

Supplementary Information

A target-disease network model of second-generation BCR-ABL inhibitor action in Ph+ ALL

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Figure S1. ABL *in vitro* kinase assay. A. Chemical structures of nilotinib, pc-nilotinib and c-nilotinib and synthetic modification of pc-nilotinib generating c-nilotinib. Boc-Gly-OH: *N*-(*tert*-Butoxycarbonyl)glycine, DCC: *N,N'*-Dicyclohexylcarbodiimide, DMAP: 4-(Dimethylamino)pyridine, TFA: Trifluoroacetic acid. **B.** *In vitro* kinase inhibition assay of nilotinib and pre-c-nilotinib (pc-nilotinib), the non-esterified precursor of c-nilotinib, using recombinant full-length c-ABL determines similarly potent inhibition of ABL by nilotinib and pc-nilotinib.

Figure S2. Ph+ ALL-specific kinome-wide drug-target maps of nilotinib, dasatinib, bosutinib and bafetinib displaying new and known targets. Ph+ ALL kinase targets of the TKI nilotinib (A), dasatinib (B), bosutinib (C) and bafetinib (D) that have been identified in this study were mapped to the phylogenetic tree of human protein kinases. Known kinase targets of the respective drugs are shown in blue, new targets in grey. Color intensities indicate the degree of amino acid (aa) sequence

coverage observed for each protein. A black dotted rim indicates independent validation by various *in vitro* assays that have been reported previously, a red dotted rim indicates validation of drug-protein interactions performed in the course of this study (see Table S4 in this file), selecting the most prominent kinase targets (based on the aa sequence coverage) without previous independent validation. The Human Kinome Map was adapted with permission from Cell Signaling Technology (www.cellsignal.com).

Figure S3. Hybrid drug-protein/protein-protein interaction networks of specific dasatinib binding proteins in the patient pool sample. The primary cellular target profile of dasatinib (red) was overlaid with PPI data from public databases. Protein kinases were considered to be direct drug binders (solid lines) and displayed in red. All other non-kinase proteins were assumed to be indirect binders (dashed lines) and are displayed in grey.

Figure S4. Measurement of ³H-thymidine uptake in BV-173 cells.

Figure S5. Measurement of ³H-thymidine uptake in Z-119 cells.

Figure S6 Measurement of ³H-thymidine uptake in SUP-B15 cells.

Figure S7. Measurement of cell apoptosis in BV-173 and Z-119 cells.

Table S1. Molecular Characteristics of patient samples. WBC: White blood cell count; Hb: Hemoglobin; Plt: Platelet count.

Table S2. Mass spectrometry data for drug affinity pulldowns in BV-173 cells. AC: Swissprot accession code. Entrez-ID: Entrez accession code. Entrez_GN: alternative gene names. PC: number of unique peptides (peptide count). SC: number of mass spectra to sequence matches (spectral count). SeqCov: percentage (1.00=100%) of amino acid sequence for individual protein that is cumulatively covered by all assigned unique peptides (sequence coverage). Numbers following drug names are indicating the individual replicates (1,2: technical replicates of experimental replicate 1; 3,4: technical replicates of experimental replicate 2). 'grp' indicates the overall peptide counts, spectral

counts or sequence coverage across all replicates. Each row represents one group of proteins, the representative of which is listed in detail.

Table S3. Mass spectrometry data for drug affinity pulldowns in Z-119 cells. For detailed description see Table S2 in this file.

Table S4. Mass spectrometry data for dasatinib affinity pulldowns in primary cells from Ph+ ALL patient pool. For detailed description see Table S2 in this file.

Table S5. IC₅₀ values (in nM) of selected new drug-kinase interactions determined by *in vitro* kinase assays.

Table S6. Mass spectrometry data for competitive drug affinity pulldowns in BV-173 cells. Competition was performed with concomitant incubation of drug beads with the respective original drug at a concentration of 20 µM. For detailed description see Table S3 in this file.

Table S7. Mass spectrometry data for competitive drug affinity pulldowns in Z-119 cells. Competition was performed with concomitant incubation of drug beads with the respective original drug at a concentration of 20 µM. For detailed description see Table S3 in this file.

