

SUPPORTING INFORMATION

IDENTIFICATION OF “PREFERRED” HUMAN KINASE INHIBITORS FOR SLEEPING SICKNESS LEAD DISCOVERY. ARE SOME KINASES BETTER THAN OTHERS FOR INHIBITOR REPURPOSING?

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Table of Contents	
Supplementary data tables	S2
Supplementary Figures	S34
References	S38

Table S1 – PKIS HTS Data

Compound	Tbb pEC₅₀	Tbb %inh (Avg)	HepG2 pTC₅₀	Selectivity (pEC₅₀-pTC₅₀)
GW778894X	8.1	100.2	<4	>4.1
GSK571989A	7.8	100.3	5.1	2.7
GSK326090A	7.8	100.2	5	2.8
GW779439X	7.8	100.0	5	2.8
GW396574X	7.5	100.7	5	2.5
GW780056X	7.5	100.0	<4	>3.5
GW806290X	7.2	100.0	5.3	1.9
GW801372X	7.2	99.5	<4	>3.2
GW305178X	7.1	101.1	<4	>3.1
GSK579289A	7.1	100.2	4.9	2.2
GW810576X	7.1	99.9	<4	>3.1
GSK1173862A	7	100.1	5.3	1.7
GSK2186269A	7	99.8	5.6	1.4
GSK1007102B	6.9	96.5	5.8	1.1
SB-732881-H	6.8	100.0	5.5	1.3
GW837331X	6.8	93.6	4.3	2.5
GSK1220512A	6.7	100.2	5.3	1.4
GSK1751853A	6.7	100.1	5.3	1.4
GW559768X	6.7	100.0	4.8	1.9
GSK978744A	6.7	100.0	<4	>2.7
GW784307A	6.6	100.2	4.8	1.8
GW806742X	6.6	100.1	5.5	1.1
SB-732881	6.6	100.1	<4	>2.6
GSK237701A	6.6	100.0	4.1	2.5
GSK2163632A	6.6	99.9	5.1	1.5
GW416981X	6.6	99.8	4.4	2.2
GW770220A	6.5	100.5	4.4	2.1
GSK317315A	6.5	100.3	4.6	1.9
GSK1713088A	6.5	100.2	5.3	1.2
SB-220025-R	6.5	99.8	<4	>2.5
GW297361X	6.5	94.8	<4	>2.5
SB-725317	6.4	100.5	4.6	1.8
SB-220025-A	6.4	100.3	<4	>2.4
GSK317314A	6.4	100.1	4.4	2
GW276655X	6.4	99.9	<4	>2.4
GSK994854A	6.4	96.1	5.1	1.3
GW784752X	6.4	93.2	<4	>2.4

SB-236687	6.3	100.3	4.2	2.1
GSK718429A	6.3	100.1	4.8	1.5
GW612286X	6.2	100.3	4.6	1.6
GSK2110236A	6.2	100.1	4.8	1.4
GW572399X	6.2	99.9	<4	>2.2
GW296115X	6.2	71.5	5.4	0.8
GW583373A	6.2	59.3	<4	>2.2
GW709042A	6.1	100.2	5.6	0.5
GSK300014A	6.1	99.8	<4	>2
SB-245392	6.1	99.8	5.1	1
GW861893X	6.1	99.3	<4	>2.1
SB-772077-B	6.1	93.5	<4	>2.1
GW644007X	6	100.3	<4	>2
SB-675259-M	6	100.0	<4	>2
SB-220455	6	99.9	<4	>2
GW827106X	6	78.1	<4	>2
SB-376719	5.9	100.1	<4	>1.9
SB-223133	5.9	100.1	<4	>1.9
SB-734117	5.9	88.2	4.3	1.6
GW406108X	5.9	87.7	4.4	1.5
GW768505A	5.8	100.5	6.3	-0.5
GW280670X	5.8	100.2	4.7	1.1
SB-226879	5.8	99.2	<4	>1.8
GSK1326255A	5.8	96.7	4.3	1.5
GW513184X	5.8	94.8	<4	>1.8
GW275944X	5.8	83.1	4.5	1.3
GSK2213727A	5.8	81.7	<4	>1.8
GW827102X	5.8	66.8	<4	>1.8
GW627834A	5.8	63.9	4.7	1.1
GW615311X	5.8	58.3	<4	>1.8
GW784684X	5.7	99.7	4.8	0.9
GW795486X	5.7	99.3	5.4	0.3
SB-242719	5.7	97.7	4.9	0.8
GW621823A	5.7	96.6	<4	>1.7
GW429374A	5.7	85.1	4.5	1.2
GW700494A	5.7	84.7	4.7	1
GW869810X	5.7	83.7	4.3	1.4
SB-390527	5.7	78.3	<4	>1.7
GSK259178A	5.7	77.9	4.3	1.4
GW810372X	5.7	74.0	<4	>1.7
GW576609A	5.7	59.7	<4	>1.7

GW576484X	5.7	53.4	4.8	0.9
GW567808A	5.7	51.6	4.4	1.3
SB-253226	5.6	99.5	4.8	0.8
GW618013A	5.6	99.1	4.6	1
GW829906X	5.6	80.6	4.3	1.3
GW683134A	5.6	72.5	5	0.6
SB-739245-AC	5.6	64.8	4.7	0.9
GW442130X	5.6	60.8	4.2	1.4
GSK938890A	5.6	58.6	4.2	1.4
GW770249A	5.6	53.8	6.4	-0.8
GW799251X	5.5	79.7	4.4	1.1
GW569530A	5.5	77.0	<4	>1.5
GSK943949A	5.5	56.1	4.7	0.8
GW654652C	5.5	56.1	<4	>1.5
GSK270822A	5.4	37.3	4.3	1.1
GW771127A	5.3	70.5	4.5	0.8
GSK317354A	5.3	43.6	<4	>1.3
GW831091X	5.2	69.8	<4	>1.3
GW809897X	5.1	54.5	4.3	0.8
GW856804X	5	81.8	4.3	0.7
GW589933X	4.9	53.3	<4	>0.9
GSK953913A	4.7	55.0	<4	>0.7
GW405841X	4.6	49.4	<4	>0.6
GSK299115A	4.6	42.3	<4	>0.6
GW814408X	ND ^a	100.2		
GW680191X	ND ^a	99.8		
GW805758X		96.0	5.6	
GW852849X		89.0	<4	
GSK269962B		85.0	4.6	
SB-686709-A		80.4	4.7	
GW876790X		67.9	<4	
GW708336X		67.5	4.6	
GW811168X		67.3	<4	
GW575533A		53.0	<4	
SB-476429-A		50.8	4.7	
GSK466317A		49.8		
SB-400868-A		49.6		
SB-736302		49.5		
GW566221A		48.7		
GW627512B		48.6		
SB-278538		48.0		

GW278681X		46.6		
GW301784X		46.5		
GW827099X		45.7		
GW335962X		45.7		
SB-750140		45.6		
GW795493X		45.1		
GW574783B		44.9		
GW416469X		44.2		
GW568377A		43.6		
SB-253228		42.6		
GW643971X		42.5		
SB-409514		41.4		
GW458787A		39.8	4.3	
GW580496A		39.3		
GSK1030061A		39.3		
GW576924A		39.2		
SB-590885-AAD		38.5	6.1	
GW284408X		38.2		
GW574782A		38.2		
GW673715X		37.9		
GSK614526A		37.7		
GW300653X		37.7		
SB-682330-A		37.4		
SB-437013		37.3		
GW833373X		37.1		
SB-221466		36.8		
GSK2220400A		35.3		
GW694590A		34.6		
GSK204925A		34.4		
GW759710A		33.1		
GW578748X		32.3		
GW633459A		31.8		
SB-251505		31.7		
GW589961A		31.1		
GW290597X		30.7		
SB-278539		30.2		
GSK3206866B		30.1		
GW549034X		30.1		
GW651576X		29.9		
GW561436X		29.9		
GW782612X		29.7		

GW301888X		29.4	4.3	
GSK1511931A		29.3		
SB-284847-BT		29.2		
GW575808A		28.3		
GW282536X		28.0		
GSK200398A		27.6		
GSK237700A		27.4		
GW830263A		26.7		
GW305074X		26.5		
GW284372X		25.4		
GW572401X		25.4		
GW827105X		24.6		
GW581744X		24.4		
GW772405X		24.3		
SB-250715		23.8		
GI261520A		23.6		
GSK238063A		23.5		
GW282974X		23.2		
GW813360X		23.2		
GW282449A		23.0		
GW831090X		22.9	<4	
GW804482X		22.7		
GW819077X		22.4		
GSK619487A		21.9		
SB-698596-AC		21.7		
GSK238583A		21.4		
GW301789X		21.4		
GW824645A		21.2		
GSK182497A		21.1		
SB-678557-A		20.3		
GW607049C		20.1		
GW569293E		19.9		
GW770249X		19.8		
GW279320X		19.8		
GW775608X		18.6		
GW693881A		18.6		
GW275616X		18.4		
GSK192082A		18.4		
GW300657X		18.2		
SB-431542-A		18.1		
SB-711237		17.8		

GW684626B		17.7		
GSK248233A		17.5		
SB-738482		17.5		
GW461104A		16.8		
SB-347804		16.2		
SB-735465		16.2		
SB-242721		16.2		
GW439255X		16.1		
SB-742865		16.1		
GW693917A		15.8		
GW406731X		15.7		
GW832467X		15.7		
GW683109X		15.6		
GW621970X		15.4		
GW695874X		15.4		
GSK312948A		15.4		
GW809885X		15.3		
GSK635416A		15.2		
GW616030X		15.0		
GW659386A		14.8		
GW683768X		14.3		
GW701427A		14.2		
GW580509X		14.0		
GW659893X		14.0		
GR105659X		13.8		
GW694234A		13.8		
GW642138X		13.7		
GW622055X		13.7		
GSK319347A		13.5		
GW434756X		13.2		
GW435821X		12.9		
GSK2219385A		12.7		
SB-251527		12.6		
GW445012X		12.4		
SB-735467		12.3		
SB-239272		12.2	>8.8	
GW432441X		12.2		
GW632046X		11.6		
GW683003X		11.3		
GW632580X		11.2	4.3	
GW785804X		11.2		

