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High Throughput Screening of a GlaxoSmithKline Protein Kinase Inhibitor Set Identifies an Inhibitor of Human Cytomegalovirus Replication that Prevents CREB and Histone H3 Post-Translational Modification

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Abstract:	To identify new compounds with anti-human cytomegalovirus (HCMV) activity and new anti-HCMV targets, we developed a high throughput strategy to screen a GlaxoSmithKline (GSK) Published Kinase Inhibitor Set (PKIS). This collection contains a range of extensively characterized compounds grouped into chemical families (chemotypes). From our screen we identified compounds within chemotypes that impede HCMV replication and identified kinase proteins associated with inhibition of HCMV replication that are potential novel anti-HCMV targets. We focused our study on a top "hit" in our screen, SB-734117, which we found inhibits productive replication of several HCMV strains. Kinase selectivity data indicated that SB-734117 exhibits polypharmacology and is an inhibitor of several proteins from the AGC and CMCG kinase groups. Using western blotting we found that SB-734711 inhibited accumulation of HCMV immediate-early proteins, phosphorylation of cellular proteins involved in immediate-early protein production (CREB and histone H3) and histone H3 lysine 36 trimethylation (H3K36me3). Therefore, we identify SB-734117 as a novel anti-HCMV compound and find that inhibition of AGC and CMCG kinase proteins during productive HCMV replication is associated with inhibition of viral protein production and prevents post-translational modification of cellular factors associated with viral protein production.

STANDARD RESEARCH ARTICLE

High Throughput Screening of a GlaxoSmithKline Protein Kinase Inhibitor Set Identifies an Inhibitor of Human Cytomegalovirus Replication that Prevents CREB and Histone H3 Post-Translational Modification

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Running Title: Screening Kinase Inhibitors Targeting HCMV

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ABSTRACT

To identify new compounds with anti-human cytomegalovirus (HCMV) activity and new anti-HCMV targets, we developed a high throughput strategy to screen a GlaxoSmithKline (GSK) Published Kinase Inhibitor Set (PKIS). This collection contains a range of extensively characterized compounds grouped into chemical families (chemotypes). From our screen we identified compounds within chemotypes that impede HCMV protein production and identified kinase proteins associated with inhibition of HCMV protein production that are potential novel anti-HCMV targets. We focused our study on a top “hit” in our screen, SB-734117, which we found inhibits productive replication of several HCMV strains. Kinase selectivity data indicated that SB-734117 exhibits polypharmacology and is an inhibitor of several proteins from the AGC and CMCG kinase groups. Using western blotting we found that SB-734711 inhibited accumulation of HCMV immediate-early proteins, phosphorylation of cellular proteins involved in immediate-early protein production (CREB and histone H3) and histone H3 lysine 36 trimethylation (H3K36me3). Therefore, we identify SB-734117 as a novel anti-HCMV compound and find that inhibition of AGC and CMCG kinase proteins during productive HCMV replication is associated with inhibition of viral protein production and prevents post-translational modification of cellular factors associated with viral protein production.

INTRODUCTION

Disease associated with human cytomegalovirus (HCMV) infection affects a range of immunodeficient individuals [1]. As yet, there is no widely available vaccine against HCMV [2] and disease management largely rests on the use of anti-HCMV drugs [1, 3]. The most widely used anti-HCMV drugs (including the frontline drug ganciclovir) target the viral DNA polymerase, thereby inhibiting HCMV replication [3]. However, there are drawbacks to the use of ganciclovir and other currently available anti-HCMV drugs, including the development of drug resistant virus [3]. Furthermore, HCMV not only undergoes productive replication but can also enter a latent state from which the virus can reactivate. Currently, there is no effective treatment to clear latent HCMV infection.

Several novel anti-HCMV drugs are under development [1, 3, 4]. One strategy to expand the range of anti-HCMV drugs available is to identify existing compounds with hitherto unappreciated anti-HCMV activity. A large number of currently available compounds inhibit protein kinases in each of the groups that comprise the human kinome. Protein kinases are involved in many aspects of HCMV replication and pathogenesis, including intracellular signaling that results in transcription from the HCMV major immediate early promoter (MIEP), which stimulates a transcriptional cascade (*immediate-early* to *early* to *late* gene transcription) required for productive HCMV replication and reactivation from latency [1]. Therefore, protein kinase inhibitors could inhibit productive HCMV replication or reactivation from latency and a number of kinase inhibitors with

anti-HCMV activity have been identified [3]. Furthermore, it is possible that the full complement of protein kinases that are required for HCMV replication have yet to be identified. Therefore, kinase inhibitors could be used as chemical probes to identify kinase proteins required for HCMV replication, many of which could be novel anti-HCMV drug targets. However, an important consideration when using kinase inhibitors is that compounds targeting the conserved ATP-binding site of a kinase protein can display polypharmacology and are capable of inhibiting several kinase proteins or proteins outside the kinome, such as G-protein coupled receptors (GPCRs) [5-7]. Therefore, knowledge of kinase selectivity is important when discussing the use of kinase inhibitors as drugs or chemical probes [5].

We utilized a high throughput screening methodology to assess the ability of compounds within a GlaxoSmithKline (GSK) Published Kinase Inhibitor Set (PKIS) [8] to inhibit HCMV protein production. This compound library contained a range of extensively characterized compounds organized into structurally related collections of compound families (chemotypes) [7, 8]. Known characteristics of compounds within this GSK PKIS collection include kinase selectivity, compound structures and off-targets effects. Therefore, screening of this compound library allowed identification of both compounds and chemotypes with anti-HCMV activity, identification of novel anti-HCMV drug targets and permitted the on and off-targets effects of compounds identified in the screening process to be considered. These data lead to investigation of the anti-HCMV activity of a top “hit” in our screen, SB-734117.

RESULTS

High throughput screening of a GSK PKIS library to identify protein kinase inhibitors with anti-HCMV activity. To identify compounds with anti-HCMV activity we utilized a high throughput screening methodology (Fig. 1(a)), similar to the approach that we have previously used to screen siRNAs in HCMV infected cells [9]. Briefly, high passage HCMV strain AD169 and compounds from the GSK PIKS collection (listed in Table S1) were added to duplicate 384-well plates seeded with human foreskin fibroblast (HFF) cells. As negative and positive controls for compound treatment several wells in each plate were treated with either DMSO or heparan sulphate (a small molecule that inhibits HCMV entry into cells [10]), respectively. At 72 hours post infection (h.p.i.) cells were stained with Hoescht 33342 to detect nuclear DNA and CellMask to detect the area of the cell, plus were treated with antibodies to detect the cytoplasmic HCMV antigen pp28. An automated microscopy system was then used to assay both the number of cells in each well and the number of infected cells in each well expressing pp28. An image of infected cells treated as described above and captured using automated microscopy is shown in Fig. 1(b).

The mean number of cells in each well per plate was determined. Where the number of cells in any well was less than 2-fold below the mean number of cells of the plate, the compound in that well was judged to be cytotoxic (listed by chemotype in Table 1 and by compound in Table S2). Data from the remaining wells on duplicate plates were combined and converted to a z-score (the number

of standard deviations from the mean of the data [11, 12]) to demonstrate the increase (positive z-score) or decrease (negative z-score) in the number of pp28 positive cells in presence of each compound (shown in Fig. 1(c), listed by chemotype in Table 1 and by compound in Table S3).

Analysis of cytotoxic compounds. We first investigated what compounds within chemotypes were judged to be cytotoxic. Approximately 40-50% of compounds in the benzimidazole N-thiophene, 2H-3 pyrimidinyl pyrazolopyridazine, 3-amino pyrazolopyridines and 6-phenyl isoquinolines chemotypes contained compounds judged to be cytotoxic to HCMV infected cells (Table 1 and Table S2). Therefore, compounds from these chemotypes are generally not suitable for further use.

We then utilized kinase selectivity data to investigate which kinase proteins were inhibited by each compound judged to be cytotoxic (Table S4). Kinase selectivity data [7] lists the ability of each compound to inhibit a panel of 224 kinase proteins from several protein groups of the human kinome (including TK, STE, AGC, S-T-PK, CAMK and CMCG groups). We found that all cytotoxic benzimidazole N-thiophenes were potent inhibitors of PLK-1, whose inhibition can lead to apoptosis, and nearly all other cytotoxic compounds from a number of chemotypes were potent inhibitors of a range of CDK proteins, which are involved in regulation of the cell cycle. In our screen cytotoxicity was judged by the number of cells detected in each well of the screening plate. Therefore, we concluded that compounds were generally judged to be cytotoxic due to

apoptosis associated with inhibition of PLK-1 or due to lack of cell division associated with inhibition of CDK function.

Analysis of compounds assigned z-scores. Next, we analyzed those compounds assigned z-scores to determine which compounds and chemotypes should be considered for further study as anti-HCMV compounds and chemical probes. We found that nearly all chemotypes contained compounds that had both positive and negative effects on pp28 production. Notably, however, the 2-aryl 3-pyridimidinyl pyrazolopyridazine and furopyrimidine chemotypes and the 3-vinyl pyridine, 2,4-diamino pyrimidine, maleimide, phenyl carboxamide and indazole-5-carboxamide chemotypes contained a large number of compounds with negative and positive effects on pp28 production, respectively (Tables 1 and S3). We sought to further characterize the results of our screen and judged any compound with a z-score between 1 to -1 to have little or no effect on pp28 production, whereas compounds with z-scores of -1 to -2 and 1 to 2 had modest negative or positive effects on pp28 production, respectively. Thusly, compounds with z-scores of less than -2 or more than 2 had the greatest negative or positive effect on pp28 production, respectively. Therefore, three compounds (GW575808A, GW874091X and GW627512B) from three different chemotypes (2,4-diamino pyrimidines, imidazotriazines, 2-amino oxazoles, respectively) had strong positive effects on pp28 production, while four compounds (GW297361X, SB-734117, SB-220025-R and GW795493X) from four chemotypes (oxindoles, furazan benzimidazoles, 4-pyrimidinyl ortho-aryl azoles, furopyrimidines,

160 respectively) had strong negative effects on pp28 production (Figs. 1(c) and
161 1(d)).
162
163 **Examination of kinase protein inhibition by compounds assigned z-**
164 **scores.** We then examined kinase selectivity data of compounds assigned z-
165 scores (Table S5). The data from Table S5 is presented in Figure 2 as a
166 “heatmap” of kinase inhibition. Nearly all compounds assigned z-scores exhibited
167 polypharmacology and could inhibit more than one kinase protein. Consistent
168 with our analysis of compounds judged to be cytotoxic (Table S2), we found that
169 less than 5% of all compounds either potently inhibited PLK-1 or were potent
170 inhibitors of several different CDK proteins (Table S5). Compounds with positive
171 or negative z-scores were inhibitors of a wide range of kinase proteins in the TK
172 kinase group (Fig. 2 and Table S5). Therefore, inhibition of TK kinases alone was
173 unlikely to positivity or negatively influence pp28 production. However, a number
174 of kinases in the STE (including MAP4K4 and MNK), CAMK (including PRKD1,
175 PRKD2 and PRKD3) and CMCG (including CLK2, HIPK1, HIPK4, DYRK1A,
176 DYRK1B, DYRK2) kinase groups were inhibited by compounds assigned z-
177 scores of less than -1 from 8, 4 and 3 different chemotypes, respectively (Figs.
178 2(a)-(c), respectively, and Table S5). Therefore, these kinase proteins, alone or
179 in combination, were likely to be important for HCMV replication and could
180 represent future anti-HCMV drug targets. A number of compounds from two
181 different chemotypes that inhibited kinases in AGC kinase family (including
182 PRKG1, PRKG2, PRKX, PKA, ROCK1, ROCK2) were assigned z-scores over 1

(Fig. 2(d)). Therefore, these kinase proteins, alone or in combination, were likely to be inhibitory to HCMV replication. Compounds targeting these kinase proteins are likely to be off little value as anti-HCMV drugs.

Compounds assigned z-scores of less than -2 (GW297361X, SB-734117, SB-220025-R and GW795493X) each had a distinct kinase selectivity profile (Fig. 2 and Table S5). Therefore, it was likely each compound inhibited pp28 production by a different mechanism. Each was a potent inhibitor of several kinase proteins from several groups, except for SB-220025-R, which was a potent inhibitor of only 2 kinase proteins: CK1a and p38α (Fig. 2 and Table S5).

Kinase inhibition of compounds assigned z-scores of greater than 2 was also examined. GW575808A and GW627512B had similar kinase selectivity profiles and were inhibitors of several TK and S-T-PK group kinases (Fig. 2 and Table S5). As inhibition of these TK and S-T-PK kinases can result in either positive or negative z-scores (Fig. 2 and Table S5), it was unlikely that inhibition of these TK and S-T-PK kinase proteins had a direct effect on pp28 production. Moreover, we found that GW874091X was not a potent inhibitor of any kinase assayed (Fig. 2 and Table S5). Therefore, GW874091X was either an inhibitor of kinase proteins not assayed in the kinase selectivity data or exerted an effect on pp28 production that did not involve inhibition of cellular kinase proteins. It, therefore, remains unclear from this analysis which kinase proteins should not be targeted in the development of future anti-HCMV drugs.

We further considered the polypharmacology of compounds tested in our screen. It has been reported that ATP-competitive kinase inhibitors can inhibit the

function of proteins other than kinases, including aminergic GPCRs [6]. GPCR agonism and antagonism of the compounds in the GSK PKIS collection has been investigated elsewhere [7]. No compound within the GSK PKIS collection is a GPCR agonist, but several are GPCR antagonists [7]. However, we observed no correlation between compounds judged to be cytotoxic, compounds assigned a z-score and GPCR antagonism (data not shown).

Inhibition of HCMV replication by SB-734117. We chose to focus our studies on SB-734117, a compound from the furazan benzimidazole chemotype that had a low z-score in our screen (Figs. 1(c) and 1(d)). First, we used viral yield reduction assays to assess the ability of SB-734117 to inhibit replication of HCMV strain AD169 compared to the frontline anti-HCMV drug ganciclovir (GCV) (Table 2, experiment 1) at up to 96 h.p.i. The 50% effective dose (ED50) of both SB-734117 and GCV was 0.5μM, indicating that SB-734117 inhibit AD169 replication as efficiently as the current frontline anti-HCMV drug. To complement and confirm this data we analyzed AD169 replication over time and found an approximately 2-fold decrease in AD169 replication from 72-96 h.p.i. in the presence of 1μM SB-734117 (Fig. 3(a)).

We also found that SB-734117 could inhibit replication of a ganciclovir resistant virus (AD169-P53) and a low passage HCMV strain (Merlin(RCMVR1111)), whose genomic content is similar to a clinical sample [13], at low or sub-micromolar ED50 values (Table 2, experiments 2 and 3,

228 respectively) at up to 96 h.p.i.. Therefore, SB-734117 was an effective inhibitor of
229 different HCMV strains.

230 To ensure that the anti-HCMV activity of SB-734117 was not due to
231 cellular cytotoxicity we used an MTT dye-uptake assay to assess cell viability and
232 cell division in uninfected cells in the presence of SB-734117. We found that the
233 50% cellular cytotoxicity (CC50) of SB-734117 after 96 hours treatment with SB-
234 734117 was greater than 10μM (data not shown). Thus, the CC50 values in
235 uninfected cells were greater than 10μM at the ED50 values for all HCMV strains
236 tested. Therefore, inhibition of HCMV replication by SB-734117 observed in
237 experiments shown in Table 2, or in the other experiments presented here, was
238 unlikely to be the result of cellular cytotoxicity or inhibition of cell division.

239

240 **Examination of HCMV immediate early protein and mRNA production**
241 **in HCMV infected cells treated with SB-734117.** We next sought to understand
242 how HCMV replication was inhibited by SB-734117. Therefore, western blotting
243 was used to analyze the accumulation of HCMV proteins in the presence or
244 absence of SB-734117 (Fig. 3(b)). Compared to treatment of infected cells with
245 DMSO (Fig. 3(b), lanes 2-4), the treatment of infected cells with SB-734117 (Fig.
246 3(b), lanes 5-7) reduced the accumulation of immediate early proteins IE1 and
247 IE2, and IE2 proteins expressed late in infection (IE2-60 and IE2-40 [14]). In this
248 and subsequent western blots the amount of β-actin in each sample was also
249 assayed, which demonstrated equivalent loading of samples in each lane.

We then quantified the relative density of the western blotting bands shown in Fig. 3(b), by determining the band intensity of bands corresponding to viral proteins relative to the intensity of the β-actin band in the same lane (Fig. 3(c)). We found an approximately 2-4 fold decrease in the accumulation of IE1 in the presence of 1 μM SB-734117, which is consistent with an ED50 of 0.5-1 μM shown in Table 2. The loss of IE2 protein production (approximately 2- to 20-fold, depending on which antibody was used (Fig. 3(c))) was greater than IE1. Consistent with loss of IE protein production and our screening results, we also observed using western blotting that treatment of cells with SB-734117 resulted reduced accumulation of the HCMV early and late proteins UL44 and pp28, respectively, compared to infected cells treated with DMSO (data not shown). To compliment these findings we assayed for differences in IE1 and IE2 mRNA expression in infected cells treated with SB-734117 compared to infected cells treated with DMSO using quantitative PCR against the two major IE RNA species (Fig. 3(d)). This analysis revealed that no obvious defect in IE1 mRNA levels was evident in the presence of SB-734117. The analysis of IE2 mRNA again did not show any overt phenotype although typically a 2 fold reduction in IE2 mRNA was observed in SB-734117 treated cells when compared with DMSO control. However, taken together the data suggest that the decrease in IE1 and IE2 protein production shown in Figs. 3(b) and 3(c) was unlikely to be the result of decreased *IE* gene expression.

Our studies thus far could not rule out that SB-734117 impacted events occurring prior to IE gene expression. Thus we addressed whether the presence

of SB-734117 may affect virus entry into the cell or translocation of the HCMV genome to the nucleus. Pre-exposure of cells to SB-734117 before infection or incubation of virus with SB-734117 before infection did not increase the inhibitory effects of the compound (data not shown). However, when we treated AD169 infected HFF cells with 1μM SB-734117 at 24 h.p.i. we found a 2-fold decrease in HCMV replication at 120 h.p.i., compared to infected cells treated with DMSO at 24 h.p.i. (Fig. 4(a)). Quantitative analysis of western blotting of infected cells treated as described above (Figs 4(a) and 4(b)) showed that, similar to data presented in Fig. 3, treatment of infected cells with SB-734117 resulted in approximately 2-fold decrease in IE2 protein production depending on which antibody was used. However, there was no obvious decrease in production of IE1 protein.

Therefore, SB-734117 had no obvious effect on cells or virus before infection, but could inhibit HCMV replication after entry of the HCMV genome and did so by reducing IE2 protein production. Thus, SB-734117 may not inhibit events during infection before expression of IE proteins, but could have inhibitory effects on HCMV replication after the initiation of IE protein production.

Inhibition of AGC and CMCG kinase proteins by SB-734711. Next, we investigated what kinases proteins are inhibited by SB-734117. SB-734117 has been reported to inhibit MSK1 [15]. However, using the kinase selectivity data shown in Fig. 2 and Table S5, we found that at SB-734117 inhibits several AGC kinase group proteins, including MSK1 (MSK1, MSK2, RSK1, RSK2, RSK3,

296 p70S6K1, PCK-η, PRKG2, ROCK1, ROCK2), and several CMCG kinase group
297 proteins (GSK3A, GSK3B, DYRK1A and DYRK1B). However, in our screen
298 potent and selective inhibitors of GSK3A and GSK3B had no obvious negative
299 effect on pp28 production (Table S5) and compounds with either positive or
300 negative z-scores were potent inhibitors of PKC-η, PRKG2, ROCK1 and ROCK2
301 (Table S5). Therefore, inhibition of these kinases proteins may not be related to
302 inhibition of pp28 production. Rather, analysis of SB-734117 kinase selectivity
303 data compared to other assigned z-scores argued that potent inhibition of MSK1,
304 MSK2, RSK1, RSK2, RSK3, p70S6K1, DYRK1A and DYRK1B was related to
305 inhibition of pp28 production.

306 A kinase inhibitor that is structurally unrelated to SB-734117, H-89, inhibits
307 a similar range of AGC and CMCG kinase proteins [16]. We found that H-89
308 inhibited productive HCMV replication and immediate-early protein production
309 (data not shown). Therefore, inhibition of AGC and CMCG kinase proteins, not
310 an unknown function of SB-734117, is likely to be responsible for the observed
311 defects in HCMV replication and protein production. Furthermore, using western
312 blotting [17], we found that SB-734117 did not inhibit autophosphorylation of the
313 HCMV encoded kinase UL97 (data not shown). Therefore, the anti-HCMV effects
314 of SB-734117 were unlikely to be due to inhibition of UL97.

315

316 **Analysis of CREB and histone H3 phosphorylation in HCMV infected**
317 **cells.** We then considered how inhibition of AGC and CMCG kinase proteins by
318 SB-734114 would affect post-translational modification of cellular proteins

thought to be involved in HCMV replication. We focused our investigation on phosphorylation of the cellular transcription factor CREB and histone H3.

CREB is thought to directly or indirectly facilitate transcription from the MIEP [18, 19] and other viral promoters [20] during productive HCMV replication and it has been reported that phosphorylation of CREB at serine residue 133 (CREB-Ser133) by MSK1 is involved in promoting changes to chromatin required for activation of the MIEP during HCMV reactivation from latency [21]. In preliminary experiments we could not detect either total cellular CREB or CREB-Ser133 before 72 h.p.i. using western blotting (data not shown). However, both proteins could only be detected at 72 h.p.i. when we increased the amount of cell lysate assayed (see Materials & Methods). Therefore, we used western blotting to assay total cellular CREB and CREB-Ser133 phosphorylation in HCMV infected cells treated with either DMSO or SB-734117 at 72 h.p.i. (Fig. 5(a)). We observed a decrease in accumulation of CREB-Ser133 and an increase in the accumulation of CREB in the presence of SB-734117 (Fig. 5(a), lane 5), compared to infected cells treated with DMSO (Fig. 5(a), lane 3). Analysis of relative band intensities (Fig. 5(b)), indicated that there was approximately a 2-fold decrease in CREB-Ser133 in infected cells treated with SB-734117, compared to those treated with DMSO and a modest increase in CREB. The 2-fold decrease in the accumulation of CREB-Ser133 in the presence of 1μM SB-734117 was consistent with the observed ED50 of 0.5-1 μM and 2-4 fold decrease in production of immediate-early HCMV protein production (Table 2 and Fig. 3). Therefore, the effect of SB-734117 on HCMV replication correlated

342 with a loss of CREB-Ser133 phosphorylation. Similar observations were made
343 when infected cells were treated with H89 (data not shown), indicating the AGC
344 and CMCG kinase proteins were involved in phosphorylation of CREB.

345 Phosphorylation of histone H3 by MSK1 or another kinase, IKKα is
346 required for binding of transcription factors to DNA in uninfected cells [22, 23].
347 We have previously demonstrated that phosphorylation of histone H3 at serine
348 residue 10 (H3S10p) by IKKα is associated with immediate-early protein
349 production during productive HCMV replication [17]. Also, it has been
350 demonstrated that H3S10 phosphorylation by MSK1 is associated with
351 immediate-early gene expression during reactivation of HCMV from latency [21].
352 We decided to assay H3S10 phosphorylation in the presence of SB-734117.
353 Using western blotting we analyzed accumulation of H3 and H3S10
354 phosphorylation in uninfected HFF cells (Fig. 5(c), lane 1) and AD169 infected
355 HFF cells treated with either DMSO or SB-734117 (Fig. 5(c), lanes 2-4 and 5-7,
356 respectively, at 24-72 h.p.i.). Similar levels of H3 were found in each sample,
357 however, over time we observed a decrease in H3S10p in infected cells treated
358 with SB-734117 to near undetectable levels, compared to infected cells treated
359 with DMSO. Therefore, inhibition of H3S10 phosphorylation during productive
360 HCMV replication may have contributed to the anti-HCMV activity of SB-734117.
361 Similar results were found when infected cells were treated with H89 (data not
362 shown), indicating that AGC and CMCG kinase proteins were involved in
363 phosphorylation of H3S10.

364 Phosphorylation of histone H3 at serine residue 28 (H3S28) by MSK1 is
365 also known to be associated with gene expression in uninfected cells [22]. We
366 also used western blotting to investigate H3S28 phosphorylation during HCMV
367 replication. However, we could not detect H3S28p in either uninfected HFF cells,
368 AD169 infected HFF treated with either DMSO or SB-734117, or uninfected HFF
369 cells treated with either anisomycin, which can stimulate H3S28 phosphorylation,
370 or phosphatase inhibitor okadaic acid, which can prevent dephosphorylation of
371 histones (data not shown). Therefore, we suggest that inhibition of H3S28
372 phosphorylation did not contribute to the anti-HCMV activity of SB-734117.
373
374 **Analysis of histone H3 post-translational modifications in HCMV**
375 **infected cells.** H3S10 phosphorylation by either MSK1 or IKKα is associated
376 with the presence of acetyl modifications of H3, including at acetylation (ac) of
377 lysine 14 (H3K14ac) [24-26]. There is a relationship during transcriptional
378 activation between the presence of H3S10p and H3K14ac and the association of
379 transcription factors with DNA [23, 27]. As the presence of H3K14ac is
380 associated with transcriptional activation in HCMV infected cells [28], H3K14ac
381 may be required for HCMV replication. We have previously demonstrated that
382 during HCMV replication inhibition or depletion of IKKα leads to loss of total
383 cellular H3S10 phosphorylation, but not loss of total cellular H3K14ac [17]. Thus,
384 we assayed whether treatment of HCMV infected cells by SB-734117 would lead
385 to loss of H3S10p or H3K14ac. We used western blotting to assay total cellular
386 levels of H3, H3S10p and acetylation of H3 on a number of commonly studied H3

lysine residues including K14 (H3K9ac, H3K14ac, H3K18ac, H3K27ac) in either uninfected HFF cells (Fig. 5(c), lane 1) or HFF cells infected with HCMV and treated with either DMSO or SB-734117 (Fig. 5(c), lanes 2-4 and 5-7, respectively). Treatment of infected cells with SB-734117 had a slight effect (less than 2-fold (data not shown)) on accumulation of H3K14ac and no detectable effect on detection of H3K9ac, H3K18ac, or H3K27ac. Therefore, treatment of infected cells with SB-734117 was associated with loss of total cellular H3S10p, but not loss of the total cellular H3 acetylation modifications we assayed, including H3K14ac.

The relationship between H3S10p and dimethylation (me2) and trimethylation (me3) of H3 and H3 phosphorylation is not well characterized, but it has been reported that in a murine model there is a relationship between the presence of H3S10p and the presence of H3K36me3 [29] and in *Drosophila melanogaster* loss of the MSK1/2 homologue JIL-1 results in loss of H3S10p, H3 acetylation and H3 methylation, including H3K36me3 [30]. Therefore, we asked if loss of total cellular H3S10p in HCMV infected cells was associated with me2 and me3 modification of H3 lysine residues. Western blotting was used to assay the presence of H3 and H3S10p, plus me2 (H3K4me2, H3K27me2, H3K36me2) or me3 (H3K4me3, H3K9me3, H3K27me3, H3K36me3) modifications of H3 in uninfected HFF cells (lane 1, Figs. 5(d) and 5(e), respectively) or HFF cells infected with HCMV and treated with either DMSO or SB-734117 (lanes 2-4 and 5-7, Figs. 5(d) and 5(e), respectively). We observed that SB-734117 had no effect on total cellular accumulation of any me2 modification of H3 (Fig. 5(d)) or

410 accumulation of H3K4me3, H3K9me3 or H3K27me3 (Fig. 5(e)). However, we
411 observed a near total loss of detectable H3K36me3 over time in infected cells
412 treated with SB-734117 (Fig. 5(e), lane 7) compared to infected cells treated with
413 DMSO (Fig. 5(e), lane 4). Similarly, a near total loss of detectable H3K36me3
414 was observed in infected cells treated with H89 (data not shown), suggesting that
415 loss of H3K36me3 is related to inhibition of AGC and CMCG kinase proteins.
416 Thus, inhibition of H3K36me3 was associated with loss of total cellular H3S10p
417 and was likely the result of inhibition of AGC and CMCG kinase proteins inhibited
418 by SB-734117. Loss of both total cellular H3S10p and total cellular H3K36me3
419 may have contributed to the anti-HCMV activity of SB-734117.
420
421 **Investigation of HCMV MIEP transcriptional activation.** Loss of CREB
422 and H3S10 phosphorylation (Figs. 5(a)-(e)) suggested that SB-734117 acted by
423 inhibiting activation of the HCMV MIEP. However, our analysis of IE1 and IE2
424 gene expression (Fig. 3(d)) indicated that transcription from the MEIP was not
425 obviously compromised in the presence of SB-734117. To investigate this in
426 more detail we utilized chromatin immunoprecipitation (ChIP) to assay the
427 presence of H3K14ac, a marker of MIEP transcriptional activation [28], at the
428 MIEP in the presence of either DMSO or SB-734117 (Fig. 6). The data showed
429 that no overt impact on H3K14ac at the MIEP between 24-72hpi in DMSO or SB-
430 734117 treated cells. Indeed, we noted that SB-734117 treated cells actually
431 showing higher levels of H3K14ac at the MIEP at late times post infection when
432 compared to control. Therefore, in agreement with our analysis of IE1 and IE2

433 gene expression (Fig. 3(d)), there was no obvious defect in MIEP transcriptional
434 activation in the presence of SB-734177. Thus, the observed defects in HCMV
435 immediate-early protein production (Figs 3 and 4) could not be explained by
436 defects in transcription from the MIEP.
437
438

DISCUSSION

Our overall analysis of the chemotypes screened indicated that each chemotype contained compounds with anti-HCMV activity, however modest that anti-HCMV activity may have been. As the structure of each compound in each chemotype is known, structure-activity relationships derived from our data could form the basis of future studies in the discovery of compounds with anti-HCMV activity from each chemotype.

Our survey of the GSK PKIS kinase selectivity data argued that several proteins from several kinase groups, alone or in combination, were required for pp28 production. These proteins kinases include those from the STE (including MAP4K4 and MNK), CAMK (including PRKD1, PRKD2 and PRKD3) and CMCG (including CLK2, HIPK1, HIPK4, DYRK1A, DYRK1B, DYRK2) kinase groups. The function of these protein kinases in productive HCMV replication is unclear or unknown. Therefore, it is possible that our data identified novel cellular factors required for productive HCMV replication. However, the polypharmacology of the compounds tested makes it difficult to identify specific kinases required for productive HCMV replication. Thus, each of the aforementioned kinases will have to be tested individually to identify their roles in HCMV infected cells. With this information these kinases could be exploited as novel anti-HCMV drug targets.

We chose to pursue studies of SB-734117 as this compound had one of the greatest negative effects on pp28 production in our screen, with no obvious cytotoxic effects, and was an effective inhibitor of a number of HCMV strains.

462 Moreover, the function of the AGC and CMCG kinase proteins inhibited by SB-
463 734117 in productive HCMV replication was unknown or unclear.

464 SB-734117 was originally described as an inhibitor of MSK1 [15].
465 However, like other MSK1 inhibitors [16], SB-734117 displays polypharmacology
466 and can inhibit several kinases whose roles in productive HCMV replication are
467 unknown or unclear. Thus, to understand how SB-734117 inhibits HCMV
468 replication it will be necessary to understand if a particular kinase or a
469 combination of kinase proteins is required for productive HCMV replication. A
470 truly selective inhibitor of MSK1 has yet to be found. Structure-activity
471 relationships involving SB-734117 and other furazan benzimidazole compounds
472 could be explored to generate compounds with improved anti-HCMV activity and
473 kinase selectivity. However, we could discern no obvious relationship between
474 inhibition of HCMV replication, kinase selectivity and the structures of
475 compounds within the furazan benzimidazole chemotype analyzed here due to
476 the small number of furazan benzimidazole compounds that returned low
477 negative z-scores in our screen (data not shown). An improved compound
478 related to SB-734117 would have value as an anti-HCMV drug, as it would have
479 the potential to inhibit both productive HCMV replication and reactivation of
480 HCMV from latency. Plus, based on our observations, an improved compound
481 should be as effective an inhibitor of HCMV replication as ganciclovir and be able
482 to inhibit replication of ganciclovir resistant HCMV strains.

483 Perhaps the most intriguing observations we make concern modification of
484 histone H3 in the presence of SB-734117. Previous observations from our

485 laboratory have indicated that IKKα was required for H3S10 phosphorylation in
486 AD169 infected HFF cells [17], which is consistent with data presented
487 elsewhere indicating that H3S10 is substrate of IKKα [24, 25, 31-33]. We note
488 that inhibition of IKKα results in loss of H3S10p early in HCMV replication (24
489 h.p.i. onwards) [17], whereas treatment with SB-734117 leads to a loss of
490 H3S10p later in HCMV replication (48-72 h.p.i.). SB-734117 does not inhibit
491 IKKα (Table S5). Therefore, we propose that in HCMV infected cells a
492 mechanism exists wherein IKKα does not phosphorylate H3S10 during treatment
493 with SB-734117. Conversely, kinases inhibited by SB-734117 do not
494 phosphorylate H3S10 when IKKα is inhibited or depleted. This mechanism may
495 ensure appropriate regulation of H3S10 phosphorylation that is necessary for
496 productive HCMV replication.

497 It has been reported that in uninfected cells from humans and mice loss of
498 H3S10p can lead to loss of H3K14ac [24-26]. However, we did not observe loss
499 of total cellular H3K14ac upon treatment of HCMV infected cells with SB-734117
500 or in our previous study where inhibition or depletion of IKKα resulted in loss of
501 H3S10p [17]. We speculate, as we have done previously [17], that an as yet
502 unrecognized mechanism exists in HCMV infected cells that maintains total
503 H3K14ac when total H3S10p levels are lowered to near undetectable levels.