Table S8. Eluate abundance scores A for each specific drug-binding protein identified in BV-173 cells. AC: Swissprot accession code. ID: Uniprot identifier. Individual scores were calculated as the product of the mean spectral count and the 'grp' sequence coverage extracted from Table S3 in this file.

Table S9. Eluate abundance scores A for each specific drug-binding protein identified in Z-119 cells. AC: Swissprot accession code. ID: Uniprot identifier. Individual scores were calculated as the product of the mean spectral count and the 'grp' sequence coverage extracted from Table S4 in this file.

Table S10. Gene copy numbers of the 11 Ph+ ALL disease genes as reported in the Cancer Cell Line Encyclopedia (CCLE).

Table S11. Distances between each specific drug-binding protein and the deleted disease nodes within the Ph+ ALL disease-modified PPI network. AC: Swissprot accession code. ID: Uniprot identifier. 'NA' indicates proteins that were not represented in any PPI database and were therefore not mapped onto the network.

Table S12. Expression analysis of BTK, LYN, ILK and TEC by qPCR in individual Ph+ ALL patient samples and cell lines.

Structural characterization of coupleable drug analogues

pc-Nilotinib

M = 587.59 g/mol ($C_{31}H_{28}F_3N_7O_2$)

LC/MS Purity: 99%

MS (pos.-ESI) m/z 588.0 $[M+H]^+$ (66), 294.6 $[M+2H]^{2+}$ (100).

1H -NMR (400 MHz, CD_3OD): δ 9.09 (bs, 1H), 8.55 (s, 1H), 8.50 (s, 1H), 8.49 (d, 1H), 8.46 (s, 1H), 8.25 (s, 1H), 8.13 (s, 1H), 8.11 (s, 1H), 7.71 (d, 1H), 7.61 (s, 1H), 7.43 (d, 1H), 7.41 (d, 1H), 7.37 (s, 1H), 3.52 (t, 2H), 2.81 (t, 2H), 2.43 (s, 3H), 2.27 (s, 3H), 1.85 (m, 2H).

c-Dasatinib

M = 487.02 g/mol ($C_{22}H_{27}ClN_8OS$)

LC/MS Purity: 96%

MS (pos.-ESI) m/z 487.3/489.2 $[M+H]^+$ (100/35).

1H -NMR (400 MHz, CD_3OD): δ 8.19 (s, 1H), 7.35 (dd, 1H), 7.26-7.22 (m, 1H), 7.24-7.20 (m, 1H), 6.34 (s, 1H), 3.94 (b, 4H), 3.35-3.29 (m, 2H), 3.21-3.14 (m, 6H), 2.54 (s, 3H), 2.31 (s, 3H).

c-Bosutinib

M = 696.93 g/mol ($C_{29}H_{36}Cl_2N_6O_3 \cdot 3HCl$), free base 587.54 g/mol ($C_{29}H_{36}Cl_2N_6O_3$)

LC/MS Purity: 96%

MS (pos.-ESI) m/z 587.1/589.0 $[M+H]^+$ (56/41).

$^1\text{H-NMR}$ (300 MHz, DMSO- d_6): δ 12 (bs, 1H), 11.15 (bs, 1H), 8.97 (s, 1H), 8.31 (s, 1H), 8.03 (bs, 2H), 7.84 (s, 1H), 7.59 (s, 1H), 7.51 (s, 1H), 6.1-5.1 (b, 2H), 4.34 (t, 2H), 4.04 (s, 3H), 3.88 (s, 3H), 3.66 (bs, 6H), 3.56 (bs, 4H), 3.35 (m, 2H), 2.81 (m, 2H), 2.36 (bs, 2H), 1.81 (bs, 2H), 1.64 (bs, 2H).