GW734508X		11.2		
GW641155A		11.1		
SB-409513		11.0		
GW830365A		10.9		
GW820759X		10.7		
GW678313X		10.6		
SB-633825		10.6		
GW829115X		10.5		
GW703087X		10.3		
GW807930X		10.3		
SB-264866		10.2		
GW711782X		10.0		
GSK969786A		10.0	<4	
SB-744941		10.0		
SB-210313		9.9		
SB-742864		9.7		
SB-657836-AAA		9.7		
GW830900A		9.5		
GW743024X		9.3	4.7	
SB-610251-B		9.3		
GSK620503A		9.3		
GW682841X		9.1		
GSK466314A		9.1		
SB-630812		9.0	<4	
GW829055X		9.0		
GW827396X		8.7		
SB-264865		8.4		
SKF-62604		8.2		
GW829877X		8.1		
GW781673X		8.0		
SB-759335-B		7.9		
SB-614067-R		7.9		
GSK561866B		7.8		
GW607117X		7.7		
SKF-86002-A2		7.7		
GW631581B		7.6		
GW679410X		7.4		
SB-751148		7.3		
GSK1030059A		7.1		
SB-360741		6.8		
GW769076X		6.7		

GW410563A		6.6		
SB-361058		6.4		
GSK1023156A		6.3		
GW817394X		6.2		
GW782907X		6.0		
SB-741905		6.0		
SB-739452		6.0		
GW846105X		5.9	<4	
GW796921X		5.9		
GW794726X		5.8		
GW785974X		5.8		
SB-242718		5.7		
GW794607X		5.6		
GSK605714A		5.5		
GSK625137A		5.2		
SB-390523		5.2		
GW786460X		5.2		
GW853609X		5.1		
GW549390X		5.1		
GW811761X		4.9		
GW572738X		4.9		
GSK1030058A		4.8		
GW780159X		4.7		
GW300660X		4.7		
SB-736290		4.7		
GW445014X		4.6		
GW441756X		4.4		
SB-254169		4.4		
SB-216385		4.4		
GW843682X		4.3		
GW807982X		4.1		
GSK1392956A		4.1		
SB-738561		3.9		
GW829874X		3.8		
SB-732941		3.4		
SB-431533		3.3		
GSK586581A		3.3		
GW874091X		3.2		
GW445017X		3.1		
GSK1000163A		3.0		
GW427984X		2.7		

SB-358518		2.5		
GW407323A		2.4		
GW785404X		2.0		
GW577921A		1.7		
GSK180736A		1.7		
GW853606X		1.6	4.4	
GSK949675A		1.2		
SB-751399		0.9		
GW796920X		0.8		
GW445015X		0.6		
GW459057A		0.5		
GW680908A		0.5		
GW782912X		0.1		
GSK711701A		0.1		
GSK1030062A		0.1		
SB-242717		0.0		
GW828525X		-0.2		
GW693481X		-0.3		
GW708893X		-0.4		
GR269666A		-0.8		
SB-814597		-0.9		
GW642125X		-1.0		
GW568326X		-1.4		
SB-285234-W		-1.6		
GSK980961A		-1.8	4.1	
GW620972X		-2.1		
GW680975X		-2.1		
GW441806A		-2.2		
GW701032X		-2.3		
GW806776X		-2.6		
GW817396X		-2.7		
GW819230X		-2.8		
SB-743899		-3.1		
GSK554170A		-3.1		
GW450241X		-3.8		
SB-333612		-5.2		
GSK1819799A		-5.7		
GW828529X		-6.6		
GW458344A		-6.9		
SB-737198		-9.5		
SKF-86055		-10.9		

^a ND=pEC50 data not obtained.

Table S2. Structures of purchased inhibitors of preferred kinases selected for purchase and screening, with *T. brucei* potency data.

#	NEU	Name	Tbb pEC50	SMILES
1	NEU-838	Crizotinib	6.36	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>
2	NEU-844	TAE684	7.00	<chem>COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1CCN(C)CC1</chem>
3	NEU-893	GSK1838705A	5.70	<chem>CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4=C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C1F</chem>
4	NEU-967	NVP-AEW541	5.74	<chem>NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1</chem>
5	NEU-968	BMS-265246	6.34	<chem>CCCCOC1=C2C=NNC2=NC=C1C(=O)C1=C(F)C=C(C)C=C1F</chem>
6	NEU-969	PHA-848125	7.57	<chem>CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21</chem>
7	NEU-970	GSK1904529A	5.86	<chem>CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(CC1)S(C)(=O)=O</chem>
8	NEU-971	JNJ-7706621	6.55	<chem>NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F</chem>
9	NEU-973	ON-01910	<5.5	<chem>COC1=CC(OC)=C(C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1</chem>
10	NEU-974	CH5424802	<5.5	<chem>CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O</chem>
11	NEU-975	Dinaciclib	7.41	<chem>CCC1=C2N=C(C=C(NCC3=CC=C[N+](O-)=C3)N2N=C1)N1CCCC[C@H]1CCO</chem>
12	NEU-976	Linsitinib	<5.5	<chem>C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=CN=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1</chem>
13	NEU-977	Roscovitine	<5.5	<chem>CC[C@H](CO)NC1=NC(NCC2=CC=CC=C2)=C2N=CN(C(C)C)C2=N1</chem>
14	NEU-978	CHIR-98014	<5.5	<chem>NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2)C2=CC=C(Cl)C=C2Cl)=CC=C1N(=O)=O</chem>
15	NEU-979	Volasertib	<5.5	<chem>CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3OC)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O</chem>
16	NEU-980	BI 2536	6.22	<chem>CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O</chem>
17	NEU-982	AT7519	6.50	<chem>C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1</chem>
18	NEU-984	SNS-032	6.93	<chem>CC(C)(C)C1=CN=C(CSC2=CN=C(NC(=O)C3CCNCC3)S2)O1</chem>
19	NEU-985	AZD5438	7.48	<chem>CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1</chem>
20	NEU-986	SB 415286	6.05	<chem>OC1=C(Cl)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1</chem>
21	NEU-987	Flavopiridol	6.75	<chem>CN1CC[C@@H]([C@H](O)C1)C1=C(O)C=C(O)C2=C1OC(=CC2=O)C1=CC=CC=C1C</chem>
22	NEU-989	TWS119	5.96	<chem>NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1</chem>
23	NEU-990	SB 216763	<5.5	<chem>CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(Cl)C=C(Cl)C=C1</chem>
24	NEU-991	Tideglusib	<5.5	<chem>O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=CC=CC2=CC=C1</chem>
25	NEU-1007	PHA-793887	5.73	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>
26	NEU-1049	Harmine	<5.5	<chem>COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC=C1</chem>

Table S3. Human kinase potency data for the inhibitors of preferred human kinases and tested against protozoan pathogens and host cells.

NEU number	NEU-838	NEU-844	NEU-893	NEU-967	NEU-968	NEU-969
Name	Crizotinib ¹	TAE684 ²	GSK1838705A ³	NVP-AEW541 ⁴	BMS-265246 ⁵	PHA-848125 ⁶
T brucei EC50	0.432±0.075	0.1±0.046	1.98±0.083	1.82±0.348	0.457±0.163	0.027±0.0043
PIK1						
IGF-1R			0.002	0.15		
ALK	0.024	0.003	0.0005			
GSK-3α						
GSK-3β						
CDK1/cyc B					0.006	
CDK1						
CDK2						
CDK2/cyc E					0.009	0.363
CDK2/cyc A						0.045
CDK3/Cyc E						
CDK4						
CDK4/cyc D1					0.23	0.16
CDK5						
p35/CDK5						0.265
p25/CDK5						
CDK6						
CDK6/CycD3						
CDK7						
CDK7/cyc H						0.15
CDK9						
CDK9/cyc T						
Aurora-A						
Aurora-B						
CLK1						
CLK2						
CLK3						
CLK4						
DYRK1A						
DYRK1B						

NEU number	NEU-970	NEU-971	NEU-973	NEU-974	NEU-975
Name	GSK1904529A ⁷	JNJ-7706621 ⁸	ON-01910 ⁹	CH5424802 ¹⁰	Dinaciclib ¹¹
T brucei EC50	1.38±0.362	0.283±0.044	>3	>3	0.039±0.0056
PIK1			0.009		
IGF-1R	0.027				
ALK				0.0019	
GSK-3α					
GSK-3β					
CDK1/cyc B		0.009			
CDK1					0.003
CDK2					0.001
CDK2/cyc E		0.003			
CDK2/cyc A		0.004			
CDK3/Cyc E					
CDK4					
CDK4/cyc D1					
CDK5					
p35/CDK5					0.001
p25/CDK5					
CDK6					
CDK6/CycD3					
CDK7					
CDK7/cyc H					
CDK9					0.004
CDK9/cyc T					
Aurora-A		0.011			
Aurora-B		0.015			
CLK1					
CLK2					
CLK3					
CLK4					
DYRK1A					
DYRK1B					

NEU number	NEU-976	NEU-977	NEU-978	NEU-979	NEU-980
Name	Linsitinib ¹²	Roscovitine ¹³	CHIR-98014 ¹⁴	Volasertib ¹⁵	BI 2536 ¹⁶
T brucei EC50	>3	>3	>3	>3	0.6±0.091
PIK1				0.00087	0.00083
IGF-1R	0.035				
ALK					
GSK-3α			0.00065		
GSK-3β			0.00058		
CDK1/cyc B					
CDK1					
CDC/cyc B		0.65			
CDK2					
CDK2/cyc E		0.7			
CDK2/cyc A		0.7			
CDK3/Cyc E					
CDK4					
CDK4/cyc D1					
CDK5					
p35/CDK5		0.16			
p25/CDK5					
CDK6					
CDK6/CycD3					
CDK7					
CDK7/cyc H					
CDK9					
CDK9/cyc T					
Aurora-A					
Aurora-B					
CLK1					
CLK2					
CLK3					
CLK4					
DYRK1A					
DYRK1B					