504 We observed that treatment of HCMV infected cells with SB-734117
505 resulted in loss of H3K36me3. We have previously found that depletion of IKKα
506 in HCMV infected cells leads to loss of H3S10p, but not H3K36me3 [17].
507 Therefore, the loss of H3K36me3 in HCMV infected cells is related to loss of

H3S10p during inhibition of AGC and CMCG kinases, but not during inhibition of IKKα. This may be related to regulation of H3S10 phosphorylation by different kinases, as we discuss above. We propose that, as in mice and *Drosophila* [29, 30], the presence of H3K36me3 in HCMV infected cells is related to the presence of H3S10p, potentially via phosphorylation of H3 by MSK1. Alternatively, there may be a substrate of kinase proteins inhibited by SB-734117 whose phosphorylation directly or indirectly mediates H3K36 tri-methylation.

Treatment of HCMV infected cells with SB-734117 impacted on immediate early protein production and caused loss of total cellular levels of post-translational modification of cellular factors potentially involved in transactivation of the HCMV MIEP. However, in the presence of SB-734117 we did not find obvious defects in activation of transcription from the HCMV MIEP or defects in immediate-early gene transcription. Therefore, the loss of total cellular levels of CREB and H3S10 phosphorylation or H3K36me3 had no direct impact on transcription from the HCMV MIEP. This interpretation would be consistent with previous studies that have shown that the deletion of CREB binding sites from the MIEP has little impact on productive HCMV replication [21, 34]. During reactivation, it is hypothesized the H3S10p is important as it drives the transition of the MIEP from a repressed to active promoter, a mechanism also proposed for HSV reactivation [35] Thus, during productive HCMV replication at high MOI, where the MIEP is associated with active, not repressed, chromatin very early post infection [28], H3S10p may not be essential for transcription. However, it remains possible that H3S10p has a role in the release of Early and Late HCMV

promoters from repression as infection proceeds. Thus, future challenges will include mapping of CREB, H3S10p and H3K36me3 to viral and cellular promoters to understand in more detail to understand their possible involvement in productive HCMV replication.

We propose that the greatest impact of SB-734117 on productive HCMV replication is on production of IE proteins. It will be important to investigate if SB-734117 impacts on additional phosphorylation events that are required for production of both proteins. Post-translational modification of both IE1 and IE2 is not yet completely characterized. Thus, SB-734117 could directly or indirectly inhibit phosphorylation of these proteins, which leads to their loss. Further investigation of IE protein production and the roles of IE post-translational modification are required in order to fully understand the mechanism of action of SB-734117 during productive HCMV replication.

MATERIALS & METHODS

Compounds. The GSK PIKS library (version 1) was supplied to the Institute of Chemistry and Chemical Biology-Longwood at Harvard Medical School by GSK. SB-734117 was a kind gift from GlaxoSmithKline. Ganciclovir was obtained from SIGMA. H89 and heparan sulphate were obtained from Calbiochem. All drugs were resuspended in dimethyl sulfoxide (DMSO).

Cells and viruses. Human foreskin fibroblast (HFF) cells (clone Hs29) were obtained from American Type Culture Collection no. CRL-1684 (ATCC, Manassas, VA) and maintained in Dulbeccos Modified Eagles Medium (DMEM) (Gibco) containing 5% fetal bovine serum (FBS) (Gibco), plus penicillin and streptomycin. High passage HCMV strain AD169 was a gift from Don Coen (Harvard Medical School). Low passage strain Merlin R1111 (derived from BACmid pAL1111, which does not express RL13 and UL128)[36] was a gift from Richard Stanton (Cardiff University). Ganciclovir resistant virus AD169-P53 was supplied by the National Institute of Health (NIH) AIDS Reagent Program.

Screening of GSK PKIS collection and analysis of screening data. See supplementary material.

Characterization of compounds within the GSK PKIS collection. See supplementary material.

568

569 **Viral yield reduction assays.** Assays were performed essentially as described
570 in [37]. HFF cells were plated at 5 × 10^4 cells per well in 24-well plates. After
571 overnight incubation, cells were infected with HCMV at a multiplicity of infection
572 (MOI) of 1. After virus adsorption for 1 hour at 37°C, cells were washed and
573 incubated with 0.5 ml of media containing DMSO or compounds at a range of
574 concentrations in duplicate. Plates were incubated for 4 days at 37°C. Titers
575 were determined by serial dilution of viral supernatant onto HFF monolayers
576 which were covered in DMEM containing 5% FBS, 0.6% methylcellulose and
577 antibiotics. Cultures were incubated for 14 days, cells were stained, with crystal
578 violet and plaques were counted. Data shown represents the mean value of
579 duplicate plaque counts. The final concentration of DMSO in all samples was
580 maintained at <1% (v/v).

581

582 **MTT cytotoxicity assays.** Assays were performed essentially as described [37].
583 HFF cells were seeded at 1 × 10^4 cells per well into 96-well plates. After
584 overnight incubation to allow cell attachment, cells were treated for the time
585 indicated in the text with at range of concentrations concentrations in duplicate.
586 The highest concentration of compound tested was 10 μM. Cell viability was then
587 determined with an MTT assay according to the manufacturer's instructions (GE
588 Healthcare). Data shown represents the mean value of duplicate readings. The
589 final concentration of DMSO in all samples was maintained at <1% (v/v). As a

590 positive control, in all experiments a 2-fold dilution series of HFF cells starting at
591 1 × 10^4 cells per well was included. In each experiment we found a linear
592 relationship between the number of cells per well and output from the MTT assay
593 (data not shown).

594

595 **Western blotting.** At time points indicated in the text cells were washed
596 once with PBS and resuspended in 100 μl Laemmli buffer containing 5% β-
597 mercaptoethanol. Proteins were separated on 8% or 10% polyacrylamide gels.
598 Typically, a volume of cell lysate corresponding to 1 x 10^4 HFF cells was
599 analyzed, except when blotting for CREB or CREB-Ser133 when a volume of cell
600 lysate corresponding to 5 x 10^5 HFF cells was analyzed. Antibodies used are
601 listed in the supplementary material. Relative band intensity (band intensity
602 relative to β-actin signal in the same lane) was analyzed using ImageJ software,
603 obtained from the National Institutes of Health (USA).

604

605 **RNA analysis and Quantitative PCR.** Quantitative PCR was performed
606 using a SYBR green qPCR kit (Qiagen) and analysed using the ΔΔCT method to
607 compare DMSO versus SB-734117 treated cells. Briefly, cDNA was prepared
608 from RNA extracted from infected cells at timepoints indicated in the Figure.
609 cDNA and no RT controls were amplified in technical duplicates from multiple
610 experiments using a constant primer in exon 3 (UL122-123) and a primer from

611 exon 4 (UL123) or exon 5 (UL122). Cellular RNA was amplified using 18S RNA
612 primers.
613 Exon 3: ACG AGA ACC CCG AGA AAG ATG; exon 4: CGC CAG TGA ATT
614 TCT CTT C; exon 5: CCG GGG AGA GGA GTG TTA GT; 18S for: GTA ACC
615 CGT TGA ACC CCA; 18S rev: CCA TCC AAT CGG TAG TAG CG.
616 qPCR was performed using cycling conditions: 95^{o}C (15s) then 40 cycles of 94^{o}C
617 (15s), 55^{o}C (30s) and 72^{o}C (30s).
618
619 **Chromatin immunoprecipitation.** All procedures were performed
620 essentially as previously described [21]. Briefly, HFFs were fixed with 1%
621 formaldehyde (10 mins) and then enzymatically digested to fragment DNA as
622 described by manufacturer (Pierce chromatin preparation kit). DNA associated
623 with histones was immunoprecipitated with control serum (Sigma) or anti-acetyl-
624 histone H3-lysine 14 (1:150 dilution of antibody – see supplementary material).
625 For detection of the HCMV MIEP, DNA from disrupted nucleosomes was
626 precipitated and amplified by SYBR green qPCR kit (Qiagen) using 5′ - TGG
627 GAC TTT CCT ACT TGG (sense) and 5′ - CCA GGC GAT CTG ACG GTT (anti-
628 sense) primers. Specific immuno-precipitation of sequences was expressed as
629 enrichment from Input.
630

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632

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646

CONFLICTS OF INTEREST

The authors declare no conflicts of interest.

ABBREVIATIONS

AGC: containing PKA, PKG, PKC families group, **CAMK**: calcium/calmodulin-dependent protein kinase group, **CDK**: cyclin-dependent kinase, **CLK2**: cyclin-dependent kinase-like kinase 2, **CK**: casein kinase, **CMCG**: containing CDK, MAPK, GSK3, CLK families group, **CREB**: cAMP response element-binding protein, **GCV**: ganciclovir, **DYRK**: dual-specificity tyrosine phosphorylation-regulated kinase, **GSK**: glycogen synthase kinase, **HCMV**: human cytomegalovirus, **HIPK**: homeodomain interacting protein kinase, **MAPK4K4**: mitogen-activated protein kinase kinase kinase kinase 4, **MNK1**: MAP kinase-interacting serine/threonine-protein kinase 1, **MSK**: mitogen and stress kinase, **PCK-η**: protein kinase C-η, **PLK-1**: polo-like kinase 1, **PRKD**: protein kinase D, **PRKG**: protein kinase, cGMP-Dependent, **PRKX**: protein kinase, x-linked, **p70S6K1**: ribosomal protein S6 kinase beta-1, **ROCK**: rho-associated, coiled-coil-containing protein kinase 1, **RSK**: ribosomal s6 kinase, **STE**: homologs of yeast Sterile 7, Sterile 11, Sterile 20 kinases group, **S-T-PK**: serine/threonine protein kinase group, **TK**: tyrosine kinase group, **TKL**: tyrosine kinase-like group.

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FIGURE LEGENDS

Fig. 1 High throughput screening of the GSK PKIS collection. (a) Diagram of screening process. (b) A representative example of a microscopy image from an Image Express Micro microscope of infected HFF cells treated with Hoecsht 33342 (blue), Deep Red Cell Mask (Red) and primary and secondary antibodies to detect HCMV pp28 (green). The large white box is a magnified image of the area identified by the small white box. (c) Plot of z-scores where each data point represents a single compound. The compounds with highest and lowest z-scores are identified and their z-scores are stated in parentheses. (d) Structures of compounds with z-scores ((i)-(iv)) lower than -2 and ((v)-(vii)) greater than 2.

Fig. 2 Kinase selectivity of compounds assigned z-scores. The full list of kinase selectivity data is shown in Table S5. Table S5 is shown here as a "heatmap" of kinase selectivity wherein the potency of each compound at 1 μM concentration against a particular kinase is represented in colour as indicated at the bottom of the figure (less than 0% inhibition – blue, 0-50% inhibition – green, 51-75% inhibition – yellow, 76-90% inhibition – orange, greater than 91% inhibition – red). Each row represents a compound and each column represents the kinase tested. The z-scores of each compound are indicated to the left of the figure. The kinase groups of each kinase tested are indicated above the figure. (a)-(c) Kinase inhibition of compounds with z-scores of less than -1 not found in

807 compounds with z-scores greater than 1. (d) Kinase inhibition of compounds with
808 z-scores greater than 1 not found in compounds with z-scores of less than -1.
809
810 **Fig. 3 Analysis of HCMV replication and protein production in infected HFF**
811 **cells treated with DMSO or SB-734117 at the time of infection.** (a) HFF cells
812 were infected at MOI1 with AD169 then treated with 1μM SB-734117 or the
813 equivalent volume of DMSO. Viral titre (plaque forming units (p.f.u.)/ml)) was
814 determined at the indicated time points (hours post infection (h.p.i.)). Data points
815 and error bars represent the mean and standard deviation, respectively, from
816 three experiments. (b) HFF cells were infected with AD169 at an MOI of 1, then
817 treated with either 1μM SB-734117 or the equivalent volume of DMSO. Cell
818 lysates were prepared for western blotting at the time points (hours post infection
819 (h.p.i.)) indicated above the figure. Uninfected cells harvested at the time of
820 infection are shown as 0 h.p.i.. Proteins recognized by the antibodies used are
821 indicated to the right of each figure. The positions of molecular mass markers
822 (kDa) are indicated to the left of each figure. (c) Relative band intensity of
823 immediate-early protein bands relative to β-actin signal in the same lane in
824 Figure 3A, as quantified using ImageJ. Band intensities of 0-1, 1-2 and greater
825 than 2 are highlighted in light grey, dark grey and black, respectively. (d) HFF
826 cells were infected at MOI1 with AD169 then treated with 1μM SB-734117 or the
827 equivalent volume of DMSO. Samples were prepared for quantitative PCR
828 analysis of *IE1* and *IE2* mRNA expression, respectively, at the time points
829 indicated in the figures. Data and error bars represent the mean and standard

deviation of three PCR replicates from each sample, respectively (n=2). Change in gene expression relative to DMSO is shown for each timepoint using ΔΔCT method.

Fig. 4 Analysis of HCMV replication and protein production in infected HFF cells treated with DMSO or SB-734117 at 24 hours post infection. (a) HFF cells were infected at MOI1 with AD169 then treated with 1μM SB-734117 or the equivalent volume of DMSO at 24 hours post infection. Viral titre (plaque forming units (p.f.u.)/ml)) was determined at 120 hours post infection (h.p.i.). (b) HFF cells were infected with AD169 at an MOI of 1, then treated with either 1μM SB-734117 or the equivalent volume of DMSO at 24 hours post infection. Cell lysates were prepared for western blotting at the time points (hours post infection (h.p.i.)) indicated above the figure. Infected cells harvested at 24 h.p.i. that were not treated with either SB-734117 or DMSO were also assayed. Proteins recognized by the antibodies used are indicated to the right of each figure. The positions of molecular mass markers (kDa) are indicated to the left of each figure. (c) Relative band intensity of immediate-early protein bands relative to β-actin signal in the same lane in Figure 3A, as quantified using ImageJ. Band intensities of 0-1, 1-2 and greater than 2 are highlighted in light grey, dark grey and black, respectively.

Fig. 5 Inhibition of phosphorylation of cellular proteins by SB-734117 ((a), (c)-(3)) HFF cells were infected with AD169 at an MOI of 1, then treated with

853 either 1μM SB-734117 or the equivalent volume of DMSO (as indicated above
854 each Figure). Cell lysates were prepared for western blotting at (a) 72 h.p.i. or
855 ((c)-(e)) as indicated above the figure. Uninfected cells harvested at the time of
856 infection are shown as 0 h.p.i. in (c)-(e). In (a) no lysate was analyzed in lanes 2
857 and 4. Proteins recognized by the antibodies used are indicated to the right of
858 each figure. The positions of molecular mass markers (kDa) are indicated to the
859 left of each figure. (b) Relative band intensity of CREB and CREB-Ser133 bands
860 relative to β-actin signal in the same lane in Fig. 4(a), as quantified using ImageJ.
861 Band intensities of 0-1, 1-2 and greater than 2 are highlighted in light grey, dark
862 grey and black, respectively.
863
864 **Fig. 6 H3K14ac at the MIEP is unaffected in SB-734117 treated cells.** DNA
865 was immune-precipitated from infected cells (24-72hpi) treated with either DMSO
866 or SB-734117 using an anti-H3K14ac antibody (K14) or isotype control (C), then
867 amplified in an MIEP qPCR. Enrichment of MIEP sequences was expressed
868 relative to amplification in Input sample. Data and error bars represent the mean
869 and standard deviation of three PCR replicates from each sample, respectively

TABLES

Table 1

Chemotype	Total no. of compounds in chemotype	No. of compounds excluded due to cytotoxicity	No. of compounds assigned z-scores.
4-pyrimidinyl ortho-aryl azoles	31	0	31
Oxindoles	30	3	27
Furazan benzimidazoles	25	1	24
4-anilino quinazolines and related	25	0	25
Benzimidazole N-thiophenes	21	9	12
4-pyridyl ortho-aryl azoles	18	0	18
2H-3 pyrimidinyl pyrazolopyridazines	16	7	9
2-amino oxazoles	15	0	15
4-hydrazinly pyrazolopyrimidines	15	0	15
2,4-dianilino pyrrolopyrimidines	15	1	14
Biaryl amides	14	0	14
3-vinyl pyridines	13	0	13
Anilino thienopyrimidines	12	0	12
Benzimidazolyl diaryl ureas	12	2	10
2-aryl 3-pyridimidinyl pyrazolopyridazines	12	0	12
2,4-diamino pyrimidines	12	0	12
Maleimide	11	0	11
Furopyrimidines and related	9	0	9
Indazole-3-carboxamides	7	1	6
3-amino pyrazolopyridines	7	3	4
2-pyridinyl imidazoles and related	7	0	7
4-anilino 5-alkynyl pyrimidines	7	0	7
3-cyano thiophenes	6	2	4
Phenyl carboxamides	6	0	6
Indazole-5-carboxamides	6	0	6
3-amino pyrazolopyridazines	4	1	3
3-amino pyrazoles	3	0	3
Imidazotriazine	3	0	3
4-anilino quinolones	2	0	2
6-phenyl isoquinolines	2	1	1
3-benzyl pyrimidines	1	0	1

877 Table 2

878

Experiment	Viral Strain	Compound	ED50* (μM)
1	AD169	SB-734117	0.5
	AD169	GCV†	0.5
2	AD169	SB-734117	0.4
	AD169-P53	SB-734117	1.3
3	AD169	SB-734117	1
	Merlin(RCMV1111)	SB-734117	2

879 *50% effective dose
880 †Ganciclovir

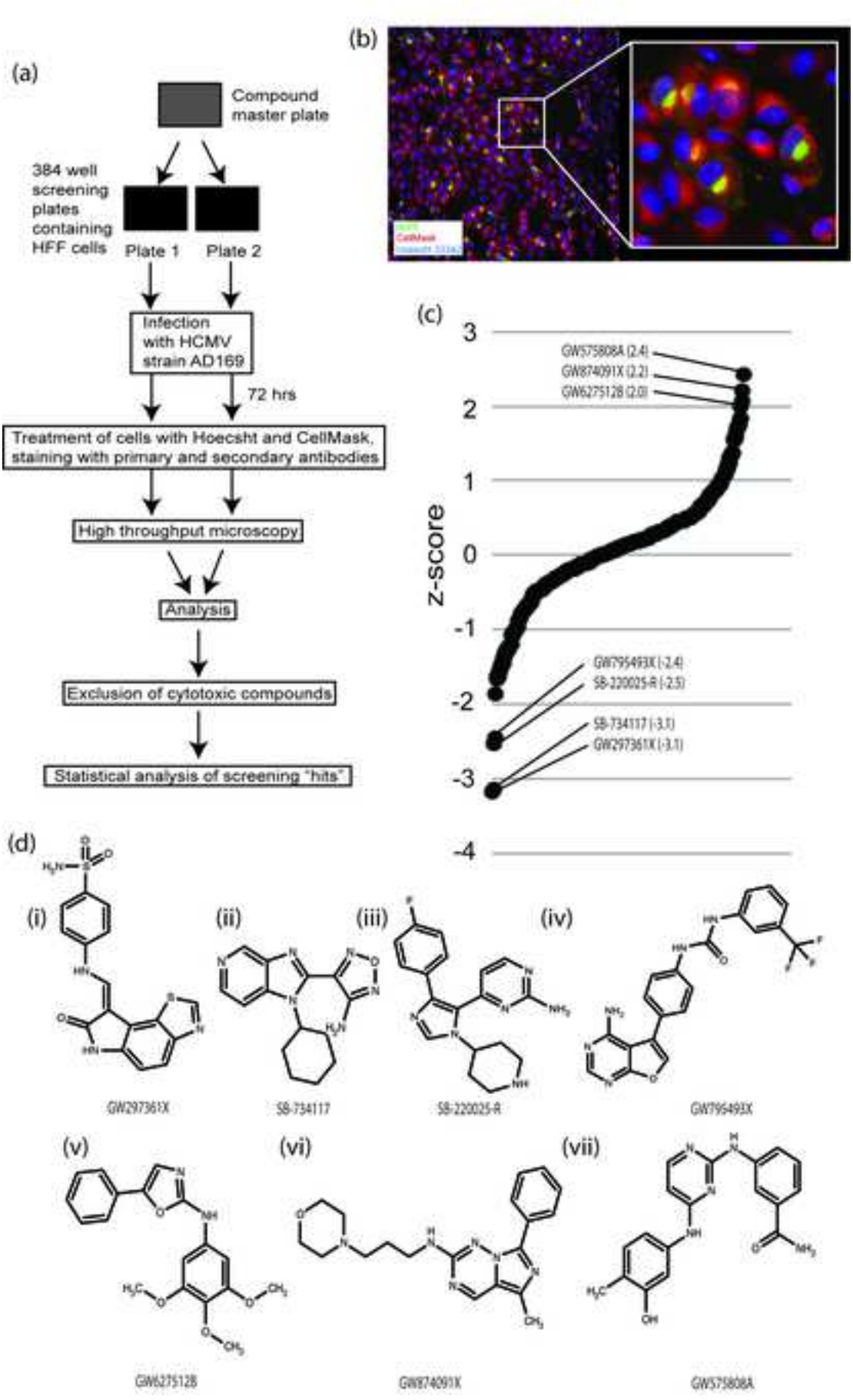


Fig. 1

Figure2

Click here to download Figure Screen2.tif

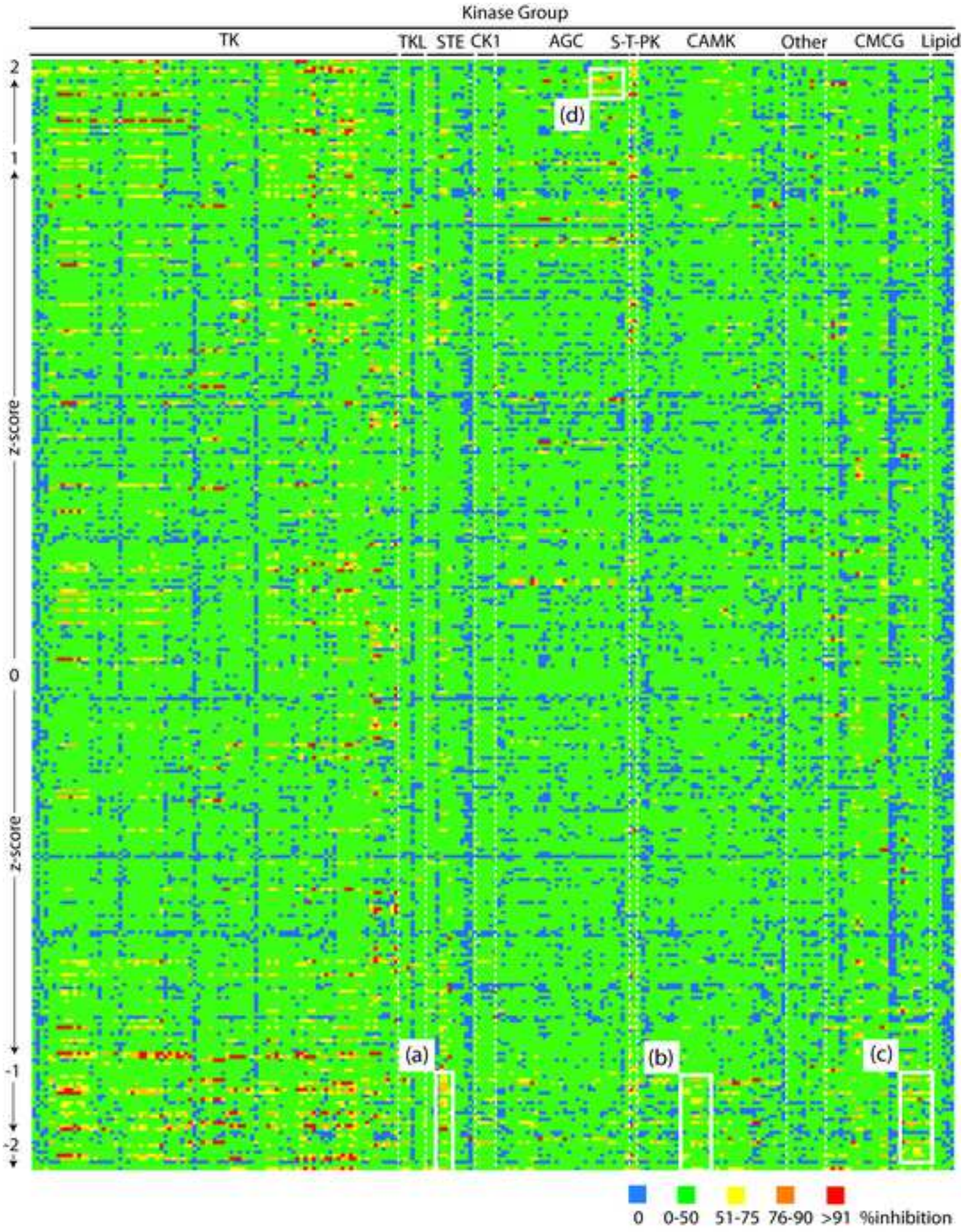
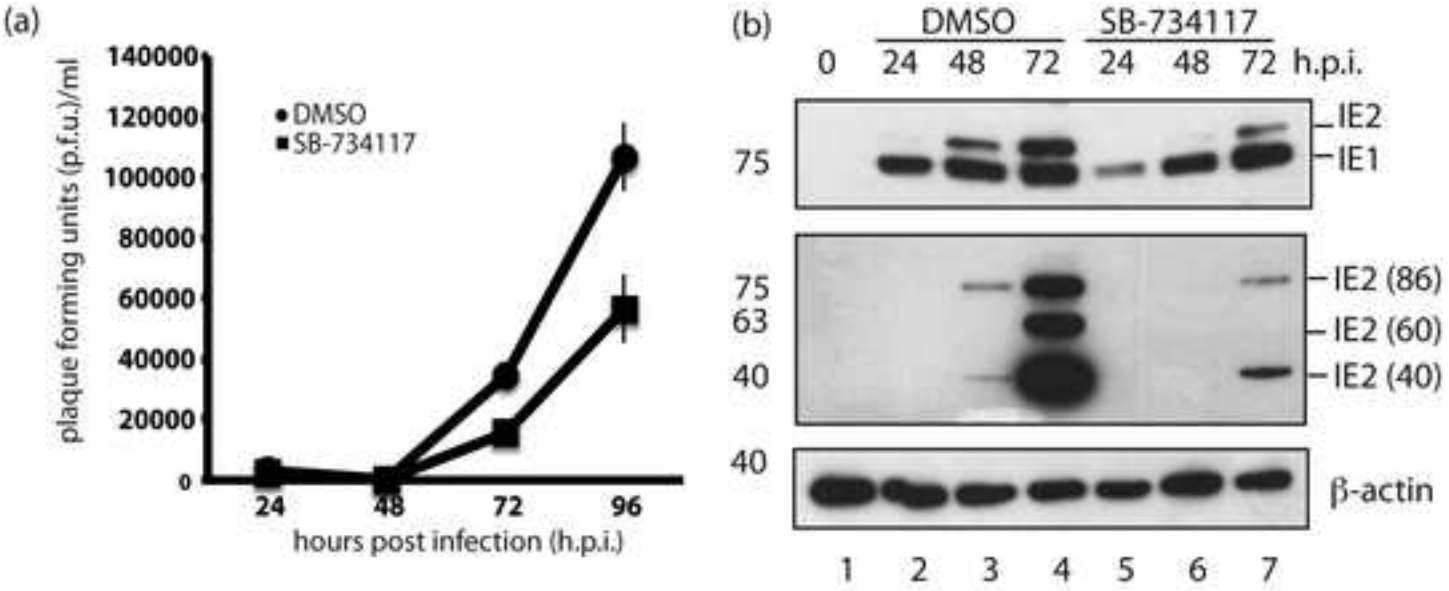


Fig. 2



(c)

	DMSO			SB-734117		
	h.p.i.			h.p.i.		
Protein	24	48	72	24	48	72
IE1	0.51	1.65	2.25	0.16	0.52	1.38
IE2	0	1.46	4.19	0	0	1.50
IE2(86)	0	0.21	6.28	0	0	0.37
IE2(60)	0	0	6.98	0	0	0
IE2(40)	0	0.03	5.72	0	0	1.27

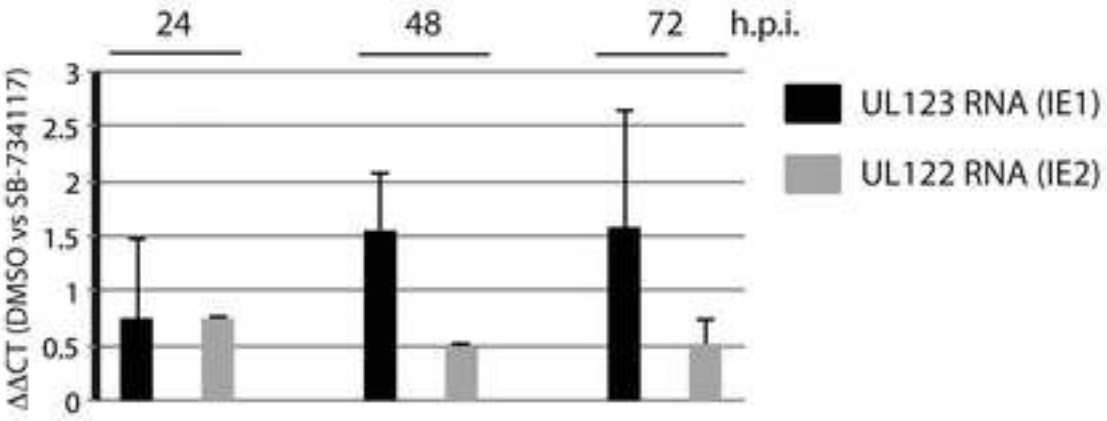
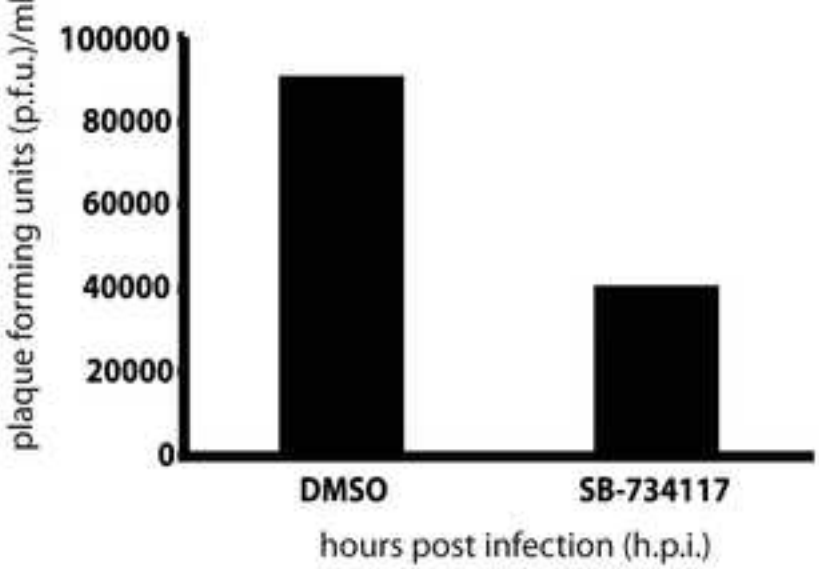
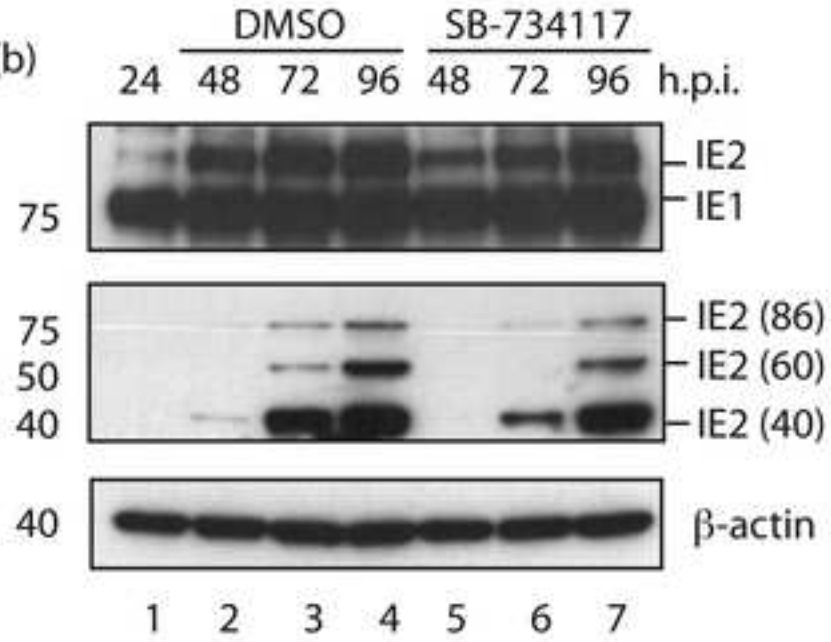


Fig. 3

(a)



(b)



(c)

Protein	h.p.i.	DMSO h.p.i.			SB-734117 h.p.i.		
	24	24	48	72	24	48	72
IE1	1.10	1.10	1.00	1.02	1.02	0.81	0.87
IE2	0.11	0.81	1.32	1.08	0.62	1.32	1.74
IE2(86)	0	0	1.10	2.06	0	0.61	2.64
IE2(60)	0	0	0.23	3.66	0	0	2.92
IE2(40)	0	0.09	1.86	2.06	0	0.90	2.14