pc-Bafetinib

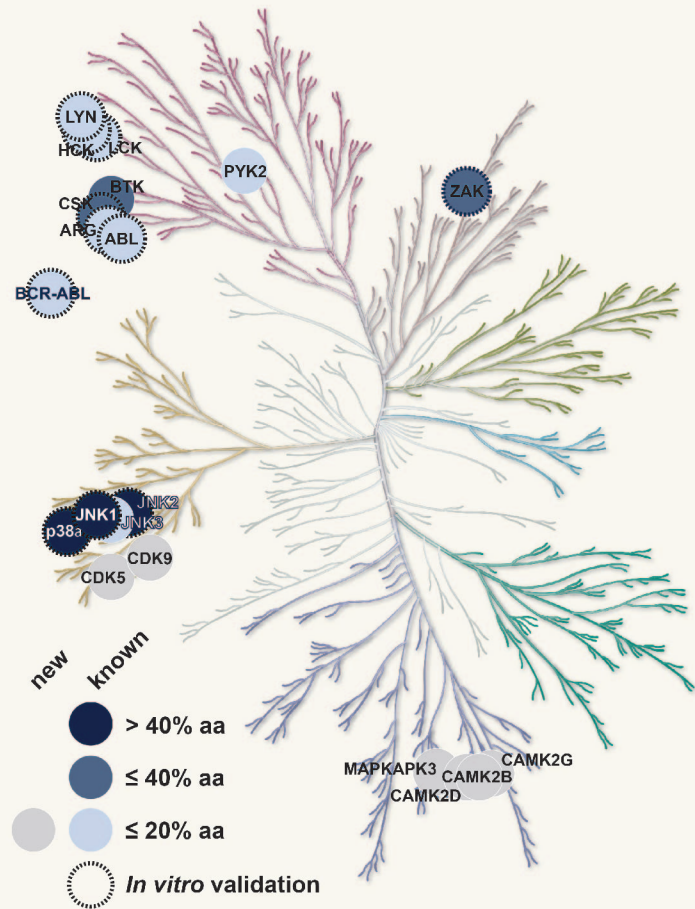
M = 633.71 g/mol ($\text{C}_{34}\text{H}_{38}\text{F}_3\text{N}_7\text{O}_2$)

LC/MS Purity: 96%

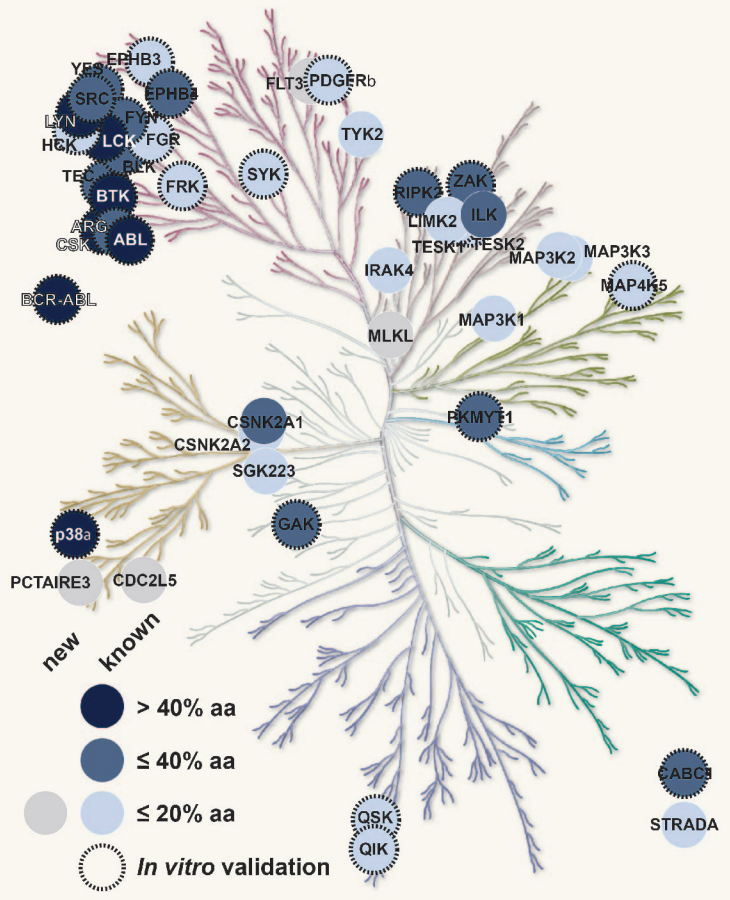
MS (pos.-ESI) m/z 634.3 $[M+H]^+$ (37), 317.7 $[M+2H]^{2+}$ (100).

