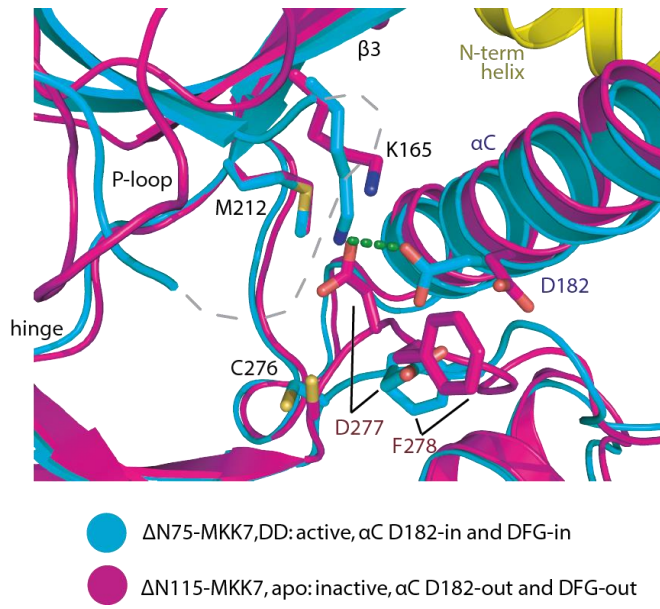
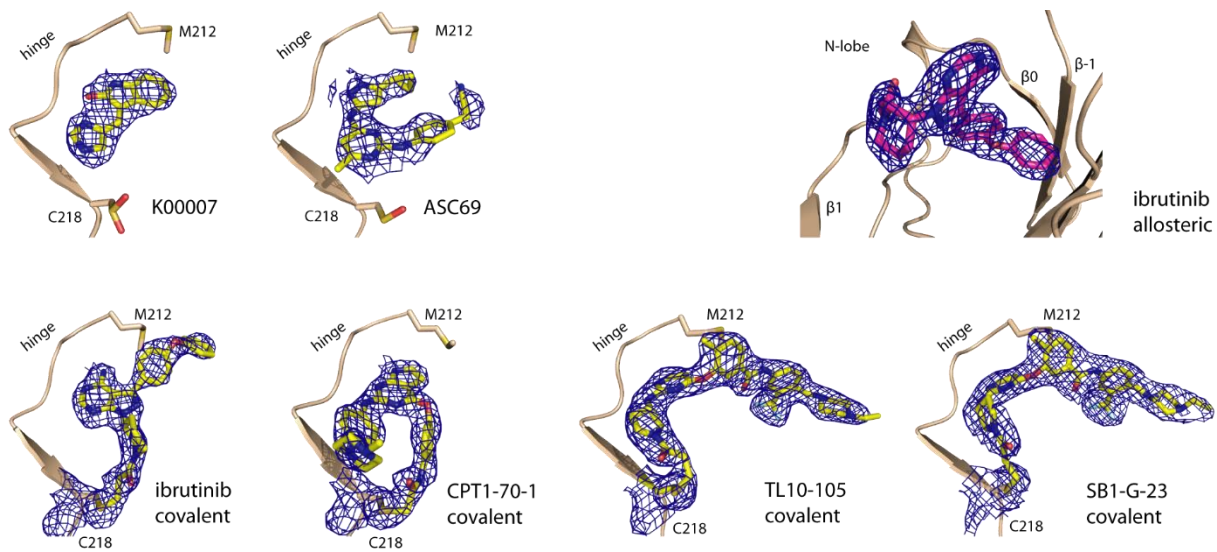


MKK7	-----MAA-----SSLEQKLSRLEA-KL	17
MEK1	-----	0
MEK2	-----	0
MEK4	-----	0
MEK5	MLWLALGPFAMENQVLVIRIKIPNSGAVDWTVHSGPQLLFRDVLVIGQVLEPATTAF	60
MEK6	-----	0
MKK7	KQENREARRRIDLNLDISPQRPRPIIVITLSPAPAPSQRAALQLPLANDGGSRSPPSSESS	77
MEK1	-----MPK-----KKPTP--I	9
MEK2	-----MLAR-----RKPVLPAL	12
MEK4	-----MAAPSPSGGGGS--GGGSGSGTTPGVPVSPA	28
MEK5	EYE-DEGDRIITVRSDEEMKAMLSYYSYTVME-----QQVNGQLIEPL	102
MEK6	-----	0
MKK7	PQHPTPPA---RPRHMLGLPSTLFTPR-----SMESIEI-----D-QKL	112
MEK1	QLNP-APD-----GSAVNGTSSAETNLEALQKKLELEELD	43
MEK2	TINPTIAE-----GPSPTSEGASEANLVDLQKKLELEELD	47
MEK4	PGHPAVSSMQGKRKALKLNFPANPPFKSTARFTLNPNPTGVQNPHE-----E-RLR	77
MEK5	QIFPRACKPPGERNIHGLKVNTRA-----GPSQHSSPAV-----SDSLP	141
MEK6	-----MSQSKGKKRNPGLKIPKEAFEQ-----PQT-----S-STP	29
MKK7	-QEIMKQTYLTIIGGQRYQAEINDLENLGMGSGTCGQVVKMRFRKTGHVIAVKQMRRS	171
MEK1	EQQQRKLEAFLTQKQKVGELKDDDFEKISELGAGNGGVVFKVSHKPSGLVMARKLIHLEI	103
MEK2	EQQQRKLEAFLTQKAKVGELKDDDFERISELGAGNGGVVTKVQHRPSGLIMARKLIHLEI	107
MEK4	THSIESSGKLIKISPEQHWDFTAEDLKDLEIGRGAAGSVNKMVHKPSGQIMAVKRIRSTV	137
MEK5	SNSLKKSSAELKKILANGQMNQDQIRYRDTLGHGNGGTVYKAYHVPVSGKILAVKVIILDI	201
MEK6	PRDLDSKACI-SIGNQNFVKKADLEPIMELGRGAYGVVEKMRHVPSGQIMAVKRIRATV	88
MKK7	NKEENKRILMDLDVVVKSHDCPYIVQCFGFTITNTDVFIAAMELMTCAEKLKRR----MQ	227
MEK1	KPAIRNQIIRELQVLHE-CNSPYIVGFYGFYSDGEISICMEHMDGGSLDQVLK----KA	158
MEK2	KPAIRNQIIRELQVLHE-CNSPYIVGFYGFYSDGEISICMEHMDGGSLDQVLK----EA	162
MEK4	DEKEQQLMLMDLDVVMRSDCCPYIVQFYGALFREGDCWICMELMSTSFDFKYKYVYVSLD	197
MEK5	TLLELQKIMSELEILYK-CDSSYIIGFYGAFVFNRSICTEFMDGGSLDVYR-----	253
MEK6	NSQEQRRLMLDLDISMRVTDCPFTVTFYGFALFREGDVVVICMELMDSLKDFYKVIDK-G	147
MKK7	GPIPERILGKMTVAIVKALYLLKEKHGVIHRDVKPSNILLDERGQIKLDFGISGRLVDS	287
MEK1	GRIPQILGKVSIAVIGKGLTYLREKHKIMHRDVKPSNILLVNSRGEIKLDFGVSGQLIDS	218
MEK2	KRIPEEILGKVSIAVLRGLAYLREKHQIMHRDVKPSNILLVNSRGEIKLDFGVSGQLIDS	222
MEK4	DVIPLEILGKITLATVKALNHLKENLKIHRDIKPSNILLDRSGNIKLDFGISGRLVDS	257
MEK5	-KMPEHVLGRIAVAVVKGGLTYLW-SLKILHRDVKPSNMLVNRGQVKLDFGVSTQLVNS	311
MEK6	QTIPELILGKIAVSVKALEHLHSLKSLVIHRDVKPSNVLINALGQVKMDFGISGYLVD	207
MKK7	KAKTRSAGCAAYMAPERIDPPDTPKPDYDIRADVWSLGISLVELATGQFPYKNCNT----	343
MEK1	MANSF-VGTRSYMSPERLQG----THYSVQSDIWSMGLSLVEMAVGRYI PPPDAKELE	272
MEK2	MANSF-VGTRSYMAPERLQG----THYSVQSDIWSMGLSLVELAVGRYI PPPDAKELE	276
MEK4	IAKTRDAGCRPYMAPERIDPSA-SRQGYDVRSDVWSLGITLYELATGRFPYKPNWS----	312
MEK5	IAKTY-VGNAYMAPERISG----EQYGIHSDVWSLGISFMELALGRFPYPIQIKN----	362
MEK6	VAKTI DAGCKPYMAPERINPEL-NQKGYSVKSDIWSLGITMIELAILRFPYDSWGT----	262
MKK7	-----DFEVLTKVLQEEPPPLPHG	362
MEK1	LMFGCQV---EGDAAETPPRPTGRPLSSYGMDSRPPMAIFELLDYIVNEPPPKLPS-	327
MEK2	AIFGRPVVDGEEGEPHSISPRPRPPGRPVSGHGMDSRPAMAI FELLDYIVNEPPPKLPS-	335
MEK4	-----VFDQLTQVVKGDPPQLSNS	331
MEK5	-----QGSMLPLQLQCIVDEDSVLPV-	385
MEK6	-----PFQQLKQVVEEPSQLPA-	280
MKK7	--MGFSGDFQSFKDCLTKDHRKRPKYNKLEHSFIKRYETLE-VDVASWFKDVMKATES	419
MEK1	--GVFSLEFQDFVNKCLIKNPAERADLKQIMVHAFIKRSDAEE-VDFAGWLCSTIGLNQP	384
MEK2	--GVFTPDFQEFVNKCLIKNPAERADLKMLTNHTFIKRSEVEE-VDFAGWLCSTIGLNQP	392
MEK4	EEREFSPSFINFVNLCCLKDESKRPKYKELLKHPFILMYEERA-VEVACYVCKIILDQMPA	390
MEK5	--GEFSEPFVHFITQCMRQPKERPAPEELMGHPFIVQFNDGNAAVVMWVCRALERRS	443
MEK6	--DKFSAEFVDFTSQCLKKNKERPTYPELMOHPFFTLHESKG-TDVASVFKLILGD---	334
MKK7	-PRTSGVLSQPHLPFFR	435
MEK1	STPTHAAGV-----	393
MEK2	GTPTRTAV-----	400
MEK4	-TPSSPMYVD-----	399
MEK5	-QQGPP-----	448
MEK6	-----	334

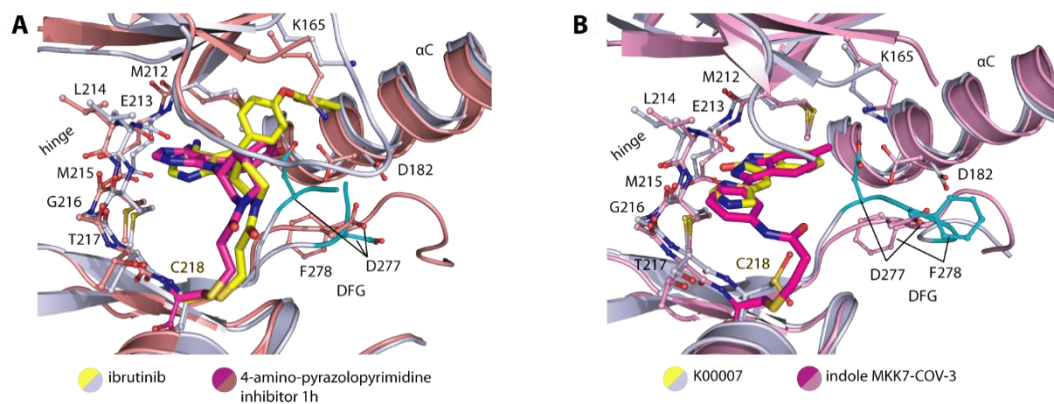
Supplementary figure S1. Sequence alignment of MAP2K family members. Green boxes indicate predicted MAPK docking domains, and pink boxes indicate the starting point of the C-terminal kinase domains. The N-terminal regulatory helices of MEK1 and MKK7 evident from the crystal structures are highlighted in yellow boxes.



Supplementary figure S2. Structural superimposition of the inactive, apo kinase domain and active $\Delta N75$ -MKK7 harboring S287D and T291D mutations reveals potential steric clashes upon an in-swing of the αC Asp182 in the active form to the DFG-out Asp277 in the apo state.



Supplementary figure S3. Omitted $|2F_o| - |F_c|$ electron density maps contoured at 1σ for the bound ligands and Cys218 in the case of covalent binding.



Supplementary figure S4. Comparison of inhibitor interactions in MKK7 between ibrutinib and 4-amino-pyrazolopyrimidine 1h (A) and K0007 and indole MKK7-COV-3 (B) reveals similar binding modes of the hinge interacting moieties in the pairs.

Supplementary table 1. Data collection and refinement statistics for MKK7 structures.

Complex	Apo Δ N115-MKK7, wild type	Apo Δ N115-MKK7, DD	Δ N75-MKK7, DD	Δ N115-MKK7, wild type: ibrutinib	Δ N115-MKK7, wild type: ibrutinib (allosteric only)
PDB accession code	6YFZ	6YG0	6YG1	6YG2	6YZ4
Beamline	Diamond, i04	Diamond, i02	Diamond, i02	Diamond, i04	Diamond, i04
Data Collection					
Resolution ^a (Å)	30.41-1.90 (2.00-1.90)	36.19-2.00 (2.11-2.00)	64.83-2.22 (2.34-2.22)	19.55-2.00 (2.11-2.00)	25.58-1.70 (1.79-1.70)
Spacegroup	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>C</i> 2	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
Cell dimensions	a=57.5, b=74.5, c=81.8 Å $\alpha=\beta=\gamma=90.0^\circ$	a=60.4, b=69.8, c=84.6 Å $\alpha=\beta=\gamma=90.0^\circ$	a=127.2, b=67.9, c=142.8 Å $\alpha=\gamma=90.0^\circ, \beta=114.8^\circ$	a=53.1, b=75.0, c=86.7 Å $\alpha=\beta=\gamma=90.0^\circ$	a=53.5, b=74.7, c=87.2 Å $\alpha=\beta=\gamma=90.0^\circ$
No. unique reflections ^a	28,220 (4,047)	24,828 (3,550)	54,756 (7,970)	24,057 (3,473)	39,163 (5,630)
Completeness ^a (%)	99.6 (99.6)	100.0 (100.0)	99.8 (99.8)	99.9 (100.0)	99.9 (99.9)
I/ σ ^a	9.2 (2.0)	13.8 (2.0)	8.2 (2.0)	12.1 (2.2)	13.1 (2.3)
R _{merge} ^a	0.103 (0.843)	0.066 (0.952)	0.090 (0.661)	0.106 (0.901)	0.085 (0.781)
CC (1/2)	0.996 (0.621)	0.997 (0.693)	0.996 (0.675)	0.997 (0.734)	0.999 (0.552)
Redundancy ^a	6.1 (6.1)	6.7 (6.8)	3.7 (3.5)	7.3 (7.4)	6.5 (6.5)
Refinement					
No. atoms in refinement (P/L/O) ^b	2,386/ -/ 233	2,229/ -/ 89	7,344/ -/ 353	2,333/ 66/ 230	2,332/ 33/ 362
B factor (P/L/O) ^b (Å ²)	38/ -/ 43	61/ -/60	64/ -/55	38/ 37/44	28/ 24/ 38
R _{fact} (%)	19.2	19.4	20.4	17.9	16.9
R _{free} (%)	23.7	24.5	23.2	23.0	20.6
rms deviation bond ^c (Å)	0.016	0.015	0.014	0.015	0.016
rms deviation angle ^c (°)	1.7	1.4	1.4	1.5	1.6
Molprobrity Ramachandran					
Favour (%)	96.23	98.18	98.05	98.58	97.18
Outlier (%)	0	0	0.32	0	0
Crystallization condition	19% PEG3350, 0.15 M ammonium acetate, 0.1 M tris, pH 7.8	16% PEG3350, 0.25 M ammonium acetate, 0.1 M tris, pH 8.2	27% PEG3350, 0.2 M potassium thiocyanate, 10% ethylene glycol, 0.1 M bis-tris propane, pH 7.5	19% PEG3350, 0.1 M ammonium acetate, 0.1 M tris, pH 7.8	16% PEG3350, 0.25 M ammonium acetate, 0.1 M tris, pH 7.8

^a Values in brackets show the statistics for the highest resolution shells; ^b P/L/O indicate protein, ligand molecules of interest, and other (water and solvent molecules), respectively; ^c rms indicates root-mean-square.

Supplementary table 1 cont. Data collection and refinement statistics for MKK7 structures.