Fig. 4

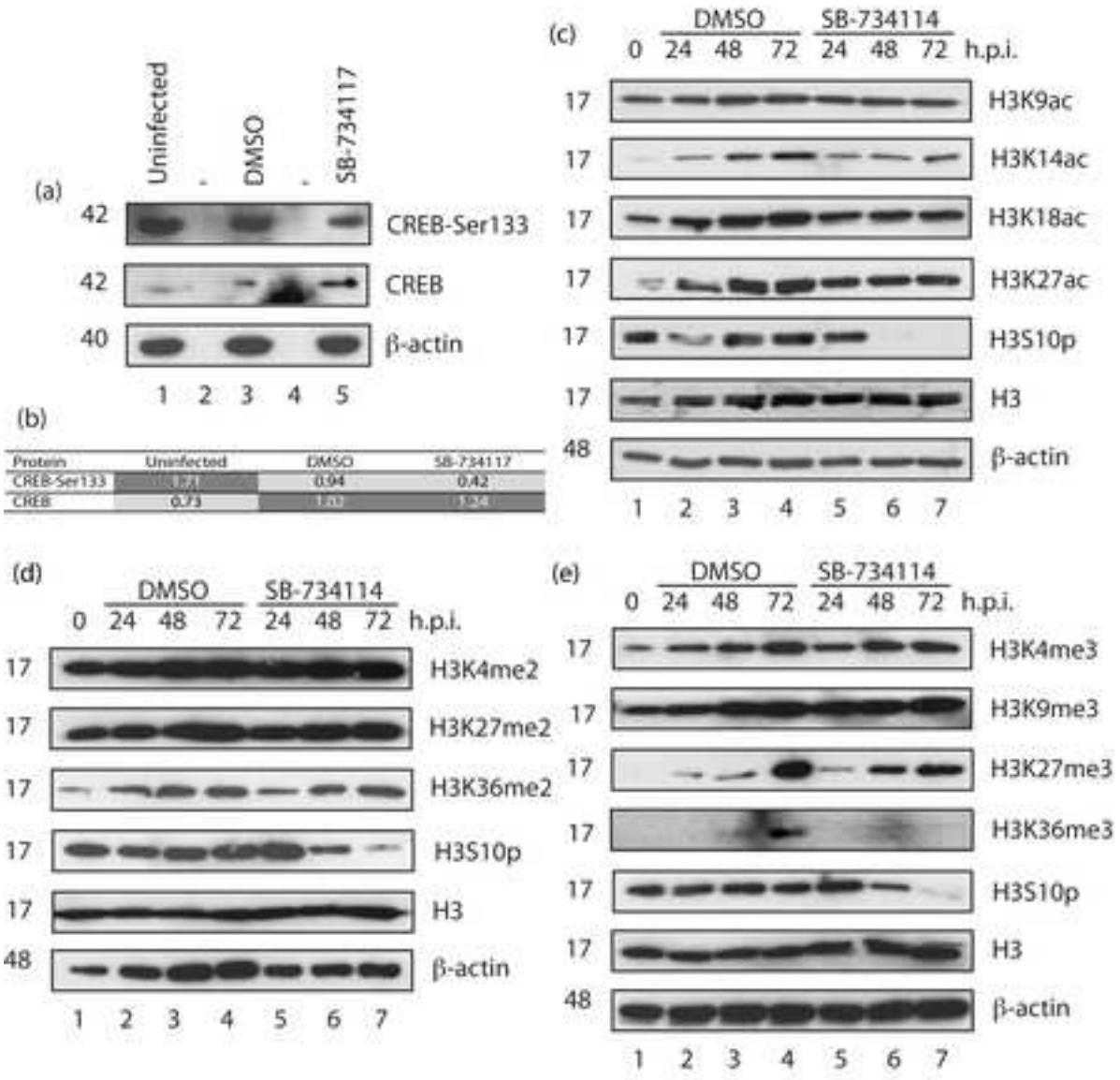


Fig. 5

Figure 5

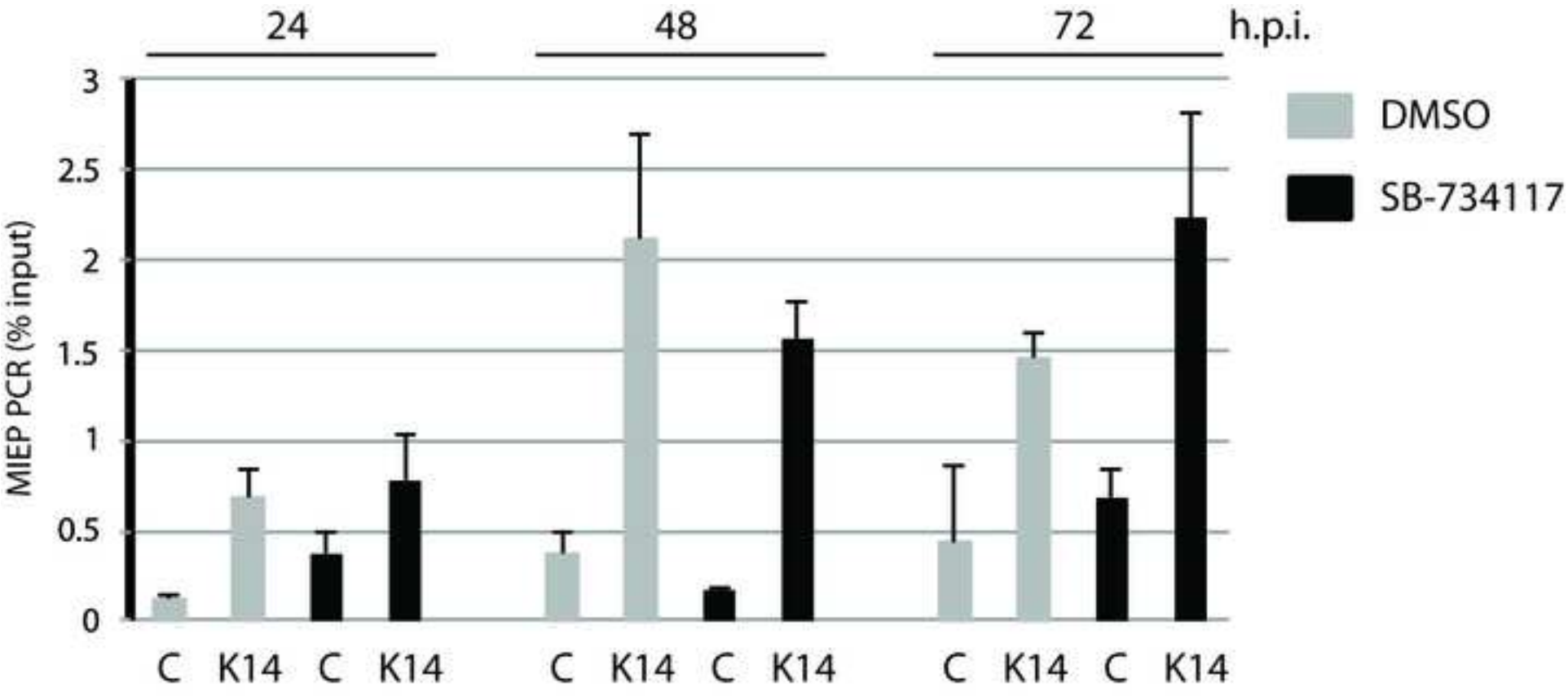


Fig. 6

SUPPLEMENTARY MATERIAL

High Throughput Screening of a GlaxoSmithKline Protein Kinase Inhibitor Set Identifies an Inhibitor of Human Cytomegalovirus Replication that Prevents CREB and Histone H3 Post-Translational Modification

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Matthew B Reeves[2] & Blair L Strang[1,4]

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Compound treatment and infection of cells for high throughput screening. The GSK PKIS library [1] (stock concentration of 3.3 mM of each compound in DMSO) was screened in duplicate. Twenty four hours before infection 2000 HFF cells were seeded in each well of each Corning 384 plate. Unless stated otherwise, liquid was added to wells using a WellMate apparatus. At the time of infection, media was removed with a suction manifold and 30 μl of complete media was added to each well. Compounds were added to the plate containing HFF cells using a 100 nl pin transfer on a liquid handling robot. Negative and

positive controls (water+0.3% DMSO or heparin sulfate (5 μg/ml) + 0.3% DMSO, respectively) were added to plates by hand (12 wells of each). Cells were then infected with HCMV strain AD169 (MOI 1) in a total volume of 5 μl. Thus, the final concentration of compound in each well was 9.4 μM. Infected cells were incubated for 72 hours at 37°C, then prepared for analysis.

Preparation of screening plates for high throughput microscopy analysis. Cell culture media was removed from infected cells and replaced with 20 μl Hoecsht 33342 (SIGMA) diluted in PBS to a final concentration of 10 μg/ml. After incubation for 1 hour at 37°C, 20 μl of Deep Red Cell Mask (Invitrogen) (diluted in PBS to a concentration of 5 μg/ml) was added to each well. Cells were incubated for a further 5 min at 37°C. Cells were then fixed by removing PBS containing Hoescht and Cell Mask and adding 50 μl of 3.5%Formaldyhyde (SIGMA) in PBS to each well. After incubating at room temperature for 10 min, fixative was removed and 50 μl of PBS containing 0.5% TritonX-100 was added per well to permeablize cells. After 10 min incubation at room temperature, PBS containing detergent was removed, and cells was washed once with PBS. PBS was removed and replaced with 20 μl MAb P207 recognizing pp28 (Virusys) (dilution 1:1000) and anti-mouse secondary antibody conjugated to flurophore Alexa488 (Molecular Probes) (dilution 1:1000). Plates were incubated at 37°C for 1 hour. After incubation, PBS containing antibodies was removed and replaced with 50 μl of PBS. Plates were then analyzed using automated microscopy for the presence of pp28 protein.

Microscopy analysis of screening plates. Infected cells stained with antibody to detect pp28 were imaged on an Image Express Micro (IXM) microscope (Molecular Devices) at 10x magnification to detect 3 wavelengths; 488 nm to detect antibody recognizing pp28, 568nm to detect Deep Red CellMask and 350 nm to detect Hoescht 33342 stain bound to nuclear DNA. Three images were captured from each wavelength in each well of the 384-well plate. The number of cells positive at all 3 wavelengths and percentage of pp28 positive cells in each well was determined using the Metamorph Multiwavelength Cell Scoring software (Molecular Devices). Typically, approximately 60% of cells were infected in wells treated with negative control, DMSO (data not shown).

Analysis of screening results. To assess the quality of data that could be returned from the screening protocol we calculated the Z'-factor [2, 3] derived from the positive (heparan sulphate treated infected cells) and negative (DMSO treated infected cells) control wells. The screening controls returned Z'-factors of greater than or equal to 0.5, indicating a robust separation of difference in the data derived from positive and negative controls (data not shown). Thus, the screening protocol could be reliably used to screen the compound collection.

After screening of the compound collection, data was discarded from any well in which the number of cells stained with Hoescht 33342 fell below 2-fold of the mean of the number of cells in each well of the plate. The data from the remaining wells from each plate was converted to a z-score (the number of

standard deviations from the mean of the data [2, 3]) and the average z-score from data in duplicate plates was determined. Images chosen at random were visually inspected throughout image capture and analysis to ensure raw data was consistent with z-scores.

Characterization of compounds within the GSK PKIS collection. Characterization of compounds has been reported by Elkins and co-workers [4]. Kinase profiling was previously performed by using the Nanosyn microfluidics capillary electrophoresis technology (based on the change in electrophoretic mobility of a substrate upon phosphorylation) to determine each compounds ability to inhibit a panel of 224 recombinant kinase proteins. GPCR screening using calcium mobility assays was carried out as previously described [4]. The structure of each compound is available at ChEMBL (https://www.ebi.ac.uk/chembl/) [1].

Primary and secondary antibodies used in western blotting. Membranes were probed with antibodies recognizing IE1/2, UL44, pp28, UL84 (all Virusys, 1:1000 dilution), IE2 proteins (clone 5A8.2, Millipore, 1:1000 dilution), β-actin (SIGMA, 1:5000 dilution), CREB (product no. 06-863) or CREB-Ser133 (product no. 06-519) (both Millipore, 1:500 dilution). Antibody recognizing UL97 [5] was a kind gift from Donald Coen (Harvard Medical School, USA), respectively. All antibodies recognizing histone proteins were obtained from Cell Signaling Technology (products #9927, #9847, #9783) and used as per suppliers instructions. All primary antibodies were detected using anti-mouse- or anti-

rabbit-horseradish peroxidase (HRP) conjugated antibodies (Millipore and Cell Signaling Technology, respectively). Chemiluminescence solution (GE Healthcare) was used in each case to detect secondary antibodies using film.

1. **Drewry DH, Willson TM, Zuercher WJ.** Seeding collaborations to advance kinase science with the GSK Published Kinase Inhibitor Set (PKIS). Current topics in medicinal chemistry. 2014;14:340-342.

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4. **Elkins JM, Fedele V, Szklarz M, Abdul Azeez KR, Salah E, et al.** Comprehensive characterization of the Published Kinase Inhibitor Set. Nat Biotechnol. 2016;34:95-103.

5. **Kamil JP, Coen DM.** Human cytomegalovirus protein kinase UL97 forms a complex with the tegument phosphoprotein pp65. J Virol. 2007;81:10659-10668.

Table S1. Compounds in GSK PKIS collection.

COMPOUND	CHEMOTYPE	SMILES	ORIGINAL TARGET
GI261520A	04:4-anilino_quinazolines_and_related	Cl.COc1ccc2ncnc(N	EGFR/ErbB2
GR105659X	02:Oxindoles	Oc1ccc2c(CC\C2=C	TRKA
GR269666A	04:4-anilino_quinazolines_and_related	Cl.C(c1nc2ccc(Nc3	EGFR/ErbB2
GSK1000163A	03:Furazan_benzimidazoles	CCn1c(nc2c(nc(CN	AKT
GSK1007102B	03:Furazan_benzimidazoles	OC(=O)C(F)(F)F.C	AKT
GSK1023156A	05:Benzimidazole_N-thiophenes	NC(=O)c1sc(cc1OC	PLK
GSK1030058A	05:Benzimidazole_N-thiophenes	COC(=O)c1sc(cc1C	PLK
GSK1030059A	05:Benzimidazole_N-thiophenes	COc1cc2ncn(-c3cc	PLK
GSK1030061A	05:Benzimidazole_N-thiophenes	CNC(=O)c1sc(cc1C	PLK
GSK1030062A	05:Benzimidazole_N-thiophenes	COc1cc2ncn(-c3cc	PLK
GSK1173862A	10:2,4-dianilino_pyrrolopyrimidines	CCCN1CCCC(C1)c	IGF-1R
GSK1220512A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc(ccc1Nc1nc	IGF-1R
GSK1326255A	10:2,4-dianilino_pyrrolopyrimidines	CCCN1CCC(CC1)c	IGF-1R
GSK1392956A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc(ccc1Nc1nc	IGF-1R
GSK1511931A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc(ccc1Nc1nc	IGF-1R
GSK1713088A	10:2,4-dianilino_pyrrolopyrimidines	CCCN1CCC(CC1)C	IGF-1R
GSK1751853A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc2CCN(C(=C	IGF-1R
GSK180736A	25:Indazole-5-carboxamides	CC1=C(C(NC(=O)N	RHO
GSK1819799A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc(ccc1Nc1nc	IGF-1R
GSK182497A	13:Anilino_thienopyrimidines	CN(C)C(=O)O[C@H	EGFR/ErbB2
GSK192082A	13:Anilino_thienopyrimidines	CCNC(=O)O[C@H]	EGFR/ErbB2
GSK200398A	13:Anilino_thienopyrimidines	Cl.O=C(O[C@H]1C	EGFR/ErbB2
GSK204925A	05:Benzimidazole_N-thiophenes	COc1cc2ncn(-c3cc	PLK
GSK2110236A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc2CCCN(C(=	IGF-1R
GSK2163632A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc2c(cc1Nc1r	IGF-1R
GSK2186269A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc2CCN(C(=C	IGF-1R
GSK2213727A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc(C)c(NC(=C	IGF-1R
GSK2219385A	10:2,4-dianilino_pyrrolopyrimidines	COc1cc(C)c(cc1Nc	IGF-1R
GSK2220400A	10:2,4-dianilino_pyrrolopyrimidines	CNC(=O)c1ncccc1N	IGF-1R
GSK237700A	05:Benzimidazole_N-thiophenes	COc1cc2ncn(-c3cc	PLK
GSK237701A	05:Benzimidazole_N-thiophenes	COc1cc2ncn(-c3cc	PLK
GSK238063A	13:Anilino_thienopyrimidines	CN(C)C(=O)O[C@(	EGFR/ErbB2
GSK238583A	13:Anilino_thienopyrimidines	OC(=O)C(F)(F)F.O	EGFR/ErbB2
GSK248233A	03:Furazan_benzimidazoles	CCn1c(nc2cnc(Oc3	RHO
GSK259178A	13:Anilino_thienopyrimidines	OC(=O)C(F)(F)F.Fc	EGFR/ErbB2
GSK269962B	03:Furazan_benzimidazoles	Cl.CCn1c(nc2cnc(C	RHO
GSK270822A	25:Indazole-5-carboxamides	CC1=C(C(CC(=O)N	RHO
GSK299115A	25:Indazole-5-carboxamides	CC1=C(C(CC(=O)N	RHO
GSK300014A	13:Anilino_thienopyrimidines	CS(=O)(=O)CCNCc	EGFR/ErbB2
GSK312948A	05:Benzimidazole_N-thiophenes	COc1cc2ncn(-c3cc	PLK
GSK317314A	05:Benzimidazole_N-thiophenes	COc1ccc2ncn(-c3c	PLK
GSK317315A	05:Benzimidazole_N-thiophenes	COc1ccc2ncn(-c3c	PLK
GSK317354A	25:Indazole-5-carboxamides	CC1=C(C(N=C(N1)	RHO
GSK319347A	05:Benzimidazole_N-thiophenes	COc1cc2ncn(-c3cc	IKK
GSK326090A	05:Benzimidazole_N-thiophenes	C[C@@H](Oc1cc(s	PLK
GSK466314A	25:Indazole-5-carboxamides	Cc1n[nH]c2ccc(NC	RHO
GSK466317A	25:Indazole-5-carboxamides	CC1=C(C(CC(=O)N	RHO
GSK554170A	03:Furazan_benzimidazoles	OC(=O)C(F)(F)F.C	AKT

GSK561866B	03:Furazan_benzimidazoles	OC(=O)C(F)(F)F.C(	AKT
GSK571989A	05:Benzimidazole_N-thiophenes	C[C@@H](Oc1cc(s	PLK
GSK579289A	05:Benzimidazole_N-thiophenes	C[C@@H](Oc1cc(s	PLK
GSK586581A	24:Phenyl_carboxamides	CS(=O)(=O)Nc1ccc	IKK
GSK605714A	24:Phenyl_carboxamides	COc1ccc(cc1C(N)=	IKK
GSK614526A	03:Furazan_benzimidazoles	OC(=O)C(F)(F)F.C(	AKT
GSK619487A	03:Furazan_benzimidazoles	OC(=O)C(F)(F)F.C(	AKT
GSK620503A	24:Phenyl_carboxamides	NC(=O)c1cc(cc(-c2	IKK
GSK625137A	24:Phenyl_carboxamides	NC(=O)c1cc(cc(-c2	IKK
GSK635416A	24:Phenyl_carboxamides	CNC(=O)c1cc(cc(-c	IKK
GSK711701A	24:Phenyl_carboxamides	COc1c(cc(cc1-c1cc	IKK
GSK718429A	06:4-pyridyl_ortho-aryl_azoles	CCn1cc(c(n1)-c1cc	RAF
GSK938890A	03:Furazan_benzimidazoles	CCn1c(nc2c(nc(OC	AKT
GSK943949A	03:Furazan_benzimidazoles	CCn1c(nc2c(nc(OC	AKT
GSK949675A	03:Furazan_benzimidazoles	Cl.CCn1c(nc2c(nc(	AKT
GSK953913A	30:6-phenyl_isoquinolines	NS(=O)(=O)c1ccc(	IKK
GSK969786A	13:Anilino_thienopyrimidines	Fc1cccc(COc2ccc(I	EGFR/ErbB2
GSK978744A	05:Benzimidazole_N-thiophenes	C[C@@H](Oc1cc(s	PLK
GSK980961A	30:6-phenyl_isoquinolines	NS(=O)(=O)c1cccc	IKK
GSK994854A	10:2,4-dianilino_pyrrolopyrimidines	CCCN1CCC=C(C1	IGF-1R
GW275616X	02:Oxindoles	NS(=O)(=O)c1cccc	TRKA
GW275944X	02:Oxindoles	Cc1ccc2NC(=O)\C(	CDK2
GW276655X	02:Oxindoles	NS(=O)(=O)c1ccc(N	CDK2
GW278681X	02:Oxindoles	CS(=O)(=O)Nc1ccc	TRKA
GW279320X	02:Oxindoles	Cc1cc(Cl)cc2C(=N	CDK2
GW280670X	02:Oxindoles	NS(=O)(=O)c1ccc(N	CDK2
GW282449A	04:4-anilino_quinazolines_and_related	Cl.COc1cc2ncnc(N	EGFR/ErbB2
GW282536X	02:Oxindoles	Cc1cccc2c1NC(=O	CDK2
GW282974X	04:4-anilino_quinazolines_and_related	CN(C)c1cc2c(Nc3c	EGFR/ErbB2
GW284372X	04:4-anilino_quinazolines_and_related	C(Oc1ccc(Nc2ncnc	EGFR/ErbB2
GW284408X	02:Oxindoles	O=C1Nc2ccccc2\C	TRKA
GW290597X	02:Oxindoles	NS(=O)(=O)c1ccc(N	CDK2
GW296115X	17:Maleimide	COc1ccc2[nH]c3c4	PDGFR
GW297361X	02:Oxindoles	NS(=O)(=O)c1ccc(N	CDK2
GW300653X	02:Oxindoles	CC(C)c1ccc2c(NC(	CDK2
GW300657X	02:Oxindoles	NS(=O)(=O)c1ccc(N	CDK2
GW300660X	02:Oxindoles	NS(=O)(=O)c1ccc(N	CDK2
GW301784X	02:Oxindoles	CC(C)(CO)CNC(=C	CDK2
GW301789X	02:Oxindoles	O=C1Nc2ccccc2\C	TRKA
GW301888X	04:4-anilino_quinazolines_and_related	CN(C)c1cc2c(Nc3c	EGFR/ErbB2
GW305074X	02:Oxindoles	Oc1c(Br)cc(C=C2C	RAF
GW305178X	02:Oxindoles	NS(=O)(=O)c1ccc(N	CDK2
GW335962X	02:Oxindoles	C\C(Nc1ccc(cc1)S(	CDK2
GW352430A	02:Oxindoles	Cl.NS(=O)(=O)c1cc	CDK2
GW396574X	02:Oxindoles	CC(C)=Cc1cccc2N	CDK2
GW405841X	02:Oxindoles	COC(=O)c1ccc2NC	RAF
GW406108X	02:Oxindoles	Oc1c(Cl)cc(C=C2C	RAF
GW406731X	12:3-vinyl_pyridines	COC(=O)c1cncc(\C	RAF
GW407323A	02:Oxindoles	Cl.Nc1nc(cs1)-c1cc	RAF
GW410563A	04:4-anilino_quinazolines_and_related	Cl.COc1cc2ncnc(N	VEGFR
GW416469X	02:Oxindoles	CN(C)c1ccc2NC(=(	CDK2

GW416981X	02:Oxindoles	CC(C)COC(=O)c1c	CDK2
GW427984X	12:3-vinyl_pyridines	CN(C)C(=O)c1cncc	RAF
GW429374A	02:Oxindoles	Cl.Oc1c(Br)cc(C=C	RAF
GW432441X	12:3-vinyl_pyridines	CNC(=O)Oc1cc(C)(	RAF
GW434756X	06:4-pyridyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1nn2(	P38
GW435821X	12:3-vinyl_pyridines	Cc1cc(O)cc(C)c1\C	RAF
GW439255X	12:3-vinyl_pyridines	Cc1cc(O)cc(C)c1\C	RAF
GW440139A	29:4-anilino_quinolines	Cl.Cc1ccc(O)cc1Nc	RET
GW441756X	02:Oxindoles	Cn1cc(C=C2C(=O)I	TRKA
GW441806A	12:3-vinyl_pyridines	Cl.Cc1cc(O)cc(C)c1	RAF
GW442130X	02:Oxindoles	COc1ccccc1-c1cc(\	TRKA
GW445012X	12:3-vinyl_pyridines	CNC(=O)c1cncc(\C	RAF
GW445014X	12:3-vinyl_pyridines	CNC(=O)c1cncc(\C	RAF
GW445015X	12:3-vinyl_pyridines	CNC(=O)c1cncc(\C	RAF
GW445017X	12:3-vinyl_pyridines	CNC(=O)c1cncc(\C	RAF
GW450241X	12:3-vinyl_pyridines	CCc1cccc(CC)c1\C	RAF
GW458344A	12:3-vinyl_pyridines	Cl.Cc1cc(cc(C)c1\C	RAF
GW458787A	04:4-anilino_quinazolines_and_related	Cl.CS(=O)(=O)CCN	EGFR/ErbB2
GW459057A	12:3-vinyl_pyridines	Cl.Cc1cc(cc(C)c1\C	RAF
GW461104A	04:4-anilino_quinazolines_and_related	Cl.CS(=O)(=O)CCN	EGFR/ErbB2
GW513184X	09:4-hydrazinly_pyrazolopyrimidines	COc1cc(C=NNc2nc	GSK3
GW549034X	03:Furazan_benzimidazoles	CCn1c(nc2ccccc12	MSK
GW549390X	08:2-amino_oxazoles	N(c1ncc(o1)-c1ccc(	VEGFR
GW559768X	29:4-anilino_quinolines	Cc1ccc(O)cc1Nc1c	RET
GW561436X	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1nn2(	P38
GW566221A	04:4-anilino_quinazolines_and_related	Cl.CS(=O)(=O)CCN	EGFR/ErbB2
GW567808A	04:4-anilino_quinazolines_and_related	Cl.CS(=O)(=O)CCN	EGFR/ErbB2
GW568326X	01:4-pyrimidinyl_ortho-aryl_azoles	Nc1nccc(n1)-c1c(n	P38
GW568377A	04:4-anilino_quinazolines_and_related	Cl.CS(=O)(=O)CCN	EGFR/ErbB2
GW569293E	01:4-pyrimidinyl_ortho-aryl_azoles	OC(=O)\C=C\C(O)=	P38
GW569530A	04:4-anilino_quinazolines_and_related	Cl.CS(=O)(=O)CCN	EGFR/ErbB2
GW572399X	08:2-amino_oxazoles	NS(=O)(=O)c1ccc(N	VEGFR
GW572401X	08:2-amino_oxazoles	CCN(CC)S(=O)(=O	VEGFR
GW572738X	23:3-cyano_thiophenes	Fc1ccccc1C(=O)Nc	JNK
GW574782A	04:4-anilino_quinazolines_and_related	Cl.CS(=O)(=O)CCN	EGFR/ErbB2
GW574783B	04:4-anilino_quinazolines_and_related	Cl.CS(=O)(=O)CCN	EGFR/ErbB2
GW575533A	08:2-amino_oxazoles	Cl.COc1ccc(Nc2nc(	VEGFR
GW575808A	16:2,4-diamino_pyrimidines	Cl.Cc1ccc(Nc2ccnc	LCK
GW576484X	04:4-anilino_quinazolines_and_related	CS(=O)(=O)CCNC(	EGFR/ErbB2
GW576609A	04:4-anilino_quinazolines_and_related	OC(=O)C(F)(F)F.Fc	EGFR/ErbB2
GW576924A	04:4-anilino_quinazolines_and_related	Cl.Fc1cc(Nc2ncnc3	EGFR/ErbB2
GW577921A	08:2-amino_oxazoles	Cl.COc1ccccc1Nc1	VEGFR
GW578748X	09:4-hydrazinly_pyrazolopyrimidines	COc1cc(\C=N\Nc2r	GSK3
GW580496A	04:4-anilino_quinazolines_and_related	Cl.CS(=O)(=O)CCN	EGFR/ErbB2
GW580509X	08:2-amino_oxazoles	CCS(=O)(=O)c1ccc	VEGFR
GW581744X	01:4-pyrimidinyl_ortho-aryl_azoles	NC(=O)c1ccc2c(c(r	P38
GW583373A	04:4-anilino_quinazolines_and_related	Cl.Clc1cc(Nc2ncnc2	EGFR/ErbB2
GW589933X	02:Oxindoles	NS(=O)(=O)c1ccc(N	CDK2
GW589961A	14:Benzimidazolyl_diaryl_ureas	Cl.COC(=O)Nc1nc2	TIE2/VEGFR2
GW607049C	14:Benzimidazolyl_diaryl_ureas	OS(O)(=O)=O.COC	TIE2/VEGFR2
GW607117X	11:Biaryl_amides	Cc1nnc(o1)-c1ccc((	p38

GW612286X	16:2,4-diamino_pyrimidines	COc1cc(Nc2nccc(N	VEGFR
GW615311X	04:4-anilino_quinazolines_and_related	Fc1cccc(COc2ccc(I	EGFR/ErbB2
GW616030X	04:4-anilino_quinazolines_and_related	CS(=O)(=O)CCN(C	EGFR/ErbB2
GW618013A	01:4-pyrimidinyl_ortho-aryl_azoles	CS(O)(=O)=O.CN(C	P38
GW620972X	23:3-cyano_thiophenes	O=C(Nc1sc2CCCC	JNK
GW621431X	08:2-amino_oxazoles	CCS(=O)(=O)c1ccc	VEGFR
GW621823A	04:4-anilino_quinazolines_and_related	Cl.CCCN(CCS(C)(=	EGFR/ErbB2
GW621970X	08:2-amino_oxazoles	CCS(=O)(=O)c1ccc	VEGFR
GW622055X	08:2-amino_oxazoles	CCS(=O)(=O)c1ccc	VEGFR
GW627512B	08:2-amino_oxazoles	COc1cc(Nc2ncc(o2	VEGFR
GW627834A	08:2-amino_oxazoles	Cl.N#Cc1cccc(Nc2r	VEGFR
GW631581B	08:2-amino_oxazoles	COc1cc(Nc2ncc(o2	VEGFR
GW632046X	08:2-amino_oxazoles	Cc1cccc(Nc2ncc(o2	VEGFR
GW632580X	31:3-benzyl_pyrimidines	COc1ccc(COc2ccc	CSF
GW633459A	04:4-anilino_quinazolines_and_related	Cl.Fc1cccc(COc2cc	EGFR/ErbB2
GW641155A	08:2-amino_oxazoles	Cl.N(c1ncc(o1)-c1c	VEGFR
GW642125X	18:Furopyrimidines_and_related	COc1ccc(cc1)-c1cc	TIE2/VEGFR2
GW642138X	18:Furopyrimidines_and_related	COc1ccc(cc1)-c1cc	TIE2/VEGFR2
GW643971X	09:4-hydrazinly_pyrazolopyrimidines	COc1cc(C=NNc2nc	GSK3
GW644007X	09:4-hydrazinly_pyrazolopyrimidines	COc1cc(ccc1O)\C=	GSK3
GW651576X	22:4-anilino_5-alkynyl_pyrimidines	Fc1cccc(COc2ccc(I	EGFR/ErbB2
GW654652C	16:2,4-diamino_pyrimidines	Cl.CCS(=O)(=O)c1(	VEGFR
GW659386A	14:Benzimidazolyl_diaryl_ureas	Cl.COC(=O)Nc1nc2	TIE2/VEGFR2
GW659893X	22:4-anilino_5-alkynyl_pyrimidines	Nc1ccc(cc1)C#Cc1	EGFR/ErbB2
GW673715X	14:Benzimidazolyl_diaryl_ureas	CCc1cccc(NC(=O)N	TIE2/VEGFR2
GW678313X	08:2-amino_oxazoles	CCS(=O)(=O)c1ccc	VEGFR
GW679410X	06:4-pyridyl_ortho-aryl_azoles	COc1ccc(cc1)-c1cc	TGFBR
GW680191X	04:4-anilino_quinazolines_and_related	CS(=O)(=O)CCNC(	EGFR/ErbB2
GW680908A	14:Benzimidazolyl_diaryl_ureas	Cl.COC(=O)Nc1nc2	TIE2/VEGFR2
GW680975X	06:4-pyridyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1cc(c	TGFBR
GW682841X	06:4-pyridyl_ortho-aryl_azoles	CC(C)c1ccc(cc1)-c:	TGFBR
GW683003X	07:2H-3_pyrimidinyl_pyrazolopyridazines	FC(F)(F)CNc1nccc	CDK
GW683109X	07:2H-3_pyrimidinyl_pyrazolopyridazines	C(CNc1nccc(n1)-c1	CDK
GW683134A	14:Benzimidazolyl_diaryl_ureas	Cl.Fc1ccc(cc1NC(=	TIE2/VEGFR2
GW683768X	07:2H-3_pyrimidinyl_pyrazolopyridazines	CCc1nn2ncccc2c1-	CDK
GW684626B	13:Anilino_thienopyrimidines	Fc1cccc(COc2ccc(I	EGFR/ErbB2
GW693481X	21:2-pyridinyl_imidazoles_and_related	Nc1nc(c(s1)-c1ccc2	TGFBR
GW693881A	13:Anilino_thienopyrimidines	Cl.Fc1cccc(COc2cc	EGFR/ErbB2
GW693917A	14:Benzimidazolyl_diaryl_ureas	Cl.COC(=O)Nc1nc2	TIE2/VEGFR2
GW694234A	14:Benzimidazolyl_diaryl_ureas	Cl.COC(=O)Nc1nc2	TIE2/VEGFR2
GW694590A	14:Benzimidazolyl_diaryl_ureas	Cl.COC(=O)Nc1nc2	TIE2/VEGFR2
GW695874X	06:4-pyridyl_ortho-aryl_azoles	C(CN1CCOCC1)Oc	TGFBR
GW700494A	14:Benzimidazolyl_diaryl_ureas	Cl.CN1CCN(CCCN	TIE2/VEGFR2
GW701032X	11:Biaryl_amides	COc1ccc(CNC(=O)	p38
GW701427A	14:Benzimidazolyl_diaryl_ureas	Cl.COC(=O)Nc1nc2	TIE2/VEGFR2
GW703087X	22:4-anilino_5-alkynyl_pyrimidines	CC(=O)Nc1cccc(c1	EGFR/ErbB2
GW708336X	07:2H-3_pyrimidinyl_pyrazolopyridazines	C1CC1Nc1nccc(n1	CDK
GW708893X	11:Biaryl_amides	Cc1nnc(o1)-c1ccc((	p38
GW709042A	14:Benzimidazolyl_diaryl_ureas	Cl.Fc1ccc(cc1NC(=	TIE2/VEGFR2
GW711782X	06:4-pyridyl_ortho-aryl_azoles	C(Cn1ccnc1)Oc1cc	TGFBR
GW734508X	11:Biaryl_amides	Cc1nnc(o1)-c1cccc	p38

