1G	CAMK1G	83	1000
CAMK2A	CAMK2A	100	1000
CAMK2B	CAMK2B	87	1000
CAMK2D	CAMK2D	100	1000
CAMK2G	CAMK2G	100	1000
CAMK4	CAMK4	73	1000
CAMKK1	CAMKK1	100	1000
CAMKK2	CAMKK2	100	1000
CASK	CASK	84	1000
CDC2L1	CDC2L1	92	1000
CDC2L2	CDC2L2	100	1000
CDC2L5	CDC2L5	100	1000
CDK11	CDC2L6	100	1000
CDK2	CDK2	91	1000
CDK3	CDK3	100	1000
CDK4-cyclinD1	CDK4	100	1000
CDK4-cyclinD3	CDK4	100	1000
CDK5	CDK5	100	1000
CDK7	CDK7	94	1000
CDK8	CDK8	97	1000
CDK9	CDK9	100	1000
CDKL1	CDKL1	100	1000
CDKL2	CDKL2	100	1000
CDKL3	CDKL3	100	1000
CDKL5	CDKL5	100	1000
CHEK1	CHEK1	85	1000
CHEK2	CHEK2	73	1000
CIT	CIT	38	1000
CLK1	CLK1	60	1000
CLK2	CLK2	52	1000
CLK3	CLK3	87	1000
CLK4	CLK4	53	1000
CSF1R	CSF1R	81	1000
CSK	CSK	95	1000
CSNK1A1	CSNK1A1	97	1000
CSNK1A1L	CSNK1A1L	100	1000
CSNK1D	CSNK1D	97	1000
CSNK1E	CSNK1E	87	1000

CSNK1G1	CSNK1G1	84	1000
CSNK1G2	CSNK1G2	73	1000
CSNK1G3	CSNK1G3	82	1000
CSNK2A1	CSNK2A1	77	1000
CSNK2A2	CSNK2A2	52	1000
CTK	MATK	89	1000
DAPK1	DAPK1	96	1000
DAPK2	DAPK2	100	1000
DAPK3	DAPK3	97	1000
DCAMKL1	DCLK1	87	1000
DCAMKL2	DCLK2	100	1000
DCAMKL3	DCLK3	94	1000
DDR1	DDR1	98	1000
DDR2	DDR2	100	1000
DLK	MAP3K12	100	1000
DMPK	DMPK	95	1000
DMPK2	CDC42BPG	95	1000
DRAK1	STK17A	100	1000
DRAK2	STK17B	100	1000
DYRK1A	DYRK1A	70	1000
DYRK1B	DYRK1B	100	1000
DYRK2	DYRK2	100	1000
EGFR	EGFR	87	1000
EGFR(E746-A750del)	EGFR	89	1000
EGFR(G719C)	EGFR	96	1000
EGFR(G719S)	EGFR	96	1000
EGFR(L747-E749del, A750P)	EGFR	88	1000
EGFR(L747-S752del, P753S)	EGFR	97	1000
EGFR(L747-T751del,Sins)	EGFR	100	1000
EGFR(L858R)	EGFR	100	1000
EGFR(L858R,T790M)	EGFR	100	1000
EGFR(L861Q)	EGFR	100	1000
EGFR(S752-I759del)	EGFR	97	1000
EGFR(T790M)	EGFR	100	1000
EIF2AK1	EIF2AK1	100	1000
EPHA1	EPHA1	100	1000
EPHA2	EPHA2	100	1000
EPHA3	EPHA3	95	1000
EPHA4	EPHA4	100	1000
EPHA5	EPHA5	100	1000
EPHA6	EPHA6	95	1000
EPHA7	EPHA7	93	1000
EPHA8	EPHA8	91	1000