Complex	Δ N115-MKK7, wild type: CPT1-70-1	Δ N115-MKK7, wild type: K00007	Δ N115-MKK7, wild type: ASC69	Δ N75-MKK7, DD: TL10-105	Δ N75-MKK7, DD: SB1-G-23
PDB accession code	6YG3	6YG4	6YG5	6YG6	6YG7
Beamline	Diamond, i03	Diamond, i04	Diamond, i04	Diamond, i02	Diamond, i03
Data Collection					
Resolution ^a (Å)	30.38-2.05 (2.16-2.05)	38.46-2.30 (2.42-2.30)	39.64-2.40 (2.53-2.40)	47.33-2.15 (2.27-2.15)	61.83-2.20 (2.32-2.20)
Spacegroup	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁	<i>P</i> 2 ₁
Cell dimensions	a=58.2, b=64.5, c=85.5 Å $\alpha=\beta=\gamma=90.0^\circ$	a=54.1, b=72.6, c=83.1 Å $\alpha=\beta=\gamma=90.0^\circ$	a=59.7, b=68.0, c=84.7 Å $\alpha=\beta=\gamma=90.0^\circ$	a=72.7, b=69.93, c=73.8 Å $\alpha=\gamma=90.0^\circ, \beta=119.4^\circ$	a=72.1, b=69.2, c=72.3 Å $\alpha=\gamma=90.0^\circ, \beta=117.9^\circ$
No. unique reflections ^a	20,596 (2,930)	15,049 (2,162)	13,948 (2,013)	35,192 (5,117)	32,046 (4,662)
Completeness ^a (%)	99.1 (98.4)	99.6 (99.8)	99.5 (99.6)	99.9 (99.9)	99.9 (99.9)
I/ σ ^a	10.7 (2.0)	11.2 (2.1)	12.5 (2.0)	10.0 (2.2)	10.2 (2.0)
R _{merge} ^a (%)	0.098 (0.935)	0.066 (0.745)	0.061 (0.730)	0.101 (0.906)	0.070 (0.770)
CC (1/2)	0.998 (0.494)	0.998 (0.691)	0.997 (0.766)	0.996 (0.659)	0.998 (0.740)
Redundancy ^a	6.6 (6.6)	4.6 (4.7)	4.7 (4.7)	5.3 (5.1)	4.9 (4.9)
Refinement					
No. atoms in refinement (P/L/O) ^b	2,122/ 34/ 153	2,064/ 16/ 58	2,060/ 26/ 13	4,536/ 92/ 179	4,438/ 92/ 84
B factor (P/L/O) ^b (Å ²)	44/ 45/ 51	65/ 56/ 70	77/ 100/ 72	63/ 47/ 56	66/ 48/ 56
R _{fact} (%)	18.8	21.1	23.1	20.4	20.7
R _{free} (%)	23.5	25.5	28.2	23.9	25.1
rms deviation bond ^c (Å)	0.015	0.012	0.008	0.012	0.014
rms deviation angle ^c (°)	1.5	1.3	1.2	1.3	1.5
Molprobability Ramachandran					
Favour (%)	98.47	95.97	92.80	97.65	97.23
Allowed (%)	0	0	0.8	0	0
Crystallization condition	19% PEG3350, 0.25 M ammonium acetate, 0.1 M tris, pH 8.2	19% PEG3350, 0.1 M ammonium acetate, 0.1 M tris, pH 8.2	16% PEG3350, 0.2 M ammonium acetate, 0.1 M tris, pH 7.8	19% PEG3350, 0.15 M ammonium acetate, 0.1 M tris, pH 8.2	25% PEG3350, 0.1 M ammonium acetate, 0.1 M tris, pH 8.5

^a Values in brackets show the statistics for the highest resolution shells; ^b P/L/O indicate protein, ligand molecules of interest, and other (water and solvent molecules), respectively;

^c rms indicates root-mean-square.

Supplementary table 2. Tm shift values from screening MKK7 against an in-house library of 360 compounds

No.	ΔTm WT	ΔTm C202S	compound ID	compound names	source	smile
1	24.8	11.2	K06214a	TL10-105	in-house collection	CCN1CCN(CC1)Cc1ccc(cc1C(F)F)NC(c1ccc(C)c(c1)O)c1cnc(N[C@H]2CCN(C2)C(C=C)O)n1=O
2	14.1	8.2	K06669a	SB1-G-23	in-house collection	CCN1CCN(CC1)Cc1ccc(cc1C(F)F)NC(c1ccc(C)c(c1)O)c1cnc(N[C@H]2CCN(C2)C(C=C)O)n1=O
3	13.2	0.6	K05736a	ibrutinib	SelleckChem	C=CC(N1[C@H]N2N=C(C3=CC=C(OC4=CC=CC=C4)C=C3)C5=C(N)N=CN=C52)CCC1=O
4	12.4	10.8	K05783a	OTSSP167	SelleckChem	C1C=CC(C2=CC=C(N=CC(C1)=O)=C3N[C@H]4CC(C[C@H])(CN(C)C)CC4)C3=N2=CC(C1)=C1O
5	10.8	6.2	K06774a	CPT1-70-1	in-house collection	CN1CCN(CC1)C1ccc(cc1)Nc1nc(c2cc(nH)c2n1)O1ccc(cc1)NC(C1)I)=O
6	9.3	7.1	K05737a	HYJ-2-002-1	in-house collection	CCN1CCN(CC1)Cc1ccc(cc1C(F)F)NC(c1ccc(C)c(c1)O)c1cnc3c(cc(nH)3)c2OC)c1=O
7	8.8	6.2	K03428	HG-6-71-01	in-house collection	COC=C1CN(C=C)NC(C=C)C(C2C(F)F)CN(CCN3CC)CC3)C=2)=O=CC2)C=2)C(C(=N=C1)N1)C=C1
8	8.7	5.1	K03434a	XMD15-46	in-house collection	O=C(NC(=C(C(F)F)F)=C(CCN(CN)C1)C1)C=C1)C=CC(=CN=C(CN=C1)C12)C=2)=C(C1C1)C=C1
9	5.5	3.5	K03427	HG-6-64-01	in-house collection	CC(=CC=C1CN(C=C)C(C2C(F)F)CN(CCN3CC)CC3)C=2)=O=C(C1)C=CC(=C(C(=N1)C2)C=2)OC)C=N1
10	3.4		K02079a	KH-HP04	in-house collection	C1C=C(C1)C=CC=C1/C=C=2NC(C/C2=O)=C(C3=CC(Br)=C(O)C(Br)=C3)=O
11	3.2	2.3	K00007	K00007	Calbiochem (EMD)	C1C=CC=C(C1=N1)C(C1=O)=CC(N=CN1)=C1
12	2.7	4.9	K00609	ASC69	MolPort	C(=C(N1)C)C(=NC=1NC1C=CC=C1)CCN)NC(=N1)C(C2)C2)C=C1
13	2.6		K03010a	GSK1326255A	GSK	CCCN(CCC1C(C=CC(NC(N=C(NC(C=C)F)F)C2)C=2)C(N)=O)C(C=CN2)=C23)=N3=C2OC)C2)CC1
14	2.6		K00980a	GSK 650394	Tocris	N1C=C(C=C(C1=N1)C=C1)C=C(C1)C(O)=O(CCC2)C2)C1=C=CC=C1)C=1
15	2.3		K02255a	229_0248_0168	BioFocus	N(C=C1)C(C=C2OC(F)F)F)=CC=C2)(N=C2NCCO)C(=N1)C=C2
16	2.3		K00781a	5361852	ChemBridge	C(C=N=C1NC(C=C2)C=CC=2OC)C=C1)(N(C1)C2)C=C=C2)=C(N1)C.[Br].[Br]
17	2.2		K00777a	JNK Inhib IX	SelleckChem	O=C(C1=CC=CC2=C1C=CC=C2)NC3=C(C#N)C4=C(S3)CCCC4
18	2.2		K00772	TO503-6573	Enamine	FC(F)F)C1C=C(SC1=N2)C=C3C=CN=C3)C#N=C2=C1
19	2.2		K00984a	BX-795	Axon Ligands	C1=NC=C(C1NCCNC(C=C)C2)S2)=O)))(N1)NC(=CC=C1)NC(NCC2)C2)=O)C=1
20	2.2		K02259a	229_0236_0196	BioFocus	N(C=C1)C(C=C2OC)C=CN=C2)(N=C2NCC3=C(C1)C(O4)=CC=3)OC4)C(N1)C=C2
21	2.1		K00524	294_0046_0333	BioFocus	C=C(C1)C(C=C2)C=CC=2N)(N=C2NC(C=C3)C1)=CC=C3)N(N1)C=C2
22	2.1	3.3	K00040	TBB (218697)	Calbiochem (EMD)	C=C(C=C(C1=N2)[Br])[Br])[Br])(C1=N2)[Br]
23	2.1		K02245a	229_0131_0068	BioFocus	N(C=C1)C(C=C(C1)C2)C=CC=C2)C3)C(N=C2NCC3=CC=C(C=C3)OC)OC)C(=N1)C=C2
24	2.1		K02250a	229_0033_0135	BioFocus	N(C=C1)C(C=C2N(C)C)C=C=C2)(N=C2NCCO)C(=N1)C=C2
25	2.0		K02128a	032_0036_0715	BioFocus	C=CC1(C=C2)=CC=C2CC(C)C(N=CN=1)NC1=CC(=C(C1)OC)OC
26	2.0		K02227a	190_0027_0168	BioFocus	C(N(C1C(C=C2OC(F)F)F)=CC=C2)C2)=NC=1)C(=NC=2)NC(C=C1OC(C(F)F)F)=CC=C1
27	2.0		K02240a	179_0223_0312	BioFocus	N(C=C1C(C=C2C(F)F)F)=CC=C2)N2)(N=C1)C(=CC=2)NCC(=CC1)C1)C=CC=1
28	1.9		K00488	229_0153_0279	BioFocus	N(C=C1)C(C=C2)C1)=CC=C2)(N=C2NC(CO)C)C(=N1)C=C2
29	1.9		K02257a	229_0131_0280	BioFocus	N(C=C1)C(C=C2)=CC=C2OC)(N=C2NCC3=CC=C(C=C3)OC)OC)C(=N1)C=C2
30	1.9		K02234a	190_0141_0079	BioFocus	C(N(C1C(C=C2)OC)OC)C=2)C2)=NC=1)C(=NC=2)NC(C=C1OC(C(F)F)F)=CC=C1
31	1.9		K00523	294_0046_0068	BioFocus	C=C(C1)C(C=C(C1)C2)C=CC=C2)C3)C(N=C2NC(C=C3)C1)=CC=C3)N(N1)C=C2
32	1.9		K02272a	229_0146_0160	BioFocus	N(C=C1)C(C=C2)=CC=C2)C1)=CC=C2)C(N=C2NCC(C3)C=CC=3)C(=N1)C=C2
33	1.8		K02231a	190_0235_0284	BioFocus	C(N(C1C(C=C2OC)C=CC=C2)C2)=NC=1)C(=NC=2)NC(C=C1C(F)F)F)=CC=C1
34	1.8		K00582a	AM-807/14961157	Specs	C=C(N1)N)SC=1NC1=CC=C(C=C1)C1)C1)C1)C(=C=C2)F)C=C1=O
35	1.8		K00575a	AK-777/36504023	Specs	C=C(N1)N)SC=1NC(C=C1)=CC=C1)C(C=C1)C=C=C1)C1)=O
36	1.8		K02288a	382_0087_0284	BioFocus	C1(C=C2C(C=CC3O)C=CC=3)C(=NC=2)N)C=C(C=C1)OC)OC
37	1.8		K00515	229_0254_0284	BioFocus	N(C=C1)C(C=C2OC)C=CC=C2)(N=C2NC(C(C)C)C)C(=N1)C=C2
38	1.8		K00027	Oxindole I	Calbiochem (EMD)	C=C(C1(N1)=O)C(C=C1C=C1)C=C1)C1)C1)C1)C(=CC=C1)N1
39	1.8		K00046	Genistein	Calbiochem (EMD)	C1=C(C=C(C=C1O1)C(C=C1)C(C=C(C1)O)C=1)=O)O
40	1.7		K02220a	184_0219_0168	BioFocus	N(C1NC(C=C2)C=CC=2OC)N2)C(=CN=1)C(C=C1OC(F)F)F)=CC=C1)C=C2
41	1.7		K02129	032_0049_0005	BioFocus	C=CC1(C=C2N)=CC=C2)(N=CN=1)NC(=CC1)C=C=C1)C1
42	1.7		K02256a	229_0131_0204	BioFocus	N(C=C1)C(C=C(C1)C2)C=CC=C2)C3)C(N=C2NCC3=CC=C(C=C3)OC)OC)C(=N1)C=C2
43	1.7		K00517	229_0254_0313	BioFocus	N(C=C1)C(C=C2F)=CC=C2)(N=C2NC(C(C)C)C)C(=N1)C=C2
44	1.7		K00060a	SB 218078	Tocris	C1=C=CC(=C1N1)C2C3)C=C1C1N4C(O2)C3)C=C(C=C1=C4C1)C=C=C1)C1=O)C(N1)=O
45	1.7		K02246a	229_0236_0004	BioFocus	N(C=C1)C(C=C2)C=CC=2N(O)C(N=C2NCC3=C(C1)C(O4)=CC=3)OC4)C(=N1)C=C2
46	1.7		K00572a	AK-777/09836058	Specs	C=C(N1)N)SC=1NC(C=C1)=CC=C1)C(=CC=C1)F)C=C1=O
47	1.7		K02226a	190_0021_4139	BioFocus	C(N(C1C(C=C2)=CC=C2)C2)=NC=1)C(=NC=2)NC1=CC(=C(C1)OC)OC
48	1.7		K02416a	081_0283_0078	BioFocus	C(C=NC1)C2=CC=1)C(=CC1NC(C=C3)=CC=C3(C)C)C(=NC=1)=CC=C2
49	1.6	0.6	K00828	PI3Kg inhib II (528108)	Calbiochem (EMD)	C=C(C1)OC2(F)C(C=C1)C=C(SC1(N)=O)C1=O)O2
50	1.6		K00565a	Pfmrk Inhibitor (538140)	Calbiochem (EMD)	C(C=C1)[Br]=CC=C1(C1=O)=CC(C=C2)F)=CC=C2)=O)N1
51	1.6		K02236a	190_0141_4145	BioFocus	C(N(C1C(C=C2C(=O)C)C=CC=C2)C2)=NC=1)C(=NC=2)NC(C=C1OC(C(F)F)F)F)=CC=C1
52	1.6		K00052	Lavendustin A	Tocris	OC1=CC=C(O)C=C1CN(C3=C(O)C=CC=C3)C2=CC=C(O)C(C(O)=O)=C2
53	1.6		K02438a	382_0341_0280	BioFocus	C=CC1(C=C2)=CC=C2OC)C(=NC=1)N)C(=CC1)C=CC=1OCOC
54	1.5		K02265a	229_0131_4038	BioFocus	N(C=C1)C(C=C(F)C2)C=CC=C2)(N=C2NCC3=CC=C(C=C3)OC)OC)C(=N1)C=C2
55	1.5		K00478	229_0033_0279	BioFocus	N(C=C1)C(C=C2)C1)=CC=C2)(N=C2NCCO)C(=N1)C=C2
56	1.5		K02124a	032_0100_0085	BioFocus	C(OC(C=1)C=CC=C1C(C=C1)C=C1NC(C=C2)=CC=C2N(CCO)C)C=NC=N1)F)F)F
57	1.5		K02214a	174_0213_0339	BioFocus	C=NC1(C=C2)C=CC=2)N(C2)CCN2CCO)C(=NC=1)N
58	1.5		K00518	229_0254_4145	BioFocus	N(C=C1)C(C=C2C(=O)C)C=CC=C2)(N=C2NC(C(C)C)C)C(=N1)C=C2
59	1.5		K00519	229_4051_0139	BioFocus	N(C=C1)C(C=C2C(=O)O)C=CC=C2)(N=C2NCC(C3)C3)C(=N1)C=C2
60	1.5		K00507	229_0242_4145	BioFocus	N(C=C1)C(C=C2C(=O)C)C=CC=C2)(N=C2NC(C3)CCO3)C(=N1)C=C2
61	1.5		K02244a	229_0131_0005	BioFocus	N(C=C1)C(C=C2N)C=CC=C2)(N=C2NCC3=CC=C(C=C3)OC)OC)C(=N1)C=C2
62	1.4		K00776a	Wee1/Chk1 inhibitor	Calbiochem (EMD)	C1=C=C(C=C1)C2=CC3=C(C4=C(N3)C=CC(=C4)O)C5=C(C=O)NC5=O.O
63	1.4		K02122a	032_0118_0071	BioFocus	C=CC1(C=C2)=CC=C2)(N(C2)CCN2CC(N(C=C2)C=CC=C2)C=O)N=CN=1
64	1.4		K02217a	174_1002_0061	BioFocus	C(N=C1C(C=C2)C=CC=C2)(N(C2)CC2C(=O)O)C(=N=C1)N
65	1.4		K02285a	382_0005_4038	BioFocus	C=CC1(C=C(F)C2)C=CC=C2)(C=NC=1)N)C(=CC1N)C=CC=1