GW743024X	11:Biaryl_amides	Cc1ccc(NC(=O)c2c	p38
GW759710A	16:2,4-diamino_pyrimidines	Cl.NC(=O)c1cccc(N	LCK
GW768505A	18:Furopyrimidines_and_related	Cl.COc1ccc(cc1)-c1	TIE2/VEGFR2
GW769076X	11:Biaryl_amides	Cc1ccc(NC(=O)c2c	P38
GW770220A	16:2,4-diamino_pyrimidines	Cl.CN(c1ccc2c(C)n	VEGFR
GW770249A	18:Furopyrimidines_and_related	Cl.Nc1ncnc2occ(-c1	TIE2/VEGFR2
GW770249X	18:Furopyrimidines_and_related	Cl.Nc1ncnc2occ(-c1	TIE2/VEGFR2
GW771127A	16:2,4-diamino_pyrimidines	Cl.CN(c1ccc2c(C)n	VEGFR
GW772405X	22:4-anilino_5-alkynyl_pyrimidines	CNC(=O)c1cccc(c1	EGFR/ErbB2
GW775608X	11:Biaryl_amides	Cc1ccc(NC(=O)c2c	P38
GW778894X	07:2H-3_pyrimidinyl_pyrazolopyridazines	N#Cc1cccc(Nc2ncc	CDK
GW779439X	07:2H-3_pyrimidinyl_pyrazolopyridazines	CN1CCN(CC1)c1c(	CDK
GW780056X	07:2H-3_pyrimidinyl_pyrazolopyridazines	CCN(CC)Cc1ccc(N	CDK
GW780159X	21:2-pyridinyl_imidazoles_and_related	Nc1nc(c(s1)-c1ccc2	TGFBR
GW781673X	07:2H-3_pyrimidinyl_pyrazolopyridazines	Clc1ccc(CNc2nccc(	CDK
GW782612X	16:2,4-diamino_pyrimidines	NC(=O)c1cccc(Nc2	LCK
GW782907X	11:Biaryl_amides	Cc1ccc(cc1-c1ccc(	p38
GW782912X	11:Biaryl_amides	Cc1ccc(cc1-c1ccc(	p38
GW784307A	09:4-hydrazinly_pyrazolopyrimidines	Cl.COc1cccc(c1)-n1	GSK3
GW784684X	13:Anilino_thienopyrimidines	CN1CCN(Cc2ccc(o	EGFR/ErbB2
GW784752X	09:4-hydrazinly_pyrazolopyrimidines	COc1cccc(c1)-n1nc	GSK3
GW785404X	03:Furazan_benzimidazoles	CCn1c(nc2ccc(F)cc	MSK
GW785804X	21:2-pyridinyl_imidazoles_and_related	Nc1nc(c(s1)-c1ccc2	TGFBR
GW785974X	11:Biaryl_amides	CC(C)NC(=O)c1cc(	p38
GW786460X	21:2-pyridinyl_imidazoles_and_related	Cc1cccc(n1)-c1n[nH	TGFBR
GW794607X	09:4-hydrazinly_pyrazolopyrimidines	CCCNc1cccc(c1)-n	GSK3
GW794726X	22:4-anilino_5-alkynyl_pyrimidines	CC(=O)Nc1cccc(n1	EGFR/ErbB2
GW795486X	18:Furopyrimidines_and_related	Nc1ncnc2occ(-c3cc	TIE2/VEGFR2
GW795493X	18:Furopyrimidines_and_related	Nc1ncnc2occ(-c3cc	TIE2/VEGFR2
GW796920X	11:Biaryl_amides	Cc1ccc(NC(=O)CC	p38
GW796921X	11:Biaryl_amides	CCC(=O)Nc1ccc(C	p38
GW799251X	22:4-anilino_5-alkynyl_pyrimidines	Nc1nccc(n1)C#Cc1	EGFR/ErbB2
GW801372X	07:2H-3_pyrimidinyl_pyrazolopyridazines	COc1cc(Nc2nccc(n	GSK3
GW804482X	05:Benzimidazole_N-thiophenes	COc1cccc(COc2cc	PLK
GW805758X	07:2H-3_pyrimidinyl_pyrazolopyridazines	CC(C)c1ccc(Nc2nc	CDK
GW806290X	07:2H-3_pyrimidinyl_pyrazolopyridazines	C1COc2cc(Nc3ncc	GSK3
GW806742X	16:2,4-diamino_pyrimidines	CN(c1ccc(NC(=O)N	VEGFR
GW806776X	11:Biaryl_amides	O=C(NCC1CC1)c1	p38
GW807930X	22:4-anilino_5-alkynyl_pyrimidines	CC(=O)NCc1cccc(c	EGFR/ErbB2
GW807982X	07:2H-3_pyrimidinyl_pyrazolopyridazines	CCOc1ccc2c(cnn2n	GSK3
GW809885X	09:4-hydrazinly_pyrazolopyrimidines	COc1cccc(c1)-n1nc	GSK3
GW809897X	16:2,4-diamino_pyrimidines	CN(c1ccc(NC(=O)N	VEGFR
GW810372X	07:2H-3_pyrimidinyl_pyrazolopyridazines	COc1ccc2c(cnn2n1	GSK3
GW810576X	07:2H-3_pyrimidinyl_pyrazolopyridazines	COc1cccc(Nc2nccc	GSK3
GW811168X	09:4-hydrazinly_pyrazolopyrimidines	COc1cccc(c1)-n1nc	GSK3
GW811761X	07:2H-3_pyrimidinyl_pyrazolopyridazines	CCOc1ccc2c(cnn2n	GSK3
GW813360X	09:4-hydrazinly_pyrazolopyrimidines	COc1cccc(c1)-n1cn	GSK3
GW814408X	09:4-hydrazinly_pyrazolopyrimidines	COc1cccc(c1)-c1c[n	GSK3
GW817394X	09:4-hydrazinly_pyrazolopyrimidines	COc1cccc(c1)-n1nc	GSK3
GW817396X	09:4-hydrazinly_pyrazolopyrimidines	COc1cccc(c1)-n1nc	GSK3
GW819077X	07:2H-3_pyrimidinyl_pyrazolopyridazines	FC(F)(F)c1cccc(Nc	GSK3

GW819230X	18:Furopyrimidines_and_related	Cc1ccc(cc1)-c1cc2(	GSK3
GW820759X	11:Biaryl_amides	Cc1ccc(cc1-c1ccc2	P38
GW824645A	27:3-amino_pyrazoles	Cl.NS(=O)(=O)c1cc	CDK2
GW827099X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	Fc1ccc(cc1)-c1nn2(	GSK3
GW827102X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	FC(F)(F)c1cccc(c1)	GSK3
GW827105X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	COc1ccc(cc1)-c1nr	GSK3
GW827106X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	COc1ccc(cc1)-c1nr	GSK3
GW827396X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	COc1ccc(cc1)-c1nr	GSK3
GW828525X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	FC(F)(F)c1ccc(cc1)	GSK3
GW828529X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	Fc1ccc(Nc2nccc(n2	GSK3
GW829055X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	Clc1ccc(cc1)-c1nn2	GSK3
GW829115X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	COc1ccc(cc1)-c1nr	GSK3
GW829874X	09:4-hydrazinly_pyrazolopyrimidines	COc1cccc(\C=N\Nc	GSK3
GW829877X	09:4-hydrazinly_pyrazolopyrimidines	COc1cccc(c1)-n1nc	GSK3
GW829906X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	Cc1ccc2c(c(nn2n1)	GSK3
GW830263A	16:2,4-diamino_pyrimidines	Cl.CN(c1ccc(NC(=(	VEGFR
GW830365A	16:2,4-diamino_pyrimidines	Cl.CN(c1ccc(NC(=(	VEGFR
GW830900A	16:2,4-diamino_pyrimidines	Cl.CN(C)CCNC(=O	VEGFR
GW831090X	27:3-amino_pyrazoles	NS(=O)(=O)c1ccc(N	CDK2
GW831091X	27:3-amino_pyrazoles	NS(=O)(=O)c1ccc(N	CDK2
GW832467X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	Cc1ccc2c(c(nn2n1)	GSK3
GW833373X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines	Cc1ccc2c(c(nn2n1)	GSK3
GW837331X	28:Imidazotriazine	COc1cc(Nc2ncc3c(	PLK
GW843682X	05:Benzimidazole_N-thiophenes	COc1cc2ncn(-c3cc	PLK
GW846105X	23:3-cyano_thiophenes	O=C(Nc1sc2N(CC(	JNK
GW852849X	05:Benzimidazole_N-thiophenes	COc1cc2ncn(-c3cc	PLK
GW853606X	05:Benzimidazole_N-thiophenes	NC(=O)c1sc(cc1OC	PLK
GW853609X	05:Benzimidazole_N-thiophenes	NC(=O)c1sc(cc1OC	PLK
GW856804X	18:Furopyrimidines_and_related	Nc1ncc(-c2cccc(c2)	TIE2/VEGFR2
GW861893X	28:Imidazotriazine	COc1cc(Nc2ncc3c(	PLK
GW869810X	13:Anilino_thienopyrimidines	Fc1cccc(COc2ccc(N	EGFR/ErbB2
GW874091X	28:Imidazotriazine	Cc1nc(-c2ccccc2)n	PLK
GW876790X	03:Furazan_benzimidazoles	CCn1c(nc2cncc(C(=	AKT
SB-210313	06:4-pyridyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1ncn(	P38
SB-216385	01:4-pyrimidinyl_ortho-aryl_azoles	Nc1nccc(n1)-c1c(n(	P38
SB-220025-A	01:4-pyrimidinyl_ortho-aryl_azoles	Cl.Nc1nccc(n1)-c1c	P38
SB-220025-R	01:4-pyrimidinyl_ortho-aryl_azoles	Cl.Nc1nccc(n1)-c1c	P38
SB-220455	01:4-pyrimidinyl_ortho-aryl_azoles	CN1CCC(CC1)n1cn	P38
SB-221466	01:4-pyrimidinyl_ortho-aryl_azoles	CC1(C)CC(CC(C)(C	P38
SB-223133	01:4-pyrimidinyl_ortho-aryl_azoles	Nc1nccc(n1)-c1c(n(	P38
SB-226879	01:4-pyrimidinyl_ortho-aryl_azoles	CN1CCC(CC1)n1cn	P38
SB-236687	01:4-pyrimidinyl_ortho-aryl_azoles	CN1CCC(CC1)n1cn	P38
SB-239272	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1ncn(	P38
SB-242717	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(Oc2nccc(n2	P38
SB-242718	01:4-pyrimidinyl_ortho-aryl_azoles	NC(=O)c1ccc(Oc2n	P38
SB-242719	01:4-pyrimidinyl_ortho-aryl_azoles	CCc1ccc(Oc2nccc(	P38
SB-242721	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1ncn(	P38
SB-245392	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1ncn(	P38
SB-250715	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1ncn(	P38
SB-251505	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1ncn(	P38
SB-251527	01:4-pyrimidinyl_ortho-aryl_azoles	COc1ccccc1Oc1nc(	P38

SB-253226	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1ncn(	P38
SB-253228	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1ncn(	P38
SB-254169	01:4-pyrimidinyl_ortho-aryl_azoles	CS(=O)(=O)c1ccc((	P38
SB-264865	01:4-pyrimidinyl_ortho-aryl_azoles	NC(=O)Cc1ccccc1(	P38
SB-264866	01:4-pyrimidinyl_ortho-aryl_azoles	NC(=O)CCc1ccccc	P38
SB-278538	01:4-pyrimidinyl_ortho-aryl_azoles	CC(C)(C)c1ccc(Oc2	P38
SB-278539	01:4-pyrimidinyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1ncn(	P38
SB-284847-BT	01:4-pyrimidinyl_ortho-aryl_azoles	OC(=O)C(F)(F)F.C(	P38
SB-285234-W	01:4-pyrimidinyl_ortho-aryl_azoles	[Li+].[O-]C(=O)c1cc	P38
SB-333612	17:Maleimide	Clc1ccc(cc1)C1=C(	GSK3
SB-347804	23:3-cyano_thiophenes	Fc1ccc(cc1)C(=O)N	JNK
SB-358518	17:Maleimide	Oc1c(Cl)cc(NC2=C	GSK3
SB-360741	17:Maleimide	OC(=O)c1cc(NC2=(	GSK3
SB-361058	17:Maleimide	COc1ccc(cc1)C1=C	GSK3
SB-376719	17:Maleimide	COc1ccccc1C1=C(	GSK3
SB-390523	17:Maleimide	Oc1c(Cl)cc(NC2=C	GSK3
SB-390527	17:Maleimide	Oc1cccc(NC2=C(C	GSK3
SB-400868-A	21:2-pyridinyl_imidazoles_and_related	Cl.C1Cc2nc(c(-c3c(	TGFBR
SB-409513	17:Maleimide	OC(=O)c1cc(NC2=(	GSK3
SB-409514	17:Maleimide	Oc1ccc(NC2=C(C(=	GSK3
SB-431533	21:2-pyridinyl_imidazoles_and_related	OCc1ccc(cc1)-c1nc	TGFBR
SB-431542-A	21:2-pyridinyl_imidazoles_and_related	Cl.NC(=O)c1ccc(cc	TGFBR
SB-437013	06:4-pyridyl_ortho-aryl_azoles	COc1ccc2cc(ccc2c	TIE2
SB-476429-A	06:4-pyridyl_ortho-aryl_azoles	Cl.NCc1ccc(cc1)-c1	RAF
SB-590885-AAD	06:4-pyridyl_ortho-aryl_azoles	O.Cl.CN(C)CCOc1(	RAF
SB-610251-B	06:4-pyridyl_ortho-aryl_azoles	Cl.Oc1cccc(c1)-c1n	RAF
SB-614067-R	06:4-pyridyl_ortho-aryl_azoles	Cl.ON=C1CCc2cc((	RAF
SB-630812	06:4-pyridyl_ortho-aryl_azoles	COc1ccc2cc(ccc2c	TIE2
SB-633825	06:4-pyridyl_ortho-aryl_azoles	COc1ccc2cc(ccc2c	TIE2
SB-657836-AAA	23:3-cyano_thiophenes	OC(=O)C(O)=O.O=	JNK
SB-675259-M	26:3-amino_pyrazolopyridazines	OC(=O)C(F)(F)F.O	GSK3
SB-678557-A	26:3-amino_pyrazolopyridazines	Cl.CN1CCC(CC1)C	GSK3
SB-682330-A	06:4-pyridyl_ortho-aryl_azoles	Cl.CN(C)CCOc1cc(	RAF
SB-686709-A	26:3-amino_pyrazolopyridazines	Cl.CCN1CCC(CC1)	GSK3
SB-698596-AC	26:3-amino_pyrazolopyridazines	O[C@H]([C@@H]((	GSK3
SB-711237	20:3-amino_pyrazolopyridines	COc1ccc(cc1)-c1cc	GSK3
SB-725317	20:3-amino_pyrazolopyridines	Oc1ccc(cc1)-c1nc2	GSK3
SB-732881	20:3-amino_pyrazolopyridines	CN1CCC(CC1)C(=(	GSK3
SB-732881-H	20:3-amino_pyrazolopyridines	OC(=O)\C=C/C(O)=	GSK3
SB-732941	19:Indazole-3-carboxamides	O=C(Nc1n[nH]c2cc	GSK3
SB-734117	03:Furazan_benzimidazoles	Nc1nonc1-c1nc2cn	MSK
SB-735465	19:Indazole-3-carboxamides	Fc1ccc(F)c(c1)-c1c	GSK3
SB-735467	19:Indazole-3-carboxamides	Fc1ccc(cc1)-c1ccc2	GSK3
SB-736290	03:Furazan_benzimidazoles	Cn1c(nc2cnccc12)-	MSK
SB-736302	03:Furazan_benzimidazoles	Nc1nonc1-c1nc2cn	MSK
SB-737198	03:Furazan_benzimidazoles	CCOc1nccc2n(CC)	MSK
SB-738482	19:Indazole-3-carboxamides	NS(=O)(=O)c1ccc((	GSK3
SB-738561	03:Furazan_benzimidazoles	CCn1c(nc2ccncc12	MSK
SB-739245-AC	20:3-amino_pyrazolopyridines	O[C@H]([C@@H]((	GSK3
SB-739452	20:3-amino_pyrazolopyridines	Brc1cc2c(NC(=O)C	GSK3
SB-741905	19:Indazole-3-carboxamides	NS(=O)(=O)c1cccc(	GSK3

SB-742864	19:Indazole-3-carboxamides	CS(=O)(=O)Nc1ccc	GSK3
SB-742865	19:Indazole-3-carboxamides	CS(=O)(=O)Nc1ccc	GSK3
SB-743899	20:3-amino_pyrazolopyridines	O=C(Nc1n[nH]c2nc	GSK3
SB-744941	03:Furazan_benzimidazoles	CCn1c(nc2c(nccc1	MSK
SB-750140	03:Furazan_benzimidazoles	NCc1ccc(cc1)-n1c(	MSK
SB-751148	03:Furazan_benzimidazoles	CCc1nccc2n(CC)c(	MSK
SB-751399	03:Furazan_benzimidazoles	CN(C)CCCn1c(nc2	MSK
SB-759335-B	03:Furazan_benzimidazoles	Cl.CCn1c(nc2cncc(	AKT
SB-772077-B	03:Furazan_benzimidazoles	Cl.CCn1c(nc2cncc(	RHO
SB-814597	23:3-cyano_thiophenes	Fc1ccc(C(=O)Nc2s	JNK
SKF-62604	17:Maleimide	O=C1NC(=O)C(=C	GSK3
SKF-86002-A2	06:4-pyridyl_ortho-aryl_azoles	Cl.Fc1ccc(cc1)-c1n	P38
SKF-86055	06:4-pyridyl_ortho-aryl_azoles	Fc1ccc(cc1)-c1c(nc	TGFBR

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Table S2. Compounds excluded for cytotoxicity. Each chemotype is labbeled with a different colc

COMPOUND	CHEMOTYPE	REFERENCE
GSK1007102B	03:Furazan_benzimidazoles	Aminofurazans as potent inhib
GSK2110236A	10:2,4-dianilino_pyrrolopyrimidines	Optimization of a series of 4,6-
GSK237700A	05:Benzimidazole_N-thiophenes	Design of potent thiophene inh
GSK237701A	05:Benzimidazole_N-thiophenes	Design of potent thiophene inh
GSK317314A	05:Benzimidazole_N-thiophenes	Design of potent thiophene inh
GSK317315A	05:Benzimidazole_N-thiophenes	Design of potent thiophene inh
GSK326090A	05:Benzimidazole_N-thiophenes	Design of potent thiophene inh
GSK579289A	05:Benzimidazole_N-thiophenes	Design of potent thiophene inh
GSK953913A	30:6-phenyl_isoquinolines	Discovery of 6-Aryl-7-alkoxyisc
GSK978744A	05:Benzimidazole_N-thiophenes	Design of potent thiophene inh
GW305178X	02:Oxindoles	Oxindole-Based Inhibitors of C
GW416981X	02:Oxindoles	Oxindole-Based Inhibitors of C
GW589933X	02:Oxindoles	Oxindole-Based Inhibitors of C
GW589961A	14:Benzimidazolyl_diaryl_ureas	Discovery of Novel Benzimidaz
GW620972X	23:3-cyano_thiophenes	N-(3-Cyano-4,5,6,7-tetrahydrc
GW694590A	14:Benzimidazolyl_diaryl_ureas	Discovery of Novel Benzimidaz
GW778894X	07:2H-3_pyrimidinyl_pyrazolopyridazines	Synthesis and evaluation of py
GW779439X	07:2H-3_pyrimidinyl_pyrazolopyridazines	Synthesis and evaluation of py
GW780056X	07:2H-3_pyrimidinyl_pyrazolopyridazines	Synthesis and evaluation of py
GW801372X	07:2H-3_pyrimidinyl_pyrazolopyridazines	N-Phenyl-4-pyrazolo[1,5-b]pyri
GW805758X	07:2H-3_pyrimidinyl_pyrazolopyridazines	Synthesis and evaluation of py
GW806290X	07:2H-3_pyrimidinyl_pyrazolopyridazines	N-Phenyl-4-pyrazolo[1,5-b]pyri
GW810576X	07:2H-3_pyrimidinyl_pyrazolopyridazines	N-Phenyl-4-pyrazolo[1,5-b]pyri
GW843682X	05:Benzimidazole_N-thiophenes	Design of potent thiophene inh
GW852849X	05:Benzimidazole_N-thiophenes	Design of potent thiophene inh
SB-675259-M	26:3-amino_pyrazolopyridazines	5-Aryl-pyrazolo[3,4-b]pyridazin
SB-725317	20:3-amino_pyrazolopyridines	6-Heteroaryl-pyrazolo[3,4-b]py
SB-732881	20:3-amino_pyrazolopyridines	6-Aryl-pyrazolo[3,4-b]pyridines
SB-732881-H	20:3-amino_pyrazolopyridines	6-Aryl-pyrazolo[3,4-b]pyridines
SB-742864	19:Indazole-3-carboxamides	6-Heteroaryl-pyrazolo[3,4-b]py
SB-814597	23:3-cyano_thiophenes	N-(3-Cyano-4,5,6,7-tetrahydrc

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Table S3. Comounds with z-scores. Each chemotype is labbeled with a different col

Z-SCORE	COMPOUND	CHEMOTYPE
-3.169797691	GW297361X	02:Oxindoles
-3.140110193	SB-734117	03:Furazan_benzimidazoles
-2.530824545	SB-220025-R	01:4-pyrimidinyl_ortho-aryl_azoles
-2.453957701	GW795493X	18:Furopyrimidines_and_related
-1.850126041	GW814408X	09:4-hydrazinly_pyrazolopyrimidines
-1.669248959	GW683003X	07:2H-3_pyrimidinyl_pyrazolopyridazines
-1.615567914	GW781673X	07:2H-3_pyrimidinyl_pyrazolopyridazines
-1.614579425	GW829906X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-1.585815461	GSK1173862A	10:2,4-dianilino_pyrrolopyrimidines
-1.526063338	GSK938890A	03:Furazan_benzimidazoles
-1.524934645	GW786460X	21:2-pyridinyl_imidazoles_and_related
-1.467016484	GSK718429A	06:4-pyridyl_ortho-aryl_azoles
-1.459262622	GW856804X	18:Furopyrimidines_and_related
-1.443746972	GW770249A	18:Furopyrimidines_and_related
-1.440607043	GSK1326255A	10:2,4-dianilino_pyrrolopyrimidines
-1.369339564	SKF-86055	06:4-pyridyl_ortho-aryl_azoles
-1.356463631	GW833373X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-1.301473159	GW770249X	18:Furopyrimidines_and_related
-1.275839775	GW775608X	11:Biaryl_amides
-1.26667381	GW679410X	06:4-pyridyl_ortho-aryl_azoles
-1.26461248	GW695874X	06:4-pyridyl_ortho-aryl_azoles
-1.225914986	GSK994854A	10:2,4-dianilino_pyrrolopyrimidines
-1.21511901	GW683109X	07:2H-3_pyrimidinyl_pyrazolopyridazines
-1.207651294	GW784307A	09:4-hydrazinly_pyrazolopyrimidines
-1.184965891	GW806742X	16:2,4-diamino_pyrimidines
-1.08262417	GW711782X	06:4-pyridyl_ortho-aryl_azoles
-1.068060494	GW296115X	17:Maleimide
-1.039715515	GSK1220512A	10:2,4-dianilino_pyrrolopyrimidines
-1.029006859	SB-732941	19:Indazole-3-carboxamides
-1.021493927	SB-736290	03:Furazan_benzimidazoles
-1.00668174	GW572399X	08:2-amino_oxazoles
-0.994882477	GW429374A	02:Oxindoles
-0.977988237	GSK625137A	24:Phenyl_carboxamides
-0.946694707	GSK2186269A	10:2,4-dianilino_pyrrolopyrimidines
-0.867427492	GW768505A	18:Furopyrimidines_and_related
-0.862303156	GW440139A	29:4-anilino_quinolines
-0.847844226	SB-242721	01:4-pyrimidinyl_ortho-aryl_azoles
-0.794219247	SB-735467	19:Indazole-3-carboxamides
-0.773771855	SB-751148	03:Furazan_benzimidazoles
-0.75651772	GW709042A	14:Benzimidazolyl_diaryl_ureas
-0.754454018	GW581744X	01:4-pyrimidinyl_ortho-aryl_azoles

-0.752829798	GW769076X	11:Biaryl_amides
-0.743648528	GW680975X	06:4-pyridyl_ortho-aryl_azoles
-0.725887923	GW784752X	09:4-hydrazinly_pyrazolopyrimidines
-0.715805908	SB-711237	20:3-amino_pyrazolopyridines
-0.705276988	GW827106X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-0.66025709	GW804482X	05:Benzimidazole_N-thiophenes
-0.6584495	SB-743899	20:3-amino_pyrazolopyridines
-0.655339844	GW406108X	02:Oxindoles
-0.654900974	GW708336X	07:2H-3_pyrimidinyl_pyrazolopyridazines
-0.63805317	GW569530A	04:4-anilino_quinazolines_and_related
-0.621275354	GW827102X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-0.581024151	GW693881A	13:Anilino_thienopyrimidines
-0.544290577	SB-735465	19:Indazole-3-carboxamides
-0.525284667	GSK312948A	05:Benzimidazole_N-thiophenes
-0.511565687	SB-686709-A	26:3-amino_pyrazolopyridazines
-0.501225216	SB-630812	06:4-pyridyl_ortho-aryl_azoles
-0.493156603	GW827396X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-0.483248881	GW641155A	08:2-amino_oxazoles
-0.482833885	GW830263A	16:2,4-diamino_pyrimidines
-0.47912894	GW301888X	04:4-anilino_quinazolines_and_related
-0.475340924	GW405841X	02:Oxindoles
-0.472863321	SB-476429-A	06:4-pyridyl_ortho-aryl_azoles
-0.469364336	GW827099X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-0.459316596	GW621823A	04:4-anilino_quinazolines_and_related
-0.45858838	GW682841X	06:4-pyridyl_ortho-aryl_azoles
-0.450324767	GSK1023156A	05:Benzimidazole_N-thiophenes
-0.43775124	GW282974X	04:4-anilino_quinazolines_and_related
-0.430397951	GW832467X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-0.42058237	SB-400868-A	21:2-pyridinyl_imidazoles_and_related
-0.411014998	SB-633825	06:4-pyridyl_ortho-aryl_azoles
-0.39196538	GW572738X	23:3-cyano_thiophenes
-0.388028691	SB-744941	03:Furazan_benzimidazoles
-0.382452669	GW782912X	11:Biaryl_amides
-0.371165097	SB-347804	23:3-cyano_thiophenes
-0.366706546	GW569293E	01:4-pyrimidinyl_ortho-aryl_azoles
-0.358964461	SB-742865	19:Indazole-3-carboxamides
-0.357765135	GW708893X	11:Biaryl_amides
-0.355798615	GW784684X	13:Anilino_thienopyrimidines
-0.349584468	GR269666A	04:4-anilino_quinazolines_and_related
-0.338467482	GW632580X	31:3-benzyl_pyrimidines
-0.326166984	SB-431533	21:2-pyridinyl_imidazoles_and_related
-0.324498832	GW819230X	18:Furopyrimidines_and_related
-0.309045451	GW576609A	04:4-anilino_quinazolines_and_related
-0.306755798	GW694234A	14:Benzimidazolyl_diaryl_ureas

-0.306313009	GW282536X	02:Oxindoles
-0.298703659	GW819077X	07:2H-3_pyrimidinyl_pyrazolopyridazines
-0.292348425	SB-614067-R	06:4-pyridyl_ortho-aryl_azoles
-0.289660875	SB-737198	03:Furazan_benzimidazoles
-0.28761919	SB-254169	01:4-pyrimidinyl_ortho-aryl_azoles
-0.273680305	GW807982X	07:2H-3_pyrimidinyl_pyrazolopyridazines
-0.271673073	GW651576X	22:4-anilino_5-alkynyl_pyrimidines
-0.258966214	GW416469X	02:Oxindoles
-0.255477575	GW659893X	22:4-anilino_5-alkynyl_pyrimidines
-0.254453414	GW785974X	11:Biaryl_amides
-0.243445401	SKF-86002-A2	06:4-pyridyl_ortho-aryl_azoles
-0.234040406	SB-698596-AC	26:3-amino_pyrazolopyridazines
-0.223827153	SB-216385	01:4-pyrimidinyl_ortho-aryl_azoles
-0.221689675	SB-220455	01:4-pyrimidinyl_ortho-aryl_azoles
-0.216367548	GW811761X	07:2H-3_pyrimidinyl_pyrazolopyridazines
-0.214816612	GW642125X	18:Furopyrimidines_and_related
-0.210306441	GW829115X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-0.19767302	GW513184X	09:4-hydrazinly_pyrazolopyrimidines
-0.195548743	SB-431542-A	21:2-pyridinyl_imidazoles_and_related
-0.190878672	GW683768X	07:2H-3_pyrimidinyl_pyrazolopyridazines
-0.187090916	GSK300014A	13:Anilino_thienopyrimidines
-0.186679269	GW796921X	11:Biaryl_amides
-0.184062033	GW275616X	02:Oxindoles
-0.183580329	GW809885X	09:4-hydrazinly_pyrazolopyrimidines
-0.177207824	GW561436X	01:4-pyrimidinyl_ortho-aryl_azoles
-0.171340775	GW607117X	11:Biaryl_amides
-0.170363151	GSK1392956A	10:2,4-dianilino_pyrrolopyrimidines
-0.159820042	GW817394X	09:4-hydrazinly_pyrazolopyrimidines
-0.155215129	GW574783B	04:4-anilino_quinazolines_and_related
-0.151425963	GW817396X	09:4-hydrazinly_pyrazolopyrimidines
-0.151329371	GW794726X	22:4-anilino_5-alkynyl_pyrimidines
-0.144143449	GW828525X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-0.139956334	GW782907X	11:Biaryl_amides
-0.118978477	GW622055X	08:2-amino_oxazoles
-0.118080311	GW734508X	11:Biaryl_amides
-0.113913232	GW407323A	02:Oxindoles
-0.111006185	GSK1713088A	10:2,4-dianilino_pyrrolopyrimidines
-0.110626749	SB-221466	01:4-pyrimidinyl_ortho-aryl_azoles
-0.108256361	GW305074X	02:Oxindoles
-0.107876368	GW700494A	14:Benzimidazolyl_diaryl_ureas
-0.10656013	GW785804X	21:2-pyridinyl_imidazoles_and_related
-0.101559189	SB-678557-A	26:3-amino_pyrazolopyridazines
-0.096659801	GW680908A	14:Benzimidazolyl_diaryl_ureas
-0.093363938	GW795486X	18:Furopyrimidines_and_related

-0.08619167	GW549034X	03:Furazan_benzimidazoles
-0.084854293	GW583373A	04:4-anilino_quinazolines_and_related
-0.058910114	SB-242718	01:4-pyrimidinyl_ortho-aryl_azoles
-0.056006538	GSK1030059A	05:Benzimidazole_N-thiophenes
-0.055808935	GW829055X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-0.054655478	GW282449A	04:4-anilino_quinazolines_and_related
-0.049924633	GW434756X	06:4-pyridyl_ortho-aryl_azoles
-0.040894659	GW703087X	22:4-anilino_5-alkynyl_pyrimidines
-0.038089205	GW300660X	02:Oxindoles
-0.024796258	SB-285234-W	01:4-pyrimidinyl_ortho-aryl_azoles
-0.009674542	GW618013A	01:4-pyrimidinyl_ortho-aryl_azoles
-0.009181085	GW827105X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
-0.005620923	GW461104A	04:4-anilino_quinazolines_and_related
-0.004208573	GW820759X	11:Biaryl_amides
-0.003643629	GSK238063A	13:Anilino_thienopyrimidines
0.003870959	GW824645A	27:3-amino_pyrazoles
0.00963596	GSK238583A	13:Anilino_thienopyrimidines
0.011790396	GW693481X	21:2-pyridinyl_imidazoles_and_related
0.012723882	SB-390523	17:Maleimide
0.014117095	SB-657836-AAA	23:3-cyano_thiophenes
0.015615266	GW780159X	21:2-pyridinyl_imidazoles_and_related
0.026661965	GW785404X	03:Furazan_benzimidazoles
0.027306967	SB-610251-B	06:4-pyridyl_ortho-aryl_azoles
0.028573384	GW445014X	12:3-vinyl_pyridines
0.031804031	SB-242717	01:4-pyrimidinyl_ortho-aryl_azoles
0.032816577	GW811168X	09:4-hydrazinly_pyrazolopyrimidines
0.033856669	GW680191X	04:4-anilino_quinazolines_and_related
0.046024276	SB-250715	01:4-pyrimidinyl_ortho-aryl_azoles
0.046480444	GSK1030062A	05:Benzimidazole_N-thiophenes
0.048958032	GW615311X	04:4-anilino_quinazolines_and_related
0.056876417	GW633459A	04:4-anilino_quinazolines_and_related
0.057016401	GW276655X	02:Oxindoles
0.058390532	GW807930X	22:4-anilino_5-alkynyl_pyrimidines
0.063406682	GSK605714A	24:Phenyl_carboxamides
0.066222036	GSK182497A	13:Anilino_thienopyrimidines
0.07078921	GW568377A	04:4-anilino_quinazolines_and_related
0.08089029	GW580509X	08:2-amino_oxazoles
0.091498657	GW796920X	11:Biaryl_amides
0.09462216	GW290597X	02:Oxindoles
0.100998808	GW459057A	12:3-vinyl_pyridines
0.10173642	GW441806A	12:3-vinyl_pyridines
0.104342308	GSK635416A	24:Phenyl_carboxamides
0.107170069	SB-738482	19:Indazole-3-carboxamides
0.113248866	GW813360X	09:4-hydrazinly_pyrazolopyrimidines