$^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 9.00 (d, 1H), 8.68 (bs, 1H), 8.53 (d, 1H), 8.50 (d, 1H), 8.40 (bs, 1H), 8.16 (s, 1H), 8.07 (s, 1H)*, 8.02 (d, 1H), 7.92 (d, 1H), 7.28-7.20 (m, 2H), 7.18 (d, 1H), 7.06 (s, 1H)*, 3.82 (dd, 1H), 3.71 (dd, 1H), 3.47 (m, 2H), 2.81 (m, 1H), 2.79 (m, 2H), 2.73-2.60 (m, 3H), 2.48 (m, 1H), 2.29 (s, 3H), 2.17 (s, 6H), 2.05-1.90 (m, 1H), 1.88-1.75 (m, 3H).

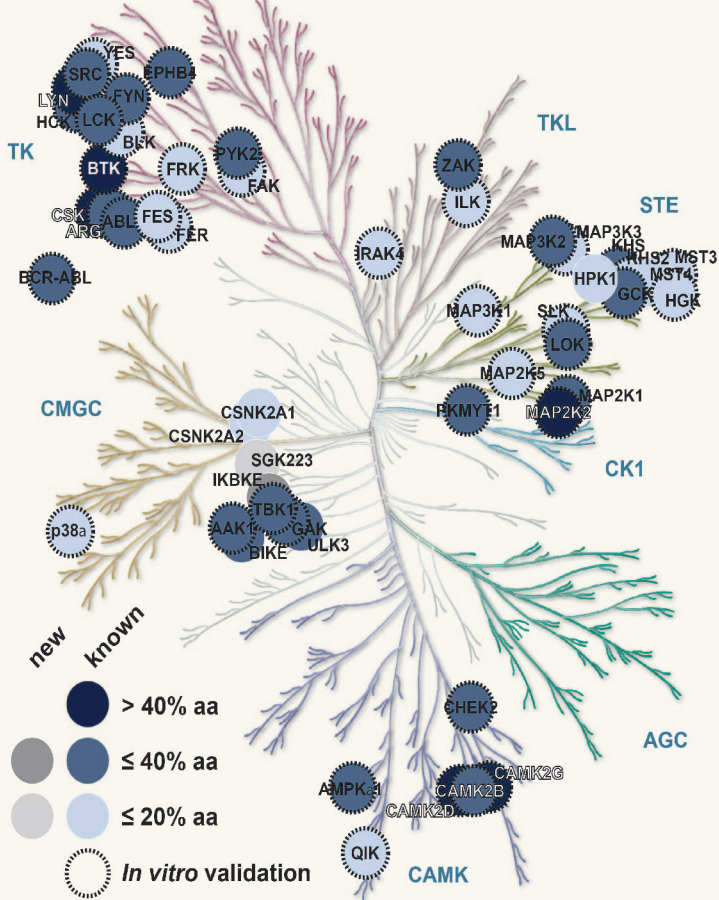
A Nilotinib



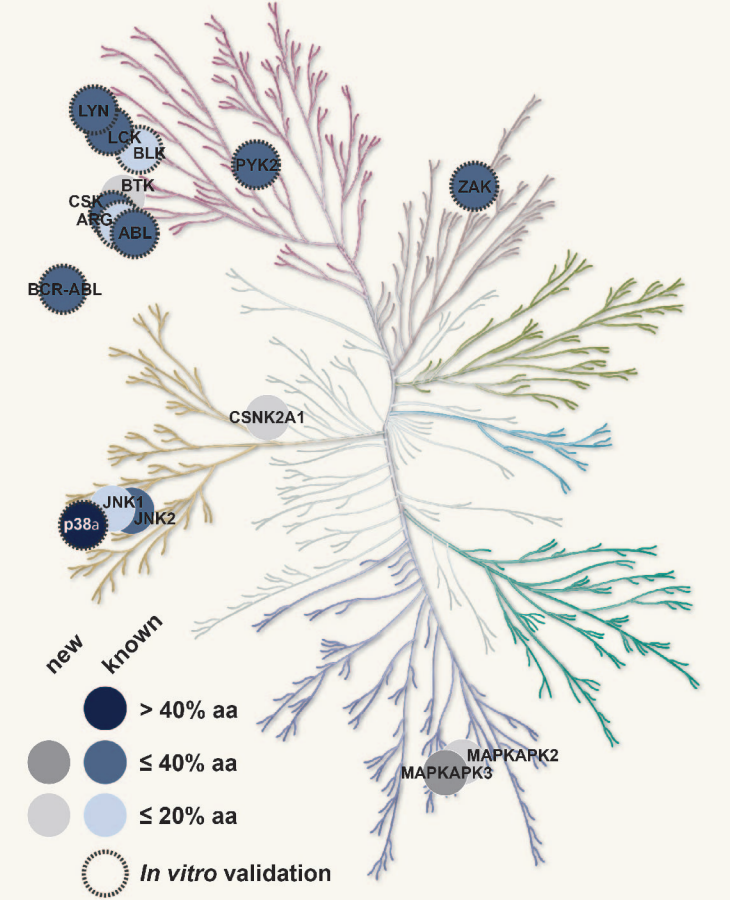
B Dasatinib



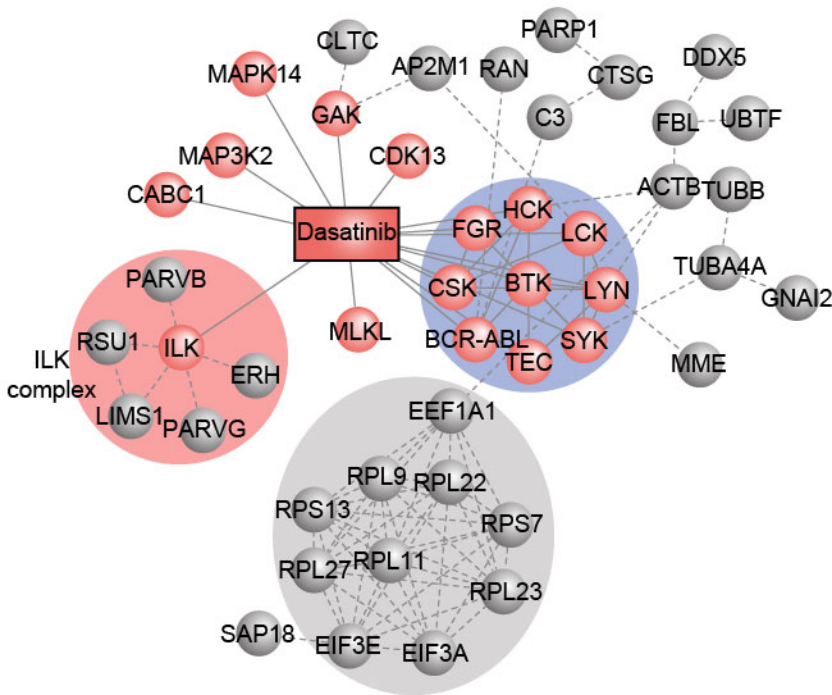
C Bosutinib



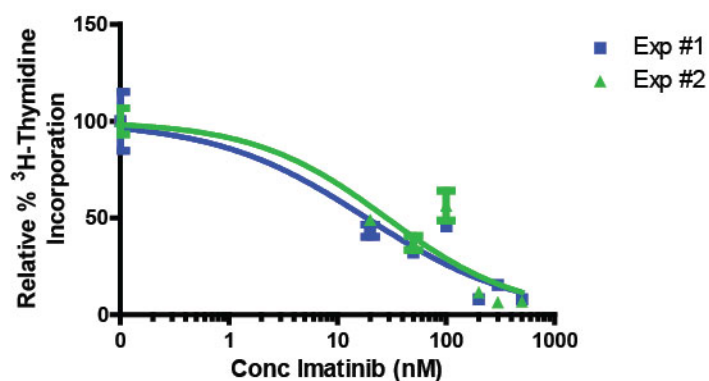
D Bafetinib



Rix et al., Supplementary Figure 3

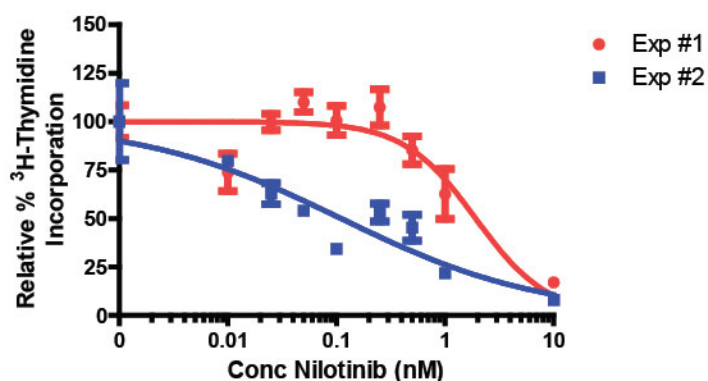


Effect of Imatinib on ³H-Thymidine Incorporation by BV173 Cells



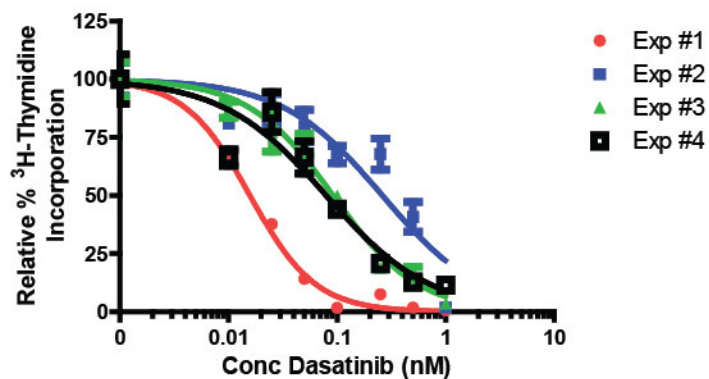