66	1.4	K02239a	179_0236_4139	BioFocus	N(C=C1C(=CC2)C=CC=2)N2(N=C1)C(=CC=2)NCC1C=C(C(O)2)=CC=1)OC2
67	1.4	K02160a	093_0220_0168	BioFocus	C(N(C1=C2)N=C2)(=CC(=N1)C(C=C1OC(F)F)F)=CC=C1)N(CCN1)CCN1C
68	1.4	K00510	229_0254_0086	BioFocus	N(C=C1)C(=CC2)C=CC=2)C#N(N=C2N(C(C)C)CO)C(=N1)C=C2
69	1.4	K00584a	AM-807/41062770	Specs	C(=C(N1)N)C(NC(=NO2)C=C2)O)SC=1NC(C=C1)=CC=C1F
70	1.4	K00585a	AM-807/41930348	Specs	C(=C(N1)N)SC=1NC1C=C(C(=CC=1)F)C(C)C(=CC=C1OC)C=C1=O
71	1.4	K02228a	190_0254_0085	BioFocus	C(N(C1C=C2)=CC=C2OC(F)F)C2(=NC=1)C(=NC=2)NC(C)C)CO
72	1.3	K00827	PI3Kg inhibitor (528106)	Calbiochem (EMD)	N1=CC=NC(=C1C1)C=C(C=1)C=C(SC(N1)=O)C1=O
73	1.3	K02253a	229_0244_0139	BioFocus	N(C=C1)C(=CC2C(=O)O)C=CC=2(N=C2NCC(=CC3)C=CC=3OC)C(=N1)C=C2
74	1.3	K00932a	Lapatinib	Sequoia Research Products	C(=N1)NC2=C(C(=C(OC(C=C3F)=CC=C3)C=C2)C)C(C(=C2OC3CNCCS(=O)O)C=CC=3)=C(N=C1)C=C2
75	1.3	K00586	AM-807/41930350	Specs	C(=C(N1)N)SC=1NC1C=C(C(=CC=1)F)C(C)C(=CC1OC)C=CC=1=O
76	1.3	K02213a	225_1008_0280	BioFocus	N(C(NC(=O)C(=CC1)C=CN=1)=C1C)C(=N1)C1)C(C(=N1)C(=CC1)C=CC=1OC
77	1.3	K00576a	AM-807/12426021	Specs	C(=C(N1)N)SC=1NC(=CC=C1OC)C=C1)C(C(=CC1OC)C=CC=1=O
78	1.3	K00768a	T0512-1192	Enamine	FC(F)F)C1C=CC(N=C(S2)C=C3=C(C=3)C#N)C=C2=1
79	1.3	K02736a	Scorzoalhydrostilbene A	in-house collection	O[C@H]1[C@@H](O)[C@H](O)[C@H](O)C2=CC=C(O)C(CCC3=CC=C(O)C(OC)=C2C(C)=O)[C@H]1CO
80	1.3	K00513	229_0254_0196	BioFocus	N(C=C1)C(=C2OC)C=CN=2(N=C2N(C(C)C)CO)C(=N1)C=C2
81	1.3	K02267a	229_0231_0062	BioFocus	N(C=C1)C(=C2C3)C=CC=3)=CC=C2(N=C2NCC(C=CN3)C=CC=3)C(=N1)C=C2
82	1.3	K02241a	179_0236_4027	BioFocus	N(C=C1C=C(C)C)C(=CC=2)N2(N=C1)C(=CC=2)NCC1C=C(C(=N1)C)OC2
83	1.2	K02218a	174_0221_0192	BioFocus	C(N=C1C(=CC2C(=O)NCCO)C=CC=2)(N(C2)CCN2CCN(C)C)C(=N1)N
84	1.2	K00483	229_0153_0081	BioFocus	N(C=C1)C(=CC2N(=O)C)C=CC=2(N=C2N(C)CO)C(=N1)C=C2
85	1.2	K00244b	GSK inhibitor XIII	Calbiochem (EMD)	CC1=CC(NC2=NC(C3=CC=CC=3)=NC4=C2CC(C4)=NN1
86	1.2	K02437a	382_0327_0087	BioFocus	C(=CC1C2=CC(=C(C2)OC)OC)C(=NC=1)N)C(C=C1)=CC=C1(=O)NCCN(C)C
87	1.2	K02264a	229_0131_4027	BioFocus	N(C=C1)C(=C(C)C)C2=C=CC=2(N=C2NCC3=C(C(=C3)OC)OC)OC(C(=N1)C)C=C2
88	1.2	K00491	229_0153_0311	BioFocus	N(C=C1)C(=C2)C=CC=2OC(N=C2N(C)CO)C(=N1)C=C2
89	1.2	K00063	Tyrphostin A23	in-house collection	OC1=C(O)C=C(C#N)C#N)C=C1
90	1.2	K02225a	190_4059_0083	BioFocus	N(C=N1)C2N(C(=C(OC(=CC3)C=CC=3)C)C(=C1)C(=C(OC)C)C=CC=1)C=CN=2
91	1.2	K02130a	032_0045_0280	BioFocus	C(=CC1C(=C2)=CC=C2OC(N=CN=1)N1C=C(C(=N2)=CC=1)C=C2
92	1.2	K00152b	229_0242_0279	BioFocus	N(C=C1)C(=C2C)C(=CC=2)N(C2)CCN2CC(C)C(=N1)C=C2
93	1.2	K02441a	378_0021_0134	BioFocus	C(=CC1C(NC2=CC(=C(C2)OC)OC)O)N(C2)CCN2CCN(C)CC)N=CN=1
94	1.2	K02221a	184_0219_0176	BioFocus	N(C(C1NC(=CC2)C=CC=2OC)N2)C(=CN=1)C(=CC1C(=O)NCCN(C)C)C=C1)C=C2
95	1.1	K02125a	032_0106_0068	BioFocus	C(=CC1C(=C(C(O)2)=C3)OC2)=C3(N=CN=1)NC(=C1N(C)C)C=CC=1
96	1.1	K00239b	SU11652	Calbiochem (EMD)	C(=C1)=CC(=C1N1)C(C1=O)=CC(=C(C1C)C(=O)NCCN(C)C)C(=N1)C=C1
97	1.1	K02242a	179_0134_0286	BioFocus	N(C=C1C(=C(C2)C)C)C(=C(C2)OC)N2)(N(C)CC3CCN(C)CC)C=CC=2)N=C1
98	1.1	K02258a	229_0131_0285	BioFocus	N(C=C1)C(=C2)C=CC=2OC(N=C2NCC3=CC(=C(C3)OC)OC)OC(C(=N1)C)C=C2
99	1.1	K00578a	AM-807/12739008	Specs	C(=C(N1)N)SC=1NC(=CC1C(F)F)C=CC=1)C(=O)C(=CC=C1)C=C1
100	1.1	K03424a	ALW-II-41-27	in-house collection	CCN(CCN1CC(=C(C)F)F)C=C(NC(C=CC=C(C)C2N(C)C(=CC(=C(C=CC=C3)S3)=CN3)C=3)=O)C2)C=CC1
101	1.1	K00531	5387887	ChemBridge	N(C(N1)=O)C(C(C1=O)=CNC(C=C1N(C)C)=CC=C1)O)C(C=C1)=CC=C1F
102	1.1	K02159a	093_0215_0063	BioFocus	C(N(C1=C2)N=C2)(=CC(=N1)C(=C(OC(=CC1)C=C=C=1)C1)C=C=C=1)N(CCN1C)CCC1
103	1.1	K02224a	190_6937_0087	BioFocus	C(N(C1C2=C(C(=C(C=2)OC)OC)OC)C2)=NC=1)C(=NC=2)NC(C=C1)=CC=C1C(C)C
104	1.1	K01737a	KH-CARB2	in-house collection	C(C=C1C=C2N(C)C3=C1C(C#N)C(C)C)N3=O)C2C1
105	1.1	K02121a	032_0134_0060	BioFocus	C(=CC1C(=C2C(F)F)F)C(=CC(C)F)F)C2(N(C2)CCN2CCN(C)CC)N=CN=1
106	1.1	K00844a	STOCK65-33492	InterBioScreen	C(N=C1N)=(C(C=N1)N)N=C1)NC(C=C1)=CC=C1C1
107	1.0	K02119a	032_0113_0058	BioFocus	C(=CC1C(=C2C(C=C3)=CC=C3)=CC=C2)(N(C2)CCN2CCN(C)CC)C2)O)N=CN=1
108	1.0	K02716a	7K-3165	Key Organics	C(=CC=C1C(=NN=C(C2OC)C(=CC=C3)N=2)C=1
109	1.0	K00496	229_0242_0081	BioFocus	N(C=C1)C(=CC2N(C=O)C)C=CC=2(N=C2N(C)CC)CCO3)C(=N1)C=C2
110	1.0	K02268a	229_0237_0062	BioFocus	N(C=C1)C(=C2C3)C=CC=3)=CC=C2(N=C2NCC(=CC3)C=CN=3)C(=N1)C=C2
111	1.0	K00712a	F0676-0387	Life Chemicals	N(C=N1)C(=CC2F)C=CC=2)(C(=N1)N)N=C(C=C1)SCC(N(C=C1)C=CC=1)C1)O
112	1.0	K02237a	190_0021_0004	BioFocus	C(N(C1C(=C2)C=CC=2N(C)C)C2)=NC=1)C(=NC=2)NCC1=CC(=C(C1)OC)OC)OC
113	1.0	K00573a	AK-777/09836063	Specs	C(=C(N1)N)SC=1NC(=CC1)C=CC=1)C(=O)C(C=C1)=CC=C1
114	1.0	K02238a	179_0236_0313	BioFocus	N(C=C1C(=C2F)C=CC=2)N2(N=C1)C(=CC=2)NCC1C=C(C(O)2)=CC=1)OC2
115	1.0	K00606b	ASC65	in-house collection	N#CCC1C=CC(C=C1)=Nc1nc(Nc2c1[nH]n2)C2C2)c2ccccc2n1
116	1.0	K02262a	229_0131_0311	BioFocus	N(C=C1)C(=CN2)C=CC=2OC(N=C2NCC3=CC(=C(C3)OC)OC)OC(C(=N1)C)C=C2
117	1.0	K02219a	174_0213_0289	BioFocus	C(N=C1C(=CC2=CC(=O)O)C=CC=2)(N(C2)CCN2CCO)C(=N1)N
118	1.0	K00581	AM-807/14961123	Specs	C(=C(N1)N)SC=1NC(C)F=C1=CC=C1)C(=CC1)C=CC=1)Br)O
119	1.0	K02261a	229_0131_0294	BioFocus	N(C=C1)C(=C(CO)C2)C=CC=2)(N=C2NCC3=CC(=C(C3)OC)OC)OC(C(=N1)C)C=C2
120	1.0	K00089	piceatannol	Sigma Aldrich	OC1=CC(\C=C)C2=C(C(O)=C(O)C2)=CC(O)=C1
121	0.9	K00564a	Syk Inhibitor	Calbiochem (EMD)	C(=CC1)(C=C(C=12)C(N2)=O)=CC(=C1)C(=C2N1)C(=CC=C2)S(=O)(=O)N
122	0.9	K00230	Debromohymenialdisine	Calbiochem (EMD)	C1(NC(C(N=1)=O)=C(CCN1)C(=C2C1=O)C=CN2)N
123	0.9	K00521	229_4051_0284	BioFocus	N(C=C1)C(=CC2O)C=CC=2)(N=C2NCC(C3)C)C(=N1)C=C2
124	0.9	K02120a	032_0118_0079	BioFocus	C(=CC1C(=CC(=C2)OC)OC)C=2)(N(C2)CCN2CCN(C)C(=CC2)C=CC=2)O)N=CN=1
125	0.9	K02927	GW806742X	GSK	O=S(C1=CC=CC(NC2=NC=CC(N(C)C3=CC=C(C(NC4=CC=C(OC(F)F)F)C=C4)=O)C3)=N2)=C1)N)O
126	0.9	K00225c	JAK Inhibitor I	Calbiochem (EMD)	CC(C)C1=N=C2=C(N1)C3=C(C=C(C=3)F)C4=C2=C(NC4=O
127	0.9	K00853a	STOCK65-36822	InterBioScreen	C(N=C1N)=(C(C=N1)N)N=C1)NC(C=C1F)=CC=C1
128	0.9	K03184a	PF4708671	Tocris	C1=NC=NC(=C1C)N(CCN(C)C)CC(NC(=C2C3)C=CC=3(C)F)F)N2)C1
129	0.8	K02271a	229_0144_0087	BioFocus	N(C1=C(=CC(=C(C1)OC)OC)OC)C1)N=C2NCC(OC3)=CC=3)C(=N1)C=C2
130	0.8	K03001b	GSK978744A	in-house collection	C[C@H](O)C1cc(sc1C(=O)N)N2cnc3ccc(OC[C@H](O)CO)c2c3c4ccccc4C1
131	0.8	K00835a	STOCK65-32440	InterBioScreen	C(C=C1N2)N=C2)=NC(=N1)N)N(CCN1)CCN1
132	0.8	K00119	190_0027_4139	BioFocus	C(N(C1C(=C2)=CC=C2)C2)=NC=1)C(=NC=2)NC(=CC1)C=CC=1O
133	0.8	K02243a	229_0033_0004	BioFocus	N(C=C1)C(=C2)C=CC=2N(C)C(N=C2NCCO)C(=N1)C=C2
134	0.8	K02222	184_0088_0057	BioFocus	N(C(C1NC(=CC2)C=CC=2N(C)CCO2)=N2)C(=CN=1)C(=CC(=C(C1)C=C3)C=C3)C=C1)C=C2
135	0.8	K00597b	Sorafenib	LC Labs	C(=C(C=CC1)C)C(F)F)C=1NC(NC(=CC=C(C1)OC(=CC(=NC2)C(NC)=O)C2)C=C1)=O