NEU number	NEU-982	NEU-984	NEU-985	NEU-986	NEU-987
Name	AT7519 ¹⁷	SNS-032 ^{18, 19}	AZD5438 ²⁰	SB 415286 ²¹	Flavopiridol ²²
T brucei EC50	0.314±0.036	0.118±0.01	0.033±0.0027	0.89±0.684	0.177±0.072
PIK1					
IGF-1R					
ALK					
GSK-3α				0.078	
GSK-3β	0.089				
CDK1/cyc B	0.21		0.016		
CDK1		0.48			0.04
CDK2		0.038			0.04
CDK2/cyc E			0.006		
CDK2/cyc A	0.047	0.038	0.045		
CDK3/Cyc E	0.36	0.048			
CDK4		0.925			0.04
CDK4/cyc D1	0.1				
CDK5					
p35/CDK5	0.013				
p25/CDK5			0.014		
CDK6					0.04
CDK6/CycD3	0.17		0.021		
CDK7					
CDK7/cyc H		0.062	0.821		0.3
CDK9					
CDK9/cyc T		0.004	0.020		
Aurora-A					
Aurora-B					
CLK1					
CLK2					
CLK3					
CLK4					
DYRK1A					
DYRK1B					

NEU number	NEU-989	NEU-990	NEU-991	NEU-1007	NEU-1049
Name	TWS119 ²³	SB 216763 ²¹	Tideglusib ²⁴	PHA-793887 ²⁵	Harmine ²⁶
T brucei EC50	1.102±0.134	>3	>3	1.88±0.332	>3
PIK1					
IGF-1R					
ALK					
GSK-3α		0.0343			>10
GSK-3β	0.03		0.06	0.079	>10
CDK1/cyc B				0.06	18
CDK1					
CDK2					
CDK2/cyc E				0.008	
CDK2/cyc A				0.008	>30
CDK3/Cyc E					
CDK4					
CDK4/cyc D1				0.062	
CDK5					
p35/CDK5					
p25/CDK5				0.005	8
CDK6					
CDK6/CycD3					
CDK7					
CDK7/cyc H				0.01	>10
CDK9					
CDK9/cyc T				0.138	0.72
Aurora-A					
Aurora-B					
CLK1					0.072
CLK2					0.28
CLK3					>10
CLK4					0.05
DYRK1A					0.085
DYRK1B					0.028

Table S4. Tanimoto analysis of purchased compounds versus PKIS inhibitors of the same primary human kinase.

Cmpd	Inhibitor_SMILES	Primary Human Target	PKIS Compound >70% at 0.1 uM	PKIS_Parent_Smiles	Tanimoto
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK1173862A	<chem>CCCN1CCCC(C1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1</chem>	0.444095
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK2213727A	<chem>COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(Nc2cccc(F)c2C(N)=O)c2cc[nH]c2n1</chem>	0.435692
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK1326255A	<chem>CCCN1CCC(CC1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1</chem>	0.427394
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK2163632A	<chem>COc1cc2c(cc1Nc1nc(Nc3ccsc3C(N)=O)c3cc[nH]c3n1)N(CCC2(C)C)C(=O)CN(C)C</chem>	0.476852
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK2220400A	<chem>CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12</chem>	0.463869
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK2186269A	<chem>COc1cc2CCN(C(=O)CN(C)C)c2cc1Nc1nc(N2CCc3cccc23)c2cc[nH]c2n1</chem>	0.458775
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK1220512A	<chem>COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(N)=O)c2cc[nH]c2n1)N1CCN(CC1)C(C)C</chem>	0.427307
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK2110236A	<chem>COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1</chem>	0.461673
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK1392956A	<chem>COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(=O)NC[C@@H](O)CO)c2cc[nH]c2n1)N1CCN(CC1)C(C)C</chem>	0.445879
NEU-838	<chem>C[C@@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1=C(Cl)C=CC(F)=C1Cl</chem>	ALK	GSK994854A	<chem>CCCN1CCC=C(C1)c1ccc(Nc2nc(Nc3cccc3C(N)=O)c3cc[nH]c3n2)c(C)c1</chem>	0.398472
NEU-844	<chem>COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1</chem>	ALK	GSK1173862A	<chem>CCCN1CCCC(C1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1</chem>	0.512115
NEU-844	<chem>COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1</chem>	ALK	GSK2213727A	<chem>COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(Nc2cccc(F)c2C(N)=O)c2cc[nH]c2n1</chem>	0.530372
NEU-844	<chem>COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1</chem>	ALK	GSK1326255A	<chem>CCCN1CCC(CC1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1</chem>	0.512375
NEU-844	<chem>COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1</chem>	ALK	GSK2163632A	<chem>COc1cc2c(cc1Nc1nc(Nc3ccsc3C(N)=O)c3cc[nH]c3n1)N(CCC2(C)C)C(=O)CN(C)C</chem>	0.542444
NEU-844	<chem>COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1</chem>	ALK	GSK2220400A	<chem>CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12</chem>	0.524788
NEU-844	<chem>COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1</chem>	ALK	GSK2186269A	<chem>COc1cc2CCN(C(=O)CN(C)C)c2cc1Nc1nc(N2CCc3cccc23)c2cc[nH]c2n1</chem>	0.534238
NEU-844	<chem>COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1</chem>	ALK	GSK1220512A	<chem>COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(N)=O)c2cc[nH]c2n1)N1CCN(CC1)C(C)C</chem>	0.570637

	CN(C)CC1				
NEU-844	COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1	ALK	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1 nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	0.53865
NEU-844	COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1	ALK	GSK1392956A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(=O)N C[C@@H](O)CO)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.566689
NEU-844	COC1=CC(=CC=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1)N1CCC(CC1)N1C CN(C)CC1	ALK	GSK994854A	CCCN1CCC=C(C1)c1ccc(Nc2nc(Nc3cccc c3C(N)=O)c3cc[nH]c3n2)c(C)c1	0.454845
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK1173862A	CCCN1CCCC(C1)c1ccc(Nc2nc(Nc3cc(F) ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.737441
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK2213727A	COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(N c2cccc(F)c2C(N)=O)c2cc[nH]c2n1	0.875803
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK1326255A	CCCN1CCC(CC1)c1ccc(Nc2nc(Nc3cc(F) ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.72962
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK2163632A	COc1cc2c(cc1Nc1nc(Nc3ccsc3C(N)=O)c 3cc[nH]c3n1)N(CCC2(C)C)C(=O)CN(C)C	0.798484
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK2220400A	CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc 3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12	0.829857
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK2186269A	COc1cc2CCN(C(=O)CN(C)C)c2cc1Nc1nc (N2CCc3ccccc23)c2cc[nH]c2n1	0.832122
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK1220512A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(N)=O)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.736735
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1 nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	0.815995
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK1392956A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(=O)N C[C@@H](O)CO)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.75814
NEU-893	CNC(=O)C1=C(NC2=C3C=CNC3=NC(NC3=CC4 =C(CCN4C(=O)CN(C)C)C=C3OC)=N2)C=CC=C 1F	ALK	GSK994854A	CCCN1CCC=C(C1)c1ccc(Nc2nc(Nc3cccc c3C(N)=O)c3cc[nH]c3n2)c(C)c1	0.647059
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C 3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC= C1	IGF-1R	GSK1173862A	CCCN1CCCC(C1)c1ccc(Nc2nc(Nc3cc(F) ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.474952
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C	IGF-1R	GSK2213727A	COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(N	0.465839

	3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1			c2cccc(F)c2C(N)=O)c2cc[nH]c2n1	
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1	IGF-1R	GSK1326255A	CCCN1CCC(CC1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.46873
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1	IGF-1R	GSK2163632A	COc1cc2c(cc1Nc1nc(Nc3ccsc3C(N)=O)c3cc[nH]c3n1)N(CCC2(C)C)C(=O)CN(C)C	0.502914
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1	IGF-1R	GSK2220400A	CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12	0.498819
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1	IGF-1R	GSK2186269A	COc1cc2CCN(C(=O)CN(C)C)c2cc1Nc1nc(N2CCc3cccc23)c2cc[nH]c2n1	0.482534
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1	IGF-1R	GSK1220512A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(N)=O)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.45727
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1	IGF-1R	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	0.49674
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1	IGF-1R	GSK1392956A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(=O)N[C@@H](O)CO)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.473358
NEU-967	NC1=C2C(=CN([C@@H]3C[C@H](CN4CCC4)C3)C2=NC=N1)C1=CC(OCC2=CC=CC=C2)=CC=C1	IGF-1R	GSK994854A	CCCN1CCC=C(C1)c1ccc(Nc2nc(Nc3cccc3C(N)=O)c3cc[nH]c3n2)c(C)c1	0.461235
NEU-968	CCCCOC1=C2C=NNC2=NC=C1C(=O)C1=C(F)C=C(C)C=C1F	CDK1/cyc B	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.302113
NEU-968	CCCCOC1=C2C=NNC2=NC=C1C(=O)C1=C(F)C=C(C)C=C1F	CDK1/cyc B	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+](O-)=O)=CC=C3C)=O	0.377409
NEU-968	CCCCOC1=C2C=NNC2=NC=C1C(=O)C1=C(F)C=C(C)C=C1F	CDK1/cyc B	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.352594
NEU-968	CCCCOC1=C2C=NNC2=NC=C1C(=O)C1=C(F)C=C(C)C=C1F	CDK1/cyc B	GW806290X	C1COc2cc(Nc3nccc(n3)-c3cnn4ncccc34)ccc2O1	0.326923
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.404077
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+](O-)=O)=CC=C3C)=O	0.439955
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.492982
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW396574X	CC(C)=Cc1cccc2NC(=O)C(=N/Nc3ccc(cc3)S(N)(=O)=O)c12	0.43714

NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW290597X	NS(=O)(=O)c1ccc(N\N=C2/C(=O)Nc3ccc(cc23)C(=O)NCCc2ccnc2)cc1	0.45711
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW305178X	NS(=O)(=O)c1ccc(N\N=C2/C(=O)Nc3ccc4ncccc4c23)cc1	0.454702
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW589933X	NS(=O)(=O)c1ccc(NC=C2C(=O)Nc3ccc4ncsc4c23)cc1	0.488474
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW301784X	CC(C)(CO)CNC(=O)c1ccc2NC(=O)C(=N/Nc3ccc(cc3)S(N)(=O)=O)c2c1	0.439861
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW276655X	NS(=O)(=O)c1ccc(N\N=C2/C(=O)Nc3ccc(cc23)-c2cnco2)cc1	0.45879
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW300657X	NS(=O)(=O)c1ccc(N\N=C2/C(=O)Nc3ccc(cc23)C(=O)NCCc2ccncc2)cc1	0.440281
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW297361X	NS(=O)(=O)c1ccc(N\C=C2/C(=O)Nc3ccc4ncsc4c23)cc1	0.488474
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW416981X	CC(C)COC(=O)c1ccc2NC(=O)C(=C/Nc3ccc(cc3)S(N)(=O)=O)c2c1	0.422093
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW300660X	NS(=O)(=O)c1ccc(N\N=C2/C(=O)Nc3ccc(cc23)C(=O)NCCc2c[nH]cn2)cc1	0.459178
NEU-969	CNC(=O)C1=NN(C)C2=C1C(C)(C)CC1=CN=C(NC3=CC=C(C=C3)N3CCN(C)CC3)N=C21	CDK2/cyc A	GW810576X	COc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.402278
NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK1173862A	CCCN1CCCC(C1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.555866
NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK2213727A	COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(Nc2cccc(F)c2C(N)=O)c2cc[nH]c2n1	0.572225
NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK1326255A	CCCN1CCC(CC1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.541104
NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK2163632A	COc1cc2c(cc1Nc1nc(Nc3ccsc3C(N)=O)c3cc[nH]c3n1)N(CCC2(C)C)C(=O)CN(C)C	0.640389
NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK2220400A	CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12	0.625813
NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK2186269A	COc1cc2CCN(C(=O)CN(C)C)c2cc1Nc1nc(N2CCc3cccc23)c2cc[nH]c2n1	0.620011

NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK1220512A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(N)=O)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.561753
NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	0.626158
NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK1392956A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(=O)NC[C@@H](O)CO)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.586689
NEU-970	CCC1=CC(NC2=NC=CC(=N2)C2=C(N=C3C=CC=CN23)C2=CC(C(=O)NC3=C(F)C=CC=C3F)=C(OC)C=C2)=C(OC)C=C1N1CCC(CC1)N1CCN(C1)S(C)(=O)=O	IGF-1R	GSK994854A	CCCN1CCC=C(C1)c1ccc(Nc2nc(Nc3cccc3C(N)=O)c3cc[nH]c3n2)c(C)c1	0.49721
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.327977
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+])([O-])=O)=CC=C3C)=O	0.386286
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.358099
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	GW806290X	C1COc2cc(Nc3nccc(n3)-c3cnn4ncccc34)ccc2O1	0.331232
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	GW396574X	CC(C)=Cc1cccc2NC(=O)C(=N/Nc3ccc(cc3)S(N)(=O)=O)c12	0.378151
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	GW305178X	NS(=O)(=O)c1ccc(N/N=C2/C(=O)Nc3ccc4ncccc4c23)cc1	0.386364
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	GW589933X	NS(=O)(=O)c1ccc(NC=C2C(=O)Nc3ccc4ncsc4c23)cc1	0.40617
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	GW300657X	NS(=O)(=O)c1ccc(N/N=C2/C(=O)Nc3ccc(cc23)C(=O)NCc2ccncc2)cc1	0.380884
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	GW297361X	NS(=O)(=O)c1ccc(N/C=C2/C(=O)Nc3ccc4ncsc4c23)cc1	0.40617
NEU-971	NC1=NC(NC2=CC=C(C=C2)S(N)(=O)=O)=NN1C(=O)C1=C(F)C=CC=C1F	CDK2/cyc E	GW300660X	NS(=O)(=O)c1ccc(N/N=C2/C(=O)Nc3ccc(cc23)C(=O)NCc2c[nH]cn2)cc1	0.385149
NEU-972	COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+])([O-])C=C2)C=CC=C1	PLK1	GSK2213727A	COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(Nc2ccc(F)c2C(N)=O)c2cc[nH]c2n1	0.430979
NEU-972	COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+])([O-])C=C2)C=CC=C1	PLK1	GSK2220400A	CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12	0.440555
NEU-972	COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+])([O-])C=C2)C=CC=C1	PLK1	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	0.436441
NEU-972	COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+])([O-])C=C2)C=CC=C1	PLK1	GSK571989A	C[C@@H](OC1cc(sc1C(N)=O)-	0.401979

	<chem>\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>			<chem>n1cnc2ccc(OCC3CCN(C)CC3)cc12)c1ccc cc1Cl</chem>	
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GSK317315A	<chem>COc1ccc2ncn(- c3cc(O[C@H](C)c4ccccc4C(F)(F)F)c(s3) C(N)=O)c2c1</chem>	0.394393
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GSK237701A	<chem>COc1cc2ncn(- c3cc(O[C@H](C)c4ccccc4Cl)c(s3)C(N)=O c2cc1OC</chem>	0.397252
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GSK579289A	<chem>C[C@@H](Oc1cc(sc1C(N)=O)- n1cnc2ccc(OC3CCN(C)CC3)cc12)c1cccc c1Cl</chem>	0.395923
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GSK317314A	<chem>COc1ccc2ncn(- c3cc(O[C@H](C)c4ccccc4Cl)c(s3)C(N)=O c2c1</chem>	0.39103
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GW852849X	<chem>COc1cc2ncn(- c3cc(OCc4ccccc4Cl)c(s3)C(N)=O)c2cc1O C</chem>	0.38648
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GW843682X	<chem>COc1cc2ncn(- c3cc(OCc4ccccc4C(F)(F)F)c(s3)C(N)=O)c 2cc1OC</chem>	0.386751
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GSK978744A	<chem>C[C@@H](Oc1cc(sc1C(N)=O)- n1cnc2ccc(OC[C@H](O)CO)cc12)c1cc ccc1Cl</chem>	0.395392
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GSK326090A	<chem>C[C@@H](Oc1cc(sc1C(N)=O)- n1cnc2ccc(OCC3CCN(C)CC3)cc12)c1ccc cc1C(F)(F)F</chem>	0.405257
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GSK237700A	<chem>COc1cc2ncn(- c3cc(O[C@@H](C)c4ccccc4Cl)c(s3)C(N) =O)c2cc1OC</chem>	0.397252
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GSK312948A	<chem>COc1cc2ncn(- c3cc(OCc4cccs4)c(s3)C(N)=O)c2cc1OC</chem>	0.379576
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GW853606X	<chem>NC(=O)c1sc(cc1OCc1ccccc1Br)- n1cnc2ccc(cc12)C(F)(F)F</chem>	0.387716
NEU-972	<chem>COC1=CC=C(C=C1)S(=O)(=O)N(C(C)=O)C1=C(\C=C\C2=CC=[N+][([O-])C=C2]C=CC=C1</chem>	PLK1	GSK1023156A	<chem>NC(=O)c1sc(cc1OCc1ccccc1Br)- n1cnc2ccccc12</chem>	0.362376
NEU-973	<chem>COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(\OC)C(NCC(=O)O[Na])=C2)C(OC)=C1</chem>	PLK1	GSK2213727A	<chem>COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(N c2cccc(F)c2C(N)=O)c2cc[nH]c2n1</chem>	0.338076
NEU-973	<chem>COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(\OC)C(NCC(=O)O[Na])=C2)C(OC)=C1</chem>	PLK1	GSK2220400A	<chem>CNC(=O)c1cccc1Nc1nc(Nc2cc3N(CCCc 3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12</chem>	0.351317
NEU-973	<chem>COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(\OC)C(NCC(=O)O[Na])=C2)C(OC)=C1</chem>	PLK1	GSK2110236A	<chem>COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1 nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1</chem>	0.341693
NEU-973	<chem>COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(\OC)C(NCC(=O)O[Na])=C2)C(OC)=C1</chem>	PLK1	GSK571989A	<chem>C[C@@H](Oc1cc(sc1C(N)=O)- n1cnc2ccc(OCC3CCN(C)CC3)cc12)c1ccc cc1Cl</chem>	0.309723

NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GSK317315A	COc1ccc2ncn(-c3cc(O[C@H](C)c4ccccc4C(F)(F)F)c(s3)C(N)=O)c2c1	0.309602
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GSK237701A	COc1cc2ncn(-c3cc(O[C@H](C)c4ccccc4Cl)c(s3)C(N)=O)c2cc1OC	0.315824
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GSK579289A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OC3CCN(C)CC3)cc12)c1cccc1Cl	0.314527
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GSK317314A	COc1ccc2ncn(-c3cc(O[C@H](C)c4ccccc4Cl)c(s3)C(N)=O)c2c1	0.309176
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GW852849X	COc1cc2ncn(-c3cc(OCc4ccccc4Cl)c(s3)C(N)=O)c2cc1OC	0.311486
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GW843682X	COc1cc2ncn(-c3cc(OCc4ccccc4C(F)(F)F)c(s3)C(N)=O)c2cc1OC	0.309127
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GSK978744A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OC[C@@H](O)CO)cc12)c1ccc1Cl	0.312418
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GSK326090A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OC3CCN(C)CC3)cc12)c1ccc1C(F)(F)F	0.312579
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GSK237700A	COc1cc2ncn(-c3cc(O[C@@H](C)c4ccccc4Cl)c(s3)C(N)=O)c2cc1OC	0.315824
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GSK312948A	COc1cc2ncn(-c3cc(OCc4cccs4)c(s3)C(N)=O)c2cc1OC	0.305385
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GW853606X	NC(=O)c1sc(cc1OCc1ccccc1Br)-n1cnc2ccc(cc12)C(F)(F)F	0.297587
NEU-973	COC1=CC(OC)=C(\C=C\S(=O)(=O)CC2=CC=C(OC)C(NCC(=O)O[Na])=C2)C(OC)=C1	PLK1	GSK1023156A	NC(=O)c1sc(cc1OCc1ccccc1Br)-n1cnc2ccccc12	0.28042
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK1173862A	CCCN1CCCC(C1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.5
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK2213727A	COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(Nc2cccc(F)c2C(N)=O)c2cc[nH]c2n1	0.502278
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK1326255A	CCCN1CCC(CC1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.486911
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK2163632A	COc1cc2c(cc1Nc1nc(Nc3ccsc3C(N)=O)c3cc[nH]c3n1)N(CCC2(C)C)C(=O)CN(C)C	0.581949
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK2220400A	CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12	0.573743
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK2186269A	COc1cc2CCN(C(=O)CN(C)C)c2cc1Nc1nc	0.555928