0.116372525	GSK1030061A	05:Benzimidazole_N-thiophenes
0.116452925	GW794607X	09:4-hydrazinly_pyrazolopyrimidines
0.132284718	GW673715X	14:Benzimidazolyl_diaryl_ureas
0.134319539	SB-739245-AC	20:3-amino_pyrazolopyridines
0.137881548	SB-736302	03:Furazan_benzimidazoles
0.137942567	GW445017X	12:3-vinyl_pyridines
0.14045169	SB-284847-BT	01:4-pyrimidinyl_ortho-aryl_azoles
0.146870804	GW410563A	04:4-anilino_quinazolines_and_related
0.149992537	GW607049C	14:Benzimidazolyl_diaryl_ureas
0.15348926	GW575533A	08:2-amino_oxazoles
0.153636166	SB-361058	17:Maleimide
0.154774724	GSK1030058A	05:Benzimidazole_N-thiophenes
0.155921837	GW300657X	02:Oxindoles
0.159360267	SB-245392	01:4-pyrimidinyl_ortho-aryl_azoles
0.173660255	SB-739452	20:3-amino_pyrazolopyridines
0.17588616	GSK192082A	13:Anilino_thienopyrimidines
0.179075798	SB-741905	19:Indazole-3-carboxamides
0.181324731	GSK561866B	03:Furazan_benzimidazoles
0.182207285	SB-264865	01:4-pyrimidinyl_ortho-aryl_azoles
0.183751685	GSK554170A	03:Furazan_benzimidazoles
0.186973957	SB-759335-B	03:Furazan_benzimidazoles
0.18906862	SB-278539	01:4-pyrimidinyl_ortho-aryl_azoles
0.190801839	GW701032X	11:Biaryl_amides
0.197750718	GW853606X	05:Benzimidazole_N-thiophenes
0.198345425	GW572401X	08:2-amino_oxazoles
0.200085932	GW643971X	09:4-hydrazinly_pyrazolopyrimidines
0.200699667	SB-333612	17:Maleimide
0.202586534	GW684626B	13:Anilino_thienopyrimidines
0.211741808	GW549390X	08:2-amino_oxazoles
0.213932603	GW828529X	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
0.2157848	SB-409513	17:Maleimide
0.215814392	GSK711701A	24:Phenyl_carboxamides
0.22033482	GSK2213727A	10:2,4-dianilino_pyrrolopyrimidines
0.228366784	GW654652C	16:2,4-diamino_pyrimidines
0.229040796	GW284372X	04:4-anilino_quinazolines_and_related
0.229127852	SB-226879	01:4-pyrimidinyl_ortho-aryl_azoles
0.233980709	SB-242719	01:4-pyrimidinyl_ortho-aryl_azoles
0.242543243	SB-251527	01:4-pyrimidinyl_ortho-aryl_azoles
0.267721433	SB-253226	01:4-pyrimidinyl_ortho-aryl_azoles
0.27686594	SB-239272	01:4-pyrimidinyl_ortho-aryl_azoles
0.27792719	GW441756X	02:Oxindoles
0.279417194	SB-278538	01:4-pyrimidinyl_ortho-aryl_azoles
0.284848288	GW810372X	07:2H-3_pyrimidinyl_pyrazolopyridazines
0.285259829	GSK1000163A	03:Furazan_benzimidazoles

0.285278237	GW458344A	12:3-vinyl_pyridines
0.289825206	GW279320X	02:Oxindoles
0.2934662	GSK943949A	03:Furazan_benzimidazoles
0.294081916	GSK2219385A	10:2,4-dianilino_pyrrolopyrimidines
0.29941706	GW829877X	09:4-hydrazinly_pyrazolopyrimidines
0.307163031	GW567808A	04:4-anilino_quinazolines_and_related
0.312440941	GW743024X	11:Biaryl_amides
0.312643751	GW458787A	04:4-anilino_quinazolines_and_related
0.314241725	GW616030X	04:4-anilino_quinazolines_and_related
0.315461136	SB-253228	01:4-pyrimidinyl_ortho-aryl_azoles
0.326431814	GSK969786A	13:Anilino_thienopyrimidines
0.330210554	GSK200398A	13:Anilino_thienopyrimidines
0.337938877	GW829874X	09:4-hydrazinly_pyrazolopyrimidines
0.347513054	SB-210313	06:4-pyridyl_ortho-aryl_azoles
0.34812041	GW693917A	14:Benzimidazolyl_diaryl_ureas
0.355596334	SB-750140	03:Furazan_benzimidazoles
0.369867946	SB-264866	01:4-pyrimidinyl_ortho-aryl_azoles
0.376997383	GW642138X	18:Furopyrimidines_and_related
0.379571001	GW445015X	12:3-vinyl_pyridines
0.38067894	GSK2220400A	10:2,4-dianilino_pyrrolopyrimidines
0.383644722	SB-437013	06:4-pyridyl_ortho-aryl_azoles
0.388711016	SB-251505	01:4-pyrimidinyl_ortho-aryl_azoles
0.394813493	SB-738561	03:Furazan_benzimidazoles
0.404954289	GSK1751853A	10:2,4-dianilino_pyrrolopyrimidines
0.406475676	GW576924A	04:4-anilino_quinazolines_and_related
0.422216359	GW869810X	13:Anilino_thienopyrimidines
0.422940933	GSK204925A	05:Benzimidazole_N-thiophenes
0.431050604	GI261520A	04:4-anilino_quinazolines_and_related
0.431611511	GW439255X	12:3-vinyl_pyridines
0.433646341	GW568326X	01:4-pyrimidinyl_ortho-aryl_azoles
0.441302263	GSK1819799A	10:2,4-dianilino_pyrrolopyrimidines
0.448744243	SB-358518	17:Maleimide
0.450519081	GW806776X	11:Biaryl_amides
0.451739079	GR105659X	02:Oxindoles
0.454118697	GW280670X	02:Oxindoles
0.455652866	GW659386A	14:Benzimidazolyl_diaryl_ureas
0.457513416	GW770220A	16:2,4-diamino_pyrimidines
0.457741232	GSK620503A	24:Phenyl_carboxamides
0.460149114	GW301784X	02:Oxindoles
0.46544783	GW442130X	02:Oxindoles
0.480689646	GW574782A	04:4-anilino_quinazolines_and_related
0.490087229	GW853609X	05:Benzimidazole_N-thiophenes
0.49289653	GW831090X	27:3-amino_pyrazoles
0.493546524	GW301789X	02:Oxindoles

0.495011374	GW809897X	16:2,4-diamino_pyrimidines
0.497093129	GW284408X	02:Oxindoles
0.501601736	SB-682330-A	06:4-pyridyl_ortho-aryl_azoles
0.506057767	GSK586581A	24:Phenyl_carboxamides
0.512994518	GW580496A	04:4-anilino_quinazolines_and_related
0.521535037	GW837331X	28:Imidazotriazine
0.544034175	GW576484X	04:4-anilino_quinazolines_and_related
0.545707652	GW300653X	02:Oxindoles
0.561377631	GW427984X	12:3-vinyl_pyridines
0.564461504	GW701427A	14:Benzimidazolyl_diaryl_ureas
0.564646535	GW450241X	12:3-vinyl_pyridines
0.568347415	SB-590885-AAD	06:4-pyridyl_ortho-aryl_azoles
0.570907279	GW683134A	14:Benzimidazolyl_diaryl_ureas
0.571279027	SB-409514	17:Maleimide
0.597514284	SB-390527	17:Maleimide
0.598008002	GW578748X	09:4-hydrazinly_pyrazolopyrimidines
0.621812252	GW631581B	08:2-amino_oxazoles
0.645977877	GSK980961A	30:6-phenyl_isoquinolines
0.653197436	GSK248233A	03:Furazan_benzimidazoles
0.657401746	GW445012X	12:3-vinyl_pyridines
0.664527263	GW876790X	03:Furazan_benzimidazoles
0.693914556	GW830900A	16:2,4-diamino_pyrimidines
0.7001293	GSK259178A	13:Anilino_thienopyrimidines
0.700877947	GW406731X	12:3-vinyl_pyridines
0.708764162	SB-360741	17:Maleimide
0.709792668	SB-751399	03:Furazan_benzimidazoles
0.727202681	GSK619487A	03:Furazan_benzimidazoles
0.758488408	GW577921A	08:2-amino_oxazoles
0.763898119	GW566221A	04:4-anilino_quinazolines_and_related
0.764984642	SKF-62604	17:Maleimide
0.821603498	GSK2163632A	10:2,4-dianilino_pyrrolopyrimidines
0.829822517	SB-772077-B	03:Furazan_benzimidazoles
0.830140226	GW799251X	22:4-anilino_5-alkynyl_pyrimidines
0.84014397	GW678313X	08:2-amino_oxazoles
0.846248342	GW831091X	27:3-amino_pyrazoles
0.850147644	SB-223133	01:4-pyrimidinyl_ortho-aryl_azoles
0.874085694	GW621970X	08:2-amino_oxazoles
0.878031184	GW772405X	22:4-anilino_5-alkynyl_pyrimidines
0.908398348	GSK317354A	25:Indazole-5-carboxamides
0.918187008	GW830365A	16:2,4-diamino_pyrimidines
0.924920506	GSK180736A	25:Indazole-5-carboxamides
0.924931199	GW278681X	02:Oxindoles
0.931214464	GW644007X	09:4-hydrazinly_pyrazolopyrimidines
0.953762771	GSK269962B	03:Furazan_benzimidazoles

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1.008477028	GSK319347A	05:Benzimidazole_N-thiophenes
1.045075353	GW352430A	02:Oxindoles
1.048834639	SB-220025-A	01:4-pyrimidinyl_ortho-aryl_azoles
1.060072211	SB-376719	17:Maleimide
1.069107266	GW621431X	08:2-amino_oxazoles
1.106251272	GW846105X	23:3-cyano_thiophenes
1.152990985	SB-236687	01:4-pyrimidinyl_ortho-aryl_azoles
1.171052746	GW335962X	02:Oxindoles
1.213996207	GW771127A	16:2,4-diamino_pyrimidines
1.215675479	GSK1511931A	10:2,4-dianilino_pyrrolopyrimidines
1.240976912	GSK571989A	05:Benzimidazole_N-thiophenes
1.305668826	GW559768X	29:4-anilino_quinolines
1.323097818	GSK299115A	25:Indazole-5-carboxamides
1.333521309	GW432441X	12:3-vinyl_pyridines
1.357218661	GW275944X	02:Oxindoles
1.372460629	GSK949675A	03:Furazan_benzimidazoles
1.535310142	GW861893X	28:Imidazotriazine
1.554601222	GW632046X	08:2-amino_oxazoles
1.577146883	GW627834A	08:2-amino_oxazoles
1.616308645	GW782612X	16:2,4-diamino_pyrimidines
1.692568646	GSK466317A	25:Indazole-5-carboxamides
1.712367168	GW435821X	12:3-vinyl_pyridines
1.74269662	GW396574X	02:Oxindoles
1.748711727	GSK614526A	03:Furazan_benzimidazoles
1.833188223	GSK270822A	25:Indazole-5-carboxamides
1.838355728	GSK466314A	25:Indazole-5-carboxamides
1.985612551	GW612286X	16:2,4-diamino_pyrimidines
2.072046415	GW627512B	08:2-amino_oxazoles
2.200130929	GW874091X	28:Imidazotriazine
2.416773858	GW575808A	16:2,4-diamino_pyrimidines

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Table S4. Kinase selectivity profiles of compounds excluded due to toxicity.

The potency of each compound at 1 micromolar concentration against a pa

Compound	Comp Conc. (μM)	Chemotype	TK JAK1	TK TYK2	TK JAK2	TK JAK3	TK FER	TK FES
GW416981X	1	02:Oxindoles	13	4	12	46	11	0
GW305178X	1	02:Oxindoles	17	34	22	68	23	7
GW589933X	1	02:Oxindoles	51	64	24	64	28	17
GSK1007102B	1	03:Furazan_benzimidazoles	4	1	1	4	12	5
GSK317315A	1	05:Benzimidazole_N-thiophenes	5	-2	-1	6	4	0
GSK978744A	1	05:Benzimidazole_N-thiophenes	0	2	0	20	5	0
GW852849X	1	05:Benzimidazole_N-thiophenes	6	2	0	5	9	0
GSK237701A	1	05:Benzimidazole_N-thiophenes	22	0	7	26	17	5
GSK326090A	1	05:Benzimidazole_N-thiophenes	-2	3	3	30	4	-2
GSK579289A	1	05:Benzimidazole_N-thiophenes	0	-8	2	13	4	4
GW843682X	1	05:Benzimidazole_N-thiophenes	3	-7	2	-3	11	1
GSK237700A	1	05:Benzimidazole_N-thiophenes	3	-5	1	2	8	3
GSK317314A	1	05:Benzimidazole_N-thiophenes	2	-6	1	-5	4	2
GW801372X	1	07:2H-3_pyrimidinyl_pyrazolopyridazines	23	32	36	60	59	53
GW806290X	1	07:2H-3_pyrimidinyl_pyrazolopyridazines	20	13	21	46	44	48
GW810576X	1	07:2H-3_pyrimidinyl_pyrazolopyridazines	13	30	29	44	48	50
GW779439X	1	07:2H-3_pyrimidinyl_pyrazolopyridazines	18	8	30	49	37	40
GW778894X	1	07:2H-3_pyrimidinyl_pyrazolopyridazines	15	11	22	36	49	34
GW805758X	1	07:2H-3_pyrimidinyl_pyrazolopyridazines	9	0	9	6	16	26
GW780056X	1	07:2H-3_pyrimidinyl_pyrazolopyridazines	5	12	21	14	15	28
GSK2110236A	1	10:2,4-dianilino_pyrrolopyrimidines	2	-1	0	-2	82	87
GW694590A	1	14:Benzimidazolyl_diaryl_ureas	10	-1	1	0	3	1
GW589961A	1	14:Benzimidazolyl_diaryl_ureas	4	-1	0	0	2	1
SB-742864	1	19:Indazole-3-carboxamides	0	-1	1	3	0	1
SB-732881	1	20:3-amino_pyrazolopyridines	20	-1	1	-2	5	2
SB-732881-H	1	20:3-amino_pyrazolopyridines	3	-1	1	1	5	2
SB-725317	1	20:3-amino_pyrazolopyridines	55	18	28	62	7	4
SB-814597	1	23:3-cyano_thiophenes	11	-3	2	0	5	3
GW620972X	1	23:3-cyano_thiophenes	4	-4	2	2	2	2
SB-675259-M	1	26:3-amino_pyrazolopyridazines	3	2	0	0	1	-2
GSK953913A	1	30:6-phenyl_isoquinolines	10	-1	3	-1	8	5

TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK
ABL-E255K	ABL-H396P	ABL-M351T	ABL-Q252H	ABL-T315I	ABL-Y253F	ABL1	ARG	CSK	BMX	BTK	TXK	TEC	ITK	BRK	SRMS	PTK5	BLK	LCK	HCK
22	27	33	29	43	29	36	20	-2	-2	-1	5	7	5	-3	3	2	29	14	39
39	48	49	52	47	50	50	34	9	25	13	27	38	19	32	4	4	60	30	73
38	47	51	56	62	49	45	31	4	14	4	17	22	15	9	0	4	58	31	44
-1	0	5	0	4	1	6	7	-5	-1	0	2	6	1	-3	0	1	10	5	14
-2	2	2	2	1	-1	9	3	-2	2	-1	3	0	1	-1	1	1	2	2	2
6	10	9	8	12	10	12	8	-1	0	-1	3	0	1	0	2	2	3	6	6
22	31	32	28	27	33	32	21	5	4	1	13	8	3	8	8	2	23	19	27
28	49	48	43	58	47	47	37	10	10	6	16	19	9	4	6	2	23	28	52
1	1	3	2	14	1	3	4	-1	-2	-1	1	0	1	-4	3	1	14	34	33
8	10	5	11	8	13	7	2	5	7	-3	19	2	-2	3	-3	4	-1	4	13
13	23	19	22	14	19	18	13	9	8	-2	3	7	0	5	-1	3	18	13	29
21	34	30	28	13	26	28	11	6	7	1	6	8	3	8	-1	4	51	20	43
2	9	6	5	4	4	1	0	4	5	-3	-1	1	-3	5	-2	5	-2	-2	5
46	59	63	69	40	60	63	70	12	31	11	31	43	12	18	7	5	25	19	33
20	34	41	41	36	36	39	44	15	14	4	18	20	6	14	2	3	10	9	17
23	41	45	46	30	39	41	44	12	22	5	16	25	6	10	-2	4	14	11	17
38	62	75	74	64	62	63	57	7	14	6	21	23	14	28	3	15	16	34	33
33	52	61	57	34	50	48	44	13	40	5	24	39	21	24	15	16	26	18	36
4	9	10	12	11	10	13	11	6	6	-1	3	7	1	6	3	1	5	3	9
23	38	37	43	47	39	30	22	8	11	-1	2	3	0	16	1	4	2	15	13
-13	0	3	3	2	5	4	8	-5	1	1	-2	4	1	3	4	9	11	7	17
11	41	48	52	31	19	11	17	1	4	1	2	2	2	3	-1	2	4	5	5
9	41	56	60	42	22	13	29	6	1	0	2	2	0	0	-1	0	2	9	3
7	17	16	7	31	12	18	4	-2	2	2	3	4	2	-3	-2	0	5	6	3
13	16	14	17	23	15	11	4	8	4	-3	-1	1	-2	9	-2	2	1	8	6
7	14	10	16	16	10	12	5	4	4	0	3	3	2	6	-1	4	4	12	5
66	81	81	82	88	67	73	26	11	13	1	9	14	4	11	17	2	15	22	28
2	2	-2	3	2	5	2	7	3	6	0	3	4	1	5	-3	2	3	6	8
6	3	4	3	3	6	9	10	0	3	0	4	3	1	3	-1	1	2	4	6
1	3	4	3	3	4	7	4	-2	1	0	2	3	2	-1	1	0	3	4	3
4	7	4	5	3	4	7	6	5	5	0	1	4	0	6	2	1	4	4	6

TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK
LYNA	LYNB	FGR	FYN	SRC	YES	EPHA2	EPHA4	EPHA3	EPHB4	EPHB3	EPHB2	PYK2	SYK	ZAP70	LTK	ALK	ROS	INSR	IGF1R
24	20	32	72	39	22	-3	2	0	2	-5	-5	16	-3	1	4	5	15	2	2
44	40	42	30	71	48	10	31	12	13	-4	29	43	22	19	10	16	35	28	14
47	41	36	26	62	41	7	34	13	12	3	26	67	4	12	17	32	37	30	27
22	17	29	25	21	24	-5	-5	-1	1	-3	-10	80	1	1	77	20	11	2	0
2	2	2	5	0	1	-4	0	3	2	1	2	-10	1	3	2	2	3	1	0
4	3	4	5	5	4	-5	0	2	0	-1	-2	-1	1	0	4	5	12	0	0
26	21	19	24	21	18	-1	7	1	3	2	7	6	2	0	4	6	29	7	3
28	24	17	9	41	18	7	27	14	7	6	22	32	0	8	11	19	37	5	3
19	16	13	13	21	13	-3	-5	0	1	-1	-1	6	0	-1	3	21	7	1	-2
7	6	5	-4	19	3	-4	10	-1	-1	0	8	12	2	-1	5	5	15	-2	0
21	17	15	9	21	8	3	23	7	2	1	17	19	-8	-1	4	5	21	2	-3
29	22	32	27	30	33	1	14	6	4	4	14	14	-5	2	5	6	29	3	2
6	3	3	-3	6	1	-3	10	1	-1	0	12	10	-3	1	3	1	11	4	-7
29	24	37	40	64	40	24	45	11	26	-4	40	96	61	14	34	45	87	70	65
13	11	15	9	32	18	6	28	5	12	7	29	85	13	9	22	32	83	59	57
17	11	19	16	42	20	12	37	9	16	-4	36	87	34	12	18	32	71	54	52
33	27	48	32	63	50	-1	15	6	27	0	58	72	47	12	28	63	92	94	84
32	22	42	39	66	37	15	44	19	22	4	46	71	53	13	13	19	74	41	38
7	5	8	6	13	7	0	10	5	3	3	14	46	9	7	11	24	62	48	53
12	9	11	5	38	22	-5	15	1	8	1	27	81	0	-4	10	24	70	73	55
6	2	11	6	7	2	-1	4	0	2	1	5	96	11	2	95	85	82	100	101
9	7	3	5	8	5	3	11	1	0	2	4	7	0	1	4	2	3	7	0
14	11	4	2	1	2	41	63	9	14	5	68	5	1	2	1	2	3	1	2
1	0	5	3	4	3	2	-7	-1	1	-4	-11	3	1	1	1	1	3	4	-2
9	6	5	2	10	11	-3	11	-1	-1	2	8	13	0	2	50	32	10	5	-5
3	3	4	5	8	3	-1	9	4	5	5	9	6	0	2	46	35	2	7	3
16	13	21	15	20	27	24	39	14	29	6	38	19	0	4	92	72	11	6	6
6	5	3	2	10	4	1	7	5	4	5	7	7	2	3	4	4	9	5	6
6	4	5	4	7	2	-1	3	4	3	4	7	6	2	4	3	2	5	7	3
1	2	3	5	3	7	-3	2	0	1	2	4	2	1	2	0	2	1	2	-1
8	5	5	4	7	3	1	10	4	3	3	13	13	1	-1	15	16	11	5	2

TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK
IRR	DDR2	MUSK	TRKA	TRKB	TRKC	RON	MET	AXL	MER	TYRO3	RET	RET-V804L	RET-Y791F	FGFR1	FGFR2	FGFR3	FGFR4	FLT1	KDR
0	2	51	30	40	48	17	13	13	4	17	78	82	70	5	17	11	2	39	71
2	6	49	50	72	78	13	19	37	18	42	79	83	78	41	70	71	7	60	89
6	7	73	69	80	85	56	62	42	16	42	80	78	72	42	64	65	11	68	71
-2	0	2	0	1	1	3	0	9	1	7	90	48	80	6	1	0	1	80	75
0	-2	22	3	5	6	0	1	2	3	3	4	4	5	-1	5	4	3	1	14
-2	1	51	4	15	29	7	-4	3	4	2	7	5	11	1	8	7	0	-1	22
0	1	21	3	14	20	13	20	2	9	10	61	27	60	8	13	13	3	10	54
3	12	78	12	43	63	18	17	8	23	38	52	55	64	29	45		9	26	72
-3	-4	76	1	1	1	9	10	13	7	7	12	19	18	13	8	1	-1	0	34
3	5	41	8	8	9	10	5	-4	9	5	17	16	22	9	9	10	-1	3	40
3	7	33	5	10	10	8	20	-2	9	10	42	34	51	13	21	18	-1	9	69
4	2	14	6	19	33	3	3	-6	10	6	72	38	72	17	22	24	3	13	68
4	1	15	4	10	11	3	4	-9	4	3	10	7	9	5	5	5	-2	4	13
22	9	42	27	39	46	22	14	21	17	15	25	34	34	7	23	20	0	31	64
15	2	27	10	18	21	17	17	10	20	25	22	22	26	5	16	16	5	20	37
15	4	25	17	34	38	15	12	11	12	21	17	23	24	5	17	11	1	25	42
25	18	60	17	13	18	28	27	59	30	23	36	51	47	5	19	15	1	28	59
11	7	25	66	75	88	16	17	34	46	48	37	44	37	9	23	17	5	28	44
9	1	9	8	6	9	17	13	0	8	4	14	10	13	4	8	6	3	11	15
7	4	31	12	7	6	22	10	16	10	18	13	16	18	12	9	5	-3	16	39
97	6	29	-26	4	4	12	7	67	7	-22	14	14	7	-2	1	3	2	1	5
1	81	3	0	3	7	8	19	-4	3	5	27	14	26	1	4	4	-1	22	7
-1	85	33	42	22	26	6	12	7	3	11	74	55	80	9	3	3	0	57	63
-1	1	3	2	0	5	-6	2	2	1	18	15	-1	0	1	5	2	-2	-1	8
3	0	9	1	3	5	6	14	-3	4	7	10	30	21	-1	3	2	-3	2	24
2	3	7	2	3	1	12	7	-3	6	5	0	4	5	5	5	4	2	3	23
2	4	14	12	15	16	6	11	-7	8	41	28	21	36	21	18	13	3	18	72
1	3	5	0	2	2	5	9	-2	5	5	7	1	9	7	6	2	3	1	7
1	3	5	1	2	3	4	7	-1	2	2	6	4	2	2	5	5	0	0	10
-1	-1	-1	-1	1	0	-4	1	2	2	2	2	2	4	-1	-1	2	0	0	3
3	2	0	0	2	5	9	6	-1	2	4	9	5	9	3	4	3	5	3	8

TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK
FLT4	FMS	KIT	KIT-D816V	KIT-T6701	KIT-V560G	FLT3	FLT-3-D835Y	PDGFRα	PDGFRα-D842V	PDGFRα-T674I	PDGFRα-V561D	PDGFRβ	TIE2	TNK2	TNK1	EGFR	EGFR-L858R	EGFR-L861Q	EGFR-T790M
81	46	25	35	7	6	56	87	84	93	39	88	86	8	0	5	5	0	0	-2
86	79	91	24	69	37	73	80	82	92	74	92	83	11	8	57	7	3	-1	0
102	85	94	31	67	32	85	87	91	95	90	95	90	20	10	53	1	5	1	3
94	2	3	34	10	4	0	2	71	89	87	79	80	11	-2	-3	7	4	-2	-1
15	6	15	3	4	3	8	2	35	25	9	26	37	5	3	20	3	1	1	-1
23	9	5	2	1	2	5	8	62	41	51	50	55	15	2	18	2	1	-2	-1
55	24	16	0	8	3	4	9	90	82	70	83	86	27	7	63	9	13	5	0
81	42	27	15	32	14	25	40	100	88	97	87	95	42	28	71	3	15	5	6
19	8	0	-2	0	5	11	21	69	66	46	66	81	32	46	30	10	43	9	2
14	16	5	6	6	-3	14	12	69	54	58	65	71	12	1	18	4	4	4	1
53	29	20	8	10	3	10	15	84	80	68	85	84	21	7	59	4	13	4	2
68	10	12	6	6	3	3	4	74	77	50	81	68	24	6	80	7	27	8	2
4	14	23	8	7	0	5	3	23	12	10	17	19	7	1	24	-2	6	2	2
45	94	97	9	98	93	91	77	62	61	92	75	84	40	36	64	6	17	3	-1
22	86	106	10	93	83	76	36	51	41	75	62	67	21	22	64	4	11	6	2
30	91	99	4	95	78	79	52	49	47	81	64	70	21	22	66	6	9	4	1
26	92	108	6	97	91	86	64	79	80	103	85	91	31	9	64	6	12	4	-1
22	79	100	10	89	72	68	53	53	49	60	60	65	19	12	52	6	18	8	6
10	72	95	4	81	64	61	23	44	43	64	55	41	4	2	49	7	8	6	2
0	69	93	4	81	61	48	17	56	51	35	64	72	12	3	32	-2	-1	2	1
-17	83	-26	3	4	9	1	5	26	3	3	14	34	11	13	80	-20	21	9	55
0	22	68	12	9	68	14	2	67	5	94	85	21	9	1	4	0	4	1	3
9	45	91	-2	57	91	57	2	77	8	86	93	29	45	0	8	8	2	-1	-1
2	2	-4	0	-2	1	0	-5	13	9	-2	7	8	7	-2	-7	0	-2	-3	-1
-13	1	13	5	5	0	6	1	28	16	9	20	23	8	2	7	-2	6	2	3
2	5	9	3	0	-1	3	7	21	10	8	16	17	8	2	6	6	5	1	1
61	7	63	10	5	11	26	27	67	55	24	65	41	26	4	20	7	10	8	5
2	3	4	2	3	-1	3	-3	8	4	6	2	6	3	2	-3	12	5	4	4
-4	1	1	3	2	4	2	-3	12	5	10	7	9	6	1	-2	4	3	1	0
3	5	3	1	0	2	2	-2	6	2	6	4	5	2	2	0	2	3	-1	-1
2	2	8	4	4	0	3	2	13	5	9	6	9	3	2	16	3	13	6	4

TK	TK	TK	TKL	TKL	TKL	TKL	TKL	TKL	STE	STE	STE	STE	STE	STE	STE	STE	STE	STE	STE
EGFR-T790M-L858R	ERBB2	ERBB4	IRAK4	LRRK2	LRRK2-G2019S	CRAF	BRAF	BRAF-V599E	MAP4K2	MST1	MST2	MST4	MAP4K4	MINK	LOK	PAK1	PAK3	PAK2	PAK5
4	0	-2	1	23	64	0	33	34	14	82	78	11	65	54	13	2	0	0	6
5	-3	10	3	22	63	-13	60	61	50	89	88	73	82	76	13	8	4	4	3
10	-1	11	4	79	60	-2	61	61	66	80	78	79	79	79	27	8	7	5	5
-1	-2	4	-1	12	36	0	5	7	25	16	-25	11	20	11	20	14	16	49	62
0	-2	3	1	16	31	0	-2	-1	5	22	19	13	4	4	81	2	0	0	-1
0	1	-2	0	17	29	6	-1	0	16	34	26	1	4	3	86	1	0	0	-4
1	2	9	1	14	55	1	2	3	31	46	42	-3	57	51	99	1	1	-1	0
7	8	14	4	22	52	2	4	4	47	77	74	-21	19	17	88	5	7	0	4
19	0	0	10	26	31	2	-3	1	12	75	57	-27	1	0	91	0	0	-2	-2
6	3	7	4	7	13	1	8	3	18	20	13	-11	8	6	81	7	10	3	6
5	4	12	2	16	40	-1	5	4	18	56	53	-13	30	26	88	7	5	2	3
5	7	14	2	50	64	4	5	5	20	40	35	-7	32	29	80	10	5	3	5
5	3	4	2	10	20	1	5	3	11	13	13	-5	6	5	59	7	7	1	4
16	-1	9	19	24	63	10	29	29	73	36	30	5	79	72	27	3	3	3	9
7	3	12	8	20	61	-10	33	31	56	19	16	-1	52	40	24	5	5	3	15
10	2	3	11	21	55	-1	32	31	60	30	25	3	63	58	17	2	2	3	6
9	3	15	32	18	47	10	22	22	56	23	10	1	65	55	47	40	17	38	43
9	5	19	15	20	40	0	65	65	46	28	24	3	64	53	16	7	5	4	13
2	3	12	2	18	44	2	14	12	23	20	19	3	19	15	8	4	2	1	2
5	4	5	4	9	19	2	18	14	21	16	10	1	20	17	18	9	6	3	5
78	2	35	-1	86	61	-5	2	0	12	8	-17	0	15	17	17	1	7	2	-3
2	3	8	1	7	4	17	4	5	1	5	6	0	13	11	15	3	4	1	-4
1	5	10	0	14	7	5	17	15	7	2	4	1	4	5	27	1	2	0	4
-2	-4	8	0	5	5	16	3	3	3	4	4	1	6	7	10	3	1	0	-15
1	7	8	2	2	5	3	16	14	25	15	13	21	35	28	14	5	5	1	-9
-1	5	9	1	7	5	-8	15	9	20	2	4	20	22	15	9	3	2	-1	1
8	5	22	3	14	22	4	13	13	34	10	11	35	75	68	61	8	6	4	9
7	8	23	3	5	2	-2	7	6	2	3	6	3	3	5	7	10	5	2	-11
0	0	9	1	3	4	3	6	5	4	4	4	1	14	11	6	4	3	1	-10
0	0	2	0	5	6	-3	3	4	1	0	0	2	20	13	1	3	1	0	-1
2	4	9	1	8	8	2	6	4	2	8	6	0	7	6	9	6	4	0	-4

STE	STE	CK1	CK1	CK1	CK1	Other	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC
PAK6	MEK1	CK1a	CK1-g2	CK1-g1	CK1-g3	PLK1	GRK7	GRK6	PDK1	MSK1	MSK2	RSK1	RSK2	RSK4	RSK3	P70S6K1	AKT2	AKT1	AKT3
0	34	2	14	8	21	3	9	10	69	12	21	32	36	39	36	18	2	2	7
1	61	21	7	8	13	3	19	16	68	15	61	31	39	55	62	12	2	1	2
-2	68	22	19	18	26	7	22	36	78	23	64	53	57	77	80	26	3	0	3
68	6	4	4	7	10	0	114	2	28	51	61	72	69	23	70	58	96	96	95
-9	-1	2	-1	0	1	99	5	1	2	0	2	4	7	10	3	0	0	-1	0
-6	0	3	0	2	1	94	3	4	1	-1	2	3	6	13	3	2	0	-1	0
-8	2	1	2	2	3	96	9	6	6	-5	3	4	8	17	8	1	1	0	-1
12	4	3	3	4	3	97	11	15	15	4	14	19	16	26	11	5	2	2	2
-1	0	-1	-3	-1	-4	94	-2	-1	5	-1	3	33	52	55	31	6	-1	-1	2
-10	3	6	0	0	-4	97	4	6	4	2	6	12	22	40	20	5	-2	-4	-2
0	3	4	1	2	2	96	7	1	8	1	5	10	11	24	8	3	-3	-2	-2
-1	4	4	5	5	4	98	5	2	8	12	5	5	5	7	7	2	2	1	1
2	3	2	0	-1	-3	97	2	0	0	1	3	0	0	4	2	3	-3	-3	-1
-2	26	45	39	20	35	37	9	0	8	7	16	3	5	6	5	7	0	0	1
10	28	45	47	22	38	29	3	4	6	7	7	7	4	9	5	6	1	1	2
5	29	48	47	21	39	21	-2	0	6	4	11	4	2	4	2	4	1	0	0
7	18	92	77	61	80	6	9	4	8	22	7	19	24	28	20	8	2	0	3
-5	63	70	41	28	43	9	22	8	6	9	8	7	4	9	4	4	2	1	5
3	10	13	25	9	14	5	3	3	4	1	3	4	2	2	3	2	1	1	2
-3	13	54	14	6	11	8	4	1	3	3	7	3	2	10	4	8	-2	-2	-1
5	-6	4	-8	6	10	97	60	83	1	0	0	35	-1	16	8	1	1	0	5
-3	2	3	2	2	2	4	15	11	2	2	4	4	4	0	2	3	1	0	1
-1	1	1	2	1	1	1	17	0	-1	-1	-1	0	1	-1	1	1	1	0	2
-5	1	2	1	3	1	2	2	-1	1	1	3	-1	1	2	2	2	0	0	-3
-28	5	6	3	4	3	3	17	20	1	4	6	6	7	13	8	3	-2	-3	-1
-5	2	3	2	2	0	3	0	6	3	1	1	1	2	10	6	0	1	0	3
9	8	6	7	6	5	6	17	33	15	14	6	33	45	60	71	7	3	2	13
5	5	7	5	5	5	11	5	5	3	5	3	2	2	3	3	4	3	1	1
2	3	2	3	3	3	10	7	3	3	7	3	0	1	1	2	3	2	0	2
-5	3	-2	0	0	0	2	-1	0	-1	-1	1	0	1	0	2	0	0	-1	5
5	4	3	3	3	5	2	6	8	2	1	3	3	1	0	2	2	2	1	2

AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	S-T-PK	S-T-PK
SGK1	SGK3	SGK2	PKC-η	PKC-γ	PKC-α	PKC-β1	PKC-β2	PKC-θ	PKC-ι	PRKG2	PRKG1	PRKX	PKA	ROCK1	ROCK2	MRCK-β	MRCK-α	AURORA-B	AURORA-C
19	3	2	2	9	7	6	6	8	2	54	14	14	12	30	44	13	7	48	83
50	10	21	3	12	4	0	4	12	2	46	23	2	3	38	60	7	13	68	92
64	19	36	4	10	9	3	6	12	5	62	29	12	12	55	69	15	21	70	92
34	94	3	99	81	70	71	81	85	26	84	81	88	82	52	59	66	73	7	1
1	1	1	1	3	0	1	0	-1	0	1	1	0	1	0	0	2	3	8	0
1	1	3	0	0	3	2	2	1	1	0	0	-8	-1	1	1	4	4	1	-2
2	0	0	2	2	1	1	1	1	1	2	4	-3	-1	1	2	2	2	30	41
7	7	6	4	4	0	6	4	5	0	6	5	-16	2	4	14	1	6	38	51
2	-3	0	5	8	10	6	19	19	0	0	0	-1	1	12	12	1	5	2	1
1	2	1	5	5	1	4	8	10	3	4	4	-2	-4	5	5	3	6	2	-1
1	2	1	6	1	-2	1	2	3	3	1	1	3	-1	4	8	0	-3	27	36
5	7	4	3	2	4	5	5	3	5	5	5	4	4	3	5	3	1	39	49
2	6	2	4	2	-1	3	3	3	4	4	3	2	-1	3	3	3	1	1	2
4	2	0	4	17	64	9	17	7	1	24	57	0	11	8	15	3	3	71	94
7	0	2	8	10	20	4	5	6	2	9	19	2	7	10	19	2	1	65	97
10	2	7	8	9	43	6	7	5	-1	15	38	0	6	6	15	-2	0	72	97
18	0	3	62	37	77	26	36	57	2	61	25	0	14	26	39	22	22	56	88
10	7	5	32	31	73	20	30	14	2	26	50	3	13	5	12	1	3	64	97
3	1	3	4	5	7	2	1	3	0	3	4	1	2	11	25	-1	-1	43	75
8	3	5	7	8	18	-6	6	5	2	14	15	4	4	9	14	5	4	64	85
2	0	3	3	-10	10	2	2	10	-1	2	0	1	4	26	23	0	0	3	3
5	5	4	6	5	1	2	1	3	-1	2	3	4	2	6	17	0	3	25	43
0	1	-2	0	-1	-1	-5	1	0	0	-1	-1	-1	1	6	6	-1	-1	23	35
1	-1	0	3	2	2	0	1	-1	1	2	2	-1	1	0	-1	1	2	4	16
10	6	7	9	8	7	14	31	8	8	8	8	7	1	2	8	13	22	5	-8
4	0	6	4	9	11	10	31	3	6	4	6	2	3	-1	1	13	20	7	5
12	17	25	13	48	37	36	58	33	19	28	6	4	5	1	6	16	13	13	9
4	1	0	5	4	2	1	3	2	3	4	6	3	2	3	5	2	-1	6	5
0	2	1	4	1	1	-1	2	1	2	4	3	2	2	2	1	2	0	4	3
0	0	3	3	2	2	1	3	1	-1	7	0	0	0	1	1	1	-1	4	4
3	3	-1	4	4	2	3	2	3	0	3	5	2	1	4	6	-2	-1	4	-7

S-T-PK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK
AURORA-A	CHEK2	DCAMKL2	CAMK4	CAMK1D	PHKG1	PHKG2	CAMK2D	CAMK2A	PRAK	MAPKAPK2	MAPKAPK3	MNK2	MKNK1	PRKD3	PRKD1	PRKD2	MARK4	MARK3	PAR-1Bα
61	14	10	4	8	51	16	37	18	1	-1	-3	14	7	46	56	62	78	89	71
92	26	8	3	9	50	14	18	8	9	2	4	20	19	51	62	56	52	41	35
90	33	7	6	9	66	32	31	14	14	4	6	18	39	76	78	79	59	61	46
6	27	19	5	29	12	-1	14	2	-1	-1	0	33	6	64	62	66	91	101	91
6	0	-2	3	2	3	0	5	1	0	0	-1	4	3	0	1	2	5	2	5
2	-2	-7	1	1	4	-1	7	2	-1	-1	-1	3	3	0	0	2	5	6	5
24	-1	5	0	4	6	1	3	0	1	-4	-3	8	7	0	1	2	9	10	6
30	-1	1	-1	2	7	13	19	7	4	-1	0	12	12	3	4	4	32	37	18
0	-1	0	2	4	7	11	50	14	-1	-1	-2	4	2	17	12	22	50	58	43
0	5	-2	2	4	5	5	44	14	2	2	4	21	18	4	4	1	6	8	10
14	6	-1	-1	-2	9	7	7	0	2	1	4	8	7	0	1	-2	18	22	12
18	12	4	-4	2	8	7	5	-1	1	5	11	8	3	5	7	3	8	8	5
0	2	-3	-3	-2	8	5	4	-1	1	2	2	3	2	-1	-1	-3	2	3	0
94	14	-3	0	6	39	16	36	15	2	0	1	17	10	20	16	16	22	34	20
85	9	2	2	6	28	17	36	15	3	2	4	26	14	51	45	38	16	25	14
86	11	3	-2	5	28	19	35	14	3	0	3	23	11	41	38	37	17	30	21
74	10	39	8	19	69	26	57	23	0	1	2	25	18	84	79	81	27	46	32
74	11	1	0	4	58	22	63	35	4	2	5	33	23	55	49	47	10	13	10
66	3	-2	3	2	8	4	8	4	1	0	6	15	12	16	16	16	3	4	1
34	8	2	0	4	28	15	14	4	2	2	3	9	10	63	66	64	19	25	16
-11	12	0	12	-16	41	-1	13	-5	1	-2	6	0	0	51	20	40	1	5	5
4	3	5	-3	-1	6	6	2	2	3	1	2	4	7	3	3	2	1	3	-1
1	1	1	-1	1	5	2	0	-2	-1	-1	5	0	4	3	3	2	0	0	0
12	1	1	1	2	6	0	3	3	-1	0	1	3	14	2	2	4	3	7	3
4	6	5	-2	16	16	9	12	6	4	1	3	37	78	3	6	5	4	3	3
4	4	10	1	16	3	3	11	5	1	1	2	35	85	3	6	3	1	3	0
38	4	4	2	14	11	7	20	8	3	3	6	35	76	6	8	6	5	9	5
5	3	1	1	0	1	3	3	3	1	1	4	0	3	6	6	4	2	-4	-1
5	7	0	2	3	5	1	5	2	0	4	8	2	5	4	4	3	2	1	1
0	0	0	0	1	0	-2	1	2	0	0	0	2	0	0	1	1	1	1	2
7	5	3	2	1	8	5	5	3	2	1	7	26	18	3	3	5	2	0	-1

CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	Other	Other	Other
MARK1	SNF1LK2 (QIK)	SNF1LK (SIK)	ARK5	BRSK1	BRSK2	AMPKA1 (A1B1G1)	AMPKA2 (A2B1G1)	MELK	TSSK2	TSSK1	DAPK1	PIM2	PIM3	PIM1	CHEK1	PASK	NEK1	NEK2	NEK9
87	40	72	76	38	50	72	36	93	1	50	3	6	49	28	18	3	2	1	0
53	32	31	85	76	81	83	62	93	4	35	63	10	12	16	41	-2	6	5	41
67	41	34	70	60	64	68	53	94	4	33	25	5	13	10	48	-1	7	8	32
93	15	8	70	38	59	88	68	90	15	96	2	21	39	35	31	16	17	33	-1
6	5	16	44	26	36	3	3	3	1	2	-2	1	8	8	0	1	43	12	84
6	11	7	39	56	68	6	2	3	1	1	-5	2	22	19	-2	2	55	20	91
9	27	28	59	41	49	11	4	9	2	5	-15	5	9	3	-4	-1	15	37	55
32	25	53	72	65	69	24	9	24	4	8	-10	1	12	4	-1	5	68	49	92
51	30	66	77	61	75	33	14	22	0	22	4	2	48	68	0	3	61	69	102
8	14	19	67	58	71	22	9	27	2	10	2	-4	45	65	8	0	38	39	97
22	35	57	66	41	52	19	6	10	3	6	-4	-3	6	3	3	0	19	17	59
9	12	18	22	44	59	11	5	10	1	6	9	1	4	2	11	1	19	10	38
3	0	11	16	18	28	2	1	6	1	3	1	-3	4	3	0	1	25	10	84
32	39	32	85	5	7	17	17	44	0	17	1	7	11	6	8	0	19	12	70
24	18	20	83	7	9	12	13	52	4	18	4	4	16	8	7	1	20	15	50
28	14	21	71	7	10	11	8	52	1	13	0	2	18	7	4	-2	18	6	26
35	47	39	92	7	9	27	35	77	3	45	2	52	71	68	11	19	11	12	45
15	12	15	73	7	12	10	13	56	3	11	4	8	34	12	4	0	11	6	16
4	11	9	49	3	4	4	4	26	1	6	-2	2	6	2	-2	-1	14	8	11
21	47	24	84	3	11	10	13	55	2	26	1	-1	37	23	12	0	4	3	14
6	6	0	2	2	0	0	2	11	91	95	4	3	38	80	-12	1	1	7	-4
4	9	8	-1	0	2	3	1	2	4	4	3	1	1	0	4	1	2	2	7
3	2	4	0	0	1	1	2	-3	0	1	0	-1	-2	-1	-8	1	0	0	3
3	9	5	2	19	19	2	6	4	-1	0	3	1	-3	0	2	0	1	0	3
9	10	9	12	32	36	19	10	12	6	8	3	15	49	35	5	1	6	3	14
2	5	8	3	26	27	11	5	9	2	3	1	16	45	33	2	0	3	2	6
10	20	17	30	67	70	20	12	13	5	6	3	75	74	66	17	1	11	9	13
3	13	12	2	1	1	2	5	10	3	5	7	0	-2	1	6	-2	3	6	14
3	12	10		4	6	3	6	7	1	2	9	0	-2	0	10	-1	1	4	5
0	-2	5	1	-3	2	0	0	1	1	2	-2	29	70	75	-3	0	2	-2	1
4	4	10	0	0	3	3	2	4	3	4	1	-1	1	1	0	0	2	3	8

Other	Other	CAMK	Other	Other	Other	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC
NEK7	NEK6	TBK1	IKKE	IKKB	IKKA	CDK5/p35	CDK1/cyclinB	CDK2/cyclinA	CDK2/cyclinE	CDK3/cyclinE	CDK6/cyclinD3	CDK4/cyclinD	JNK2	P38α	P38β	P38δ	P38γ	MAPK1	MAPK3
0	9	83	93	7	3	80	76	87	83	91	69	67	11	-2	8	1	-1	31	14
8	0	50	45	26	20	83	80	87	84	99	81	76	34	12	27	10	19	56	31
14	8	66	65	19	23	75	70	109	77	98	78	71	36	19	27	9	6	47	28
1	-1	68	99	-3	-2	5	5	4	4	0	3	5	1	1	3	0	0	5	1
1	-2	-1	1	2	-6	1	3	1	1	-2	-1	3	-1	0	0	-1	0	0	0
0	-4	0	-1	-2	-3	2	3	3	4	2	0	1	-1	4	2	-3	-1	-2	-2
1	-4	29	3	1	5	4	6	6	5	-1	0	5	4	18	4	1	1	1	2
4	5	6	7	7	9	1	6	15	14	6	-1	3	4	6	5	4	4	5	5
-1	0	-1	-1	-3	-4	3	3	3	1	1	-2	1	-1	2	3	-4	-2	0	0
9	2	4	6	5	7	-2	-2	-1	2	0	-3	0	5	11	4	6	6	7	5
5	2	14	6	6	4	-1	-1	2	5	0	-2	1	2	10	8	5	6	6	4
5	1	27	8	5	9	2	3	6	7	0	2	4	8	7	2	4	4	7	3
6	0	4	4	5	6	-2	-2	-1	2	-3	-2	0	0	6	4	4	4	5	3
4	2	33	28	24	71	90	91	110	90	74	76	78	48	10	11	12	5	20	9
6	5	24	21	30	61	90	93	86	94	86	85	86	54	13	10	16	6	24	12
4	1	23	18	27	54	78	79	105	79	91	80	77	46	9	8	15	9	26	13
1	-1	57	49	18	39	92	95	93	95	91	79	93	37	14	9	21	8	14	5
4	6	22	28	20	31	87	89	121	87	100	84	84	44	15	14	47	26	59	36
5	3	14	8	23	64	51	64	79	65	39	19	39	27	28	5	5	4	9	3
9	0	12	18	18	35	67	68	82	70	79	62	70	31	13	5	9	7	16	8
10	0	25	9	-1	-1	0	7	6	-1	-1	6	6	8	-18	7	0	3	-30	2
2	1	2	6	5	9	1	2	0	3	-3	-1	1	3	7	8	1	1	2	5
2	-1	-2	1	1	6	0	0	-1	0	0	4	0	6	12	9	0	0	2	0
1	-1	4	3	4	-6	3	3	7	5	4	6	3	0	6	10	1	1	1	1
10	7	6	10	13	-2	13	44	63	39	56	77	77	17	13	18	14	7	12	7
9	1	2	5	4	2	11	43	63	33	53	74	78	14	11	9	12	7	4	1
46	15	23	12	10	12	55	64	108	73	78	75	74	19	16	39	33	17	10	6
5	1	4	6	5	12	1	1	0	6	-3	2	3	12	8	5	5	3	6	4
4	1	7	2	2	6	6	5	1	7	-1	5	7	25	5	4	4	3	4	0
2	0	1	1	1	-1	69	73	91	75	81	65	56	1	-1	2	5	3	3	1
5	3	3	2	22	9	-1	0	2	2	0	3	1	6	8	7	4	2	3	3

CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	Other	Other	Lipid	Lipid	Lipid	Lipid	Lipid
GSK3A	GSK3B	SRPK1	MSSK1	CLK3	CLK2	HIPK1	HIPK4	DYRK1B	DYRK1A	DYRK2	CK2	TTK	PI3-K-α	PI3-K-δ	PI4-K-β	SPHK1	SPHK2
81	83	-2	-2	11	72	17	17	54	57	22	47	70	-1	3	-3	2	0
81	80	-3	-1	15	72	65	40	55	62	36	32	68	7	8	0	-1	7
71	72	-2	-1	17	80	47	22	58	63	46	46	76	13	27	5	4	2
86	85	-3	-2	2	56	55	36	10	8	0	4	9	0	3	2	-1	-1
5	5	-1	-1	1	5	2	3	2	2	1	5	6	5	12	2	2	-3
4	4	-1	0	1	8	5	9	3	4	2	10	2	13	35	-1	0	0
9	10	-1	-1	4	3	5	45	0	4	3	10	1	20	18	2	-3	-5
20	23	8	8	8	5	12	30	0	4	6	20	13	36	60	-1	-4	-2
3	3	1	0	4	10	10	32	2	2	-3	7	1	13	56	0	2	0
0	0	-1	-1	-2	7	2	29	-3	1	7	8	9	20	63	4	-1	-2
5	7	0	6	-2	7	4	41	-3	2	3	9	10	19	16	2	-5	-2
6	6	-2	0	2	1	5	22	5	8	3	3	10	12	11	-6	-2	0
2	0	-1	0	-2	0	-2	6	-2	1	3	3	9	5	17	-3	-2	1
87	90	5	-1	77	100	94	76	92	91	30	43	15	20	35	15	1	0
92	91	3	2	52	98	93	80	89	88	51	48	35	30	26	9	-2	0
79	79	5	1	65	98	93	87	90	88	38	41	23	17	19	11	-2	-1
95	93	-3	-3	42	100	94	91	93	93	45	47	32	30	84	2	-3	0
89	88	23	3	78	97	89	88	87	86	72	64	35	23	21	15	-1	-6
76	75	-1	1	14	65	88	51	82	81	14	43	22	5	7	3	7	0
66	62	-1	0	5	92	72	59	69	88	26	31	29	11	40	5	8	3
1	3	-1	0	3	72	6	5	5	1	-3	38	36	-1	0	-3	0	0
8	8	-1	1	2	-1	2	2	2	3	1	8	5	0	0	2	3	1
4	5	-3	1	-1	-2	-1	15	0	-3	-2	2	3	4	4	-4	-1	0
10	10	-5	-1	0	4	1	-1	0	3	1	-4	5	-1	5	4	-1	0
83	82	1	-1	4	3	20	6	67	43	34	13	19	2	2	-1	0	1
82	80	-1	-1	5	3	19	4	67	52	34	1	6	2	1	1	-1	0
86	83	0	8	8	6	58	10	72	55	53	6	15	6	7	3	0	-1
3	1	-3	-3	3	1	0	1	0	3	5	-2	3	4	4	-1	-2	-1
7	7	-3	-3	1	0	2	2	1	4	3	0	1	5	5	-1	-1	0
82	82	0	-5	1	43	74	9	81	93	75	5	2	1	2	3	-2	-2
5	4	0	4	4	2	5	7	2	5	3	13	9	5	3	0	-2	1

Table S5. Kinase selectivity profiles of compounds assigned z-scores.

articular kinase is represented in colour (less than 0% inhibition – blue, 0-50% inhibition – gre

Compound ID	z score	Comp Conc. (μM)	Chemotype
GW575808A	2.416773858	1	16:2,4-diamino_pyrimidines
GW874091X	2.200130929	1	28:Imidazotriazine
GW627512B	2.072046415	1	08:2-amino_oxazoles
GW612286X	1.985612551	1	16:2,4-diamino_pyrimidines
GSK466314A	1.838355728	1	25:Indazole-5-carboxamides
GSK270822A	1.833188223	1	25:Indazole-5-carboxamides
GSK614526A	1.748711727	1	03:Furazan_benzimidazoles
GW396574X	1.74269662	1	02:Oxindoles
GW435821X	1.712367168	1	12:3-vinyl_pyridines
GSK466317A	1.692568646	1	25:Indazole-5-carboxamides
GW782612X	1.616308645	1	16:2,4-diamino_pyrimidines
GW627834A	1.577146883	1	08:2-amino_oxazoles
GW632046X	1.554601222	1	08:2-amino_oxazoles
GW861893X	1.535310142	1	28:Imidazotriazine
GSK949675A	1.372460629	1	03:Furazan_benzimidazoles
GW275944X	1.357218661	1	02:Oxindoles
GW432441X	1.333521309	1	12:3-vinyl_pyridines
GSK299115A	1.323097818	1	25:Indazole-5-carboxamides
GW559768X	1.305668826	1	29:4-anilino_quinolines
GSK571989A	1.240976912	1	05:Benzimidazole_N-thiophenes
GSK1511931A	1.215675479	1	10:2,4-dianilino_pyrrolopyrimidines
GW771127A	1.213996207	1	16:2,4-diamino_pyrimidines
GW335962X	1.171052746	1	02:Oxindoles
SB-236687	1.152990985	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW846105X	1.106251272	1	23:3-cyano_thiophenes
GW621431X	1.069107266	1	08:2-amino_oxazoles
SB-376719	1.060072211	1	17:Maleimide
SB-220025-A	1.048834639	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW352430A	1.045075353	1	02:Oxindoles
GSK319347A	1.008477028	1	05:Benzimidazole_N-thiophenes
GW759710A	0.968926534	1	16:2,4-diamino_pyrimidines
GSK269962B	0.953762771	1	03:Furazan_benzimidazoles
GW644007X	0.931214464	1	09:4-hydrazinly_pyrazolopyrimidines
GW278681X	0.924931199	1	02:Oxindoles
GSK180736A	0.924920506	1	25:Indazole-5-carboxamides
GW830365A	0.918187008	1	16:2,4-diamino_pyrimidines
GSK317354A	0.908398348	1	25:Indazole-5-carboxamides
GW772405X	0.878031184	1	22:4-anilino_5-alkynyl_pyrimidines
GW621970X	0.874085694	1	08:2-amino_oxazoles
SB-223133	0.850147644	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW831091X	0.846248342	1	27:3-amino_pyrazoles
GW678313X	0.84014397	1	08:2-amino_oxazoles

GW799251X	0.830140226	1	22:4-anilino_5-alkynyl_pyrimidines
SB-772077-B	0.829822517	1	03:Furazan_benzimidazoles
GSK2163632A	0.821603498	1	10:2,4-dianilino_pyrrolopyrimidines
SKF-62604	0.764984642	1	17:Maleimide
GW566221A	0.763898119	1	04:4-anilino_quinazolines_and_related
GW577921A	0.758488408	1	08:2-amino_oxazoles
GSK619487A	0.727202681	1	03:Furazan_benzimidazoles
SB-751399	0.709792668	1	03:Furazan_benzimidazoles
SB-360741	0.708764162	1	17:Maleimide
GW406731X	0.700877947	1	12:3-vinyl_pyridines
GSK259178A	0.7001293	1	13:Anilino_thienopyrimidines
GW830900A	0.693914556	1	16:2,4-diamino_pyrimidines
GW876790X	0.664527263	1	03:Furazan_benzimidazoles
GW445012X	0.657401746	1	12:3-vinyl_pyridines
GSK248233A	0.653197436	1	03:Furazan_benzimidazoles
GSK980961A	0.645977877	1	30:6-phenyl_isoquinolines
GW631581B	0.621812252	1	08:2-amino_oxazoles
GW578748X	0.598008002	1	09:4-hydrazinly_pyrazolopyrimidines
SB-390527	0.597514284	1	17:Maleimide
SB-409514	0.571279027	1	17:Maleimide
GW683134A	0.570907279	1	14:Benzimidazolyl_diaryl_ureas
SB-590885-AAD	0.568347415	1	06:4-pyridyl_ortho-aryl_azoles
GW450241X	0.564646535	1	12:3-vinyl_pyridines
GW701427A	0.564461504	1	14:Benzimidazolyl_diaryl_ureas
GW427984X	0.561377631	1	12:3-vinyl_pyridines
GW300653X	0.545707652	1	02:Oxindoles
GW576484X	0.544034175	1	04:4-anilino_quinazolines_and_related
GW837331X	0.521535037	1	28:Imidazotriazine
GW580496A	0.512994518	1	04:4-anilino_quinazolines_and_related
GSK586581A	0.506057767	1	24:Phenyl_carboxamides
SB-682330-A	0.501601736	1	06:4-pyridyl_ortho-aryl_azoles
GW284408X	0.497093129	1	02:Oxindoles
GW809897X	0.495011374	1	16:2,4-diamino_pyrimidines
GW301789X	0.493546524	1	02:Oxindoles
GW831090X	0.49289653	1	27:3-amino_pyrazoles
GW853609X	0.490087229	1	05:Benzimidazole_N-thiophenes
GW574782A	0.480689646	1	04:4-anilino_quinazolines_and_related
GW442130X	0.46544783	1	02:Oxindoles
GW301784X	0.460149114	1	02:Oxindoles
GSK620503A	0.457741232	1	24:Phenyl_carboxamides
GW770220A	0.457513416	1	16:2,4-diamino_pyrimidines
GW659386A	0.455652866	1	14:Benzimidazolyl_diaryl_ureas
GW280670X	0.454118697	1	02:Oxindoles
GR105659X	0.451739079	1	02:Oxindoles
GW806776X	0.450519081	1	11:Biaryl_amides
SB-358518	0.448744243	1	17:Maleimide
GSK1819799A	0.441302263	1	10:2,4-dianilino_pyrrolopyrimidines
GW568326X	0.433646341	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW439255X	0.431611511	1	12:3-vinyl_pyridines
GI261520A	0.431050604	1	04:4-anilino_quinazolines_and_related
GSK204925A	0.422940933	1	05:Benzimidazole_N-thiophenes
GW869810X	0.422216359	1	13:Anilino_thienopyrimidines
GW576924A	0.406475676	1	04:4-anilino_quinazolines_and_related
GSK1751853A	0.404954289	1	10:2,4-dianilino_pyrrolopyrimidines
SB-738561	0.394813493	1	03:Furazan_benzimidazoles
SB-251505	0.388711016	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-437013	0.383644722	1	06:4-pyridyl_ortho-aryl_azoles
GSK2220400A	0.38067894	1	10:2,4-dianilino_pyrrolopyrimidines

GW445015X	0.379571001	1	12:3-vinyl_pyridines
GW642138X	0.376997383	1	18:Furopyrimidines_and_related
SB-264866	0.369867946	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-750140	0.355596334	1	03:Furazan_benzimidazoles
GW693917A	0.34812041	1	14:Benzimidazolyl_diaryl_ureas
SB-210313	0.347513054	1	06:4-pyridyl_ortho-aryl_azoles
GW829874X	0.337938877	1	09:4-hydrazinly_pyrazolopyrimidines
GSK200398A	0.330210554	1	13:Anilino_thienopyrimidines
GSK969786A	0.326431814	1	13:Anilino_thienopyrimidines
SB-253228	0.315461136	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW616030X	0.314241725	1	04:4-anilino_quinazolines_and_related
GW458787A	0.312643751	1	04:4-anilino_quinazolines_and_related
GW743024X	0.312440941	1	11:Biaryl_amides
GW567808A	0.307163031	1	04:4-anilino_quinazolines_and_related
GW829877X	0.29941706	1	09:4-hydrazinly_pyrazolopyrimidines
GSK2219385A	0.294081916	1	10:2,4-dianilino_pyrrolopyrimidines
GSK943949A	0.2934662	1	03:Furazan_benzimidazoles
GW279320X	0.289825206	1	02:Oxindoles
GW458344A	0.285278237	1	12:3-vinyl_pyridines
GSK1000163A	0.285259829	1	03:Furazan_benzimidazoles
GW810372X	0.284848288	1	07:2H-3_pyrimidinyl_pyrazolopyridazines
SB-278538	0.279417194	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW441756X	0.27792719	1	02:Oxindoles
SB-239272	0.27686594	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-253226	0.267721433	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-251527	0.242543243	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-242719	0.233980709	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-226879	0.229127852	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW284372X	0.229040796	1	04:4-anilino_quinazolines_and_related
GW654652C	0.228366784	1	16:2,4-diamino_pyrimidines
GSK2213727A	0.22033482	1	10:2,4-dianilino_pyrrolopyrimidines
GSK711701A	0.215814392	1	24:Phenyl_carboxamides
SB-409513	0.2157848	1	17:Maleimide
GW828529X	0.213932603	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
GW549390X	0.211741808	1	08:2-amino_oxazoles
GW684626B	0.202586534	1	13:Anilino_thienopyrimidines
SB-333612	0.200699667	1	17:Maleimide
GW643971X	0.200085932	1	09:4-hydrazinly_pyrazolopyrimidines
GW572401X	0.198345425	1	08:2-amino_oxazoles
GW853606X	0.197750718	1	05:Benzimidazole_N-thiophenes
GW701032X	0.190801839	1	11:Biaryl_amides
SB-278539	0.18906862	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-759335-B	0.186973957	1	03:Furazan_benzimidazoles
GSK554170A	0.183751685	1	03:Furazan_benzimidazoles
SB-264865	0.182207285	1	01:4-pyrimidinyl_ortho-aryl_azoles
GSK561866B	0.181324731	1	03:Furazan_benzimidazoles
SB-741905	0.179075798	1	19:Indazole-3-carboxamides
GSK192082A	0.17588616	1	13:Anilino_thienopyrimidines
SB-739452	0.173660255	1	20:3-amino_pyrazolopyridines
SB-245392	0.159360267	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW300657X	0.155921837	1	02:Oxindoles
GSK1030058A	0.154774724	1	05:Benzimidazole_N-thiophenes
SB-361058	0.153636166	1	17:Maleimide
GW575533A	0.15348926	1	08:2-amino_oxazoles
GW607049C	0.149992537	1	14:Benzimidazolyl_diaryl_ureas
GW410563A	0.146870804	1	04:4-anilino_quinazolines_and_related
SB-284847-BT	0.14045169	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW445017X	0.137942567	1	12:3-vinyl_pyridines

SB-736302	0.137881548	1	03:Furazan_benzimidazoles
SB-736302	0.137881548	1	03:Furazan_benzimidazoles
SB-739245-AC	0.134319539	1	20:3-amino_pyrazolopyridines
GW673715X	0.132284718	1	14:Benzimidazolyl_diaryl_ureas
GW794607X	0.116452925	1	09:4-hydrazinly_pyrazolopyrimidines
GSK1030061A	0.116372525	1	05:Benzimidazole_N-thiophenes
GW813360X	0.113248866	1	09:4-hydrazinly_pyrazolopyrimidines
SB-738482	0.107170069	1	19:Indazole-3-carboxamides
GSK635416A	0.104342308	1	24:Phenyl_carboxamides
GW441806A	0.10173642	1	12:3-vinyl_pyridines
GW459057A	0.100998808	1	12:3-vinyl_pyridines
GW290597X	0.09462216	1	02:Oxindoles
GW796920X	0.091498657	1	11:Biaryl_amides
GW580509X	0.08089029	1	08:2-amino_oxazoles
GW568377A	0.07078921	1	04:4-anilino_quinazolines_and_related
GSK182497A	0.066222036	1	13:Anilino_thienopyrimidines
GSK605714A	0.063406682	1	24:Phenyl_carboxamides
GW807930X	0.058390532	1	22:4-anilino_5-alkynyl_pyrimidines
GW276655X	0.057016401	1	02:Oxindoles
GW633459A	0.056876417	1	04:4-anilino_quinazolines_and_related
GW615311X	0.048958032	1	04:4-anilino_quinazolines_and_related
GSK1030062A	0.046480444	1	05:Benzimidazole_N-thiophenes
SB-250715	0.046024276	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW680191X	0.033856669	1	04:4-anilino_quinazolines_and_related
GW811168X	0.032816577	1	09:4-hydrazinly_pyrazolopyrimidines
SB-242717	0.031804031	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW445014X	0.028573384	1	12:3-vinyl_pyridines
SB-610251-B	0.027306967	1	06:4-pyridyl_ortho-aryl_azoles
GW785404X	0.026661965	1	03:Furazan_benzimidazoles
GW780159X	0.015615266	1	21:2-pyridinyl_imidazoles_and_related
SB-657836-AAA	0.014117095	1	23:3-cyano_thiophenes
SB-390523	0.012723882	1	17:Maleimide
GW693481X	0.011790396	1	21:2-pyridinyl_imidazoles_and_related
GSK238583A	0.00963596	1	13:Anilino_thienopyrimidines
GW824645A	0.003870959	1	27:3-amino_pyrazoles
GSK238063A	-0.003643629	1	13:Anilino_thienopyrimidines
GW820759X	-0.004208573	1	11:Biaryl_amides
GW461104A	-0.005620923	1	04:4-anilino_quinazolines_and_related
GW827105X	-0.009181085	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
GW618013A	-0.009674542	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-285234-W	-0.024796258	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW300660X	-0.038089205	1	02:Oxindoles
GW703087X	-0.040894659	1	22:4-anilino_5-alkynyl_pyrimidines
GW434756X	-0.049924633	1	06:4-pyridyl_ortho-aryl_azoles
GW282449A	-0.054655478	1	04:4-anilino_quinazolines_and_related
GW829055X	-0.055808935	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
GSK1030059A	-0.056006538	1	05:Benzimidazole_N-thiophenes
SB-242718	-0.058910114	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW583373A	-0.084854293	1	04:4-anilino_quinazolines_and_related
GW549034X	-0.08619167	1	03:Furazan_benzimidazoles
GW795486X	-0.093363938	1	18:Furopyrimidines_and_related
GW680908A	-0.096659801	1	14:Benzimidazolyl_diaryl_ureas
SB-678557-A	-0.101559189	1	26:3-amino_pyrazolopyridazines
GW785804X	-0.10656013	1	21:2-pyridinyl_imidazoles_and_related
GW700494A	-0.107876368	1	14:Benzimidazolyl_diaryl_ureas
GW305074X	-0.108256361	1	02:Oxindoles
SB-221466	-0.110626749	1	01:4-pyrimidinyl_ortho-aryl_azoles
GSK1713088A	-0.111006185	1	10:2,4-dianilino_pyrrolopyrimidines