136	0.8	K02248a	229_0131_0078	BioFocus	N(C(C(C(=NC1)C2=CC=1)=CC=C2)=C1)(N=C2NC3=CC=C(C(C(=C3)OC)OC)OC)C(=N1)C=C2
137	0.8	K00580a	AM-807/14146364	Specs	C(=C(N1)N)SC=1NC(=CC1)C=CC=1OC(C(C=CC=C1(C1))C=C1)=O
138	0.8	K00490	229_0153_0291	BioFocus	N(C(=C1)C(=CC2CO)C=CC=2)(N=C2NC(CO)C)C(=N1)C=C2
139	0.8	K02247a	229_0033_0078	BioFocus	N(C(C(C(=NC1)C2=CC=1)=CC=C2)=C1)(N=C2NC(CO)C)C(=N1)C=C2
140	0.7	K00238b	IKK-2 Inhibitor VI	Calbiochem (EMD)	C(=CC=C1C(=CC(=C2NC(=O)N)C(=O)N)S2)C=C1
141	0.7	K02215a	174_1002_0060	BioFocus	C(=NC1C(=CC2(F)F)C=C(C(F)F)C=2)(N(C)C2)CCC2C(=O)O)C(=NC=1)N
142	0.7	K00041	BPDQ (4-[[3-Bromophenyl)amino]-6,7-diaminoquinazoline)	in-house collection	C1=CC(=CC(=C1)Br)NC2=NC=NC3=CC(=C(C=C32)N)N
143	0.7	K00703a	F0676-0186	Life Chemicals	N(C(=N1)C(C=C2)C=CC=2(C1))C(=N1)C1)N=C(C(=1)SCC(NC(CO)C1)CC1)=O
144	0.7	K00065	Tyrphostin B48	in-house collection	C(=C(C(=CC1CC(C(NC(=CC=C2)C=2)=O)C#N)O)O)C=C1
145	0.7	K00839a	STOCK65-42112	InterBioScreen	C(N=C1N)C(=C(N1)N)N=C1)NC(C=C1(C1))=CC=C1
146	0.7	K02533a	D481-2007	ChemDiv	N(N=C1C(C=C2)=CC=C2(C1))C(=N1)N)C(C(=NC1)C=CC=1)=O
147	0.7	K02134a	033_4009_0078	BioFocus	N(C(N(C1)CCO1)=C1)C(C(C(=NC2)C3=CC=2)=CC=C3)C=C1
148	0.7	K02260	229_6307_0279	BioFocus	N(C(=C1)C(C=C2(C1))=CC=C2)(N=C2NC(C=CC3)C=CC=3S(=O)(=O)N)C(=N1)C=C2
149	0.7	K00090	SL-327	SelleckChem	C(C(=C(N)Sc1ccc(cc1)N)c1cccc1C(F)F)F)N
150	0.6	K00579a	AM-807/12740052	Specs	C(=C(N1)N)SC=1NC(=CC1(C)F)F)C=CC=1)C(C=C1)C=CC=C1OC)=O
151	0.6	K00505	229_0242_0339	BioFocus	N(C(=C1)C(C=C2)=CC=C2F)N=C2NC(C3)CCO3)C(=N1)C=C2
152	0.6	K00621a	ATM/ATR inhibitor	Calbiochem (EMD)	C(=CC=C1C(C(NC(C(C1))C(C1))C1)NC(NC(C=C(C=C2)N+)(O)=O)F)=S)O)C(C=CC=C2)=C2)C=C1
153	0.6	K00720a	F0676-0429	Life Chemicals	N(C(=N1)C(C=C2F)C=CC=2)(C(=N1)C1)N=C(C(=1)SCC(NC(=NC1)S)C=1)=O
154	0.6	K00057	Daphnetin (7,8-Dihydroxycoumarin)	Sigma Aldrich	O=C1C=CC2=CC=C(C)O)C=C2O1
155	0.6	K00039	PD 169316	Calbiochem (EMD)	FC(C=C1)=CC=C1C2=C(C3=CC=NC=C3)NC(C4=C(C=C1)N)C=C4)C=C4)=N2
156	0.6	K01734a	C713-0187	ChemDiv	N(C(=N1)C(C=C2)=CC=C2F)(C(=N1)C1)N=C(C(=1)NCCCN(CCC)CC
157	0.6	K00798a	T5694244	Enamine	C(=NN1)C(NC(C=C2)=CC=C2F)O=C1C=C1)C=C1
158	0.6	K00616a	Aurora/Cdk Inhibitor	Calbiochem (EMD)	C(=CC1)C(C=CC=1NC1=NN(C(=N1)N)C(=O)C(C(=CC=C1)F)=C1F)S(=O)(=O)N
159	0.6	K00548a	5214367	ChemBridge	C(NC1=CC=C(C=C1)C1)C1)C1)NC(=CC1)C=CC=1OCCCCC)=O
160	0.5	K02291a	378_4051_0107	BioFocus	C(=CC1C(NC(C2)C2)=O)(N(C)C2)CCN2C=C(C(=C2)OC)OC)C=2)N=CN=1
161	0.5	K00699a	F0676-0126	Life Chemicals	N(C(=N1)C(C=C2)=CC=C2(C1))C(=N1)C1)N=C(C(=1)SCC(N(C1)CCO1)=O
162	0.5	K00080	HA-1004 (HCl)	Sigma Aldrich	O=S(C1=CC=CC2=CN=CC=C21)(NCCNC(N)=O.Cl.Cl
163	0.5	K00722a	F0676-0458	Life Chemicals	N(C(=N1)C(C=C2F)C=CC=2)(C(=N1)C1)N=C(C(=1)SCC(NC1)C=CC=1
164	0.5	K00024	Cdk4 Inhibitor C228125	Toronto Research Chemicals	C1=CC=C2C(C=C1)C3=C4C(=C5C6=C(C=C(C=C6)Br)N)C5=C3N2)C(=O)N)C4=O
165	0.5	K02216a	174_0220_0087	BioFocus	C(N=C1C2=CC(=C(C(=C2)OC)OC)OC)N(C)C2)CCN2=C(C(=N1)N
166	0.5	K00731a	F0676-0862	Life Chemicals	N(C(=N1)C(C=CC(=C(C2)OC)OC)C=2)(C(=N1)C1)N=C(C(=1)SCC(NC(=CC1)C)C=CC=1)=O
167	0.5	K00713a	F0676-0389	Life Chemicals	N(C(=N1)C(C=C2F)C=CC=2)(C(=N1)C1)N=C(C(=1)SCC(NC(C1)C)F)=CC=C1F)=O
168	0.5	K00769a	T0518-8465	Enamine	CC(=O)NC1C=CC(C(=C)C)C2=NC(C=C(C=C3)C=C3S2)=CC=1
169	0.5	K00837a	STOCK1N-70806	InterBioScreen	N1=C(C(=C(N=C1)N)NCC1=C(C=C1)OC)OC)N)N=C1
170	0.5	K00841a	STOCK1N-70809	InterBioScreen	N1=C(C(=C(N=C1)N)NCC(C=C1)=CC=C1)N)N=C1
171	0.5	K02127a	032_0131_0135	BioFocus	C(C(=C1)OC)C(=C1)CNC(C=C1)C(C=C2)N=C(C=2)N=CN=1)OC)OC
172	0.5	K00574a	AK-777/09836064	Specs	C(=C(N1)N)SC=1NC(=CC1)C=CC=1F)C(C(C=C1)=CC=C1F)=O
173	0.5	K00642a	5225597	ChemBridge	C(C1N1)=O)C(C=C1)C=C(C=C1)=NCC(C(C=C1O)=CC=C1)=O
174	0.5	K00710a	F0676-0384	Life Chemicals	N(C(=N1)C(C=C2F)C=CC=2)(C(=N1)C1)N=C(C(=1)SCC(NC(=CC1)F)C=CC=1)=O
175	0.5	K00994a	Dovitinib	LC Labs	C(=CC=C1)(C=C1)C(C=C1)OC(C(=N1)C2)C=C(C=2)N(C)N(C2)C2)N1)N)F
176	0.5	K00847a	STOCK65-41767	InterBioScreen	N1=C(C(=C(N=C1)N)NCC(=CC1(C1))C=CC=1)N)N=C1
177	0.4	K00625a	VX-680	Toocris	CN1CCN(C2=NC(S3=CC=C(C=C3)NC(C4CC4)=O)=NC(NC5=NNC(C)=C5)=C2)CC1
178	0.4	K03442a	9043251	ChemBridge	C(C(NC1=CC(=C(N2)C=C1)C=N2)=O)(C(=C1)OC)CC(=C1)C1
179	0.4	K00701a	F0676-0156	Life Chemicals	N(C(=N1)C(C=C2)=CC=C2(C1))C(=N1)C1)N=C(C(=1)SCC(NC(=CC1OC)C=CC=1)=O
180	0.4	K03453a	STOCK15-33760	InterBioScreen	C(C(=N1)S2)(C(=C2)C2)N=CN=2)=C(C(=C1N(C1)CCO1)C1)CC1
181	0.4	K00933a	Nilotinib	Sequoia Research Products	C(=CC(=CC1)C(NC(=CC(=CC2N(C=NC3C)C=3)C(F)F)C=2)=O)(C(=C1)NC(NC(=CC1)C(=CN=CC2)C=2)N)N=1
182	0.4	K00044	ML 3163 (no. 475800)	Calbiochem (EMD)	C(=CC(=CC1)F)C=1C(NC(=N1)SCC(=CC=C(C2)S(C)C=2)=C1C(=CC=NC1)C=C1
183	0.4	K00555a	6626103	ChemBridge	N(C(N1)=O)C(C1)C(=O)=CNC(C=C1)=CC=C1F)=O)C
184	0.4	K00709a	F0676-0370	Life Chemicals	N(C(=N1)C(C=C2F)C=CC=2)(C(=N1)C1)N=C(C(=1)SCC(=O)N
185	0.4	K02071a	KH-CARB3A	in-house collection	C(C=C=C1=C2N(C)C3=C1C(C#N)C4(CCCC4)N)C3=O)C2C1
186	0.4	K00498	229_0242_0139	BioFocus	N(C(=C1)C(=CC2(C=O)O)C=CC=2)(N=C2NC(C3)CCO3)C(=N1)C=C2
187	0.4	K00700a	F0676-0146	Life Chemicals	N(C(=N1)C(C=C2)=CC=C2(C1))C(=N1)C1)N=C(C(=1)SCC(NC(=CC1)F)C=CC=1)=O
188	0.4	K00721a	F0676-0454	Life Chemicals	N(C(=N1)C(C=C2F)C=CC=2)(C(=N1)C1)N=C(C(=1)SCC(C=N1)=CC=C1
189	0.4	K00050	Lavendustin C	Sigma Aldrich	Oc1ccc(O)c(CNc2ccc(O)c(e2)C(=O)O)c1
190	0.4	K00786a	7974871	ChemBridge	C(=NC(C=C2)=CC(=C2)C)C(C(=CC(=CC2)C=CN=2)C#N)N1
191	0.4	K00704a	F0676-0191	Life Chemicals	N(C(=N1)C(C=CC2)C=CC=2(C1))C(=N1)C1)N=C(C(=1)SCC(NC(=NC1)S)C=1)=O
192	0.4	K03452a	STOCK15-37479	InterBioScreen	C(C(=N1)S2)(C(=C2)C2)N=CN=2)=C(C(=C1N(C1)CCO1)C1)CC(O1)C
193	0.4	K00937d	TAE684	SelleckChem	CN1CCN(C2CCN(C3=CC=C(NC4=NC(C)C)N)C5=CC=CC=C5(C(C)C)=O)=N4)C(O)C(C3)CC2)CC1
194	0.4	K00094	040_0232_0074	BioFocus	C(C(=N1)C=CN=C1NCC(=CC1)C=CC=1)(=CS1)C=C1
195	0.4	K00849a	STOCK65-40137	InterBioScreen	C(N=C1N)C(=C(N1)N)N=C1)NC(C(OC)C1)=CC=C1
196	0.4	K01938b	9041990	ChemBridge	N(C(=C1N2)N=C)N=C(N1)(CC1)CC(O1)C
197	0.3	K00072	Cdk1 Inhibitor III	Calbiochem (EMD)	NC1=NC(NC2=CC=C(S(N)=O)O)C=2)N=1C(NC3=C(F)C=CC=C3F)=S
198	0.3	K02223	190_6937_0083	BioFocus	N(C(=N1)C2NC(C=C3)=CC=C3(C)C)C(C(=C1)C(C(OC)C)C=CC=1)C=CN=2
199	0.3	K00852a	STOCK65-36498	InterBioScreen	N1=C(C(=C(N=C1)N)NCC(C=C1)=CC=C1OC)N)N=C1
200	0.3	K00767a	T0507-3237	Enamine	CC(=C(C#N)N1)NC(C=CC=C2)S2)C=C(C1)C(=C(C1))=CC=1
201	0.3	K00757a	T5674742	Enamine	N#CC(=CC1C=CC=NC=1)C1=N(C(C=CC=C2)C=C2)S1
202	0.3	K00617a	Dasatinib	SelleckChem	CC1=NC(NC2=NC=C(C)NC3=C(C=CC=C3)C)O)S2)=CC(N4CCN(C4)CCO)=N1
203	0.3	K00702a	F0676-0180	Life Chemicals	CCOC(CNC(CSc1ccc2nnc(c3ccc(cc3)[Cl])n2n1)=O)=O

204	0.3	K00806a	O6-Benzylguanine	AXXORA	C=CC1(C=CC=1)COC(N=C1N)=C2C(=N1)NC=N2
205	0.3	K00075	HA-1077 (Fasudil; BRD7868)	Sigma Aldrich	O=S(C1=CC=CC=C1)N(C=CC=C2)N(C3CCNCCC3)=O
206	0.3	K00062	Alsterpaullone	Sigma Aldrich	O=C1CC2=C(C3=CC=CC=C3N1)NC4=C2C=C([N+])([O-])O)C=C4
207	0.3	K00048	AG 1879 (PP2)	SelleckChem	CC(C)(C)n1c2c(c3ccc(cc3)[Cl])n1c2ncn2
208	0.3	K00037	SB 202190	Calbiochem (EMD)	C=C(C=CC1C=C(NC2C=C(C=C3)O)C=3)C=C(C=C3)C=C(N2)F)C=1.[Cl]
209	0.3	K00566a	ERK Inhibitor	Calbiochem (EMD)	C=C(C1)OCCC=C(C=1)C=C(C(N(C1=O)CCN)=O)S1
210	0.3	K00846a	STOCK65-37451	InterBioScreen	N1=C(C=C(C(N=C1N)NCC1=CC=C(C=C1)[Cl]))(Cl)N1)NC=1
211	0.2	K00729a	F0676-0846	Life Chemicals	N(C=N1)C=C(C=C(C2)O)O)C=C2)(C=N1)C1N=C(C=1)SCC(=O)N
212	0.2	K03423	ALW-II-38-3	in-house collection	CC(N=CN1C=C(C(C(NC=C(C=C(C)C2NCC(C=C=CC=N3)O3)=O)C=2)=O)=CC2C(F)F)C=2)=C1
213	0.2	K02703a	Reversine	Calbiochem (Merck)	N1=C(N=C(C=C1N1)N=C1)NC(CCCC1)C1)NC=C(C=C1)N(CCOCC2)C2)C=1
214	0.2	K00058	Wedelolactone	Calbiochem (EMD)	C=CC(C=C1)OC(C=C1O1)C=C(C=C1O)C=C(C=C2)O)O)O
215	0.2	K00209	MEK1/2 Inhibitor	Calbiochem (EMD)	C1=CC=C(C=C1)C(C#N)=C(N)SC(C=C=CC1N)=CC=1)C(F)F
216	0.2	ATP			
217	0.2	K00714a	F0676-0414	Life Chemicals	N(C=N1)C=C(C=C2)C=C2)(C=N1)C1N=C(C=C1)SCC(NC=CC1NC(=O)C)C=CC=1)=O
218	0.2	K02487a	HA-156	Toronto Research Chemicals	N(CCN1S(C=C(C2=C(C3)[Cl])C=CN=C2)C=3)=O)O)CC1.[Cl].[Cl]
219	0.2	K00240a	Gefitinib	LC Labs	COc1cc2c(cc1OCCCN1CCOCC1)c(Nc1ccc(c1)[Cl])F)ncn2
220	0.2	K01786a	KH-CARB11	in-house collection	Cl(C=C=CC1=C2N(C)C3=C1C(C#N)C4(CCN(C)CC4)NC3=O)=C2Cl
221	0.1	K00760a	T0518-4225	Enamine	CC1=CC=C(C=C(C#N)C2=NC(C=CC=C3)=C3S2)O1
222	0.1	K03448a	7535026	ChemBridge	C(C=C1C=C(O)N)N(C=C(S1)N1)C=C(C=C1)CC1)C(O)C1)CC=1
223	0.1	K00705a	F0676-0216	Life Chemicals	N(C=N1)C=C(C=C2)C=C2)(C=N1)C1N=C(C=1)SCC(C=N1)=CC=C1
224	0.1	K00730a	F0676-0859	Life Chemicals	N(C=N1)C=C(C=C(C2)O)O)C=C2)(C=N1)C1N=C(C=1)SCC(N(C=C1)C=C1)=CC=C1)=O
225	0.1	K00931a	ART 17513474	Asinex	C=C(C=C1)OC=C1)N1)(C=C1N=C1)C=C1)CN(CCN1)CC1
226	0.1	K00789a	T0502-1077	Enamine	N=C(C=C(C=C1)C=C1)C#N)S1)C1)C(C=C1)=CC=C1
227	0.1	K00528	5981310	ChemBridge	N(C1N1=O)(C(C1=O)=CNC1=CC=C(C=C1)C)(Cl)=O)C(C=C1)=CC=C1
228	0.1	K00708a	F0676-0364	Life Chemicals	N(C=N1)C=C(C=C2)C=C2)(C=N1)C1N=C(C=1)SCC(N(C=C1)CCO1)=O
229	0.1	K00930a	ART 17513448	Asinex	C=C(C=C1)OC=C1)N1)(C=C1N=C1)C=C1)CN(CCO1)CC1
230	0.1	K00130	225_1008_0160	BioFocus	N(C(NC=O)C(C=C1)=CC=N1=C1)C(C=N1)C=C(N1)C=C(C=C1)CC=1[Cl]
231	0.1	K00569d	SB-220025	GSK	C1CNCCC1N2C=NC(C=C2)C3=NC(N=C=C3)N)C4=CC=C(C=C4)F
232	0.1	K02149a	093_0256_0204	BioFocus	C(N(C1=C2)N=C2)(=CC=N1)C=C(C(N1)=C2)C=C1)=C2)N(C(CO)C)CC1
233	0.1	K00719a	F0676-0424	Life Chemicals	N(C=N1)C=C(C=C2)C=C2)(C=N1)C1N=C(C=C1)SCC(NCC(O)C)CC1)=O
234	0.1	K02400a	9051337	ChemBridge	N1NC=C(C=C2N(C)C(C=O)C)C=C(C=C3)O)C=1)C=C2
235	0.1	K00547a	5809868	ChemBridge	C(C(N(C1=O)C)=O)(C1=O)=CC(NC1)=CC=1
236	0.1	K00976a	Cdk/CKI Inhibitor, (R)-DRF053	Calbiochem (EMD)	N(C=C(C=C1NC(C)CO)N2(C)C)N=C2)N1)C=C(C=C1)C(C=NC=CC2)C=2)C=1
237	0.1	K00477a	Imatinib	LC Labs	Cc1ccc(cc1Nc1ccc(c2cccnc2)n1)Nc1ccc(c2n2ccn(c)cc2)cc1)=O
238	0.1	K00938a	ML-7	Sigma Aldrich	C(CN(CCN1)S(C=C(C=C2)C3)C=C=C3)C=2)=O)O)C1
239	0.1	K02249a	229_0236_0078	BioFocus	N(C(C(C=NC1)C2=CC=1)=CC=C2)=C1)(N=C2NCC3C=C(C(O4)=CC=3)OC4)C=N1)C=C2
240	0.1	K00784a	6339039	ChemBridge	C=N1)(N(C(C1=CC1)=CC=1)C)C=C(C=C1)C=C1)C#N
241	0.1	K00707a	F0676-0361	Life Chemicals	N(C=N1)C=C(C=C2)C=C2)(C=N1)C1N=C(C=C1)SCC(N(C=C1)CC1)=O
242	0.1	K03863a	PD 166285	Tocris	CN(C1=NC(NC4=CC=C(COCCN(C)C)C=C4)=NC=C1C=C2C3=C(C)C=C(C=C3)C)C2=O.Cl.Cl
243	0.1	K02401a	9051854	ChemBridge	C(C(NC1=CC=C(N2)C=C1)C=N2)O)(C=C1O)O)C=CC=1
244	0.1	K00464	ST051029	TimTec	C(C1N1=O)(C=C(N1)=C1)=C(C1)C=C1
245	0.0	K00788a	T0501-6793	Enamine	C=N1)C=C(C=C2)C=C2)C#N)SC(C=C1)CC1)CC1C
246	0.0	K00851a	STOCK65-32524	InterBioScreen	N1=C(C=C(C=N1)N)NCC(C(C1))=C1)=CC=N1)N1)NC=1
247	0.0	K00724a	F0676-0462	Life Chemicals	N(C=N1)C=C(C=C2)C=C2)(C=N1)C1N=C(C=C1)SCC(C=C1)O)CC=C1
248	0.0	K01756a	KH-DTCMA	in-house collection	Cl(C=C=CC1=C2N(C)C3=C1C(CNC(C)O)C(C)C)N(C3=O)=C2Cl
249	0.0	K00247	Chk2 inhibitor II	Calbiochem (EMD)	NC(=O)C(C=C(C12)N=C(N2)C=C(C=C2)OC3C=CC(C=C3)Cl)=C2)=CC=1
250	0.0	K00549a	5214400	ChemBridge	C(NC1=C(C=C1)C=C1)(Cl)N(C=C1)C=C=C1)C=C(O)O)C=O
251	0.0	K00706a	F0676-0226	Life Chemicals	N(C=N1)C=C(C=C2)C=C2)(C=N1)C1N=C(C=C1)SCC(C=C1)O)C=C1
252	0.0	K00711a	F0676-0386	Life Chemicals	N(C=N1)C=C(C=C2)C=C2)(C=N1)C1N=C(C=C1)SCC(NC=CC1(C1)C=C=CC=1)=O
253	0.0	K00739a	F0676-0943	Life Chemicals	N(C=N1)C=C(C=C2)O)O)C=C2)(C=N1)C1N=C(C=C1)SCC(=O)O
254	0.0	K00233	Chelerythrine Chloride	AXXORA	C1C=C(C=C(C=1O)O)C1)C(C([N+]=1)C=C(C1C=C2O3)OC3)C=2)=CC=1
255	0.0	K00398	STOCK25-67628	InterBioScreen	C1=C(C=C(S1)N1)C=C(C=C1)C(C)C(C)CC1)N1)C(NC=1)=O
256	0.0	K00076	Indirubin-3monoxime	Calbiochem (EMD)	InChi=1S/C16H11N3O2/c20-16-13(9-5-1-3-7-11(9)18-16)15-14(19-21)10-6-2-4-8-12(10)17-15/h1-8,17,21H,(H,18,20)
257	0.0	K00077d	K252a	Tocris	[H][C@]([C@@]8(O)[C@@]9(O)O)O[C@]78C)N5C3=C2N7C1=CC=CC=C1C2=C(CNC6=O)C6=C3C4=CC=CC=C45
258	0.0	K00100	229_0224_0142	BioFocus	N(C=C1)C(C(O)C)=CC=2)(N=C2NCC(C=C3)=CC=C3)C(N1)C=C2
259	0.0	K00778a	PIM1 Inhib II	Calbiochem (EMD)	C1=C(NC(C=C1)C=C=CC1)C=C1)C#N)O)C=C(C=C1)Br)C=1O
260	0.0	K00833a	STOCK45-62175	InterBioScreen	N1C=C(C(C=NC=1)N)SCC=C(C1)Cl)C=C=CC1(C1)N1)NC=1
261	0.0	K00959a	Pazopanib	Sequoia Research Products	C=C(C=C1NC(NC=C2)N(C=C(C3)C=C(C4)C=C3)C=C2)S(O)(N)O)C=C1
262	0.0	K02251a	229_0131_0167	BioFocus	N(C=C1)C=C(C=C2)C=C2)(N=C2NCC3=CC=C(C(C=C3)O)O)O)C(N1)C=C2
263	0.0	K02252a	229_0236_0167	BioFocus	N(C=C1)C=C(C=C2)C=C2)(N=C2NCC3C=C(C(O4)=CC=3)OC4)C=N1)C=C2
264	0.0	K02254a	229_0244_0167	BioFocus	N(C=C1)C=C(C=C2)C=C2)(N=C2NCC(C=C3)C=C=CC3)C(N1)C=C2
265	0.0	K02232a	190_0144_0168	BioFocus	N(C=N1)C2NCC(O)C3=CC=3)(C=C1)C=C(C1O)C(F)F)C=C1)C=C=N2
266	0.0	K02233a	190_0141_0313	BioFocus	C(N(C1C=C(C2)C=C=C2)C2)=NC=1)C=C(NC=2)N(C=C1O)C(F)F)C=C=C1
267	0.0	K02235a	190_0141_0347	BioFocus	C(N(C1C=C(C2)C=C(O)N)C=C=C2)C2)=NC=1)C=C(NC=2)N(C=C1O)C(F)F)C=C=C1
268	0.0	K02229a	190_0235_0081	BioFocus	C(N(C1C=C(C2N(C=O)C)C=C=C2)C2)=NC=1)C=C(NC=2)N(C=C1)C(F)F)C=C=C1
269	0.0	K02263a	229_0236_0312	BioFocus	N(C=C1)C=C(C=C2)C=C2)(N=C2NCC3C=C(C(O4)=CC=3)OC4)C=N1)C=C2
270	0.0	K00525	294_0046_4140	BioFocus	C=C(C1)C=C(C2O)C=C=C2)(N=C2N(C=C3)C(C1)C=C=C3)N(N=1)C=C2
271	0.0	K00514	229_0254_0279	BioFocus	N(C=C1)C=C(C=C2)C=C2)(N=C2N(C(C)C)O)C(N1)C=C2