EPHB1	EPHB1	88	1000
EPHB2	EPHB2	100	1000
EPHB3	EPHB3	77	1000
EPHB4	EPHB4	100	1000
EPHB6	EPHB6	96	1000
ERBB2	ERBB2	92	1000
ERBB3	ERBB3	100	1000
ERBB4	ERBB4	100	1000
ERK1	MAPK3	95	1000
ERK2	MAPK1	100	1000
ERK3	MAPK6	100	1000
ERK4	MAPK4	99	1000
ERK5	MAPK7	100	1000
ERK8	MAPK15	2.5	1000
ERN1	ERN1	100	1000
FAK	PTK2	96	1000
FER	FER	100	1000
FES	FES	100	1000
FGFR1	FGFR1	97	1000
FGFR2	FGFR2	96	1000
FGFR3	FGFR3	100	1000
FGFR3(G697C)	FGFR3	100	1000
FGFR4	FGFR4	91	1000
FGR	FGR	100	1000
FLT1	FLT1	100	1000
FLT3	FLT3	76	1000
FLT3(D835H)	FLT3	63	1000
FLT3(D835Y)	FLT3	38	1000
FLT3(ITD)	FLT3	79	1000
FLT3(K663Q)	FLT3	82	1000
FLT3(N841I)	FLT3	80	1000
FLT3(R834Q)	FLT3	100	1000
FLT4	FLT4	100	1000
FRK	FRK	100	1000
FYN	FYN	100	1000
GAK	GAK	100	1000
GCN2(Kin.Dom.2,S808G)	EIF2AK4	80	1000
GRK1	GRK1	98	1000
GRK4	GRK4	92	1000
GRK7	GRK7	96	1000
GSK3A	GSK3A	89	1000
GSK3B	GSK3B	21	1000
HCK	HCK	94	1000

HIPK1	HIPK1	95	1000
HIPK2	HIPK2	52	1000
HIPK3	HIPK3	93	1000
HIPK4	HIPK4	84	1000
HPK1	MAP4K1	87	1000
HUNK	HUNK	100	1000
ICK	ICK	100	1000
IGF1R	IGF1R	100	1000
IKK-alpha	CHUK	69	1000
IKK-beta	IKBKB	100	1000
IKK-epsilon	IKBKE	93	1000
INSR	INSR	95	1000
INSRR	INSRR	100	1000
IRAK1	IRAK1	100	1000
IRAK3	IRAK3	97	1000
IRAK4	IRAK4	100	1000
ITK	ITK	99	1000
JAK1(JH1domain-catalytic)	JAK1	71	1000
JAK1(JH2domain-pseudokinase)	JAK1	99	1000
JAK2(JH1domain-catalytic)	JAK2	95	1000
JAK3(JH1domain-catalytic)	JAK3	100	1000
JNK1	MAPK8	100	1000
JNK2	MAPK9	100	1000
JNK3	MAPK10	100	1000
KIT	KIT	82	1000
KIT(A829P)	KIT	100	1000
KIT(D816H)	KIT	98	1000
KIT(D816V)	KIT	83	1000
KIT(L576P)	KIT	100	1000
KIT(V559D)	KIT	92	1000
KIT(V559D,T670I)	KIT	85	1000
KIT(V559D,V654A)	KIT	100	1000
LATS1	LATS1	93	1000
LATS2	LATS2	100	1000
LCK	LCK	98	1000
LIMK1	LIMK1	100	1000
LIMK2	LIMK2	100	1000
LKB1	STK11	100	1000
LOK	STK10	99	1000
LRRK2	LRRK2	100	1000
LRRK2(G2019S)	LRRK2	79	1000
LTK	LTK	88	1000
LYN	LYN	100	1000

LZK	MAP3K13	98	1000
MAK	MAK	91	1000
MAP3K1	MAP3K1	91	1000
MAP3K15	MAP3K15	100	1000
MAP3K2	MAP3K2	88	1000
MAP3K3	MAP3K3	100	1000
MAP3K4	MAP3K4	100	1000
MAP4K2	MAP4K2	83	1000
MAP4K3	MAP4K3	100	1000
MAP4K4	MAP4K4	100	1000
MAP4K5	MAP4K5	100	1000
MAPKAPK2	MAPKAPK2	93	1000
MAPKAPK5	MAPKAPK5	88	1000
MARK1	MARK1	81	1000
MARK2	MARK2	81	1000
MARK3	MARK3	98	1000
MARK4	MARK4	77	1000
MAST1	MAST1	100	1000
MEK1	MAP2K1	100	1000
MEK2	MAP2K2	97	1000
MEK3	MAP2K3	65	1000
MEK4	MAP2K4	75	1000
MEK5	MAP2K5	66	1000
MEK6	MAP2K6	100	1000
MELK	MELK	78	1000
MERTK	MERTK	99	1000
MET	MET	100	1000
MET(M1250T)	MET	81	1000
MET(Y1235D)	MET	95	1000
MINK	MINK1	68	1000
MKK7	MAP2K7	100	1000
MKNK1	MKNK1	74	1000
MKNK2	MKNK2	100	1000
MLCK	MYLK3	83	1000
MLK1	MAP3K9	93	1000
MLK2	MAP3K10	100	1000
MLK3	MAP3K11	100	1000
MRCKA	CDC42BPA	100	1000
MRCKB	CDC42BPB	100	1000
MST1	STK4	91	1000
MST1R	MST1R	92	1000
MST2	STK3	78	1000
MST3	STK24	99	1000