GW407323A	-0.113913232	1	02:Oxindoles
GW734508X	-0.118080311	1	11:Biaryl_amides
GW622055X	-0.118978477	1	08:2-amino_oxazoles
GW782907X	-0.139956334	1	11:Biaryl_amides
GW828525X	-0.144143449	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
GW794726X	-0.151329371	1	22:4-anilino_5-alkynyl_pyrimidines
GW817396X	-0.151425963	1	09:4-hydrazinly_pyrazolopyrimidines
GW574783B	-0.155215129	1	04:4-anilino_quinazolines_and_related
GW817394X	-0.159820042	1	09:4-hydrazinly_pyrazolopyrimidines
GSK1392956A	-0.170363151	1	10:2,4-dianilino_pyrrolopyrimidines
GW607117X	-0.171340775	1	11:Biaryl_amides
GW561436X	-0.177207824	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW809885X	-0.183580329	1	09:4-hydrazinly_pyrazolopyrimidines
GW275616X	-0.184062033	1	02:Oxindoles
GW796921X	-0.186679269	1	11:Biaryl_amides
GSK300014A	-0.187090916	1	13:Anilino_thienopyrimidines
GW683768X	-0.190878672	1	07:2H-3_pyrimidinyl_pyrazolopyridazines
SB-431542-A	-0.195548743	1	21:2-pyridinyl_imidazoles_and_related
GW513184X	-0.19767302	1	09:4-hydrazinly_pyrazolopyrimidines
GW829115X	-0.210306441	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
GW642125X	-0.214816612	1	18:Furopyrimidines_and_related
GW811761X	-0.216367548	1	07:2H-3_pyrimidinyl_pyrazolopyridazines
SB-220455	-0.221689675	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-216385	-0.223827153	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-698596-AC	-0.234040406	1	26:3-amino_pyrazolopyridazines
SKF-86002-A2	-0.243445401	1	06:4-pyridyl_ortho-aryl_azoles
GW785974X	-0.254453414	1	11:Biaryl_amides
GW659893X	-0.255477575	1	22:4-anilino_5-alkynyl_pyrimidines
GW416469X	-0.258966214	1	02:Oxindoles
GW651576X	-0.271673073	1	22:4-anilino_5-alkynyl_pyrimidines
GW807982X	-0.273680305	1	07:2H-3_pyrimidinyl_pyrazolopyridazines
SB-254169	-0.28761919	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-737198	-0.289660875	1	03:Furazan_benzimidazoles
SB-614067-R	-0.292348425	1	06:4-pyridyl_ortho-aryl_azoles
GW819077X	-0.298703659	1	07:2H-3_pyrimidinyl_pyrazolopyridazines
GW282536X	-0.306313009	1	02:Oxindoles
GW694234A	-0.306755798	1	14:Benzimidazolyl_diaryl_ureas
GW576609A	-0.309045451	1	04:4-anilino_quinazolines_and_related
GW819230X	-0.324498832	1	18:Furopyrimidines_and_related
SB-431533	-0.326166984	1	21:2-pyridinyl_imidazoles_and_related
GW632580X	-0.338467482	1	31:3-benzyl_pyrimidines
GR269666A	-0.349584468	1	04:4-anilino_quinazolines_and_related
GW784684X	-0.355798615	1	13:Anilino_thienopyrimidines
GW784684X	-0.355798615	1	13:Anilino_thienopyrimidines
GW708893X	-0.357765135	1	11:Biaryl_amides
SB-742865	-0.358964461	1	19:Indazole-3-carboxamides
GW569293E	-0.366706546	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-347804	-0.371165097	1	23:3-cyano_thiophenes
GW782912X	-0.382452669	1	11:Biaryl_amides
SB-744941	-0.388028691	1	03:Furazan_benzimidazoles
GW572738X	-0.39196538	1	23:3-cyano_thiophenes
SB-633825	-0.411014998	1	06:4-pyridyl_ortho-aryl_azoles
SB-400868-A	-0.42058237	1	21:2-pyridinyl_imidazoles_and_related
GW832467X	-0.430397951	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
GW282974X	-0.43775124	1	04:4-anilino_quinazolines_and_related
GSK1023156A	-0.450324767	1	05:Benzimidazole_N-thiophenes
GW682841X	-0.45858838	1	06:4-pyridyl_ortho-aryl_azoles
GW621823A	-0.459316596	1	04:4-anilino_quinazolines_and_related

GW827099X	-0.469364336	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
SB-476429-A	-0.472863321	1	06:4-pyridyl_ortho-aryl_azoles
GW405841X	-0.475340924	1	02:Oxindoles
GW301888X	-0.47912894	1	04:4-anilino_quinazolines_and_related
GW830263A	-0.482833885	1	16:2,4-diamino_pyrimidines
GW641155A	-0.483248881	1	08:2-amino_oxazoles
GW827396X	-0.493156603	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
SB-630812	-0.501225216	1	06:4-pyridyl_ortho-aryl_azoles
SB-686709-A	-0.511565687	1	26:3-amino_pyrazolopyridazines
GSK312948A	-0.525284667	1	05:Benzimidazole_N-thiophenes
SB-735465	-0.544290577	1	19:Indazole-3-carboxamides
GW693881A	-0.581024151	1	13:Anilino_thienopyrimidines
GW827102X	-0.621275354	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
GW569530A	-0.63805317	1	04:4-anilino_quinazolines_and_related
GW708336X	-0.654900974	1	07:2H-3_pyrimidinyl_pyrazolopyridazines
GW406108X	-0.655339844	1	02:Oxindoles
SB-743899	-0.6584495	1	20:3-amino_pyrazolopyridines
GW804482X	-0.66025709	1	05:Benzimidazole_N-thiophenes
GW827106X	-0.705276988	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
SB-711237	-0.715805908	1	20:3-amino_pyrazolopyridines
GW784752X	-0.725887923	1	09:4-hydrazinly_pyrazolopyrimidines
GW680975X	-0.743648528	1	06:4-pyridyl_ortho-aryl_azoles
GW769076X	-0.752829798	1	11:Biaryl_amides
GW581744X	-0.754454018	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW709042A	-0.75651772	1	14:Benzimidazolyl_diaryl_ureas
SB-751148	-0.773771855	1	03:Furazan_benzimidazoles
SB-735467	-0.794219247	1	19:Indazole-3-carboxamides
SB-242721	-0.847844226	1	01:4-pyrimidinyl_ortho-aryl_azoles
GW440139A	-0.862303156	1	29:4-anilino_quinolines
GW768505A	-0.867427492	1	18:Furopyrimidines_and_related
GSK2186269A	-0.946694707	1	10:2,4-dianilino_pyrrolopyrimidines
GSK625137A	-0.977988237	1	24:Phenyl_carboxamides
GW429374A	-0.994882477	1	02:Oxindoles
GW572399X	-1.00668174	1	08:2-amino_oxazoles
SB-736290	-1.021493927	1	03:Furazan_benzimidazoles
SB-732941	-1.029006859	1	19:Indazole-3-carboxamides
GSK1220512A	-1.039715515	1	10:2,4-dianilino_pyrrolopyrimidines
GW296115X	-1.068060494	1	17:Maleimide
GW711782X	-1.08262417	1	06:4-pyridyl_ortho-aryl_azoles
GW806742X	-1.184965891	1	16:2,4-diamino_pyrimidines
GW784307A	-1.207651294	1	09:4-hydrazinly_pyrazolopyrimidines
GW683109X	-1.21511901	1	07:2H-3_pyrimidinyl_pyrazolopyridazines
GSK994854A	-1.225914986	1	10:2,4-dianilino_pyrrolopyrimidines
GW695874X	-1.26461248	1	06:4-pyridyl_ortho-aryl_azoles
GW679410X	-1.26667381	1	06:4-pyridyl_ortho-aryl_azoles
GW775608X	-1.275839775	1	11:Biaryl_amides
GW770249X	-1.301473159	1	18:Furopyrimidines_and_related
GW833373X	-1.356463631	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
SKF-86055	-1.369339564	1	06:4-pyridyl_ortho-aryl_azoles
GSK1326255A	-1.440607043	1	10:2,4-dianilino_pyrrolopyrimidines
GW770249A	-1.443746972	1	18:Furopyrimidines_and_related
GW856804X	-1.459262622	1	18:Furopyrimidines_and_related
GSK718429A	-1.467016484	1	06:4-pyridyl_ortho-aryl_azoles
GW786460X	-1.524934645	1	21:2-pyridinyl_imidazoles_and_related
GSK938890A	-1.526063338	1	03:Furazan_benzimidazoles
GSK1173862A	-1.585815461	1	10:2,4-dianilino_pyrrolopyrimidines
GW829906X	-1.614579425	1	15:2-aryl_3-pyridimidinyl_pyrazolopyridazines
GW781673X	-1.615567914	1	07:2H-3_pyrimidinyl_pyrazolopyridazines

GW683003X	-1.669248959	1	07:2H-3_pyrimidinyl_pyrazolopyridazines
GW814408X	-1.850126041	1	09:4-hydrazinly_pyrazolopyrimidines
GW795493X	-2.453957701	1	18:Furopyrimidines_and_related
SB-220025-R	-2.530824545	1	01:4-pyrimidinyl_ortho-aryl_azoles
SB-734117	-3.140110193	1	03:Furazan_benzimidazoles
GW297361X	-3.169797691	1	02:Oxindoles

en, 51-75% inhibiti

Pubmed ID	JAK1	TYK2	JAK2	JAK3	FER	FES	ABL-E255K	ABL-H396P	ABL-M351T	ABL-Q252H	ABL-T315I	ABL-Y253F	ABL1	ARG	CSK	BMX
	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK
17600705	33	17	46	14	23	11	93	94	95	91	40	94	80	77	35	57
18929484	5	1	2	0	3	3	2	4	1	3	7	4	5	4	2	6
15743202	-1	7	5	13	3	-1	37	61	61	58	22	69	52	52	-1	8
18620382	67	33	72	28	36	11	67	78	76	73	14	84	70	70	68	65
17201405	71	37	82	69	3	2	3	4	5	3	3	1	9	7	6	5
17201405	29	5	26	31	7	3	4	12	15	17	22	5	7	9	8	4
18800763	2	-2	-2	0	1	4	-1	7	1	0	1	0	0	2	-1	-1
11728181	18	21	34	54	20	2	9	14	27	18	18	22	13	14	1	7
16890436	3	-1	3	1	2	2	61	70	69	68	7	74	66	59	26	37
17201405	52	-1	29	42	3	2	3	3	5	5	3	4	2	4	2	4
17600705	20	39	57	25	22	11	96	97	96	95	25	99	85	89	27	74
15743202	11	-2	0	-1	5	2	14	27	27	21	10	22	21	20	5	4
15743202	0	-4	3	0	8	3	8	19	22	13	6	20	14	18	1	6
18929484	-5	-3	3	2	7	3	2	2	2	1	3	3	4	1	1	4
19179070	3	-3	3	-1	1	4	3	5	4	5	4	5	5	4	6	7
11728181	-2	2	0	4	0	1	4	6	8	8	7	8	8	12	-7	-1
16890436	-2	0	1	-1	4	8	51	67	65	59	4	69	56	64	23	48
17201405	37	3	24	18	1	2	-2	0	1	3	3	1	7	4	4	2
17884497	12	10	2	0	19	39	96	96	94	96	18	97	85		94	93
19237286	6	-4	2	29	7	8	5	9	5	8	10	11	14	12	4	3
19081716	0	2	1	2	44	10	1	4	4	4	0	3	10	8	-2	-1
18620382	10	-3	6	0	74	56	68	82	85	84	52	83	64	63	19	17
11728181	-1	7	0	6	11	-3	3	7	15	14	12	13	12	10	-4	0
11597418	8	1	0	1	5	3	5	14	10	9	5	10	11	10	6	5
17194588	16	-5	1	-1	8	4	4	6	4	5	7	6	4	-1	8	4
15743202	7	-1	2	2	3	3	62	67	69	78	8	72	60	61	10	16
11266159	19	-2	3	54	10	4	7	18	17	17	20	8	22	10	5	4
11597418	3	1	2	3	3	0	1	1	1	3	2	5	5	19	3	0
11728181	2	-2	1	6	6	0	4	7	8	8	6	8	4	4	0	5
16997559	5	1	29	55	10	3	47	49	50	44	33	49	49	18	4	33
17600705	32	32	47	3	15	8	47	56	58	54	17	64	56	52	9	38
17201404	12	-1	1	0	2	3	4	4	3	4	4	4	11	8	3	3
15080992	14	5	1	3	7	5	71	81	81	82	48	82	74	69	-2	17
15013000	5	9	1	8	5	-2	3	11	16	11	18	12	11	9	-6	1
17201405	70	26	35	31	2	0	4	2	4	3	3	5	9	20	1	1
15990302	15	-1	10	7	21	8	14	26	37	39	30	22	22	36	13	23
18842034	2	-3	2	1	2	2	4	2	4	4	2	3	10	8	7	3
16483772	8	0	1	2	2	1	1	1	2	3	2	3	6	5	3	1
15743202	10	-2	2	0	9	5	80	86	85	86	25	90	77	75	18	33
11597418	-2	0	0	3	20	-3	17	34	37	34	43	24	37	30	-1	4
12941317	7	6	0	8	14	-1	15	27	31	20	23	36	35	17	-6	-1
15743202	2	1	2	14	2	0	84	82	87	85	18	91	78	65	5	9

16483772	2	-1	2	4	3	5	4	3	1	1	3	3	10	3	3	9
17018693	22	0	1	0	4	2	2	3	-1	2	3	4	4	7	5	1
19081716	3	-1	0	1	95	79	4	3	2	3	4	4	6	4	1	6
11266159	10	-3	4	12	6	4	8	9	8	7	7	8	15	6	4	4
16777410	1	1	2	1	1	4	0	4	2	4	4	3	7	4	5	6
15743202	5	-1	-1	-2	11	4	8	15	11	10	6	14	14	11	3	7
18800763	4	-1	2	-1	4	6	0	2	1	0	2	1	3	4	1	8
15955699	6	-2	1	0	4	3	4	1	4	3	1	5	5	-6	2	3
11266159	-8	0	0	3	2	-3	-2	2	5	2	3	1	8	7	-5	-3
16890436	4	-4	2	1	2	3	38	60	66	64	6	61	63	57	25	30
19208477	2	-1	2	0	6	4	4	9	4	4	4	4	3	1	3	5
15990302	-2	-3	3	0	12	7	10	12	15	17	14	15	20	17	1	10
18800763	2	-4	1	-2	3	5	4	7	3	6	5	8	5	4	5	5
16890436	-1	1	2	-1	3	-1	50	62	64	60	3	70	57	51	25	42
17201404	3	0	0	-1	3	1	9	2	5	2	1	6	4	2	-1	2
19348415	3	-5	1	1	4	7	4	10	8	6	3	5	12	15	5	4
15743202	6	-2	2	-2	3	4	23	40	41	34	13	51	35	29	5	7
15080992	9	4	4	3	14	7	83	88	88	88	47	87	79	66	25	32
11266159	1	-3	5	22	3	3	1	1	3	2	6	3	9	1	3	4
11266159	8	20	2	51	6	1	-1	1	1	3	0	3	8	8	-6	1
17676829	0	-4	7	-3	5	0	67	92	93	92	94	84	72	66	35	2
18621524	2	-5	1	1	6	3	17	34	30	45	42	40	41	19	3	3
16890436	-10	-4	2	1	2	2	18	37	32	12	5	22	46	13	1	5
17676829	2	0	5	1	2	1	4	9	20	14	15	8	6	4	-42	0
16890436	5	-3	3	1	2	1	5	8	7	9	1	14	18	12	7	6
11728181	1	1	0	1	1	0	12	34	38	27	7	29	33	26	1	6
16777410	13	-4	1	0	2	3	3	4	1	2	4	3	3	4	2	4
18929484	9	-1	11	5	17	5	8	13	11	13	13	16	15	13	13	12
16777410	3	-4	-1	-6	5	2	2	5	2	4	2	4	3	4	5	0
17502144	3	-3	4	1	1	2	2	4	3	3	1	3	7	7	1	1
18621524	1	0	-2	2	-1	-2	8	21	20	34	19	22	20	19	-1	1
15013000	21	19	2	9	12	5	15	23	25	26	24	23	26	19	9	8
15990302	20	2	21	3	77	23	36	69	82	72	73	56	53	55	19	73
15013000	30	12	1	6	11	3	9	13	14	13	17	13	14	8	7	5
12941317	7	-3	2	1	7	4	7	6	4	6	7	12	11	7	5	5
19097784	5	-3	0	1	6	2	3	4	3	3	2	5	4	5	-1	1
16777410	4	-4	0	-2	2	3	3	4	1	2	2	3	5	5	4	2
15013000	1	-1	3	5	9	4	22	22	20	20	5	20	28	15	4	6
11728181	2	4	1	13	-11	0	9	10	10	9	9	13	11	3	0	1
17502144	12	-3	1	-2	2	4	4	6	3	6	5	5	6	5	5	8
18620382	55	2	60	27	36	6	74	90	90	85	68	85	75	74	22	35
17676829	4	2	0	2	2	1	7	42	69	69	13	20	25	41	2	-2
11728181	12	0	2	1	7	3	6	13	13	10	12	11	11	12	7	5
15013000	13	7	4	13	22	7	9	15	15	13	16	16	15	9	4	8
18614366	-7	-6	1	0	-2	2	3	3	4	4	2	4	9	6	-4	3
11266159	5	3	-1	24	0	1	1	1	2	1	1	0	1	4	1	0
19081716	9	-3	2	1	76	64	6	4	2	5	8	6	6	5	7	4
16209527	2	-3	-2	0	7	4	-1	0	1	0	1	0	0	4	1	1
16890436	7	-2	4	6	3	2	22	35	46	53	4	38	32	36	33	47
14684309	3	-1	0	1	5	1	3	5	3	5	3	1	5	5	8	3
19097784	-6	-3	0	0	1	2	6	10	12	11	8	10	14	8	3	3
19208477	14	-4	1	-3	5	4	5	6	5	3	7	6	3	1	7	3
16777410	1	-4	1	0	6	3	3	1	0	1	-1	-1	6	4	-4	6
19071018	-4	-1	2	7	53	59	-1	1	3	4	2	1	0	-1	-3	3
15950465	7	-1	1	3	0	2	-2	0	3	0	0	1	4	-2	-5	0
11354358	3	-2	3	-1	13	4	3	7	3	5	2	6	12	12	4	6
17826092	-3	-5	2	0	3	3	2	4	3	5	12	4	9	9	-3	4
19081716	-1	-1	2	1	80	81	3	2	0	4	2	4	8	6	2	5

16890436	13	-3	1	0	5	2	17	29	23	19	4	32	26	16	10	16
15837294	8	4	3	0	2	-1	6	11	11	9	3	11	11	5	-1	3
11354358	-5	2	-2	0	1	-2	0	0	1	1	-1	0	-2	-1	-3	0
15955699	5	-3	2	2	6	13	3	0	0	2	1	3	4	7	1	5
17676829	9	1	7	1	6	1	67	92	93	91	93	76	80	74	33	3
9873686	-1	-1	1	1	-1	-1	0	0	1	0	-1	0	1	5	-6	0
15080992	4	-1	5	-3	4	3	34	42	42	55	10	50	27	15	4	6
19208477	3	1	-2	1	1	-1	0	1	0	1	0	1	3	2	4	2
19111461	4	-2	1	-2	3	3	3	5	1	2	3	4	9	7	3	2
11354358	7	-5	1	-2	4	2	1	3	0	2	2	3	-1	0	2	3
16777410	1	-4	1	-5	1	0	1	2	0	0	0	2	-3	-2	5	4
16777410	6	-3	0	-1	0	4	3	5	5	5	5	4	6	5	9	9
18614366	3	0	-1	0	0	2	0	2	2	1	2	-1	1	2	0	2
16777410	1	-4	3	0	1	4	3	4	1	5	2	4	9	8	3	6
15080992	4	-1	2	1	17	10	65	74	74	81	23	76	62	41	8	11
19071018	-5	-2	2	-3	23	11	2	0	0	0	0	1	0	-4	-2	2
19179070	0	-4	2	0	7	8	-1	2	2	2	8	3	3	4	2	5
11728181	13	1	0	1	5	0	5	8	7	7	5	6	8	8	4	3
16890436	3	3	0	0	8	2	2	4	4	4	2	4	5	9	3	3
19179070	3	-1	0	1	0	-1	0	1	3	3	1	0	3	6	-4	-2
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11354358	5	-2	2	-1	0	3	4	5	3	5	4	5	5	4	3	4
15013000	-6	1	3	5	21	2	28	37	36	33	44	49	45	21	-1	5
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11354358	8	-2	0	2	3	5	5	6	3	5	4	6	8	8	6	5
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16777410	2	-2	-1	0	4	2	0	1	2	0	1	0	1	4	2	2
18620382	5	-3	0	-2	34	6	89	90	88	90	15	92	79	74	15	23
19071018	-4	-2	0	-2	87	89	0	-1	-1	0	0	0	5	0	0	3
17502144	3	-7	3	-1	6	5	4	6	1	6	2	5	4	4	4	6
11266159	14	-1	1	9	3	3	3	6	5	5	4	3	6	0	2	3
15341487	0	-3	2	1	4	3	3	1	2	0	1	2	5	4	0	5
15743202	8	-5	2	-2	1	5	8	21	18	14	8	16	17	23	4	7
19111461	0	1	1	1	9	0	2	4	3	2	1	3	6	5	3	4
11266159	0	-4	3	1	7	7	4	3	3	4	2	5	8	8	1	6
15080992	3	-2	0	4	4	-4	83	90	89	92	62	91	72	49	3	17
15743202	0	0	2	2	5	0	28	33	38	38	9	42	28	37	5	7
19097784	11	-4	3	1	2	2	2	3	3	4	3	2	4	3	5	3
17981461	20	2	1	3	5	2	1	4	5	4	6	5	6	4	6	1
11354358	0	-3	-1	0	9	0	2	2	3	2	1	2	1	0	-1	2
18800763	5	-2	3	-1	1	5	5	5	0	5	2	5	3	4	4	9
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19111461	-1	-3	3	2	0	3	3	3	1	2	2	1	5	5	7	3
12941333	-1	-2	2	1	1	3	9	26	30	32	27	12	24	18	4	5
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11728181	10	1	1	6	5	2	10	15	13	12	13	19	15	9	8	4
19097784	0	-3	5	11	4	4	23	18	16	19	5	22	12	6	0	7
11266159	8	-6	3	2	5	5	4	5	7	6	6	3	10	12	9	5
15743202	8	5	3	11	4	4	33	54	56	45	19	54	58	57	-1	5
17676829	-5	0	2	2	1	-1	15	50	70	71	72	31	33	59	8	0
18620382	13	-3	1	2	8	4	86	87	85	82	68	89	78	65	17	13
11354358	5	-3	0	0	4	3	4	3	1	3	3	3	5	4	2	3
16890436	11	2	1	2	4	0	14	24	20	17	9	27	34	21	6	8

15950465	3	-2	1	-3	3	1	4	1	3	3	3	5	2	-3	1	2
15950465	0	-1	4	5	0	4	4	1	-1	4	3	4	8	5	2	5
12941333	-4	2	-2	2	2	-5	2	8	5	12	23	5	8	3	-5	-1
17676829	1	-2	5	1	2	1	14	52	58	61	51	27	24	45	4	2
15080992	12	4	15	8	9	6	77	86	86	84	86	86	75	62	12	13
19097784	7	-3	1	0	6	3	9	10	7	8	4	10	17	13	7	2
16460937	16	3	0	-2	5	-1	80	87	88	84	28	85	72	59	7	16
12941333	-1	-5	3	2	0	3	7	17	17	8	15	9	14	7	2	4
17502144	2	-1	3	0	2	2	2	3	1	1	2	4	5	4	2	2
16890436	5	-3	2	-4	12	4	79	80	80	82	8	86	71	69	43	66
16890436	3	-2	2	1	2	6	3	9	6	9	1	5	13	20	20	31
11728181	24	-2	5	19	-63	3	11	14	14	13	14	15	13	10	7	8
18614366	7	-3	5	2	8	4	5	4	3	5	3	5	9	8	6	5
15743202	-4	-4	2	6	4	2	81	85	86	87	26	86	78	73	11	26
16777410	-1	0	-1	1	2	0	0	0	0	2	1	-1	1	3	5	3
19111461	5	-3	2	2	0	3	3	0	0	4	1	4	8	6	3	3
17502144	3	-3	3	0	3	4	4	3	0	2	2	3	6	4	2	6
16483772	5	3	-3	4	1	1	2	-1	0	-1	2	3	3	-1	-3	0
11728181	6	9	6	24	1	0	7	16	18	13	20	13	9	10	4	6
16777410	5	-3	1	-1	5	4	4	7	3	6	3	7	10	8	7	7
16777410	2	0	0	3	-1	1	0	2	1	3	0	1	5	7	1	1
19097784	8	1	0	15	3	1	10	16	15	13	1	17	19	12	0	3
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EPHB3	EPHB2	PYK2	SYK	ZAP70	LTK	ALK	ROS	INSR	IGF1R	IRR	DDR2	MUSK	TRKA	TRKB	TRKC	RON	MET	AXL	MER
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TYRO3	RET	RET-V804L	RET-Y791F	FGFR1	FGFR2	FGFR3	FGFR4	FLT1	KDR	FLT4	FMS	KIT	KIT-D816V	KIT-T6701	KIT-V560G	FLT3	FLT-3-D835Y	PDGFRα	PDGFRα-D842V
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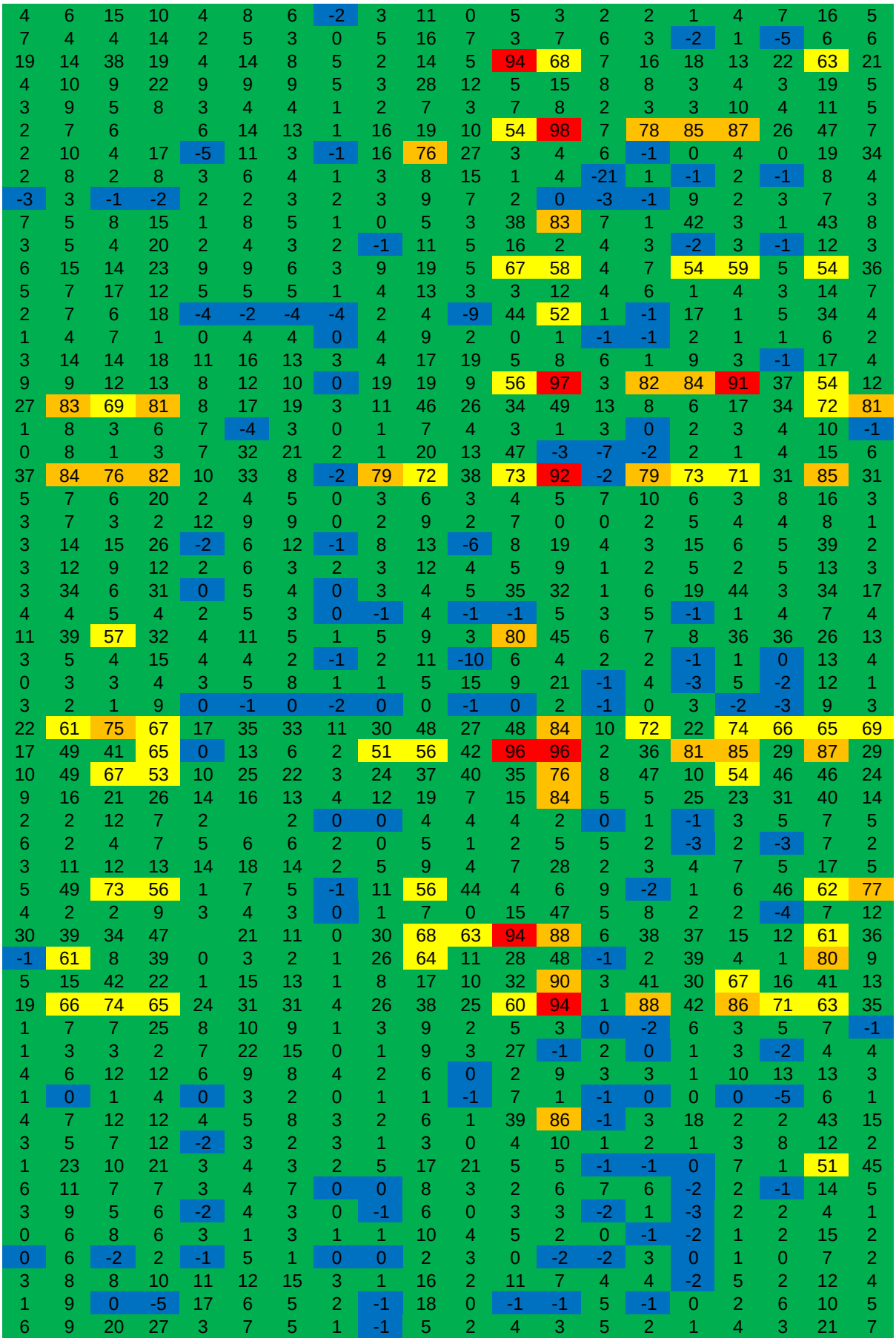