272	0.0	K00486	229_0153_0164	BioFocus	N(C=C1)C(C=C(C2)F)C1)C=2)(N=C2NC(CO)C)C(=N1)C=C2
273	0.0	K00516	229_0254_0312	BioFocus	N(C=C1)C(C=C2C(F)F)F)=CC=C2)(N=C2NC(C(C)C)CO)C(=N1)C=C2
274	0.0	K00571a	AG-690/11763552	Specs	C(=NC(=C1C(C=CC2)C=C2)C(C=C2)=CC=C2[Br])C(=CN2)C(C=C2C2)C=CC=2)N1
275	0.0	K00011	TX-1918	Calbiochem (EMD)	C(=C(C=C(C1)C)O)C)C=1=C(C(C=C1)=O)C1=O
276	0.0	K00520	229_4051_0168	BioFocus	N(C=C1)C(C=C2OC(F)F)F)=CC=C2)(N=C2NCC(C3)C3)C(=N1)C=C2
277	0.0	K02282a	382_0341_0312	BioFocus	C(C=C1C2C=C(C(=NC=2)N)C(=CC2)C=CC=2OCOC)=CC=C1)F(F)F
278	0.0	K02421a	229_0236_0062	BioFocus	N(C=C1)C(C=C2C3)C=CC=3)(N=C2NCC3C=C(C(O4)=CC=3)OC4)C(=N1)C=C2
279	0.0	K00499	229_0242_0160	BioFocus	N(C=C1)C(C=C2)=CC=C2(C1)))(N=C2NCC(C3)C3)C(=N1)C=C2
280	0.0	K02200a	040_0115_0164	BioFocus	N(C(C=CC(C1)F)C1)C=1)C=1)C(=CC(=N1)N)C(C=C1)C=C1
281	0.0	K00577a	AM-807/12426164	Specs	C(=C(N1)N)SC1NC(=CC1(C1))C=CC=1)C(C(=CC1)C=CC=1F)=O
282	0.0	K02420a	229_0131_0063	BioFocus	N(C=C1)C(C(OC(=CC2)C=CC=2)C2)C=CC=2)(N=C2NCC3=CC(=C(C=3)OC)OC)OC(C(=N1)C=C2
283	0.0	K00056	Emodin	Calbiochem (EMD)	C1=C(C=C(C(=C1C1=O)C)C(=C1C1)C(=CC=1O)O)=O)O)C
284	0.0	K00203	BIM 4	AXXORA	C(=C(C(C1=C2C)=CC=2)C=CN1)C(N1)=O)(C1=O)C1C(C=CC=C2)=C2NC=1
285	0.0	K00755a	T5675105	Enamine	N#CC(=CC1=CC=CO1)C1=NC(C=CC=C2)=C2S1
286	0.0	K02468a	7517783	ChemBridge	C(=NC(C=C1F)C=CC=1)O)=O)(N(C(C1)CCO1)C1)C=C(C(F)F)C=C1
287	0.0	K00047c	1-Na-PP1	Calbiochem (EMD)	NC1=C(C(C2=C(C=CC=C3)C3=CC=C2)=NN4C(C)C)C4=NC=N1
288	0.0	K00473	ST4022620	TimTec	C(C(N1)=O)(C=C1C1)C=CC=1)=NC(C=C1)=CC=C1C(=O)O
289	0.0	K00983a	AZD 7762	SelleckChem	FC1=CC=CC(C2=CC(NC(N)=O)=C(C(N(C@H)3CNCCC3)=O)S2)=C1
290	0.0	K00752a	T0509-1692	Enamine	N#CC(=C1CC1)C1=NC(C=C=C2)=C2S1
291	0.0	K00779a	Flt3 Inhib III	Calbiochem (EMD)	C(=CC=C1C(=CN=C2N(C=CC=C3)OCCN(CCC4)C4)C=3)S2)C=C1
292	0.0	K00862a	LY 364947	Calbiochem (EMD)	C(=CC=C(C1C2C(C(=NN3)C(=CC=CC4)N=4)C3)N=CC=2)C=C1
293	0.0	K03865a	SCH-51344	Tocris	CC1=NN=C(C3)C1=C(NC(CO)C)C2=C3C=CC(OC)=C2
294	0.0	K00956a	Axitinib	SelleckChem	O=C(NC)C1=C(C(C2=CC=C(C(C=C2)C=C=CC=C4)N=3)C3=C2)C=CC=C1
295	0.0	K00794a	T5531146	Enamine	C(=NN1)C(C=C1C=C1)C=C1)C(NC(C)OC1)=CC=1)O
296	0.0	K00613a	Aminopurvalanol	Calbiochem (EMD)	N1C(=NC(=C2C=1NC1=CC(=C(C1)N)C1)))(N(C=N2)C(C)C)NC(C)C)CO
297	-0.1	K02395a	9046662	ChemBridge	C(NC1=CC(=C(N2)C=C1)C=N2)(C(C=C1F)=CC=C1)=O
298	-0.1	K00742a	F0676-0950	Life Chemicals	N(C(=N1)C(C=CC(C2)OC)OC)C=2)(C(=N1)C1)N=C(C(=O)C)C(=O)C)C=C1
299	-0.1	K02659b	SKF-86002-A2	GSK	[C]F(C=CC=C1C(N2)=C(N3C=2SCC3)C(=CN=C2)=C2)C=C1
300	-0.1	K04080a	BIX02188	Boehringer Ingelheim	CN(C)C1c1cccc1NC(=C1C2c1cccc12)C(N)=O)O)c1cccc1
301	-0.1	K00819a	IKK-3 Inhibitor IX	Calbiochem (EMD)	C1=C(C(=CC(=C1N1)C(S(C(=C2OC)C=CC=C3)C=3)S(=O)=O)C)N)N=C1)OC)OC
302	-0.1	K00761a	T5679507	Enamine	CN1C=C(C(C#N)C2=NC(C=CC=C3)C=3S2)C=N1
303	-0.1	K00799a	T5730157	Enamine	C(=NN1)C(NC(=NC2)SC=2)=O)C(=C1C=C1)C=C1
304	-0.1	K01741a	KH-CARB9	in-house collection	C(C=C=C1C2N(C)C3=C1C(C#N)C4(COCC4)N3)C=O)C=C1
305	-0.1	K00019	2-(Morpholin-4-yl)-benzo[h]chromen-4-one	Calbiochem (EMD)	C(=CC=C1)C(=C1C(C2=O)OC(=C2)N(COCC2)C2)C=C1
306	-0.1	K01739a	KH-CARB7	in-house collection	C(C=C=C1C2N(C)C3=C1C(C#N)C4(CCCC4)N3)O)=C2C1
307	-0.1	K03447a	5919559	ChemBridge	C1=C(C(C=N2)S1)=C(C=C2N(C1)CCO1)C1)CC(C1)N(C)=O)N
308	-0.1	K00715a	F0676-0415	Life Chemicals	N(C(=N1)C(C=CC(F)C=CC=2)(C(=N1)C1)N=C(C(=1)SCC(NC(C=C1)CC=C1NC(=O)C)O)C=O
309	-0.1	K00717a	F0676-0418	Life Chemicals	N(C(=N1)C(C=CC(F)C=CC=2)(C(=N1)C1)N=C(C(=1)SCC(NC(C=O)OC)C=O
310	-0.1	K00067	ST638	Calbiochem (EMD)	OC1=C(C=C(C(C(N)=O)C#N)C=C1OC)CSC2=CC=CC=C2
311	-0.1	K00725a	F0676-0464	Life Chemicals	N(C(=N1)C(C=CC(F)C=CC=2)(C(=N1)C1)N=C(C(=O)OC)C)C=C1
312	-0.1	K02615b	JAK3 Inhibitor IV (no. 1367)	Tocris	C1C=CC(=C2C=1)C=CC(=C2)C(CCN(C1=C=CC=C1)C)C)O.[H][Cl]
313	-0.1	K02466a	7497813	ChemBridge	C(NC(C=CN1)C=CC=1)O)=(C(N(C1)CCO1)C1)C=C(C(F)F)C=C1
314	-0.1	K02845b	SB-223133	GSK	NC(N=CC=C1C(C=C2C(C=C)F)=C3)N(C=N2)C(CCC(O)C2)C=C1
315	-0.1	K00064	Tyrphostin B42	SelleckChem	C1=C(C=C(C=C1)CN(C)=O)C=C2=CC(=C(C=C2)O)C#N
316	-0.1	K00738a	F0676-0939	Life Chemicals	N(C(=N1)C(C=CC(C2)OC)OC)C=2)(C(=N1)C1)N=C(C(=O)OC)C)C=C1
317	-0.1	K00069	Cdk2 Inhibitor II	Calbiochem (EMD)	C1=CC(=CC=C1NC2=C3C=C(C=CC3=NC2=O)Br)S(=O)=O)N
318	-0.1	K02396a	9048213	ChemBridge	C(NC1=CC(=C(N2)C=C1)C=N2)(C(C=C(C(=C1)OC)OC)=C1)O
319	-0.1	K00003	H-1152	AXXORA	N(C(N1S(C(=C(C=CC2)C3)C(=CN=3)C)C=2)=O)O)C)CC1.[Cl].[Cl]
320	-0.2	K00231	(-)-Arctigenin	Calbiochem (EMD)	C1C=CC(=C(C=1)OC)OC)CC(CO1)C1=O)CC1C=CC(=C(C=1)OC)OC
321	-0.2	K00718a	F0676-0420	Life Chemicals	N(C(=N1)C(C=CC(F)C=CC=2)(C(=N1)C1)N=C(C(=1)SCC(NC(C=C1)CC=C1F)=O
322	-0.2	K00676a	F2563-0290	Life Chemicals	COC(c1cccc1NC(CS1nnc(2cccc2)n1n1cccc1)=O)=O
323	-0.2	K00740a	F0676-0945	Life Chemicals	N(C(=N1)C(C=CC(=C2)OC)OC)C=2)(C(=N1)C1)N=C(C(=O)OC)C)C=C1
324	-0.2	K00554a	5174681	ChemBridge	N(C(N1)=O)(C(C1=O)=NNC(C=C1)=CC=C1[Br])=O)C
325	-0.2	K00222	Compound 52	Calbiochem (EMD)	N(C(C(=CN1NCCO)N2(C)C)N=C2)N=1)C(=CC=C1(C1))C=C1
326	-0.2	K00005	(Z)-3-[4-(Dimethylamino)benzyl]indolin-2-one	Calbiochem (EMD)	C1C=CC(=C(C1N1)C(C1=O)=CC(=CC=C1)N(C)C)C=C1
327	-0.2	K04055a	SK1-1 (BML-EI411-0005)	Enzo	CCCCC1=CC=C(C=C(C@H)(O)C@H(NC)CO)C=C1.C1
328	-0.2	K00746a	VEGFR 2/3 Inhibitor	Calbiochem (EMD)	C(C=C1)C(C(=C1N1)C(=C1)C(=C1)O)C(=C2)C=C(C(C=2OC)OC)C(N1)=O
329	-0.2	K02399a	9051276	ChemBridge	N1NC(=C(C=C2N(C)=O)CC(C=C3)=CC=C3)F)C=C1
330	-0.3	K03183a	TCS 2002	Tocris	C1=CC(=CC(=C1O1)C(=C1)C=C=C(C1)S(C)=O)C1)C(=NN=C1)C)O1
331	-0.3	K00276	BAS 00382581	Asinex	S(C(=CC=C1N=C(C(N2)=O)C(C2C2)C=CC=2)C=C1)=O)O)N
332	-0.3	K00753a	T0507-3274	Enamine	N#CC(=C1CCN1)C1=NC(C=CC=C2)=C2S1
333	-0.3	K00785a	7818069	ChemBridge	N(C=C1F)N(C2)C(CO2)=C(N=C1)N(C=CC1)C=CC=1OC
334	-0.3	K03955a	Pazopanib	LC Labs	O=S(=O)(N)c1ccc(c1)Nc2nccc(n2)Nc4ccc3c(nnc3C)C4)C
335	-0.3	K02499a	7522605	ChemBridge	C(OC1(C=C2C)C)C=CC=2)(C(NC(=C(N)CCO2)C2)C=C(C(F)F)C=2)=O)C=C1
336	-0.3	K00758a	T0501-4046	Enamine	CN(C=CC=C1)C1=C(C#N)C1=NC(C=CC=C2)=C2S1
337	-0.3	K00747a	PD173074	Calbiochem (EMD)	N(C(=N1)NCCCN(C)C)C=CC(=C12)C=C(C(=N2)N)N(C(=O)OC)C(C)C(=CC(=C1)OC)C=C1OC
338	-0.3	K00737a	F0676-0937	Life Chemicals	N(C(=N1)C(C=CC(C2)OC)OC)C=2)(C(=N1)C1)N=C(C(=O)OC)C)C=C1
339	-0.3	K00793a	T5302202	Enamine	C(=NN1)C(C=C1C=C1)C=C1)C(NC(C)OC1)C1=O
340	-0.3	K00733a	F0676-0910	Life Chemicals	N(C(=N1)C(C=CC(C2)OC)OC)C=2)(C(=N1)C1)N=C(C(=O)OC)C)C=C1)C=C1)O