MST4	MST4	100	1000
MTOR	FRAP1	100	1000
MUSK	MUSK	100	1000
MYLK	MYLK	96	1000
MYLK2	MYLK2	68	1000
MYLK4	MYLK4	90	1000
MYO3A	MYO3A	100	1000
MYO3B	MYO3B	100	1000
NDR1	STK38	100	1000
NDR2	STK38L	99	1000
NEK1	NEK1	100	1000
NEK11	NEK11	100	1000
NEK2	NEK2	100	1000
NEK3	NEK3	100	1000
NEK4	NEK4	100	1000
NEK5	NEK5	87	1000
NEK6	NEK6	100	1000
NEK7	NEK7	100	1000
NEK9	NEK9	100	1000
NIM1	MGC42105	85	1000
NLK	NLK	100	1000
OSR1	OXSRI	100	1000
p38-alpha	MAPK14	100	1000
p38-beta	MAPK11	100	1000
p38-delta	MAPK13	76	1000
p38-gamma	MAPK12	100	1000
PAK1	PAK1	100	1000
PAK2	PAK2	64	1000
PAK3	PAK3	100	1000
PAK4	PAK4	100	1000
PAK6	PAK6	74	1000
PAK7	PAK7	97	1000
PCK1	PCK1	100	1000
PCK2	PCK2	100	1000
PCK3	PCK3	99	1000
PDGFRA	PDGFRA	100	1000
PDGFRB	PDGFRB	59	1000
PDPK1	PDPK1	95	1000
PFCDPK1(P.falciparum)	PFB0815w	96	1000
PFPK5(P.falciparum)	MAL13P1.279	94	1000
PFTAIK2	PFTK2	100	1000
PFTK1	PFTK1	90	1000
PHKG1	PHKG1	100	1000

PHKG2	PHKG2	100	1000
PIK3C2B	PIK3C2B	88	1000
PIK3C2G	PIK3C2G	100	1000
PIK3CA	PIK3CA	88	1000
PIK3CA(C420R)	PIK3CA	99	1000
PIK3CA(E542K)	PIK3CA	86	1000
PIK3CA(E545A)	PIK3CA	93	1000
PIK3CA(E545K)	PIK3CA	80	1000
PIK3CA(H1047L)	PIK3CA	100	1000
PIK3CA(H1047Y)	PIK3CA	100	1000
PIK3CA(I800L)	PIK3CA	100	1000
PIK3CA(M1043I)	PIK3CA	92	1000
PIK3CA(Q546K)	PIK3CA	95	1000
PIK3CB	PIK3CB	38	1000
PIK3CD	PIK3CD	84	1000
PIK3CG	PIK3CG	34	1000
PIK4CB	PI4KB	96	1000
PIM1	PIM1	0.7	1000
PIM2	PIM2	0.7	1000
PIM3	PIM3	0.45	1000
PIP5K1A	PIP5K1A	100	1000
PIP5K1C	PIP5K1C	100	1000
PIP5K2B	PIP4K2B	87	1000
PIP5K2C	PIP4K2C	100	1000
PKAC-alpha	PRKACA	100	1000
PKAC-beta	PRKACB	97	1000
PKMYT1	PKMYT1	100	1000
PKN1	PKN1	95	1000
PKN2	PKN2	94	1000
PKNB(M.tuberculosis)	pknB	95	1000
PLK1	PLK1	87	1000
PLK2	PLK2	88	1000
PLK3	PLK3	76	1000
PLK4	PLK4	100	1000
PRKCD	PRKCD	72	1000
PRKCE	PRKCE	72	1000
PRKCH	PRKCH	89	1000
PRKCI	PRKCI	81	1000
PRKCQ	PRKCQ	66	1000
PRKD1	PRKD1	32	1000
PRKD2	PRKD2	43	1000
PRKD3	PRKD3	34	1000
PRKG1	PRKG1	84	1000