	C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O			(N2CCc3ccccc23)c2cc[nH]c2n1	
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK1220512A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(N)=O)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.488386
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	0.563302
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK1392956A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(=O)N C[C@@H](O)CO)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.520321
NEU-974	CCC1=CC2=C(C=C1N1CCC(CC1)N1CCOCC1)C(C)(C)C1=C(C3=CC=C(C=C3N1)C#N)C2=O	ALK	GSK994854A	CCCN1CCC=C(C1)c1ccc(Nc2nc(Nc3ccccc3C(N)=O)c3cc[nH]c3n2)c(C)c1	0.471765
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK1173862A	CCCN1CCCC(C1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.421308
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK2213727A	COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(Nc2ccc(F)c2C(N)=O)c2cc[nH]c2n1	0.418702
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK1326255A	CCCN1CCC(CC1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.405009
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK2163632A	COc1cc2c(cc1Nc1nc(Nc3ccsc3C(N)=O)c3cc[nH]c3n1)N(CCC2(C)C)C(=O)CN(C)C	0.471986
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK2220400A	CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12	0.460091
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK2186269A	COc1cc2CCN(C(=O)CN(C)C)c2cc1Nc1nc(N2CCc3ccccc23)c2cc[nH]c2n1	0.452559
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK1220512A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(N)=O)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.411009
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	0.460436
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK1392956A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(=O)N C[C@@H](O)CO)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.430274
NEU-976	C[C@@]1(O)C[C@@H](C1)C1=NC(=C2N1C=C N=C2N)C1=CC=C2C=CC(=NC2=C1)C1=CC=CC=C1	IGF-1R	GSK994854A	CCCN1CCC=C(C1)c1ccc(Nc2nc(Nc3ccccc3C(N)=O)c3cc[nH]c3n2)c(C)c1	0.394165
NEU-977	CC[C@H](CO)NC1=NC(NCC2=CC=CC=C2)=C2N=CN(C(C)C)C2=N1	CDK1/cyc B	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.301565
NEU-977	CC[C@H](CO)NC1=NC(NCC2=CC=CC=C2)=C2N=CN(C(C)C)C2=N1	CDK1/cyc B	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+][O-])=O)=CC=C3C	0.340731

				=O	
NEU-977	CC[C@H](CO)NC1=NC(NCC2=CC=CC=C2)=C2 N=CN(C(C)C)C2=N1	CDK1/cyc B	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)- c2cnn3ncccc23)cc1C(F)(F)F	0.340118
NEU-977	CC[C@H](CO)NC1=NC(NCC2=CC=CC=C2)=C2 N=CN(C(C)C)C2=N1	CDK1/cyc B	GW806290X	C1COc2cc(Nc3nccc(n3)- c3cnn4ncccc34)ccc2O1	0.314777
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	GW778894X	N#Cc1cccc(Nc2nccc(n2)- c2cnn3ncccc23)c1	0.398459
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br) C=C2)(C3=CC([N+])([O-])=O)=CC=C3C) =O	0.392476
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)- c2cnn3ncccc23)cc1C(F)(F)F	0.444081
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	GW806290X	C1COc2cc(Nc3nccc(n3)- c3cnn4ncccc34)ccc2O1	0.405405
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	SB-698596-AC	CCN1CCC(CC(=O)Nc2n[nH]c3nnc(cc23)- c2cccc(F)c2F)CC1	0.349839
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	GW784752X	COc1cccc(c1)- n1ncc2c(N\N=C\c3ccncc3)ncnc12	0.361549
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	SB-686709-A	CCN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc 12)-c1cccc(F)c1F	0.355499
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	SB-725317	Oc1ccc(cc1)- c1nc2[nH]nc(NC(=O)C3CC3)c2cc1Br	0.40758
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	SB-675259-M	O=C(Nc1n[nH]c2nnc(cc12)- c1ccnc1)C1CC1	0.322408
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	SB-732881-H	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br) cc12)-c1ccc(O)cc1	0.415796
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	SB-678557-A	CN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc1 2)-c1cccc1	0.31745
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	GW814408X	COc1cccc(c1)- c1c[nH]c2c(N\N=C\c3ccncc3)ncnc12	0.365176
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	SB-732881	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br) cc12)-c1ccc(O)cc1	0.415796
NEU-978	NC1=NC(NCCNC2=NC(=C(C=N2)N2C=CN=C2) C2=CC=C(CI)C=C2Cl)=CC=C1N(=O)=O	GSK-3b	GW811168X	COc1cccc(c1)- n1ncc2c(N\N=C\c3ccc(cc3)S(C)(=O)=O)n cnc12	0.386701
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O C)C(=O)N[C@H]3CC[C@H](CC3)N3CCN(CC4 CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK2213727A	COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(N c2cccc(F)c2C(N)=O)c2cc[nH]c2n1	0.556368
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O C)C(=O)N[C@H]3CC[C@H](CC3)N3CCN(CC4 CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK2220400A	CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc 3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12	0.598246
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O C)C(=O)N[C@H]3CC[C@H](CC3)N3CCN(CC4 CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1 nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	0.600353

NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK571989A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OCC3CCN(C)CC3)cc12)c1ccc cc1Cl	0.490588
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK317315A	COc1ccc2ncn(-c3cc(O[C@H](C)c4ccccc4C(F)(F)F)c(s3)C(N)=O)c2c1	0.479107
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK237701A	COc1cc2ncn(-c3cc(O[C@H](C)c4ccccc4Cl)c(s3)C(N)=O)c2cc1OC	0.476
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK579289A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OC3CCN(C)CC3)cc12)c1ccc c1Cl	0.485747
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK317314A	COc1ccc2ncn(-c3cc(O[C@H](C)c4ccccc4Cl)c(s3)C(N)=O)c2c1	0.470283
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GW852849X	COc1cc2ncn(-c3cc(OCc4ccccc4Cl)c(s3)C(N)=O)c2cc1O C	0.460023
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GW843682X	COc1cc2ncn(-c3cc(OCc4ccccc4C(F)(F)F)c(s3)C(N)=O)c2cc1OC	0.467975
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK978744A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OC[C@@H](O)CO)cc12)c1cc ccc1Cl	0.479977
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK326090A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OCC3CCN(C)CC3)cc12)c1ccc cc1C(F)(F)F	0.496041
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK237700A	COc1cc2ncn(-c3cc(O[C@H](C)c4ccccc4Cl)c(s3)C(N)=O)c2cc1OC	0.476
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK312948A	COc1cc2ncn(-c3cc(OCc4ccccc4)c(s3)C(N)=O)c2cc1OC	0.450844
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GW853606X	NC(=O)c1sc(cc1OCc1ccccc1Br)-n1cnc2ccc(cc12)C(F)(F)F	0.463912
NEU-979	CC[C@H]1N(C(C)C)C2=NC(NC3=CC=C(C=C3O)C(=O)N[C@H]3CC[C@@H](CC3)N3CCN(CC4CC4)CC3)=NC=C2N(C)C1=O	PLK1	GSK1023156A	NC(=O)c1sc(cc1OCc1ccccc1Br)-n1cnc2ccccc12	0.434524
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK2213727A	COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(Nc2cccc(F)c2C(N)=O)c2cc[nH]c2n1	0.551681
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK2220400A	CNC(=O)c1ncccc1Nc1nc(Nc2cc3N(CCCc3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12	0.588935
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1	0.583433

	OC)C(=O)NC3CCN(C)CC3=N2)N(C)C1=O			nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK571989A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OC3CCN(C)CC3)cc12)c1ccc cc1Cl	0.472014
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK317315A	COc1ccc2ncn(-c3cc(O[C@H](C)c4ccccc4C(F)(F)F)c(s3)C(N)=O)c2c1	0.456961
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK237701A	COc1cc2ncn(-c3cc(O[C@H](C)c4ccccc4Cl)c(s3)C(N)=O)c2cc1OC	0.458068
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK579289A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OC3CCN(C)CC3)cc12)c1cccc c1Cl	0.467975
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK317314A	COc1ccc2ncn(-c3cc(O[C@H](C)c4ccccc4Cl)c(s3)C(N)=O)c2c1	0.452103
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GW852849X	COc1cc2ncn(-c3cc(OCc4ccccc4Cl)c(s3)C(N)=O)c2cc1OC	0.442488
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GW843682X	COc1cc2ncn(-c3cc(OCc4ccccc4C(F)(F)F)c(s3)C(N)=O)c2cc1OC	0.448075
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK978744A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OC[C@@H](O)CO)cc12)c1ccc cc1Cl	0.458694
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK326090A	C[C@@H](Oc1cc(sc1C(N)=O)-n1cnc2ccc(OC3CCN(C)CC3)cc12)c1ccc cc1C(F)(F)F	0.474315
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK237700A	COc1cc2ncn(-c3cc(O[C@@H](C)c4ccccc4Cl)c(s3)C(N)=O)c2cc1OC	0.458068
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK312948A	COc1cc2ncn(-c3cc(OCc4cccs4)c(s3)C(N)=O)c2cc1OC	0.434808
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GW853606X	NC(=O)c1sc(cc1OCc1ccccc1Br)-n1cnc2ccc(cc12)C(F)(F)F	0.445492
NEU-980	CC[C@H]1N(C)C2=C(C=NC(NC3=CC=C(C=C3OC)C(=O)NC3CCN(C)CC3)=N2)N(C)C1=O	PLK1	GSK1023156A	NC(=O)c1sc(cc1OCc1ccccc1Br)-n1cnc2ccccc12	0.417874
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK1173862A	CCCN1CCCC(C1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.387378
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK2213727A	COc1cc(C)c(NC(=O)CN(C)C)cc1Nc1nc(Nc2cccc(F)c2C(N)=O)c2cc[nH]c2n1	0.386536
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK1326255A	CCCN1CCC(CC1)c1ccc(Nc2nc(Nc3cc(F)ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1	0.389567
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK2163632A	COc1cc2c(cc1Nc1nc(Nc3ccsc3C(N)=O)c	0.404564