341	-0.3	K00736a	F0676-0936	Life Chemicals	<chem>N(C=N1)C(=CC(=C(C2)OC)OC)=2)(C(=N1)C1)N=C(C=1)SCC(=O)OCC</chem>
342	-0.3	K00744a	PI 3-K Inhibitor IV	Calbiochem (EMD)	<chem>C(S1)=CC(=C1C(=N1C(C=C(C2)O)=CC=2)N2CCOCC2)N=1</chem>
343	-0.3	K03964a	Bosutinib isomer	LC Labs	<chem>CN(C)Cc1cccc(e1)NC(=C1C(Nc2cc(ccc12)C(N(C)C)=O)O)c1cccc1</chem>
344	-0.3	K00727a	F0676-0840	Life Chemicals	<chem>N(C(=N1)C(=CC(=C(C2)OC)OC)=2)(C(=N1)C1)N=C(C=1)SCC(N(CC1)CCO1)=O</chem>
345	-0.3	K00999a	WZ-4-49-8	in-house collection	<chem>O=S(C1=CC=CC=C1NC2=C3C(NN=C3)=NC(NC4=CC=C(N5CCCC(N6CCCCC6)CC5)C=C4OCC)=N2)(C(C)C)=O</chem>
346	-0.4	K00745a	BAY 61-3606	SelleckChem	<chem>O=C(C1=CC=C(N=C1)NC2=NC(C3=CC=C(OC)C(OC)=O)C=C3)=CC4=NC=CN24)N</chem>
347	-0.4	K00068	JNK Inhibitor II	Calbiochem (EMD)	<chem>C1=CC=CC(=C1C1=O)C(C(=C1)C1)C(=CC=1)N1=N1</chem>
348	-0.4	K00759a	T5674810	Enamine	<chem>CN(C=CC1)C=1C=C(C#N)C1=NC(C=CC=C2)=C2S1</chem>
349	-0.5	K04081a	BIX01289	Boehringer Ingelheim	<chem>CN(C)Cc1cccc(e1)NC(=C1C(Nc2cc(ccc12)C(N(C)C)=O)O)c1cccc1</chem>
350	-0.5	K03740a	GW656282X	GSK	<chem>Cc1ccc(cc1Nc1ccnc(Nc2cccc(c2)C(N)=O)n1)O</chem>
351	-0.5	K00570b	SB 239063	Sigma Aldrich	<chem>C(=C(N=C1)C2=CC=C(C=C2)F)(N1C1CCC(CC1)O)C1=CC=NC(=N1)OC</chem>
352	-0.5	K00298	1910-5183	ChemDiv	<chem>C(C=C1C2)C=C([N+])([O-])=O)C=2)(C(N1)=O)=NC(C=C1)=CC=C1C(=O)OCC</chem>
353	-0.5	K00472	ST2029251	TimTec	<chem>C(=C(S1)N2)(C(=C1)CC(C(C)C)C1)C(NC=2)=O</chem>
354	-0.5	K00795a	T5543714	Enamine	<chem>C(=NN1)(C(=C1=C1)C=C1)C(NC(F)F)F=O</chem>
355	-0.6	K00774a	T0505-3534	Enamine	<chem>O=C(C1CC1)C(=C1)NC(C=C=C2)=C2S1)C#N</chem>
356	-0.6	K00648a	5228205	ChemBridge	<chem>C(=C(C1=O)C2O)(C(C(=C1)C=C=CC=1)O)C(=CC=2)NCCC(=O)OC</chem>
357	-0.7	K00728a	F0676-0841	Life Chemicals	<chem>N(C(=N1)C(=CC(=C(C2)OC)OC)=2)(C(=N1)C1)N=C(C=1)SCC(N(CC1)CCC1)C=O</chem>
358	-0.8	K02721a	AG-227/37195019	Specs	<chem>N=C(C1C(C=C2)=CC=C2)N(CC)CC(C(=NN=1)C(=CC1)C=CC=1)C1</chem>
359	-1.0	K03953a	Temsirolimus	Sigma Aldrich	<chem>O=C([C@H](C)C=C([C@@H](O)[C@@H](OC)C([C@@H]4C)=O)/C)C[C@]([C@H](C)C[C@@H]2[C@@H](OC)[C@@H](OC)C(CO)=O)CC2)([H])OC([C@@1]([H])N(C(C([C@@3]O)[C@H](C)CC[C@@]([C@@H](C)C=C/C=C/[C@@H](C4)C)OC)([H])O3)=O)O)CCCC1=O</chem>
360	-1.7	K03886a	FTY720	Sigma Aldrich	<chem>CCCCCCCCc1ccc(ccc(CO)CO)Nc1</chem>

Supplementary method.

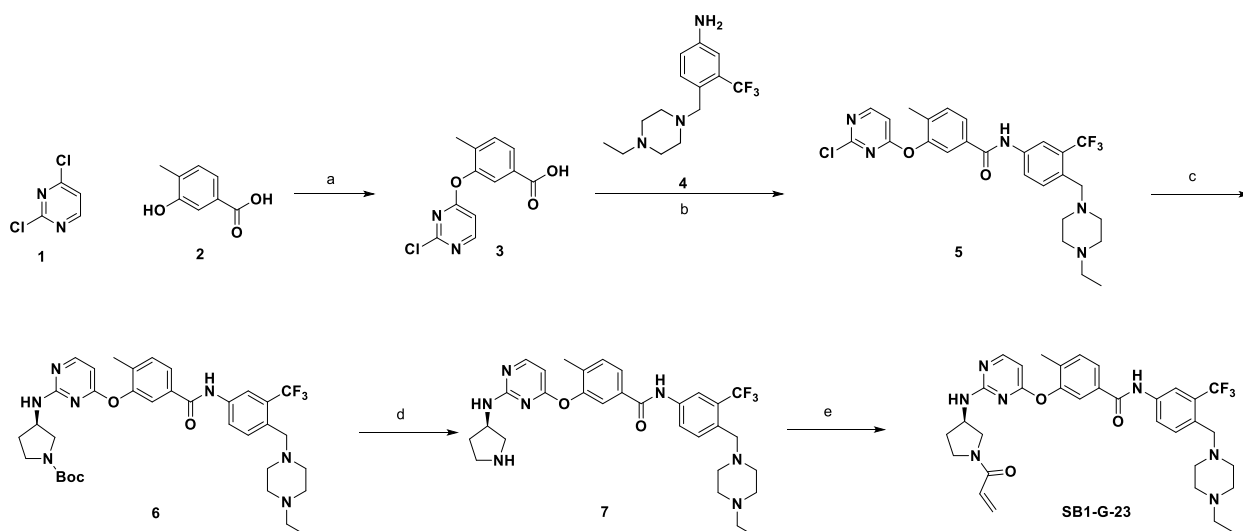
Sources and chemical syntheses of inhibitors

Inhibitors	Sources
ibrutinib	SelleckChem (Cat no. S2680)
OTSSP167	SelleckChem (Cat no. S7159)
CPT1-70-1	Reference# (Tan et al., 2017) and patent WO 2016130920
K00007	Calbiochem (Cat no. 175580)
ASC69	MolPort (Cat no. MolPort-039-333-128); Synthesis also described in patent WO2010031056A2
HG-6-64-01	Reference# (Miao et al., 2015),(Tan et al., 2015)
HG-6-71-01	Reference# (Kim et al., 2013)
HYJ-2-002-1	Reference# (Tan et al., 2015)
XMD15-46	Reference# (Deng et al., 2010)
TL10-105	Synthesis described below
SB1-G-23	Synthesis described below

Chemical syntheses of TL10-105 and SB1-G-23

Unless otherwise noted, reagents and solvents were obtained from commercial suppliers and were used without further purification. ¹H NMR spectra were recorded on 600 or 400 MHz (Varian AS600 or Bruker A400), and chemical shifts are reported in parts per million (ppm, δ) downfield from tetramethylsilane (TMS). Coupling constants (*J*) are reported in Hz. Spin multiplicities are described as s (singlet), br (broad singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). Mass spectra were obtained on a Waters Micromass ZQ instrument. Preparative HPLC was performed on a Waters Sunfire C18 column (19 x 50 mm, 5 μ M) using a gradient of 15-95% methanol in water containing 0.05% trifluoroacetic acid (TFA) over 22 min (28 min run time) at a flow rate of 20 mL/min. Purities of assayed compounds were in all cases greater than 95%, as determined by reverse-phase HPLC analysis.

Synthesis of (R)-3-((2-((1-acryloylpyrrolidin-3-yl)amino)pyrimidin-4-yl)oxy)-N-(4-((4-ethylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)-4-methylbenzamide (SB1-G-23)



Reagents and conditions: (a) Cs₂CO₃, *i*-PrOH, 55 °C, 3h, 87%; (b) oxalyl dichloride, *N,N*-dimethylformamide, CH₂Cl₂, rt, 2h; then diisopropylethylamine, CH₂Cl₂, rt, overnight, 90%; (c) tert-butyl (R)-3-aminopyrrolidine-1-carboxylate, diisopropylethylamine, *n*-butanol, 110 °C, 59%; (d) TFA, CH₂Cl₂, 94%; (e) acryloyl chloride, diisopropylethylamine, CH₃CN, rt, 4 h, 17%.

3-(2-chloropyrimidin-4-yloxy)-4-methylbenzoic acid (3)

To a solution of 2,4-dichloropyrimidine (**1**) (10 g, 67.13 mmol), 3-hydroxy-4-methylbenzoic acid (**2**) (10.22 g, 67.13 mmol) and Cs₂CO₃ (43.75 g, 134.26 mmol) in *i*-PrOH (100 mL) was stirred at 55°C for 3h. The solvent was removed under reduced pressure and water (100 mL) was added. Adjust PH of the mixture to one with 1N HCl. Filtered and dried by acetone to give **3** (15.5 g, yield: 87 %) as a white solid. LCMS (ESI) *m/z*: 265 [M+H]⁺.

3-(2-chloropyrimidin-4-yloxy)-N-(4-((4-ethylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)-4-methylbenzamide (5)

To a solution of 3-(2-chloropyrimidin-4-yloxy)-4-methylbenzoic acid (**3**) (6.5 g, 24.56 mmol) in CH₂Cl₂ (100 mL) was added *N,N*-dimethylformamide (DMF) (1 mL) and oxalyl dichloride (9.36 g, 73.68 mmol). The mixture was stirred at r.t for 2h. The solvent was removed under reduced pressure and CH₂Cl₂ (100 mL) was added. The mixture was added diisopropylethylamine (DIEA) (6.39 g, 49.44 mmol) and 4-((4-ethylpiperazin-1-yl)methyl)-3-(trifluoromethyl)aniline (**4**) (7.1 g, 24.72 mmol) and stirred at r.t for 3h. The solvent was removed under reduced pressure and the product was purified by flash column (MeOH/CH₂Cl₂ = 5% ~ 15%) to give **5** (12 g, yield: 90 %) as a brown solid. LCMS (ESI) *m/z*: 534 [M + H]⁺.

tert-butyl (R)-3-((4-(5-((4-ethylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)carbamoyl)-2-methylphenoxy)pyrimidin-2-yl)amino)pyrrolidine-1-carboxylate (6)

The mixture of **5** (600 mg, 1.12 mmol), tert-butyl (R)-3-aminopyrrolidine-1-carboxylate (550 mg, 2.95 mmol), DIEA (2 mL) in *n*-BuOH (15 mL) was stirred at 110°C overnight, after the reaction was completed the mixture was concentrated to remove the solvent, added saturated Na₂CO₃ solution (30 mL), then extracted with ethyl acetate (100 mL × 3), the organic phase was washed with brine (50 mL × 2), dried over Na₂SO₄, filtered, concentrated and purified by silica gel (MeOH/CH₂Cl₂ = 1/10) to obtain **6** (light brown solid, 450 mg, yield 59%). LCMS (ESI) *m/z*: 684 [M + H]⁺.

(R)-N-(4-((4-ethylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)-4-methyl-3-((2-(pyrrolidin-3-ylamino)pyrimidin-4-yl)oxy)benzamide (7)

The mixture of **6** (180 mg, 0.263 mmol), TFA (2 mL) in CH₂Cl₂ (5 mL) was stirred at r.t. for 4 h, concentrated to remove the solvent to get **7** (light brown solid, 120 mg, yield 94%). LCMS (ESI) *m/z*: 584 [M + H]⁺.

(R)-3-((2-((1-acryloylpyrrolidin-3-yl)amino)pyrimidin-4-yl)oxy)-N-(4-((4-ethylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)-4-methylbenzamide (SB1-G-23)

To the mixture of **7** (60 mg, 0.103 mmol), DIPEA (1 mL) in CH₃CN (10 mL) was added acryloyl chloride (12 mg, 0.133 mmol), then stirred at r.t for 4 h, concentrated to remove the solvent, the residue was purified by prep-HPLC (C18 column, CH₃CN/H₂O, containing 0.05%NH₄HCO₃) to obtain **SB1-G-23** (off-white solid, 11 mg, yield 17%). LCMS (ESI) *m/z*: 638 [M + H]⁺; ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.24 (s, 1H), 8.22 (d, *J* = 7.6 Hz, 1H), 8.15 (s, 1H), 8.01 (d, *J* = 10.8 Hz, 1H), 7.83 (d, *J* = 11.2 Hz, 2H), 7.78 (s, 1H), 7.68 (d, *J* = 12.0 Hz, 1H), 7.47 (d, *J* = 10.0 Hz, 1H), 7.20 (bs,

1H), 6.00-6.51 (m, 3H), 5.50-5.61 (m, 1H), 4.16 (bs, 1H), 3.28-3.65 (m, 7H), 2.30-2.40 (m, 8H) 2.28 (q, $J = 9.6$ Hz, 2H), 2.20 (s, 3H), 0.98 (t, $J = 9.6$ Hz, 3H).

Synthesis of (S)-3-((2-((1-acryloylpyrrolidin-3-yl)amino)pyrimidin-4-yl)oxy)-N-(4-((4-ethylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)-4-methylbenzamide (TL10-105)

TL10-105 was synthesized by similar procedure as synthesis of SB1-G-23 with tert-butyl (S)-3-aminopyrrolidine-1-carboxylate as starting material in step c. LCMS (ESI) m/z : 638 [M + H]⁺; ¹H NMR (600 MHz, DMSO-*d*₆, TFA salt) δ 10.41 (s, 1H), 9.34 (br, 1H), 8.25 (d, $J = 8.4$ Hz, 1H), 8.20 (s, 1H), 8.10 (d, $J = 7.8$ Hz, 1H), 7.85 (d, $J = 7.8$ Hz, 2H), 7.80 (s, 1H), 7.71 (d, $J = 8.4$ Hz, 1H), 7.50 (d, $J = 8.4$ Hz, 1H), 6.52 (dd, $J = 16.8, 10.8$ Hz, 1H), 6.33 (d, $J = 6.0$ Hz, 1H), 6.28 (br, 1H), 5.63 (d, $J = 6.0$ Hz, 1H), 4.33 (m, 7H), 3.69 (s, 2H), 3.46 (m, 2H), 3.15 (m, 2H), 2.88–3.04 (m, 4H) 2.41 (q, $J = 7.2$ Hz, 2H), 2.20 (s, 3H), 1.22 (t, $J = 7.2$ Hz, 3H).