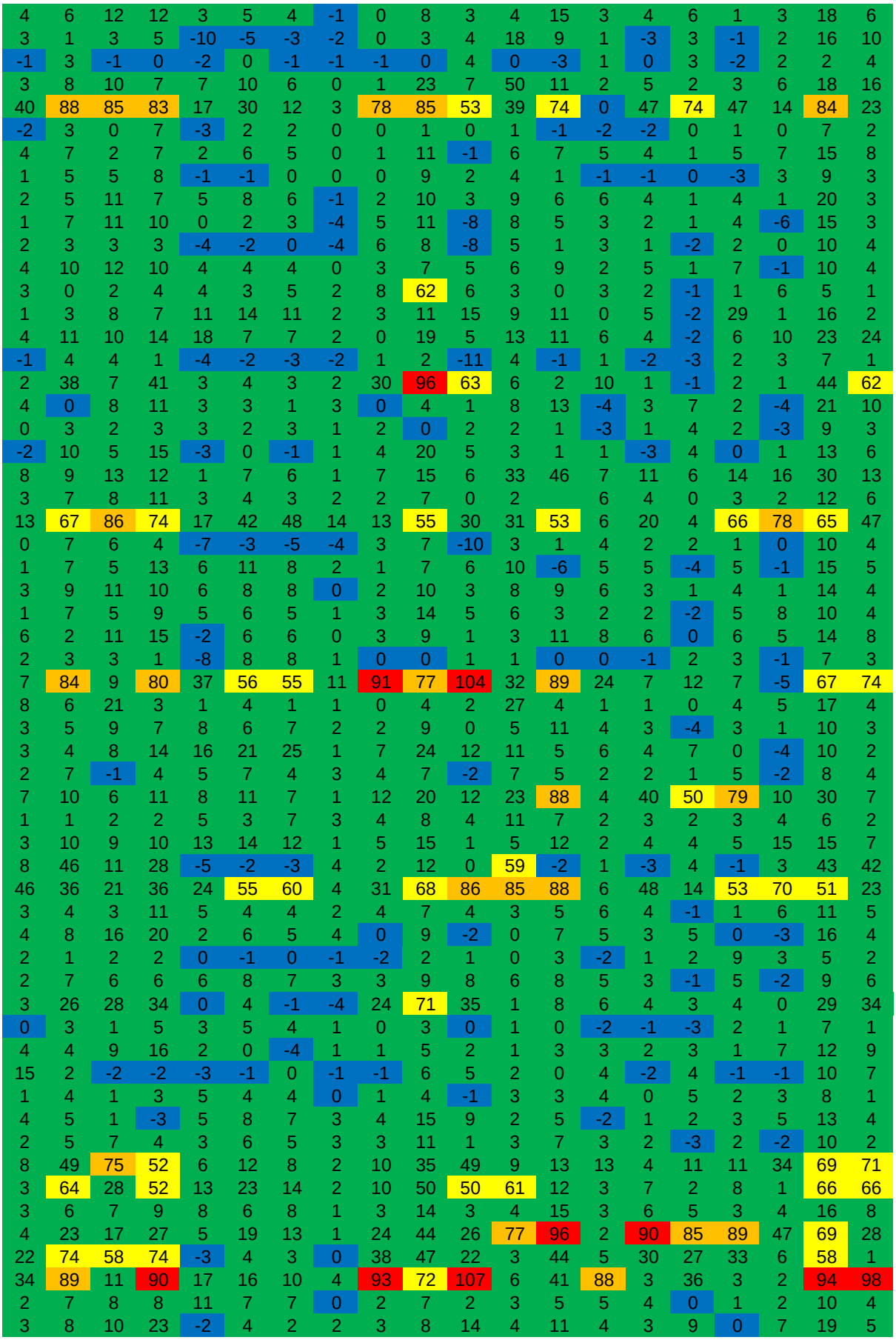

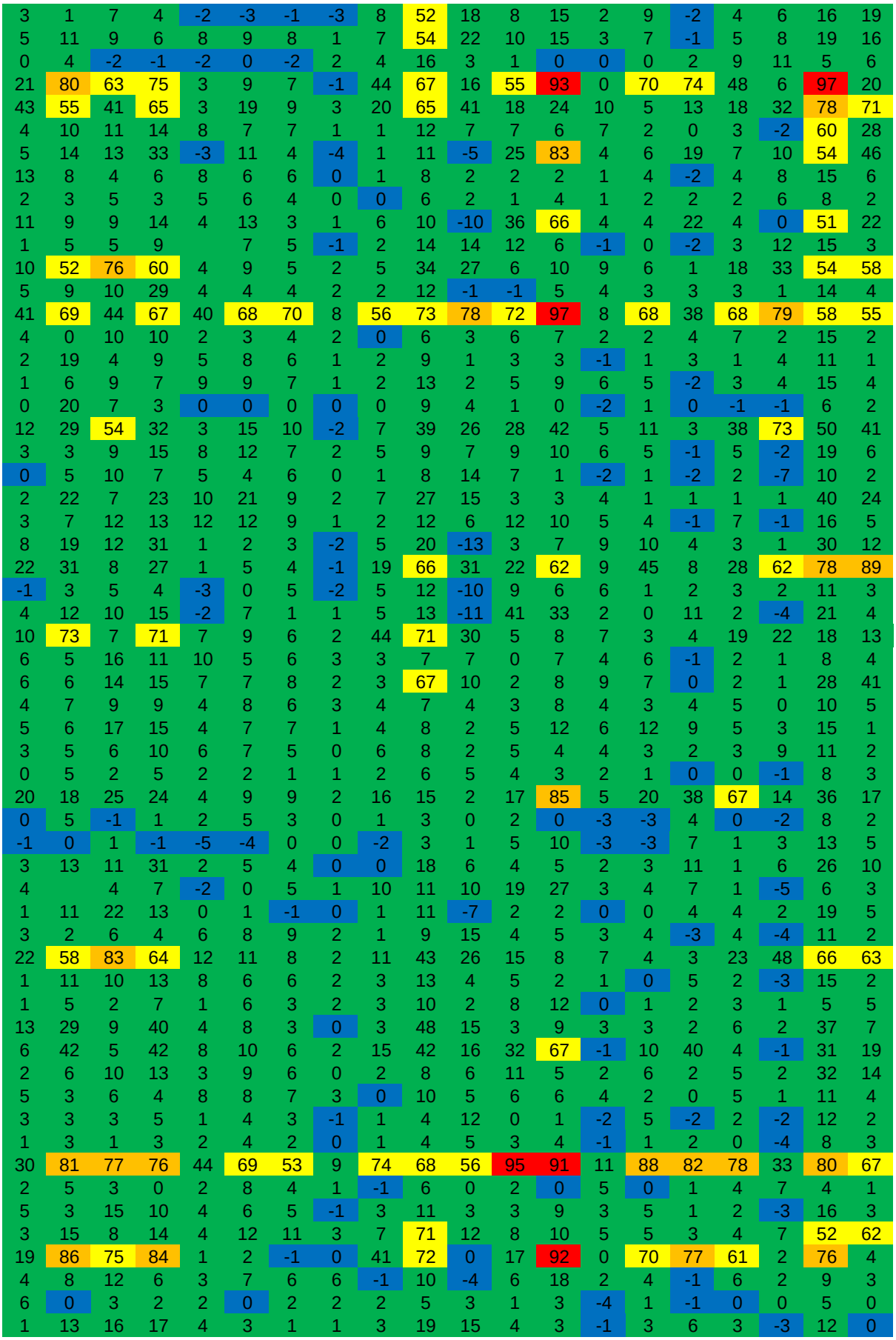

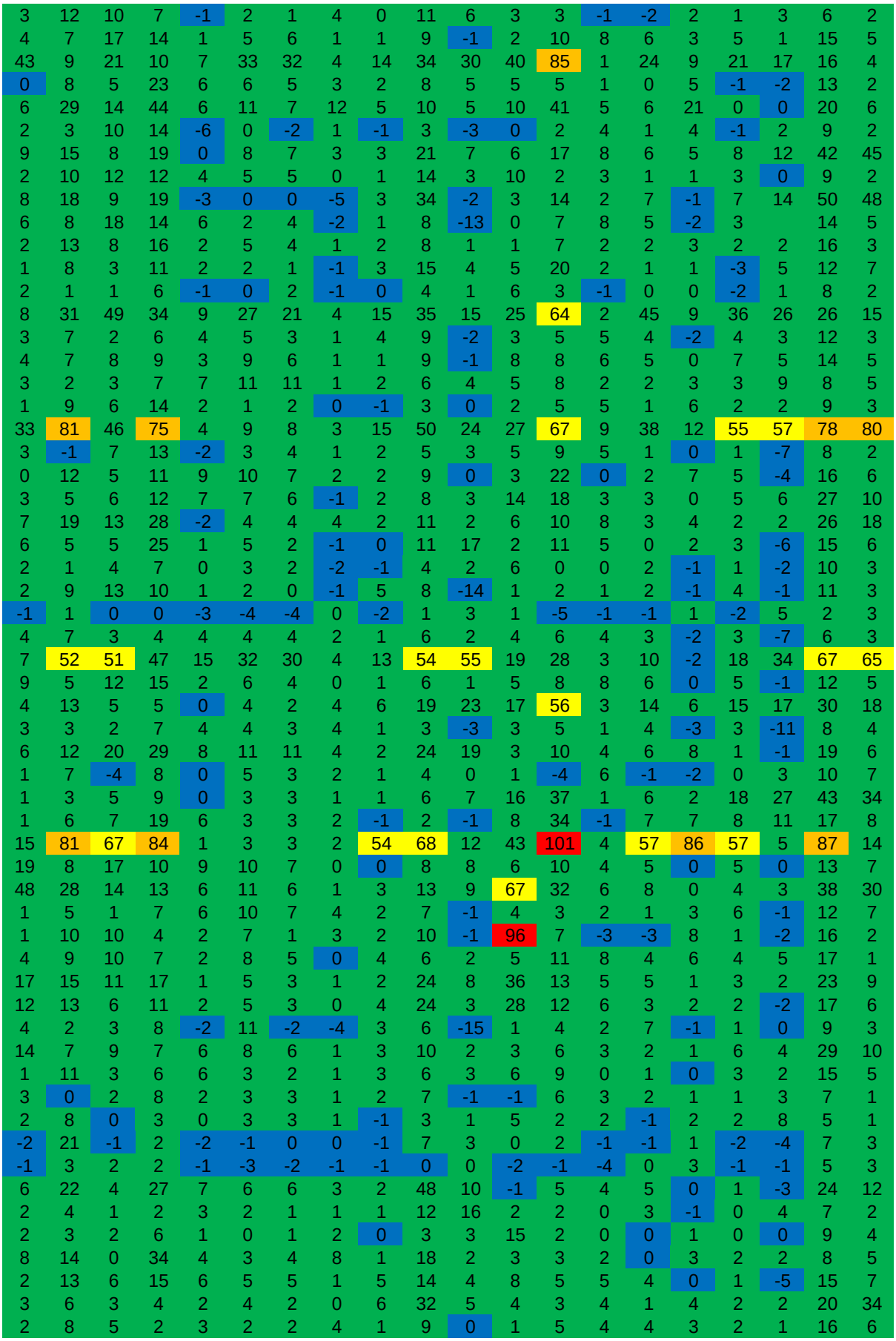

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TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TK	TKL	TKL	TKL	TKL	TKL	TKL	STE
PDGFRα-T674I	PDGFRα-V561D	PDGFRβ	TIE2	TNK2	TNK1	EGFR	EGFR-L858R	EGFR-L861Q	EGFR-T790M	EGFR-T790M-L858R	ERBB2	ERBB4	IRAK4	LRRK2	LRRK2-G2019S	CRAF	BRAF	BRAF-V599E	MAP4K2
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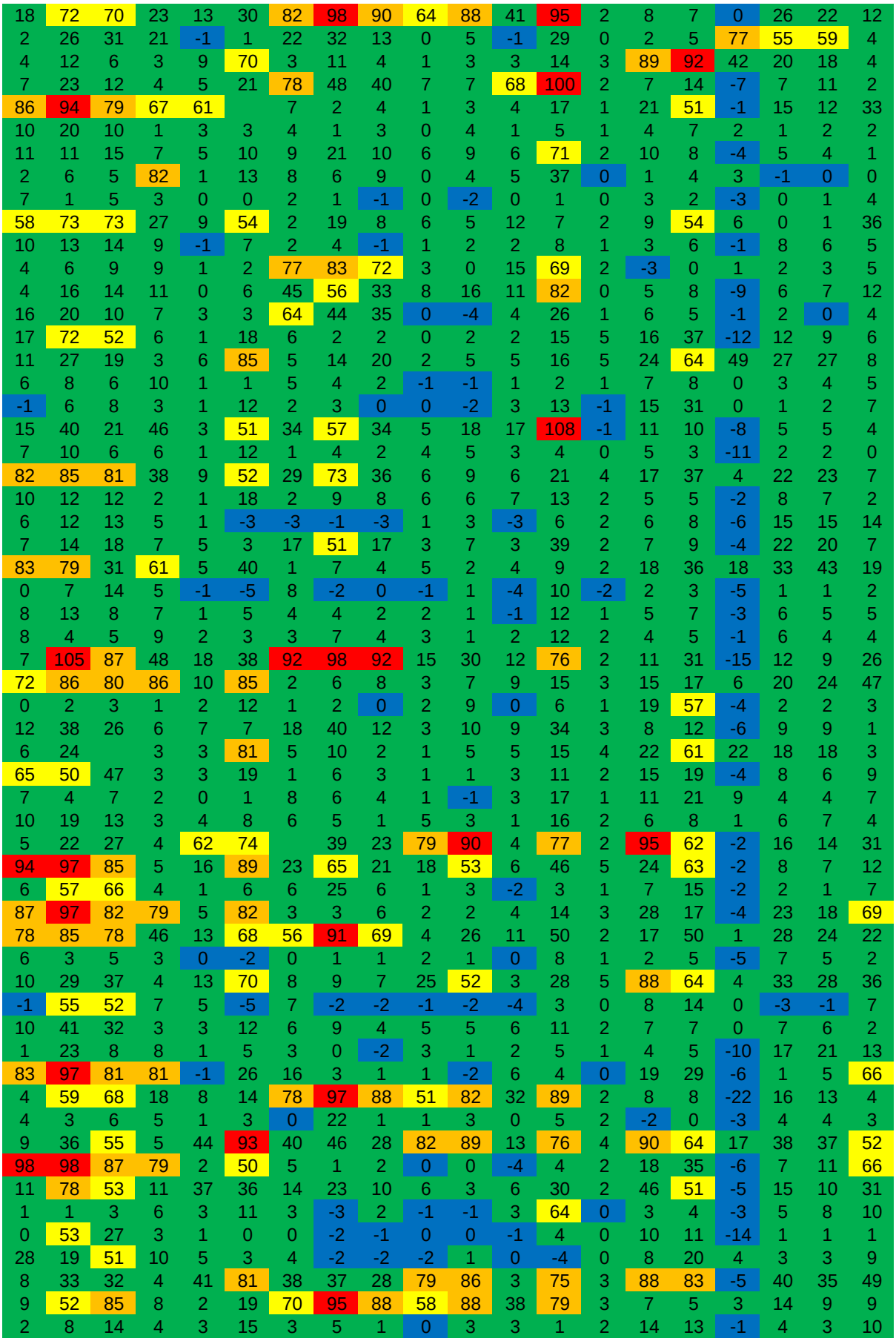

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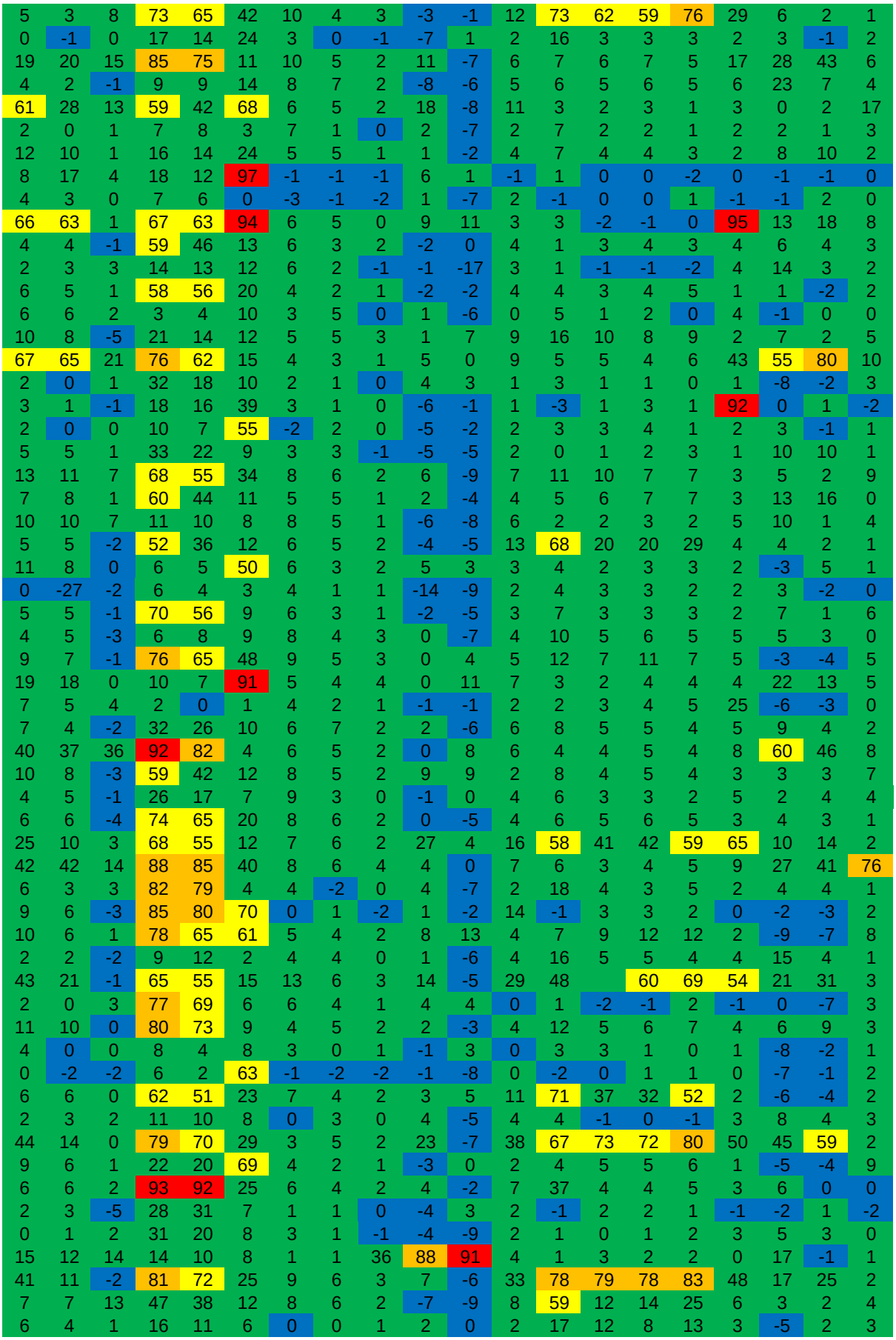

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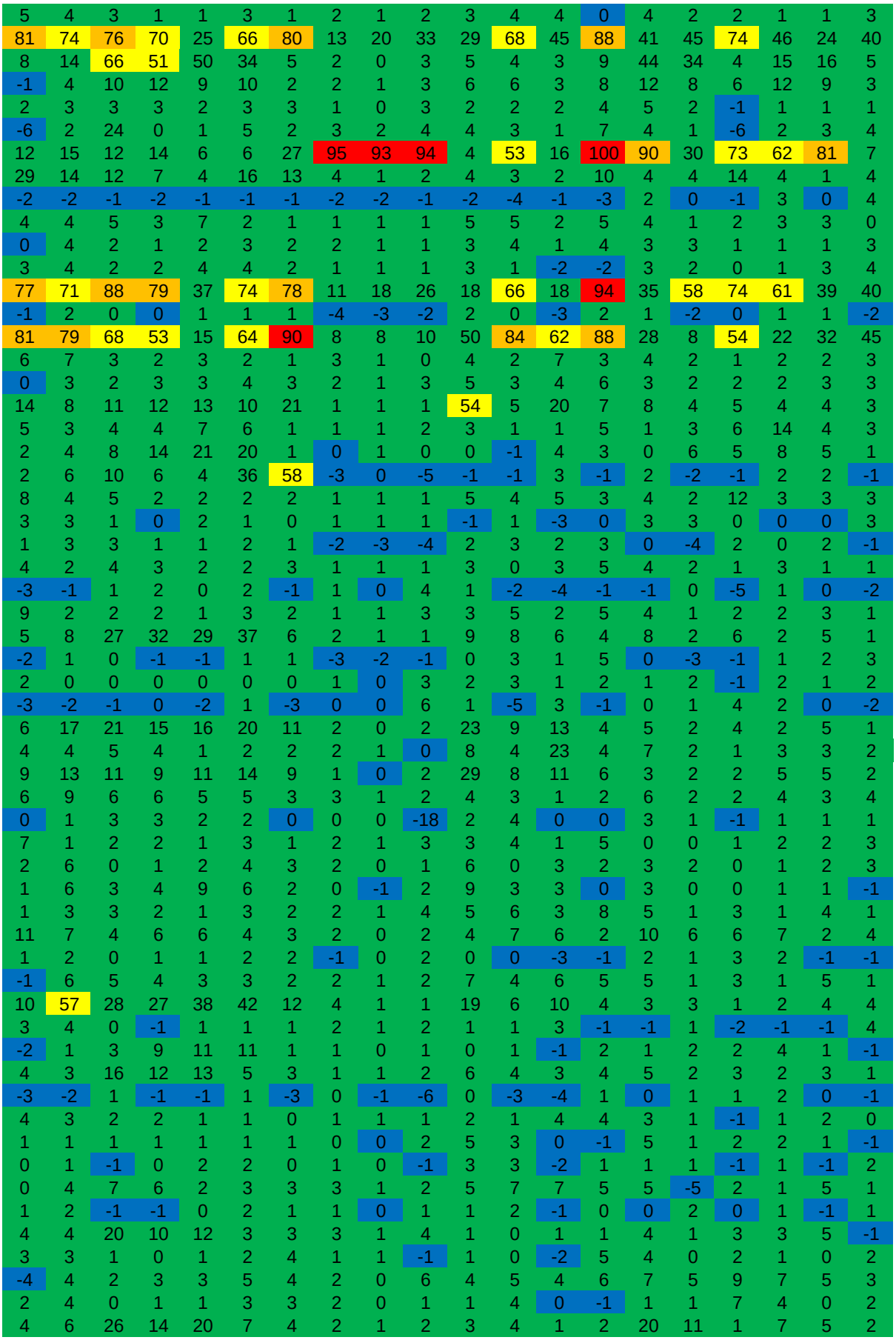

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AGC	AGC	AGC	AGC	AGC	AGC	AGC	AGC	S-T-PK	S-T-PK	S-T-PK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK
PRKG2	PRKG1	PRKX	PKA	ROCK1	ROCK2	MRCK-β	MRCK-α	AURORA-B	AURORA-C	AURORA-A	CHEK2	DCAMKL2	CAMK4	CAMK1D	PHKG1	PHKG2	CAMK2D	CAMK2A	PRAK
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CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK	CAMK
MAPKAPK2	MAPKAPK3	MNK2	MKNK1	PRKD3	PRKD1	PRKD2	MARK4	MARK3	PAR-1Bα	MARK1	SNF1LK2 (QIK)	SNF1LK (SIK)	ARK5	BRSK1	BRSK2	AMPKA1 (A1B1G1)	AMPKA2 (A2B1G1)	MELK	TSSK2
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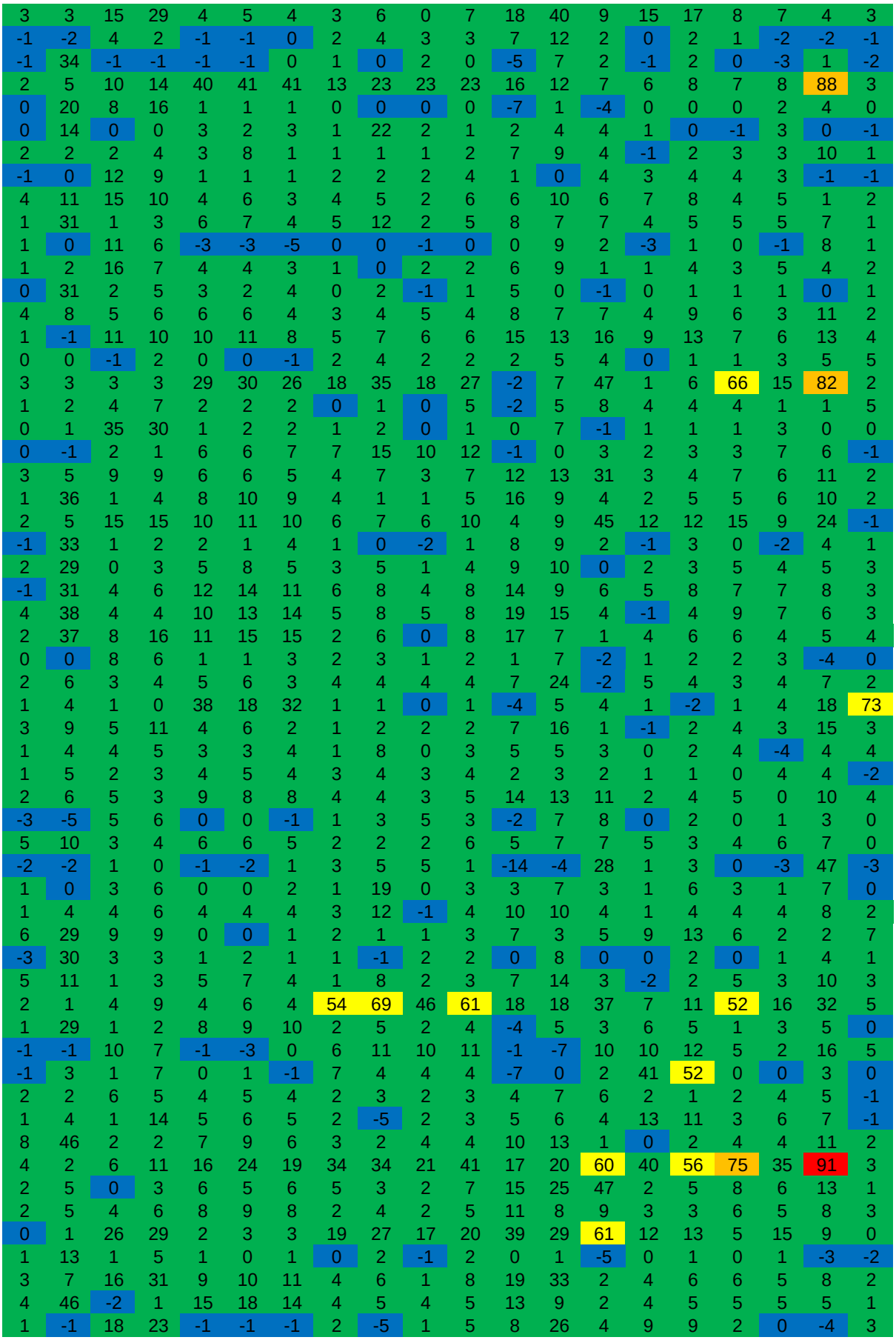

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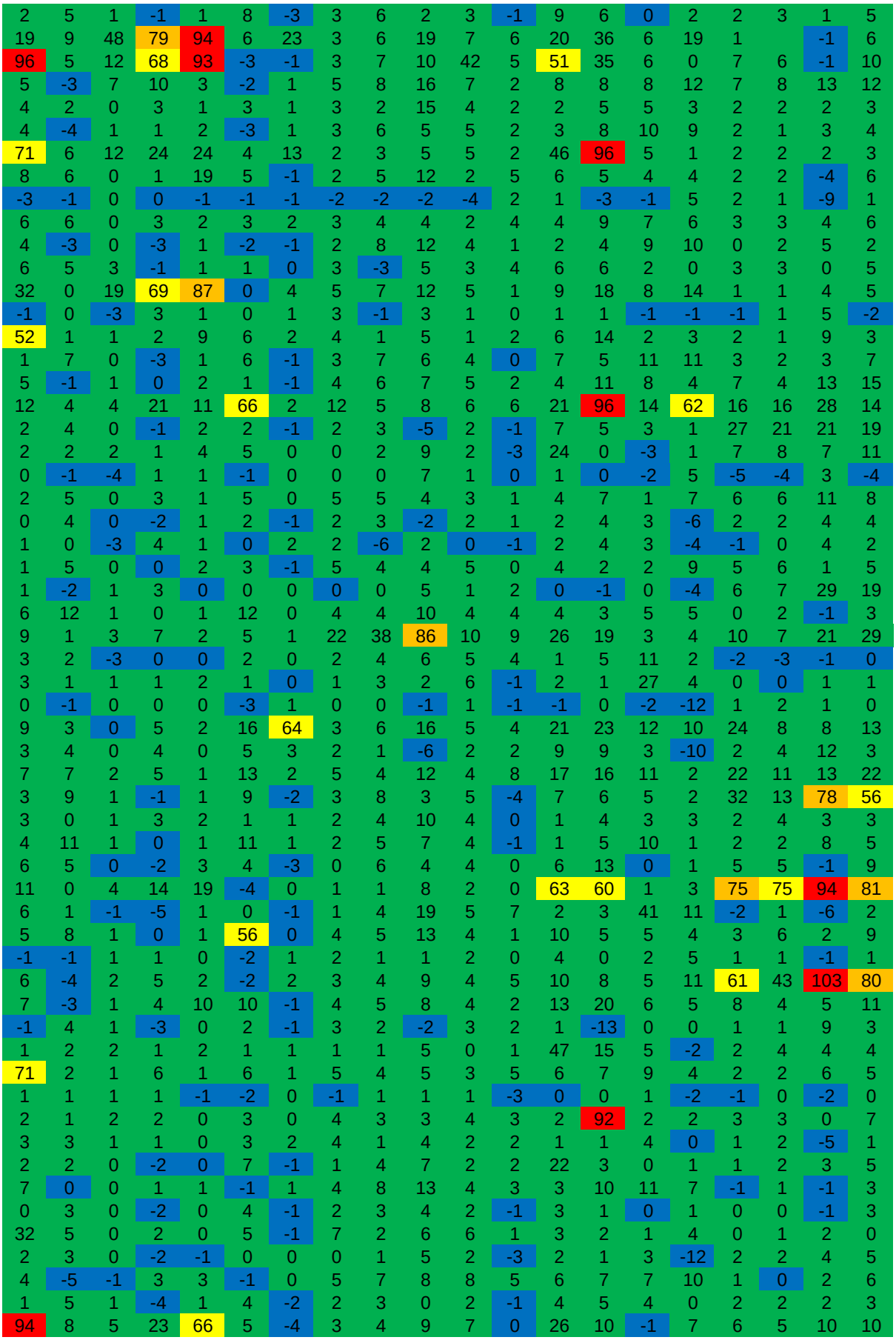

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CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC	CMGC
CDK3/cyclinE	CDK6/cyclinD3	CDK4/cyclinD	JNK2	P38α	P38β	P38δ	P38γ	MAPK1	MAPK3	GSK3A	GSK3B	SRPK1	MSSK1	CLK3	CLK2	HIPK1	HIPK4	DYRK1B	DYRK1A
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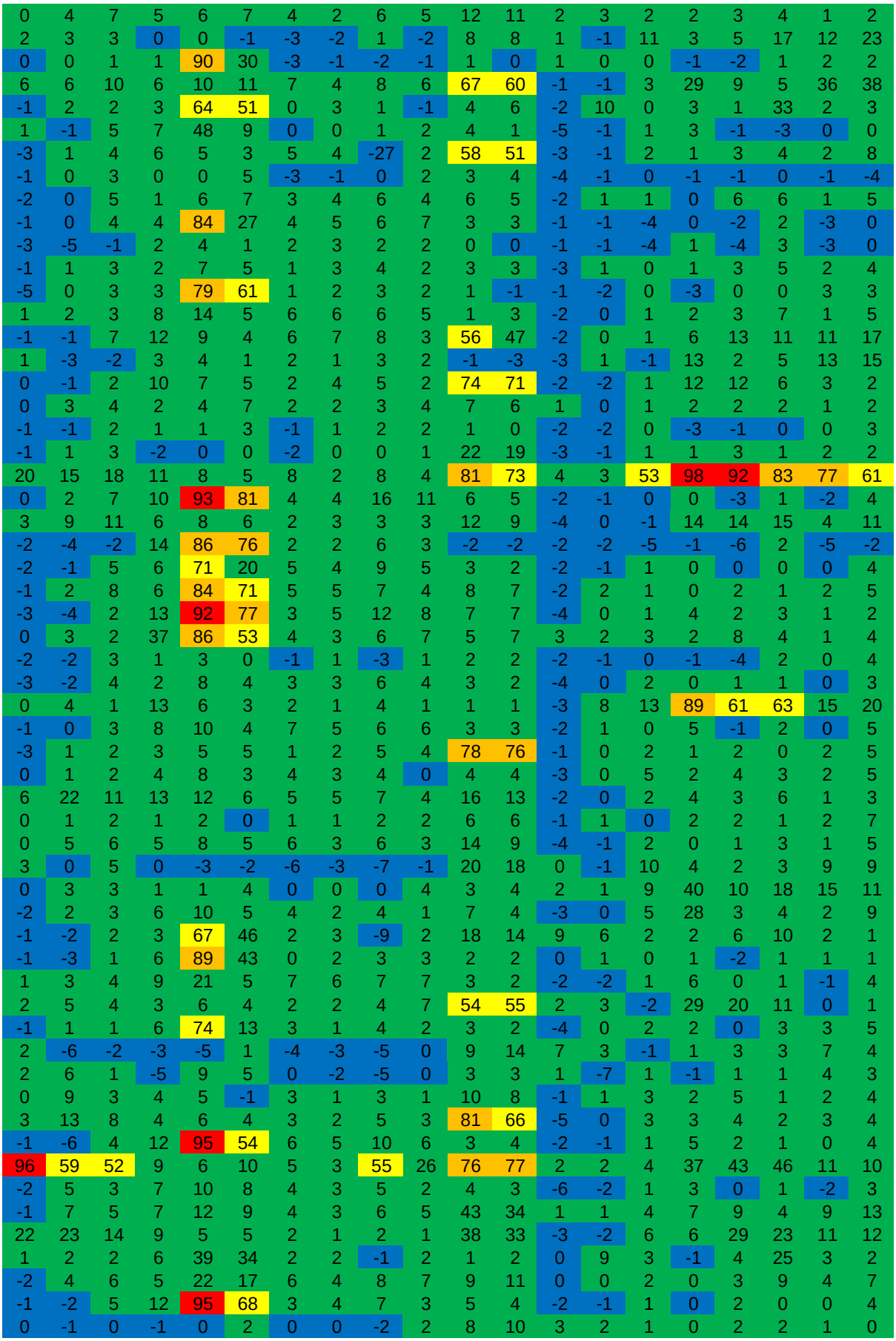

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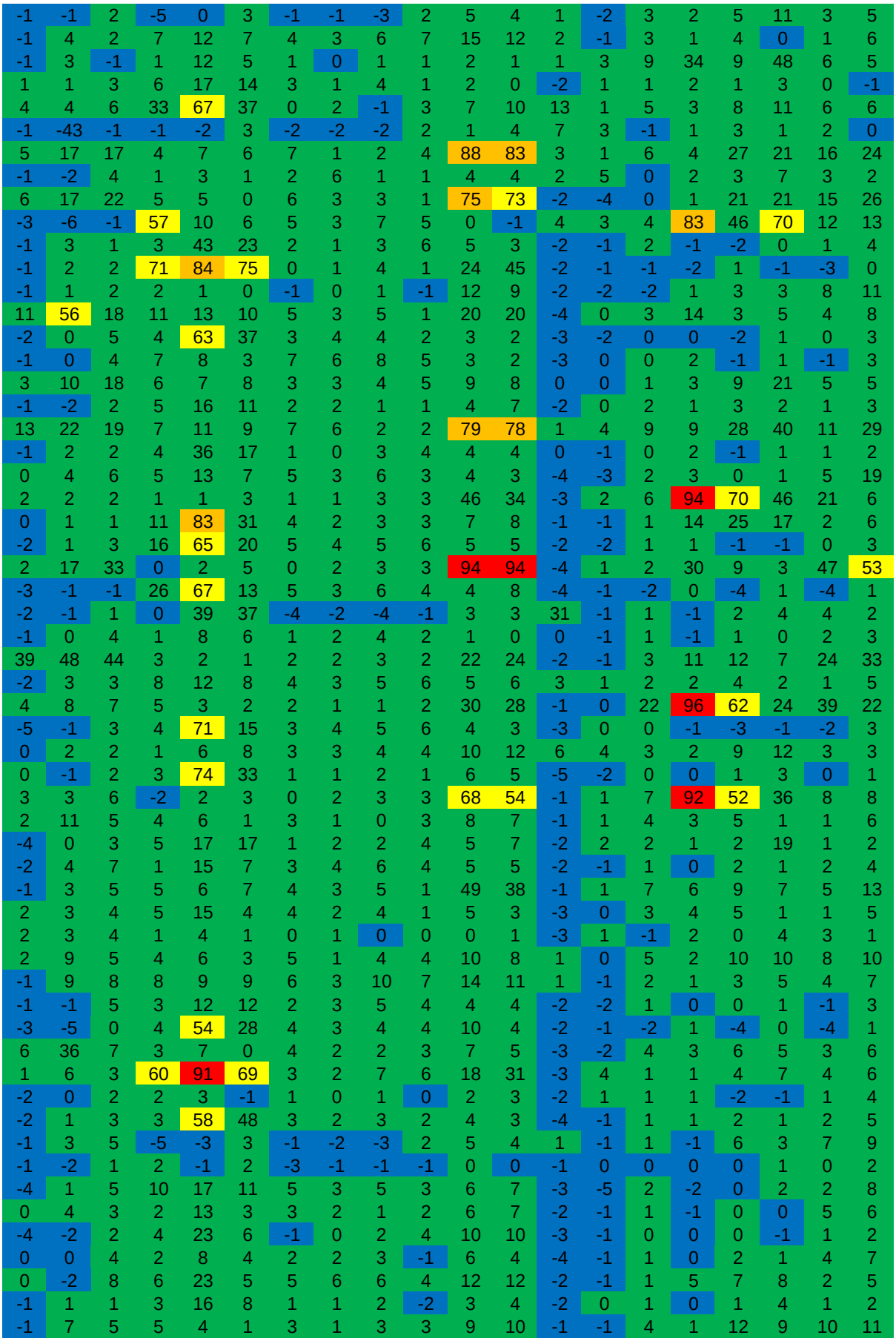

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