				3cc[nH]c3n1)N(CCC2(C)C)C(=O)CN(C)C	
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK2220400A	CNC(=O)c1cccc1Nc1nc(Nc2cc3N(CCCc3cc2OC)C(=O)CN(C)C)nc2[nH]ccc12	0.394984
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK2186269A	COc1cc2CCN(C(=O)CN(C)C)c2cc1Nc1nc(N2CCc3cccc23)c2cc[nH]c2n1	0.393082
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK1220512A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(N)=O)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.375278
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK2110236A	COc1cc2CCCN(C(=O)CN(C)C)c2cc1Nc1nc(Nc2ccsc2C(N)=O)c2cc[nH]c2n1	0.398953
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK1392956A	COc1cc(ccc1Nc1nc(Nc2ccc(F)cc2C(=O)NC[C@@H](O)CO)c2cc[nH]c2n1)N1CCN(CC1)C(C)C	0.382863
NEU-981	CC(C)(C)C1=C(O)C(Br)=CC(C=C(C#N)C#N)=C1	IGF-1R	GSK994854A	CCCN1CCC=C(C1)c1ccc(Nc2nc(Nc3cccc3C(N)=O)c3cc[nH]c3n2)c(C)c1	0.40389
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.265042
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+]([O-])=O)=CC=C3C)=O	0.293754
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)F	0.308176
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW396574X	CC(C)=Cc1cccc2NC(=O)C(=N/Nc3ccc(cc3)S(N)(=O)=O)c12	0.295422
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW290597X	NS(=O)(=O)c1ccc(N/N=C2/C(=O)Nc3ccc(cc23)C(=O)NCCn2ccnc2)cc1	0.332853
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW305178X	NS(=O)(=O)c1ccc(N/N=C2/C(=O)Nc3ccc4ncccc4c23)cc1	0.303371
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW589933X	NS(=O)(=O)c1ccc(NC=C2C(=O)Nc3ccc4nsc4c23)cc1	0.319688
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW301784X	CC(C)(CO)CNC(=O)c1ccc2NC(=O)C(=N/Nc3ccc(cc3)S(N)(=O)=O)c2c1	0.335067
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW276655X	NS(=O)(=O)c1ccc(N/N=C2/C(=O)Nc3ccc(cc23)-c2cnc2)cc1	0.312988
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW300657X	NS(=O)(=O)c1ccc(N/N=C2/C(=O)Nc3ccc(cc23)C(=O)NCCc2ccnc2)cc1	0.321694
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW297361X	NS(=O)(=O)c1ccc(N/C=C2/C(=O)Nc3ccc4nsc4c23)cc1	0.319688
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW416981X	CC(C)COC(=O)c1ccc2NC(=O)C(=C/Nc3ccc(cc3)S(N)(=O)=O)c2c1	0.284571
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW300660X	NS(=O)(=O)c1ccc(N/N=C2/C(=O)Nc3ccc(cc23)C(=O)NCCc2c[nH]cn2)cc1	0.329718
NEU-982	C1C1=CC=CC(Cl)=C1C(=O)NC1=CN=C1C(=O)NC1CCNCC1	CDK2/cyc A	GW810576X	COc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.252266
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(CDK2/cyc E	GW778894X	N#Cc1cccc(Nc2nccc(n2)-	0.421924

	C=C2)S(C)(=O)=O)=N1			c2cnn3ncccc23)c1	
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1	CDK2/cyc E	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+][O-])=O)=CC=C3C)=O	0.354041
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1	CDK2/cyc E	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.426346
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1	CDK2/cyc E	GW806290X	C1COc2cc(Nc3nccc(n3)-c3cnn4ncccc34)ccc2O1	0.435312
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1	CDK2/cyc E	GW396574X	CC(C)=Cc1cccc2NC(=O)C(=N/Nc3ccc(cc3)S(N)(=O)=O)c12	0.367647
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1	CDK2/cyc E	GW305178X	NS(=O)(=O)c1ccc(NN=C2/C(=O)Nc3ccc4ncccc4c23)cc1	0.376033
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1	CDK2/cyc E	GW589933X	NS(=O)(=O)c1ccc(NC=C2C(=O)Nc3ccc4ncsc4c23)cc1	0.380559
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1	CDK2/cyc E	GW300657X	NS(=O)(=O)c1ccc(NN=C2/C(=O)Nc3ccc(cc23)C(=O)NCc2ccncc2)cc1	0.355681
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1	CDK2/cyc E	GW297361X	NS(=O)(=O)c1ccc(NC=C2/C(=O)Nc3ccc4ncsc4c23)cc1	0.380559
NEU-985	CC(C)N1C(C)=NC=C1C1=CC=NC(NC2=CC=C(C=C2)S(C)(=O)=O)=N1	CDK2/cyc E	GW300660X	NS(=O)(=O)c1ccc(NN=C2/C(=O)Nc3ccc(cc23)C(=O)NCc2c[nH]cn2)cc1	0.358711
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.337893
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+][O-])=O)=CC=C3C)=O	0.394754
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.396263
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	GW806290X	C1COc2cc(Nc3nccc(n3)-c3cnn4ncccc34)ccc2O1	0.364793
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	SB-698596-AC	CCN1CCC(CC(=O)Nc2n[nH]c3nnc(cc23)-c2cccc(F)c2F)CC1	0.338101
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	GW784752X	COc1cccc(c1)-n1ncc2c(NN=C1c3ccncc3)ncnc12	0.34702
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	SB-686709-A	CCN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc(F)c1F	0.339562
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	SB-725317	Oc1ccc(cc1)-c1nc2[nH]nc(NC(=O)C3CC3)c2cc1Br	0.365789
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	SB-675259-M	O=C(Nc1n[nH]c2nnc(cc12)-c1cccnc1)C1CC1	0.302826
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	SB-732881-H	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br)cc12)-c1ccc(O)cc1	0.380026
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	SB-678557-A	CN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc1	0.31105
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	GW814408X	COc1cccc(c1)-	0.337398

	CC=C2)N(=O)=O)C=C1			c1c[nH]c2c(N/N=C\c3ccncc3)ncnc12	
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	SB-732881	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br)cc12)-c1ccc(O)cc1	0.380026
NEU-986	OC1=C(CI)C=C(CC2=C(C(=O)NC2=O)C2=C(C=CC=C2)N(=O)=O)C=C1	GSK-3b	GW811168X	COc1cccc(c1)-n1ncc2c(N/N=C\c3ccc(cc3)S(C)(=O)=O)ncnc12	0.371745
NEU-987	CN1CC[C@@H]([C@H](O)C1)C1=C(O)C=C(O)C2=C1OC(=CC2=O)C1=CC=CC=C1C	CDK1/cyc B	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.346926
NEU-987	CN1CC[C@@H]([C@H](O)C1)C1=C(O)C=C(O)C2=C1OC(=CC2=O)C1=CC=CC=C1C	CDK1/cyc B	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+]([O-])=O)=CC=C3C)=O	0.388554
NEU-987	CN1CC[C@@H]([C@H](O)C1)C1=C(O)C=C(O)C2=C1OC(=CC2=O)C1=CC=CC=C1C	CDK1/cyc B	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.409594
NEU-987	CN1CC[C@@H]([C@H](O)C1)C1=C(O)C=C(O)C2=C1OC(=CC2=O)C1=CC=CC=C1C	CDK1/cyc B	GW806290X	C1COc2cc(Nc3nccc(n3)-c3cnn4ncccc34)ccc2O1	0.372226
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.335387
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+]([O-])=O)=CC=C3C)=O	0.353454
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.392144
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	GW806290X	C1COc2cc(Nc3nccc(n3)-c3cnn4ncccc34)ccc2O1	0.348806
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	SB-698596-AC	CCN1CCC(CC(=O)Nc2n[nH]c3nnc(cc23)-c2cccc(F)c2F)CC1	0.345347
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	GW784752X	COc1cccc(c1)-n1ncc2c(N/N=C\c3ccncc3)ncnc12	0.326144
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	SB-686709-A	CCN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc(F)c1F	0.35733
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	SB-725317	Oc1ccc(cc1)-c1nc2[nH]nc(NC(=O)C3CC3)c2cc1Br	0.356254
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	SB-675259-M	O=C(Nc1n[nH]c2nnc(cc12)-c1cccnc1)C1CC1	0.324417
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	SB-732881-H	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br)cc12)-c1ccc(O)cc1	0.373221
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	SB-678557-A	CN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc1	0.327562
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	GW814408X	COc1cccc(c1)-c1c[nH]c2c(N/N=C\c3ccncc3)ncnc12	0.32059
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	SB-732881	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br)cc12)-c1ccc(O)cc1	0.373221
NEU-988	O=C1NC2=C(C=CC=C2)C1=C1\NC2=CC=CC=C2C1=O	GSK-3b	GW811168X	COc1cccc(c1)-n1ncc2c(N/N=C\c3ccc(cc3)S(C)(=O)=O)n	0.345711

				cnc12	
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.353834
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+][O-])=O)=CC=C3C)=O	0.322536
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.362402
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	GW806290X	C1COc2cc(Nc3nccc(n3)-c3cnn4ncccc34)ccc2O1	0.363497
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	SB-698596-AC	CCN1CCC(CC(=O)Nc2n[nH]c3nnc(cc23)-c2cccc(F)c2F)CC1	0.368621
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	GW784752X	COc1cccc(c1)-n1ncc2c(N\N=C\c3ccncc3)ncnc12	0.322148
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	SB-686709-A	CCN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc(F)c1F	0.372075
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	SB-725317	Oc1ccc(cc1)-c1nc2[nH]nc(NC(=O)C3CC3)c2cc1Br	0.4213
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	SB-675259-M	O=C(Nc1n[nH]c2nnc(cc12)-c1cccnc1)C1CC1	0.354082
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	SB-732881-H	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br)cc12)-c1ccc(O)cc1	0.420852
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	SB-678557-A	CN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc1	0.351505
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	GW814408X	COc1cccc(c1)-c1c[nH]c2c(N\N=C\c3ccncc3)ncnc12	0.371497
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	SB-732881	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br)cc12)-c1ccc(O)cc1	0.420852
NEU-989	NC1=CC=CC(=C1)C1=CC2=C(OC3=CC=CC(O)=C3)N=CN=C2N1	GSK-3b	GW811168X	COc1cccc(c1)-n1ncc2c(N\N=C\c3ccc(cc3)S(C)(=O)=O)ncnc12	0.323297
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.339806
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+][O-])=O)=CC=C3C)=O	0.411692
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.401106
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	GW806290X	C1COc2cc(Nc3nccc(n3)-c3cnn4ncccc34)ccc2O1	0.361796
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	SB-698596-AC	CCN1CCC(CC(=O)Nc2n[nH]c3nnc(cc23)-c2cccc(F)c2F)CC1	0.379924
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	GW784752X	COc1cccc(c1)-n1ncc2c(N\N=C\c3ccncc3)ncnc12	0.367282