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Supplementary table 3

KINOMEscan	TL10-105 (1μM) % control	HYJ-2-002-1 (1μM) % control	CPT-1-70-1 (1μM) % control	ibrutinib (1μM) % control	OTSSP167 (10μM) % control	XMD15-46 (10μM) % control	HG-6-71-01 (1μM) % control	HG6-64-1 (1μM) % control	HG6-64-1 (10μM) % control
Kinases	This study	This study	This study	http://lincs.ms.harvard.edu/	http://lincs.ms.harvard.edu/	from Deng et al., 2010	from Kim et al., 2013	from Tan et al., 2015	from Tan et al., 2015
MKK7	0.9	8.2	8.1	1.6	0.3	5.4	20	39	1.4
AAK1	82	100	18	92	2.3	59	100	67	26
ABL1(E255K)-phosphorylated	1.6	0.55	90	65	0.9	0.2	1.3	0.85	1
ABL1(F317I)-nonphosphorylated	1.3	0	100	30	14	8.8	2.4	19	0.9
ABL1(F317I)-phosphorylated	7.6	34	100	39	3.2	4.9	32	22	19
ABL1(F317L)-nonphosphorylated	1.6	0	100	16	94	0	4.2	0	0
ABL1(F317L)-phosphorylated	3.3	2	99	48	7.3	0.85	0.8	3.4	2.2
ABL1(H396P)-nonphosphorylated	0	0	7.2	12	5.6	0.05	0.8	0	0.1
ABL1(H396P)-phosphorylated	2.3	0.1	100	87	0.2	0.05	0.45	0.8	0.1
ABL1(M351T)-phosphorylated	2.9	0.85	86	74	1.2	1.1	0.4	4.4	2.2
ABL1(Q252H)-nonphosphorylated	0.8	0.05	52	5.1	15	1.6	2.6	1.4	0.1
ABL1(Q252H)-phosphorylated	2.4	1	100	76	0.9	0.2	1.6	1.2	1.2
ABL1(T315I)-nonphosphorylated	5	9	46	96	12	2.4	2.5	11	0
ABL1(T315I)-phosphorylated	62	0.75	19	70	1.5	0.9	1.2	5.4	1.8
ABL1(Y253F)-phosphorylated	1	0.7	100	62	0.6	0.2	1.1	0.75	0.3
ABL1-nonphosphorylated	1	0.05	25	7.2	2.6	0.1	2.8	0	0
ABL1-phosphorylated	2	0.1	51	54	0.2	0.05	0.45	0.7	0.1
ABL2	5	0	60	38	0.2	0	0.55	0.7	0
ACVR1	100	100	100	100	0.7	100	100	100	100
ACVR1B	92	100	100	100	31	63	100	95	98
ACVR2A	94	100	100	97	100	100	100	100	100
ACVR2B	93	100	100	90	70	23	86	91	62
ACVRL1	85	100	100	100	38	100	100	100	100
ADCK3	100	100	100	100	0.1	100	100	100	100
ADCK4	96	100	91	96	85	82	100	81	100
AKT1	100	100	100	100	3.7	41	100	100	100
AKT2	98	95	100	75	1.2	4.6	93	86	48

AKT3	94	100	100	100	48	82	100	100	100
ALK	82	75	38	51	6.6	52	44	80	51
ALK(C1156Y)	100	n/a	52	74	8	n/a	n/a	n/a	n/a
ALK(L1196M)	78	n/a	100	82	4.8	n/a	n/a	n/a	n/a
AMPK-alpha1	92	87	32	75	0.5	0.8	89	25	20
AMPK-alpha2	86	100	41	100	1.4	7.2	97	61	39
ANKK1	100	9.4	93	71	2.3	7.1	5.2	6	5.7
NUAK1	83	65	9.3	100	2.5	2.5	85	100	100
ASK1	94	96	100	87	1	24	91	100	35
ASK2	87	100	100	100	0.4	11	16	87	64
AURKA	92	100	37	49	0	97	86	99	97
AURKB	98	43	61	91	0.1	4.6	54	65	16
AURKC	100	80	51	77	34	11	71	34	1.5
AXL	78	21	4.8	65	16	0.1	60	55	4.6
BIKE	96	96	18	84	3.4	30	88	25	3
BLK	0.5	0.1	1.6	0.1	0.7	0	0	0.25	0.2
BMPR1A	96	100	100	100	46	53	100	100	100
BMPR1B	93	100	100	75	0.1	72	96	95	76
BMPR2	100	98	100	89	0.8	61	84	87	14
BMX	54	8.7	9.2	14	2.6	2.6	5	1.6	6.6
BRAF	82	3.7	87	53	3.6	0.45	11	17	0.6
BRAF(V600E)	41	1.2	100	50	1.5	0.1	4	7.4	0.1
BRK	100	n/a	n/a	1	42	n/a	n/a	64	9.6
BRSK1	100	97	100	100	35	100	100	83	100
BRSK2	100	91	97	76	24	90	62	93	100
BTK	98	8.1	7	0	7.6	1.2	8.8	10	0.3
BUB1	88	n/a	85	100	13	n/a	100	n/a	n/a
CAMK1	29	80	57	77	100	20	95	94	30
CAMK1D	28	94	56	84	60	68	94	100	100
CAMK1G	60	94	50	73	23	92	87	96	100
CAMK2A	95	100	95	100	81	100	83	92	100
CAMK2B	100	74	100	95	100	100	93	93	100
CAMK2D	88	100	100	79	1.6	100	100	100	100
CAMK2G	89	100	100	81	3	92	100	98	100
CAMK4	73	100	100	100	1	100	100	100	100
CAMKK1	81	100	84	90	0.7	69	100	96	100
CAMKK2	69	100	68	73	3.5	27	96	100	100
CASK	81	100	100	59	25	100	72	96	77
CDC2L1	36	88	100	96	0.6	0	98	61	8.5
CDC2L2	37	76	100	81	3.4	0	78	70	5.4
CDC2L5	65	100	91	89	52	13	94	100	100
CDK11	0	14	100	88	0.9	4.2	32	27	4.2
CDK2	77	100	100	100	2.8	13	100	90	96

CDK3	56	99	100	95	1.4	32	95	100	100
CDK4-cyclinD1	95	80	81	96	10	29	100	100	74
CDK4-cyclinD3	100	100	100	84	0.7	65	72	77	73
CDK5	72	100	100	90	1.9	24	100	100	100
CDK7	49	44	100	86	0.3	4	97	72	41
CDK8	2.8	9.2	100	76	1.2	18	32	25	21
CDK9	72	100	90	90	7.5	31	100	92	96
CDKL1	77	94	66	72	2.6	89	72	100	61
CDKL2	19	2.3	11	100	4	4.8	2	4.2	1.6
CDKL3	24	34	100	100	0.2	1.9	71	50	4
CDKL5	74	100	100	97	0.9	28	58	100	78
CHEK1	100	100	92	100	37	88	100	100	28
CHEK2	94	63	38	96	100	22	100	82	66
CIT	61	6.7	26	65	3.1	0	18	4.6	0
CLK1	85	57	5.8	100	15	6.8	83	59	14
CLK2	98	85	22	99	100	100	90	88	71
CLK3	96	88	82	90	21	94	100	90	100
CLK4	82	69	6.5	97	3.4	32	86	98	100
CSF1R	2.8	0.45	12	75	11	0	0.55	0.75	0
CSF1R- autoinhibited	95	n/a	1.4	58	3.2	n/a	64	n/a	n/a
CSK	58	0.8	93	0.5	23	0.1	1	2	0.8
CSNK1A1	88	100	55	87	2.8	89	66	93	87
CSNK1A1L	96	100	80	99	1	75	100	95	100
CSNK1D	100	73	43	97	9.4	22	89	84	38
CSNK1E	90	75	18	42	0.2	26	95	80	45
CSNK1G1	91	93	18	86	78	100	89	87	98
CSNK1G2	97	45	0.7	92	2.2	14	90	94	39
CSNK1G3	92	65	2.6	100	3	22	99	71	48
CSNK2A1	100	94	35	57	0.9	100	31	100	90
CSNK2A2	93	100	28	52	0.1	78	69	77	95
CTK	74	91	100	40	22	45	8	60	100
DAPK1	90	98	86	100	45	94	82	77	100
DAPK2	99	92	88	92	100	100	69	99	100
DAPK3	100	100	59	91	100	96	96	87	99
DCAMKL1	99	100	100	62	4.5	100	75	100	93
DCAMKL2	75	100	92	90	22	30	100	87	100
DCAMKL3	100	84	56	82	0.4	100	100	100	3.2
DDR1	0.4	0	79	90	2.6	0	0.15	0.05	0.2
DDR2	12	0.05	100	83	22	2.8	9.9	0.2	9
DLK	90	86	78	93	85	3.8	100	74	22
DMPK	98	100	41	100	7.2	27	96	100	57
DMPK2	96	92	67	97	1.2	35	100	76	16

DRAK1	88	82	14	100	9.6	24	100	52	1.3
DRAK2	98	57	90	100	100	12	92	16	1
DYRK1A	100	62	100	83	0	100	74	100	63
DYRK1B	91	76	79	93	5.8	15	82	73	27
DYRK2	85	96	100	82	0.4	51	82	68	78
EGFR	68	5	63	1.8	13	0.3	4	7.6	0.4
EGFR(E746- A750del)	66	1	17	5.8	8.4	0.75	4.4	0.7	3.8
EGFR(G719C)	59	0.75	8	1.2	36	0	1.3	0.45	0.1
EGFR(G719S)	81	1.8	34	0.9	46	0.15	1.8	0.9	0
EGFR(L747- E749del, A750P)	52	2.2	17	4.2	4	0.25	2.6	3	1.1
EGFR(L747- S752del, P753S)	38	2.2	20	3.6	6.6	0.8	3.5	0.5	0.6
EGFR(L747- T751del,Sins)	43	3.4	14	1.1	25	0.4	0.85	1.6	0
EGFR(L858R)	84	3.2	22	2.4	1	0.25	1.6	4	0.1
EGFR(L858R,T7 90M)	94	100	0.35	6.4	1.8	100	72	100	77
EGFR(L861Q)	66	0.85	18	0.5	2.2	0	0	0.25	0
EGFR(S752- I759del)	90	0	11	1.8	56	0.75	2	1.4	0
EGFR(T790M)	90	31	0.8	0.2	1	13	39	68	9.9
EIF2AK1	91	100	100	81	68	72	67	100	78
EPHA1	87	50	79	61	0.3	0.6	72	16	2
EPHA2	70	0.6	96	86	1.8	0.35	2	1.2	1.7
EPHA3	45	15	100	100	40	0.75	19	5.7	4.8
EPHA4	85	0.55	94	94	0	0.25	10	3.7	0
EPHA5	87	8.4	100	96	1.1	0.85	9.8	21	3.6
EPHA6	98	18	100	74	1.4	0.15	36	29	0
EPHA7	97	79	62	78	0.6	0.1	100	78	16
EPHA8	12	0.8	53	52	0.1	0	1.4	0.35	0.2
EPHB1	100	3	84	86	0.2	0.35	10	11	0.5
EPHB2	91	4.4	100	100	0	0.6	5.3	5.8	0
EPHB3	99	35	100	88	6.6	2.7	19	63	4.7
EPHB4	95	37	100	86	1.4	0.8	23	21	2.7
EPHB6	76	21	44	14	2.8	0.85	12	2.8	1.8
ERBB2	95	0	57	0	40	0.3	6.2	19	0
ERBB3	98	100	53	0.1	1.3	89	63	100	100
ERBB4	98	1.2	4.6	0	24	0.1	0.75	3	0.1
ERK1	100	100	100	94	100	96	100	100	100
ERK2	87	100	100	90	100	100	100	100	100
ERK3	99	100	1	100	100	100	100	91	100
ERK4	91	100	96	100	100	26	100	77	100
ERK5	87	100	87	89	1.4	36	100	83	73
ERK8	97	85	86	91	1.5	2.6	88	87	67

ERN1	96	100	69	74	16	54	12	100	72
FAK	99	91	85	100	0.4	59	98	84	67
FER	40	56	45	100	1.3	2.6	43	21	27
FES	5.3	13	73	88	1.2	0.1	8.2	6.8	0.2
FGFR1	55	1.2	2.2	36	4.6	0.15	0.95	2.8	0.1
FGFR2	77	5.7	22	46	11	0.5	12	5.4	3.7
FGFR3	93	28	35	43	21	0.15	32	13	1.8
FGFR3(G697C)	84	29	34	28	29	0.15	42	23	2.5
FGFR4	51	4.4	60	84	81	0	15	8.1	0.5
FGR	14	0.75	4.2	3.2	0.8	0.15	1	1	0.2
FLT1	36	10	54	60	2.2	0.8	9.2	12	2.4
FLT3	7	0.5	3	18	7.6	0.15	0.2	0.15	1
FLT3(D835H)	52	7.3	10	14	9.6	0.35	3.8	2.6	0.2
FLT3(D835Y)	48	38	0.35	16	1.6	0.85	17	6.8	2.8
FLT3(ITD)	24	2.3	1.6	43	2.1	0.15	5	1.4	0.4
FLT3(K663Q)	4.2	1.6	2.4	22	5.1	0	0.55	0.15	0.1
FLT3(N841I)	20	1.5	1.2	23	100	0	0.75	2.3	0.3
FLT3(R834Q)	59	44	51	64	100	7.2	4.7	7.4	50
FLT3- autoinhibited	79	n/a	38	67	2.8	n/a	76	n/a	n/a
FLT4	62	3.8	81	35	0	0.1	11	26	0.2
FRK	11	1.4	100	14	2.4	0.15	2.2	3.6	0.6
FYN	39	2.2	90	7.8	2.2	0.25	6	5.2	1.2
GAK	52	4.8	7.9	88	32	2	3.9	7	2.2
GCN2(Kin.Dom. 2,S808G)	99	14	13	100	35	0.25	2.8	11	0.6
GRK1	79	100	82	100	0.2	88	71	100	96
GRK4	92	100	100	100	50	14	97	40	8.2
GRK7	96	100	100	69	3.1	100	98	92	77
GSK3A	72	78	100	100	31	100	100	100	100
GSK3B	96	88	98	72	5.8	90	78	100	99
HASPIN	100	n/a	100	75	56	n/a	23	n/a	n/a
HCK	5.5	0.55	85	0.6	0.8	0.15	0.45	0.5	0.5
HIPK1	21	51	52	72	0.5	48	62	74	74
HIPK2	16	84	90	91	0.3	46	56	86	41
HIPK3	18	55	74	75	0.8	25	51	80	44
HIPK4	36	2.6	74	91	7.8	1.9	22	16	5.5
HPK1	32	3.4	13	100	5.4	0.05	2.8	0.55	0
HUNK	86	79	78	81	6.2	21	100	57	18
ICK	79	100	100	98	0.5	96	54	96	99
IGF1R	95	100	62	83	31	95	100	100	100
IKK-alpha	50	0.2	85	91	11	0.45	0.6	2	0
IKK-beta	90	0.3	100	72	2.2	0.1	1	5.7	0.2
IKK-epsilon	98	94	100	100	19	92	100	100	94