PRKG2	PRKG2	100	1000
PRKR	EIF2AK2	89	1000
PRKX	PRKX	100	1000
PRP4	PRPF4B	100	1000
PYK2	PTK2B	100	1000
QSK	KIAA0999	100	1000
RAF1	RAF1	98	1000
RET	RET	99	1000
RET(M918T)	RET	100	1000
RET(V804L)	RET	100	1000
RET(V804M)	RET	96	1000
RIOK1	RIOK1	78	1000
RIOK2	RIOK2	95	1000
RIOK3	RIOK3	100	1000
RIPK1	RIPK1	90	1000
RIPK2	RIPK2	100	1000
RIPK4	RIPK4	100	1000
RIPK5	DSTKY	93	1000
ROCK1	ROCK1	100	1000
ROCK2	ROCK2	77	1000
ROS1	ROS1	100	1000
RPS6KA4(Kin.Dom.1-N-terminal)	RPS6KA4	90	1000
RPS6KA4(Kin.Dom.2-C-terminal)	RPS6KA4	90	1000
RPS6KA5(Kin.Dom.1-N-terminal)	RPS6KA5	100	1000
RPS6KA5(Kin.Dom.2-C-terminal)	RPS6KA5	100	1000
RSK1(Kin.Dom.1-N-terminal)	RPS6KA1	73	1000
RSK1(Kin.Dom.2-C-terminal)	RPS6KA1	87	1000
RSK2(Kin.Dom.1-N-terminal)	RPS6KA3	95	1000
RSK3(Kin.Dom.1-N-terminal)	RPS6KA2	80	1000
RSK3(Kin.Dom.2-C-terminal)	RPS6KA2	94	1000
RSK4(Kin.Dom.1-N-terminal)	RPS6KA6	84	1000
RSK4(Kin.Dom.2-C-terminal)	RPS6KA6	100	1000
S6K1	RPS6KB1	100	1000
SBK1	SBK1	100	1000
SgK110	SgK110	78	1000
SGK3	SGK3	68	1000
SIK	SIK1	100	1000
SIK2	SIK2	100	1000
SLK	SLK	76	1000
SNARK	NUAK2	91	1000
SNRK	SNRK	75	1000
SRC	SRC	100	1000
SRMS	SRMS	85	1000

SRPK1	SRPK1	100	1000
SRPK2	SRPK2	98	1000
SRPK3	SRPK3	100	1000
STK16	STK16	90	1000
STK33	STK33	99	1000
STK35	STK35	100	1000
STK36	STK36	97	1000
STK39	STK39	84	1000
SYK	SYK	100	1000
TAK1	MAP3K7	82	1000
TAOK1	TAOK1	38	1000
TAOK2	TAOK2	76	1000
TAOK3	TAOK3	40	1000
TBK1	TBK1	100	1000
TEC	TEC	100	1000
TESK1	TESK1	100	1000
TGFBR1	TGFBR1	100	1000
TGFBR2	TGFBR2	100	1000
TIE1	TIE1	100	1000
TIE2	TEK	100	1000
TLK1	TLK1	77	1000
TLK2	TLK2	100	1000
TNIK	TNIK	100	1000
TNK1	TNK1	100	1000
TNK2	TNK2	100	1000
TNNI3K	TNNI3K	100	1000
TRKA	NTRK1	90	1000
TRKB	NTRK2	82	1000
TRKC	NTRK3	91	1000
TRPM6	TRPM6	100	1000
TSSK1B	TSSK1B	98	1000
TTK	TTK	100	1000
TXK	TXK	97	1000
TYK2(JH1domain-catalytic)	TYK2	93	1000
TYK2(JH2domain-pseudokinase)	TYK2	88	1000
TYRO3	TYRO3	100	1000
ULK1	ULK1	100	1000
ULK2	ULK2	100	1000
ULK3	ULK3	100	1000
VEGFR2	KDR	98	1000
VRK2	VRK2	100	1000
WEE1	WEE1	100	1000
WEE2	WEE2	96	1000

YANK1	STK32A	92	1000
YANK2	STK32B	100	1000
YANK3	STK32C	100	1000
YES	YES1	100	1000
YSK1	STK25	100	1000
YSK4	YSK4	100	1000
ZAK	ZAK	100	1000
ZAP70	ZAP70	88	1000