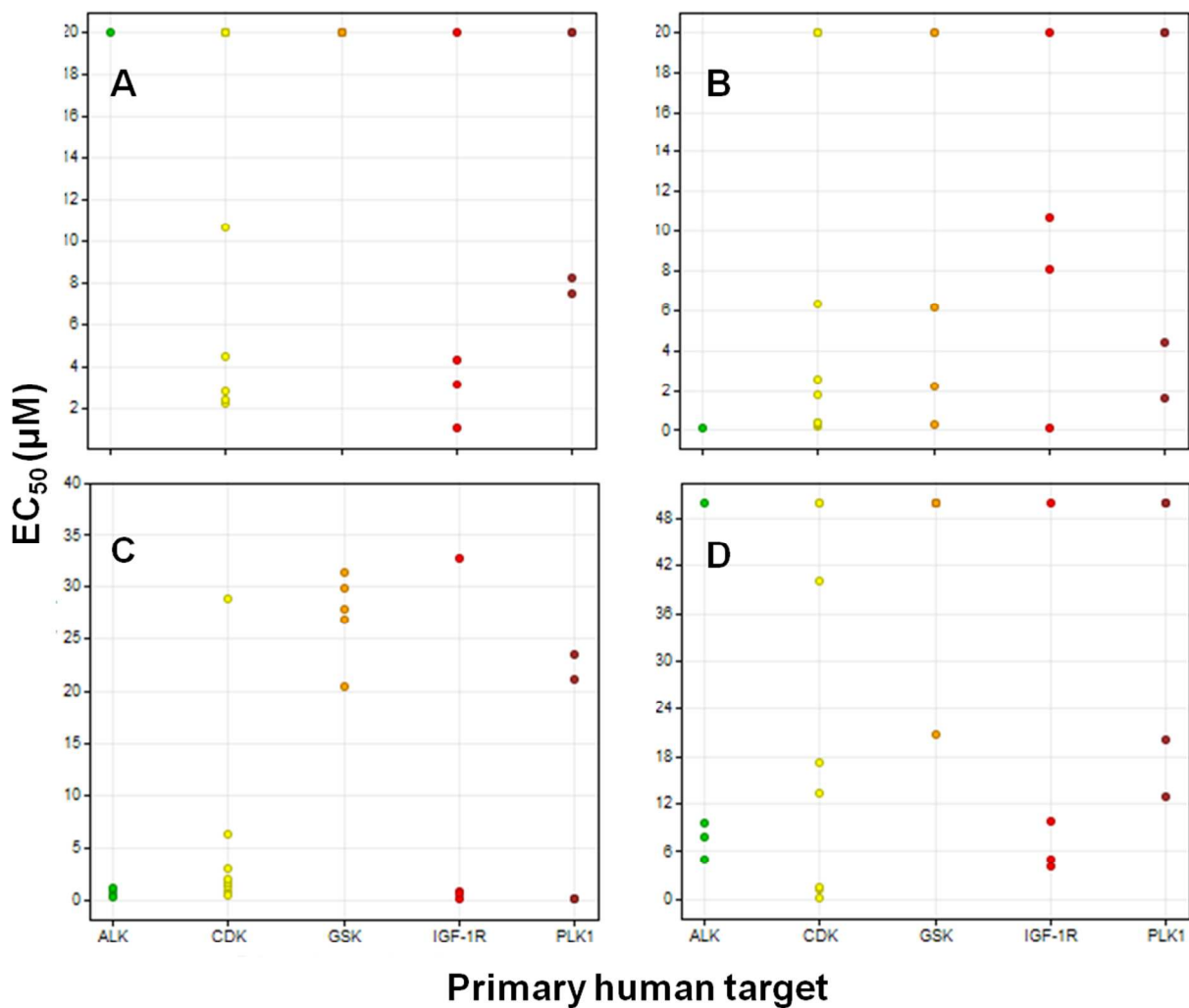
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	SB-686709-A	CCN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc(F)c1F	0.38447
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	SB-725317	Oc1ccc(cc1)-c1nc2[nH]nc(NC(=O)C3CC3)c2cc1Br	0.373041
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	SB-675259-M	O=C(Nc1n[nH]c2nnc(cc12)-c1cccnc1)C1CC1	0.342502
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	SB-732881-H	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br)cc12)-c1ccc(O)cc1	0.391682
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	SB-678557-A	CN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc1	0.340355
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	GW814408X	COc1cccc(c1)-c1c[nH]c2c(N\N=C\c3ccncc3)ncnc12	0.350582
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	SB-732881	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br)cc12)-c1ccc(O)cc1	0.391682
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	GW811168X	COc1cccc(c1)-n1nc2c(N\N=C\c3ccc(cc3)S(C)(=O)=O)ncnc12	0.381219
NEU-990	CN1C=C(C2=CC=CC=C12)C1=C(C(=O)NC1=O)C1=C(CI)C=C(CI)C=C1	GSK-3a	GW784307A	COc1cccc(c1)-n1nc2c(N\N=C\c3ccc(cc3)C(=O)NCCN(C)C)ncnc12	0.397286
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	GW778894X	N#Cc1cccc(Nc2nccc(n2)-c2cnn3ncccc23)c1	0.286136
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	PI_3-K_Inhibitor_VIII	O=S(N(C)/N=C/C1=CN=C2N1C=C(Br)C=C2)(C3=CC([N+])([O-])=O)=CC=C3C)=O	0.325253
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	GW779439X	CN1CCN(CC1)c1ccc(Nc2nccc(n2)-c2cnn3ncccc23)cc1C(F)(F)F	0.315612
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	GW806290X	C1COc2cc(Nc3nccc(n3)-c3cnn4ncccc34)ccc2O1	0.290254
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	SB-698596-AC	CCN1CCC(CC(=O)Nc2n[nH]c3nnc(cc23)-c2cccc(F)c2F)CC1	0.290909
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	GW784752X	COc1cccc(c1)-n1nc2c(N\N=C\c3ccncc3)ncnc12	0.329927
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	SB-686709-A	CCN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc(F)c1F	0.298331
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	SB-725317	Oc1ccc(cc1)-c1nc2[nH]nc(NC(=O)C3CC3)c2cc1Br	0.318246
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	SB-675259-M	O=C(Nc1n[nH]c2nnc(cc12)-c1cccnc1)C1CC1	0.275148
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	SB-732881-H	CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br)cc12)-c1ccc(O)cc1	0.325035
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	SB-678557-A	CN1CCC(CC1)C(=O)Nc1n[nH]c2nnc(cc12)-c1cccc1	0.270431
NEU-991	O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1	GSK-3b	GW814408X	COc1cccc(c1)-	0.283321