INSR	100	92	17	57	8.8	53	100	78	79
INSRR	81	100	33	90	23	68	85	100	100
IRAK1	76	62	53	74	3	6.2	100	90	26
IRAK3	93	100	89	100	100	100	100	76	65
IRAK4	81	94	94	66	1.2	64	86	100	48
ITK	98	75	0.85	6.5	0.3	2.2	100	81	18
JAK1(JH1domai n-catalytic)	62	41	77	100	5.9	2.9	66	76	39
JAK1(JH2domai n- pseudokinase)	100	93	0.75	100	10	74	100	88	41
JAK2(JH1domai n-catalytic)	84	57	1.2	77	4	3	58	32	12
JAK3(JH1domai n-catalytic)	45	2.4	0	0	2.4	3.5	12	55	1.1
JNK1	28	72	2.4	72	0.1	0.45	100	77	19
JNK2	0.35	1.8	13	60	0.2	0	9.2	6.6	0.1
JNK3	52	75	4.6	77	0.1	1.8	77	76	15
KIT	12	0	20	44	2	0	0.15	0.3	0
KIT(A829P)	12	61	75	56	100	24	3	8	64
KIT(D816H)	79	43	83	82	77	8.2	18	25	36
KIT(D816V)	66	9.2	60	77	1	0.65	22	8.8	0.7
KIT(L576P)	4.5	82	8.9	23	77	0	0.8	0.15	0
KIT(V559D)	7.5	0	15	25	3.6	0	0.1	0.05	0
KIT(V559D,T670 I)	16	0.85	28	98	9.2	0	2.8	4.9	0.1
KIT(V559D,V654 A)	51	28	100	96	47	1.4	24	7.1	2.6
KIT- autoinhibited	93	n/a	39	73	1.2	n/a	78	n/a	n/a
LATS1	100	100	77	55	4.6	3.4	100	80	32
LATS2	100	98	40	95	3.2	7	100	100	79
LCK	2.6	1.1	32	0.4	0.5	0.1	0.3	0.35	0.2
LIMK1	96	26	90	30	73	1.2	50	25	7.7
LIMK2	94	32	100	97	100	0.35	58	26	2.9
LKB1	96	100	76	100	24	60	83	58	7.9
LOK	0.35	0.75	100	40	0.1	0	0	0	0
LRRK2	94	94	7.5	85	99	6.2	97	53	12
LRRK2(G2019S)	97	83	2.6	92	100	8.8	89	71	18
LTK	84	89	100	82	5.2	2.5	74	93	62
LYN	6.5	0.15	49	11	0.5	0.05	0.4	0.45	0
LZK	100	78	73	84	56	7.8	98	82	20
MAK	66	100	100	100	69	61	80	89	100
MAP3K1	75	83	100	48	37	96	27	100	71
MAP3K15	70	100	100	92	25	72	11	100	100
MAP3K2	72	26	37	80	0.3	0.1	22	23	0.7
MAP3K3	58	1.6	16	63	1.8	1.4	4.8	2	1.4
MAP3K4	100	100	66	76	30	62	95	98	66

MAP4K2	1.8	4.6	25	79	0.4	0	5.2	3.2	0
MAP4K3	93	40	23	91	11	1.8	33	20	14
MAP4K4	2.6	11	49	93	18	1.8	0.75	1.8	4.2
MAP4K5	59	16	25	96	13	1.6	2.4	7.2	3.4
MAPKAPK2	84	100	100	96	3.6	100	100	100	100
MAPKAPK5	100	100	98	88	15	98	100	85	90
MARK1	96	100	2.1	84	84	100	72	100	94
MARK2	84	64	10	100	57	83	100	59	68
MARK3	100	100	9.2	60	5.2	42	100	100	38
MARK4	100	94	1.8	81	31	85	59	81	100
MAST1	88	99	100	67	91	100	34	96	100
MEK1	100	100	51	18	0.1	82	94	90	74
MEK2	100	22	19	20	0	37	78	74	58
MEK3	100	100	26	76	1	67	59	62	68
MEK4	94	100	35	100	3.2	25	91	100	76
MEK5	100	0.85	18	0.2	0.2	0.4	1.3	1.4	0.2
MEK6	88	91	55	100	67	88	100	100	79
MELK	85	48	16	75	5.5	6.1	73	72	20
MERTK	100	30	70	90	1.8	0.5	46	88	9.2
MET	100	59	28	98	28	9.2	82	100	40
MET(M1250T)	99	61	39	89	33	59	98	74	26
MET(Y1235D)	96	83	23	84	18	4.9	100	94	79
MINK	12	33	41	88	1.6	5.4	10	24	2.8
MKNK1	98	84	100	100	38	1.2	51	96	68
MKNK2	74	7	100	53	2.2	0.6	44	48	2.7
MLCK	96	89	100	100	2.2	18	94	100	100
MLK1	94	100	9	100	4.2	1.7	100	4.7	1.4
MLK2	100	93	56	91	52	9.5	55	53	20
MLK3	97	53	91	96	0.6	3	62	23	3.6
MRCKA	96	100	100	100	46	73	100	79	15
MRCKB	85	100	100	100	6.4	67	100	85	65
MST1	100	89	100	74	3.4	12	100	72	21
MST1R	100	100	100	100	41	76	100	81	100
MST2	93	83	86	57	100	26	41	100	5.2
MST3	88	76	93	98	2.3	3.6	87	75	20
MST4	75	98	49	62	0.4	11	25	87	18
MTOR	100	93	66	89	100	88	100	100	100
MUSK	48	1.4	8.8	97	1	0	3.9	2	0
MYLK	100	100	100	99	5.5	56	100	81	90
MYLK2	100	0.85	86	85	7.4	0.15	13	4.6	0.6
MYLK4	91	100	92	100	6.8	40	93	88	23
MYO3A	14	59	88	54	56	15	41	84	28
MYO3B	70	49	100	100	100	0	49	84	40

NDR1	99	100	37	70	4.5	33	48	89	72
NDR2	91	100	61	72	14	11	93	79	35
NEK1	100	82	100	100	95	50	63	83	89
NEK10	88	n/a	14	63	14	n/a	n/a	n/a	n/a
NEK11	99	37	95	96	100	18	51	87	32
NEK2	94	95	100	91	50	100	75	100	100
NEK3	99	100	68	96	100	49	47	79	77
NEK4	74	57	100	84	100	14	43	100	33
NEK5	93	21	82	100	85	0.65	48	47	4.3
NEK6	82	100	100	91	89	73	95	100	100
NEK7	100	100	100	94	96	50	94	92	64
NEK9	94	38	100	88	88	12	100	86	8.4
NIK	95	n/a	100	72	15	n/a	n/a	n/a	n/a
NIM1	98	100	100	100	70	98	100	99	100
NLK	49	28	100	100	36	13	28	18	17
OSR1	62	93	96	78	36	60	100	100	74
p38-alpha	0	0.25	100	100	41	0	0.9	1.7	0
p38-beta	1.4	0.35	100	100	44	0	6.4	0.3	0
p38-delta	55	66	100	100	5.6	2.6	100	67	22
p38-gamma	1.3	54	100	71	21	5.7	47	97	40
PAK1	87	100	64	64	100	62	92	100	100
PAK2	90	99	64	92	100	76	80	93	100
PAK3	78	100	50	39	100	1.1	80	66	6
PAK4	100	99	12	89	100	87	100	100	86
PAK6	93	100	74	96	100	85	100	100	54
PAK7	98	92	13	100	2.4	64	100	70	100
PCK1	93	100	100	98	0	46	100	100	98
PCK2	56	100	100	77	13	3.7	100	85	61
PCK3	76	100	97	78	2.7	12	100	84	100
PDGFRA	43	0.65	64	34	0.3	0	9	2.6	0.2
PDGFRB	6.8	0	6.9	33	1.8	0	0	0.1	0.1
PDPK1	89	72	64	71	10	60	99	100	65
PFCDPK1(P.falci parum)	1.8	0.85	100	0	2.4	0.2	2.6	4.3	0.2
PFPK5(P.falcipa rum)	97	100	100	100	100	93	100	100	93
PFTAIRE2	100	94	100	99	1	2	43	93	36
PFTK1	77	100	100	81	1	1.6	98	93	72
PHKG1	95	100	100	100	11	100	100	85	100
PHKG2	99	73	72	84	100	100	88	100	100
PIK3C2B	100	100	100	63	2.6	100	79	91	100
PIK3C2G	100	100	100	80	3	100	89	100	82
PIK3CA	100	100	100	61	5.4	93	100	100	100
PIK3CA(C420R)	100	100	100	72	3	95	68	100	100

PIK3CA(E542K)	100	100	100	72	4	96	97	100	100
PIK3CA(E545A)	100	100	79	65	2.2	93	66	100	92
PIK3CA(E545K)	100	100	84	76	4.7	98	62	100	100
PIK3CA(H1047L)	100	100	100	54	84	100	76	98	100
PIK3CA(H1047Y)	100	100	100	65	36	82	71	71	90
PIK3CA(I800L)	84	100	100	75	35	100	94	100	100
PIK3CA(M1043I)	100	100	100	65	42	100	91	100	84
PIK3CA(Q546K)	91	100	100	83	6	100	99	100	98
PIK3CB	100	100	100	59	24	85	68	100	100
PIK3CD	100	100	100	71	55	76	81	100	78
PIK3CG	100	100	100	73	0.4	100	100	100	96
PIK4CB	92	100	100	100	0.3	100	42	100	91
PIM1	98	100	100	94	87	100	100	100	100
PIM2	97	100	100	89	2.1	100	90	100	100
PIM3	99	93	81	94	75	100	100	100	100
PIP5K1A	90	77	13	97	81	10	100	21	2.6
PIP5K1C	52	100	57	13	95	100	0.9	100	84
PIP5K2B	80	90	100	83	100	7.7	100	12	0.4
PIP5K2C	76	96	63	92	100	100	20	100	100
PKAC-alpha	93	77	69	80	0.4	27	71	84	100
PKAC-beta	99	98	100	97	1.7	11	62	76	100
PKMYT1	89	96	94	100	40	48	92	68	71
PKN1	94	81	79	71	81	28	100	85	16
PKN2	99	78	100	100	27	2.2	58	35	26
PKNB(M.tuberculosis)	86	90	58	68	0.1	98	100	84	89
PLK1	88	100	100	90	0.1	56	100	98	100
PLK2	89	100	78	77	2.2	100	100	97	60
PLK3	89	100	100	69	32	92	100	100	83
PLK4	88	100	23	44	0	97	83	86	59
PRKCD	58	78	100	95	6.3	24	51	60	49
PRKCE	82	100	63	100	3.7	78	100	62	75
PRKCH	83	100	100	95	3.2	79	95	100	100
PRKCI	100	73	65	74	15	40	70	100	100
PRKCQ	72	82	100	100	100	36	100	83	31
PRKD1	100	90	52	70	6.3	63	100	100	3.5
PRKD2	89	42	70	100	6.4	13	43	81	50
PRKD3	96	67	54	100	100	6.4	72	93	52
PRKG1	97	100	100	100	5.4	100	100	86	100
PRKG2	95	100	100	54	5.1	77	100	82	91
PRKR	85	75	93	95	61	54	92	97	80
PRKX	91	78	100	100	100	19	100	57	75
PRP4	87	100	90	80	100	84	87	85	12

PYK2	84	21	66	96	4	0.15	25	19	0.8
QSK	87	100	100	98	0.8	77	52	100	100
RAF1	99	8.9	86	70	100	0.95	25	7.8	0.9
RET	29	0.15	25	18	0.1	0	0.25	0	0.1
RET(M918T)	27	0.95	13	18	0.1	0	0.2	0.05	0
RET(V804L)	97	1.4	11	91	0	0	11	3.4	0.1
RET(V804M)	65	1	2.2	90	0	0	2.2	0.8	0
RIOK1	100	100	49	77	98	53	95	20	0.8
RIOK2	86	35	5.2	95	24	2	28	61	19
RIOK3	93	100	53	69	90	38	73	27	0.4
RIPK1	56	8.2	0.15	100	100	0	28	15	0.2
RIPK2	82	5.3	100	5	28	0.3	9.6	4.5	1.8
RIPK4	90	100	100	92	0.1	8	37	100	56
RIPK5	100	86	33	9.2	1.8	8.2	100	91	36
ROCK1	100	98	29	98	100	60	100	91	43
ROCK2	82	94	26	86	100	18	100	88	34
ROS1	100	100	100	100	12	34	97	100	100
RPS6KA4(Kin.Dom.1-N-terminal)	100	99	100	100	1	3.6	70	72	50
RPS6KA4(Kin.Dom.2-C-terminal)	94	100	79	84	0	87	78	73	30
RPS6KA5(Kin.Dom.1-N-terminal)	79	76	100	100	0.4	20	69	62	34
RPS6KA5(Kin.Dom.2-C-terminal)	99	100	100	79	18	97	89	100	100
RSK1(Kin.Dom.1-N-terminal)	83	96	72	83	5.2	34	95	91	31
RSK1(Kin.Dom.2-C-terminal)	99	61	100	91	34	17	91	50	20
RSK2(Kin.Dom.1-N-terminal)	94	100	100	73	0.1	2.8	68	89	14
RSK2(Kin.Dom.2-C-terminal)	100	n/a	100	100	3.2	n/a	100	n/a	n/a
RSK3(Kin.Dom.1-N-terminal)	95	42	66	89	7.7	0.7	91	68	2.7
RSK3(Kin.Dom.2-C-terminal)	96	73	100	100	7.5	87	83	67	42
RSK4(Kin.Dom.1-N-terminal)	90	100	45	100	0.1	28	81	99	42
RSK4(Kin.Dom.2-C-terminal)	91	28	100	89	7.2	29	69	50	15
S6K1	100	55	100	63	1.6	3.2	44	46	9
SBK1	100	93	10	68	49	87	68	94	57
SGK	90	n/a	26	54	0	n/a	100	n/a	n/a
Sgk110	96	96	100	95	100	42	100	45	41
SGK2	100	n/a	100	68	1.8	n/a	n/a	n/a	n/a
SGK3	98	100	74	100	1.1	11	48	90	38
SIK	87	1.8	100	93	1.3	0.25	1.2	2.1	0.9
SIK2	87	34	57	100	48	18	52	26	30
SLK	63	9.8	77	76	1.5	0.3	2.1	13	0.6
SNARK	100	100	8.5	78	0.4	84	54	76	95

SNRK	83	100	55	60	23	60	43	100	95
SRC	16	0.2	6.6	4	0.1	0.05	0.3	2.8	0.2
SRMS	54	8.4	100	0	3.4	0.2	30	34	0.7
SRPK1	84	83	44	60	15	100	93	28	1.8
SRPK2	86	100	98	86	74	63	100	76	28
SRPK3	80	90	100	83	87	11	98	37	13
STK16	93	80	0.75	99	46	47	100	100	54
STK33	98	66	10	80	13	6.8	58	78	31
STK35	60	91	100	50	10	0.8	73	65	23
STK36	39	2.2	78	65	0.1	0.15	0.85	1.4	0.3
STK39	73	94	85	52	66	100	56	70	100
SYK	24	18	63	100	3	1	14	18	7.2
TAK1	0.4	6.6	3.6	64	6	0.25	11	1.2	4.8
TAOK1	14	34	96	84	0.5	0	46	22	0.8
TAOK2	3.7	18	65	82	0.3	0	53	16	0.5
TAOK3	2.8	0.45	71	81	0.2	0	5.2	0.75	0
TBK1	100	100	43	91	5	84	90	88	55
TEC	93	3.8	10	5.7	8.2	0.1	18	16	0.5
TESK1	96	81	83	86	43	2.4	94	100	15
TGFBR1	100	100	100	87	100	100	100	100	100
TGFBR2	84	41	100	98	0.6	1.4	94	52	5.7
TIE1	11	4.3	39	66	100	1.1	3.6	0.95	4.6
TIE2	47	0.15	100	68	5.1	0	0.35	0	0.1
TLK1	100	74	100	100	23	93	94	79	100
TLK2	100	97	100	99	3.2	100	100	100	93
TNIK	9.7	11	20	100	5.1	1.6	15	14	3.2
TNK1	93	15	0.95	99	3.7	0.8	39	6.6	1.4
TNK2	100	4.1	100	27	1.4	0.6	4.8	5.4	0.8
TNNI3K	81	6.6	100	73	9.7	0	7	5.9	1
TRKA	82	6.6	30	79	0.6	0.3	16	54	2.5
TRKB	80	4.2	28	62	1.8	2	2.3	9.4	5.2
TRKC	73	8	61	88	0.6	0.35	21	47	1
TRPM6	100	100	48	31	100	64	16	100	100
TSSK1B	99	100	25	82	100	98	78	90	100
TTK	84	64	4.8	73	100	2	78	56	6.8
TXK	100	2.1	4.6	1.4	1.4	0.25	3.2	1.4	0.7
TYK2(JH1domain-catalytic)	91	53	7.4	80	2.4	6.8	60	70	12
TYK2(JH2domain-pseudokinase)	92	100	68	100	32	96	100	47	100
TYRO3	100	40	100	41	100	38	66	76	100
ULK1	94	89	32	71	3.8	38	52	68	8.5
ULK2	100	88	29	91	0.2	61	81	81	35

ULK3	78	53	19	73	0.1	0.25	71	55	1.5
VEGFR2	45	6.4	40	52	0.3	0.35	30	14	2.6
VRK2	77	100	100	92	9.2	90	75	100	92
WEE1	97	100	88	93	100	100	99	100	100
WEE2	95	21	100	100	97	20	72	74	4.8
WNK1	86	n/a	100	76	89	n/a	81	n/a	n/a
WNK3	84	n/a	100	55	72	n/a	100	n/a	n/a
YANK1	86	100	100	45	19	98	68	100	100
YANK2	90	100	100	77	13	100	82	100	100
YANK3	93	100	100	84	100	83	89	85	100
YES	40	0.55	17	2	1	0.25	2.7	2.2	0.7
YSK1	79	87	89	96	12	12	67	100	100
YSK4	98	0.45	0.45	95	0.2	0.1	2.8	1.1	0.2
ZAK	3.1	3.9	71	34	3.8	0.25	0.6	1	0.8
ZAP70	72	69	0.2	100	31	28	45	98	52