	<chem>C=CC2=CC=C1</chem>			<chem>c1c[nH]c2c(N\N=C\c3ccncc3)ncnc12</chem>	
NEU-991	<chem>O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1</chem>	GSK-3b	SB-732881	<chem>CN1CCC(CC1)C(=O)Nc1n[nH]c2nc(c(Br) cc12)-c1ccc(O)cc1</chem>	0.325035
NEU-991	<chem>O=C1SN(C(=O)N1CC1=CC=CC=C1)C1=C2C=C C=CC2=CC=C1</chem>	GSK-3b	GW811168X	<chem>COc1cccc(c1)- n1ncc2c(N\N=C\c3ccc(cc3)S(C)(=O)=O)n cnc12</chem>	0.344925
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	GW778894X	<chem>N#Cc1cccc(Nc2nccc(n2)- c2cnn3ncccc23)c1</chem>	0.345419
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	PI_3-K_Inhibitor_VIII	<chem>O=S(N(C)/N=C/C1=CN=C2N1C=C(Br) C=C2)(C3=CC([N+][O-])=O)=CC=C3C) =O</chem>	0.399876
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	GW779439X	<chem>CN1CCN(CC1)c1ccc(Nc2nccc(n2)- c2cnn3ncccc23)cc1C(F)(F)F</chem>	0.410144
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	GW806290X	<chem>C1COc2cc(Nc3nccc(n3)- c3cnn4ncccc34)ccc2O1</chem>	0.367675
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	GW396574X	<chem>CC(C)=Cc1cccc2NC(=O)\C(=N/Nc3ccc(cc 3)S(N)(=O)=O)c12</chem>	0.404487
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	GW305178X	<chem>NS(=O)(=O)c1ccc(N\N=C2/C(=O)Nc3ccc 4ncccc4c23)cc1</chem>	0.407174
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	GW589933X	<chem>NS(=O)(=O)c1ccc(NC=C2C(=O)Nc3ccc4 ncsc4c23)cc1</chem>	0.414906
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	GW300657X	<chem>NS(=O)(=O)c1ccc(N\N=C2/C(=O)Nc3ccc(cc23)C(=O)NCc2ccncc2)cc1</chem>	0.392005
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	GW297361X	<chem>NS(=O)(=O)c1ccc(N\C=C2/C(=O)Nc3ccc 4ncsc4c23)cc1</chem>	0.414906
NEU-1007	<chem>CC(C)CC(=O)NC1=NNC2=C1CN(C(=O)C1CCN(C)CC1)C2(C)C</chem>	CDK2/cyc E	GW300660X	<chem>NS(=O)(=O)c1ccc(N\N=C2/C(=O)Nc3ccc(cc23)C(=O)NCc2c[nH]cn2)cc1</chem>	0.416082
NEU-1049	<chem>COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC=C1</chem>	DYRK1B	GSK1173862A	<chem>CCCN1CCCC(C1)c1ccc(Nc2nc(Nc3cc(F) ccc3C(N)=O)c3cc[nH]c3n2)c(OC)c1</chem>	0.424731
NEU-1049	<chem>COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC=C1</chem>	DYRK1B	GW778894X	<chem>N#Cc1cccc(Nc2nccc(n2)- c2cnn3ncccc23)c1</chem>	0.403681
NEU-1049	<chem>COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC=C1</chem>	DYRK1B	PI_3-K_Inhibitor_VIII	<chem>O=S(N(C)/N=C/C1=CN=C2N1C=C(Br) C=C2)(C3=CC([N+][O-])=O)=CC=C3C) =O</chem>	0.430839
NEU-1049	<chem>COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC=C1</chem>	DYRK1B	GW779439X	<chem>CN1CCN(CC1)c1ccc(Nc2nccc(n2)- c2cnn3ncccc23)cc1C(F)(F)F</chem>	0.435576
NEU-1049	<chem>COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC=C1</chem>	DYRK1B	GW806290X	<chem>C1COc2cc(Nc3nccc(n3)- c3cnn4ncccc34)ccc2O1</chem>	0.412941
NEU-1049	<chem>COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC=C1</chem>	DYRK1B	GW810576X	<chem>COc1cccc(Nc2nccc(n2)- c2cnn3ncccc23)c1</chem>	0.407862
NEU-1049	<chem>COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC=C1</chem>	DYRK1B	5-Iodotubercidin	<chem>C1=C(C2=C(N1C3C(C(C(O3)CO)O)O)N= CN=C2N)I</chem>	0.425439
NEU-1049	<chem>COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC=C1</chem>	DYRK1B	GW801372X	<chem>COc1cc(Nc2nccc(n2)- c2cnn3ncccc23)cc(OC)c1</chem>	0.410475

Figure S1. Contingency table analysis

		Human kinase % inhibition		
		Active (≥ 70 %inh/0.1 μ M)	Inactive (< 70 %inh/0.1 μ M)	
T. brucei pEC ₅₀	Higher (\geq cutoff)	T. brucei (+) Kinase (+) Number of compounds with T. brucei pEC ₅₀ and Human kinase % of inhibition above the two cut-off (A)	T. brucei (+) Kinase (-) Number of compounds with T. brucei pEC ₅₀ above the cut-off and Human kinase % of inhibition below the cut-off (B)	Sum of compounds with T. Brucei pIC ₅₀ above the cut-off (G) (G=A+B)
	Lower ($<$ cutoff)	T. brucei (-) Kinase (+) Number of compounds with T. brucei pEC ₅₀ below the cut-off and Human kinase % of inhibition above the cut-off (C)	T. brucei (-) Kinase (-) Number of compounds with T. brucei pEC ₅₀ and Human kinase % of inhibition below the two cut-off (D)	Sum of compounds with T. Brucei pIC ₅₀ below the cut-off (H) (H=C+D)
	Sum of compounds with activity above the considered kinase (E) (E=A+C)		Sum of compounds with activity below the considered kinase (F) (F=B+D)	

Figure S2. “Preferred” human kinase inhibitors that are enriched for activity against *T. brucei* are not enriched against *Leishmania major* (A) amastigotes or (B) promastigotes; (C) *T. cruzi*; or (D) *Plasmodium falciparum*.



Example contingency table analysis. We describe here a contingency table analysis, exemplified by that performed on the human kinase DYRK1B. In this case, we have six compounds with a % inhibition of DYRK1B $\geq 70\%$ (the definition of “Active” compounds against the human kinase), and these six compounds also show a *T. brucei* $pEC_{50} \geq 6$ (The definition of “Active” compounds against *T. brucei*.) The table below represents the contingency table for DYRK1B for the full set of compounds in Table 1. Note that 1 was added to each compound count in order to avoid zeros in any quadrant, which would provide a null ratio.

Figure S3. Contingency table analysis for DYRK1B.

		DYRK1B % inhibition		Total
		Active	Inactive	
<i>T. brucei</i> pEC_{50}	Active	<i>T. brucei</i> (+) DYRK1B (+) 6+1=7	<i>T. brucei</i> (+) DYRK1B (-) 53-(6+1)=46	53
	Inactive	<i>T. brucei</i> (-) DYRK1B (+) 0+1=1	<i>T. brucei</i> (-) DYRK1B (-) 365-(53-1)=311	312
Total		8	357	365

On this table we calculate two conditional probabilities

- $Pct1 = (TB^+ - kinase^+) / (TB^+ - kinase^+) + (TB^+ - kinase^-)$
 $= (7) / (7) + 46 = 0.13207547$
- $Pct2 = (TB^- - kinase^+) / (TB^- - kinase^+) + (TB^- - kinase^-)$
 $= (1) / (1) + (311) = 0.003205128$

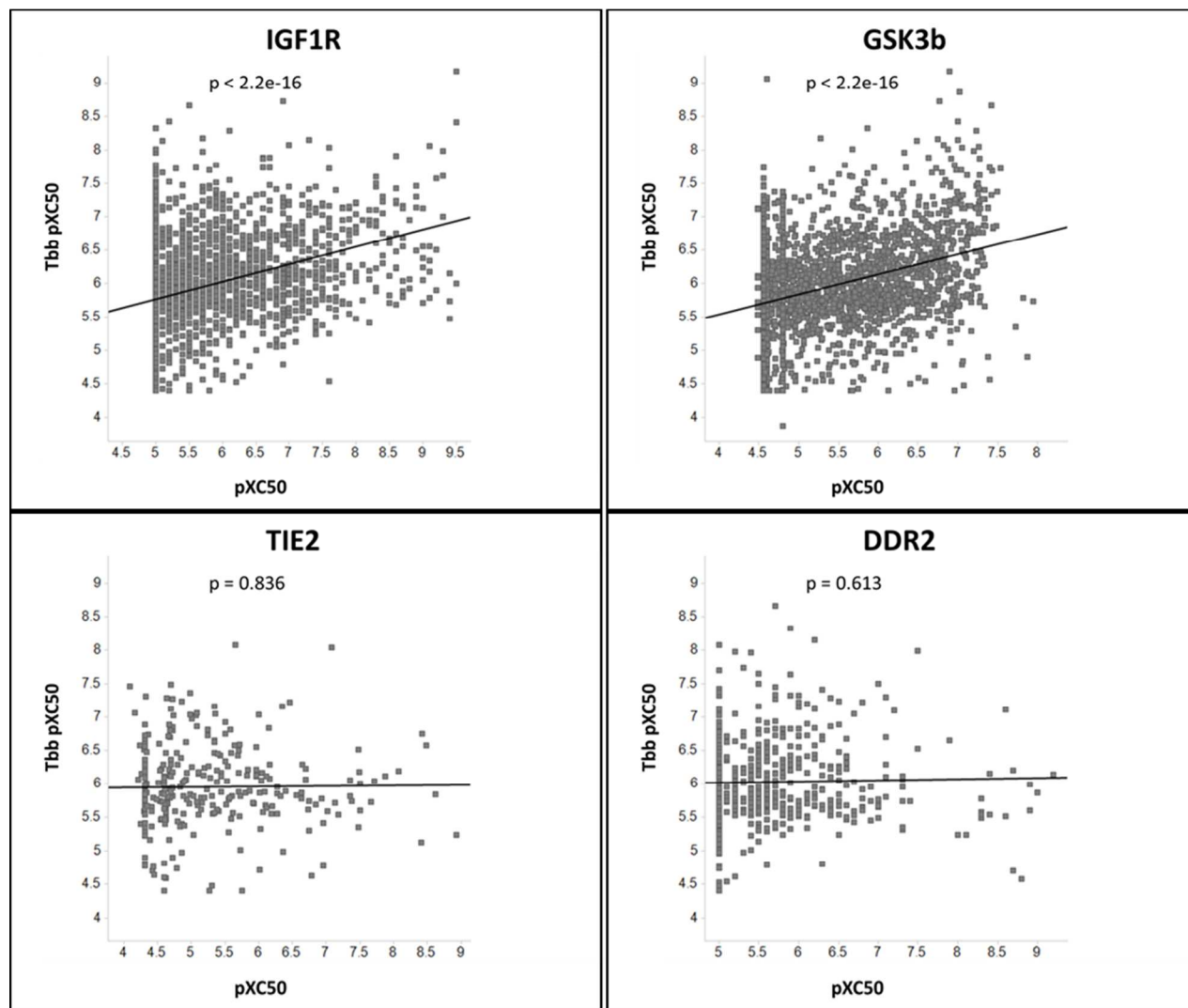
And the ratio and enrichment can be calculated:

- Ratio = $Pct1 / pct2$
- Ratio = $0.13207547 / 0.003205128 = 41.2075472$

TB ⁺ kinase ⁺	TB ⁺ kinase ⁻	TB ⁻ kinase ⁺	TB ⁻ kinase ⁻	pct1	pct2	Ratio	v.chisq
7	46	1	311	0.13207547	0.00320513	41.2075472	6.06×10^{-8}

Finally, *p*-values (chi-squared test) were calculated using R.

Figure S4. Plot of *T. brucei* pEC₅₀ versus human kinase pIC₅₀ for two preferred human kinases (IGF1R and GSK3β), and two non-preferred human kinases (TIE2 and DDR2) using non-PKIS GSK compounds. The p-value for the linear regression is shown as a statistical test for association between the *T. brucei* and human kinase activity. Only GSK3b and IGF1R give statistically significant correlations.



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