	Exp #1	Exp #2
EC50	18.50	28.41

Effect of Nilotinib on ³H-Thymidine Incorporation by BV173 Cells



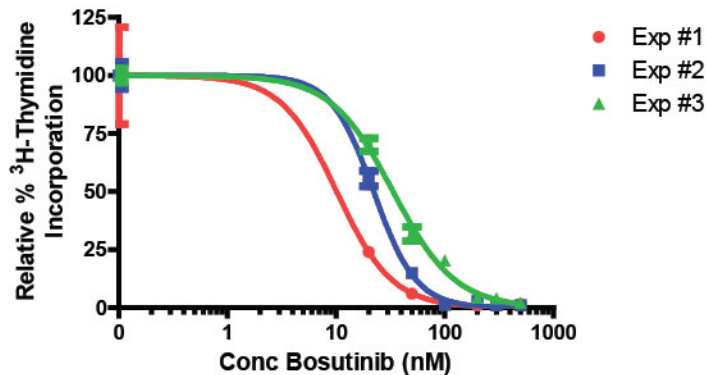
	Exp #1	Exp #2
EC50	1.921	0.1108

Effect of Dasatinib on ³H-Thymidine Incorporation by BV173 Cells



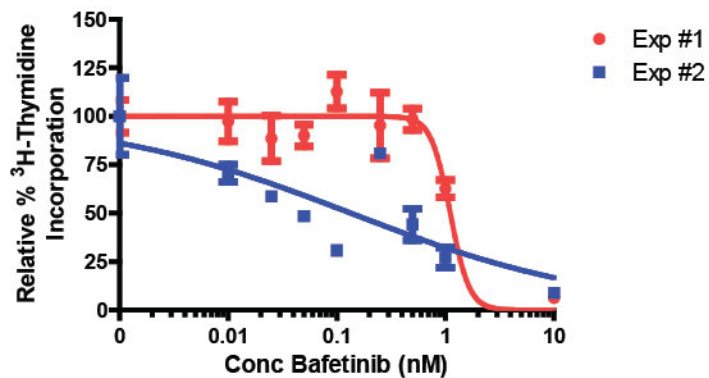
	Exp #1	Exp #2	Exp #3	Exp #4
EC50	0.01577	0.2615	0.09191	0.07953

Effect of Bosutinib on ³H-Thymidine Incorporation by BV173 Cells



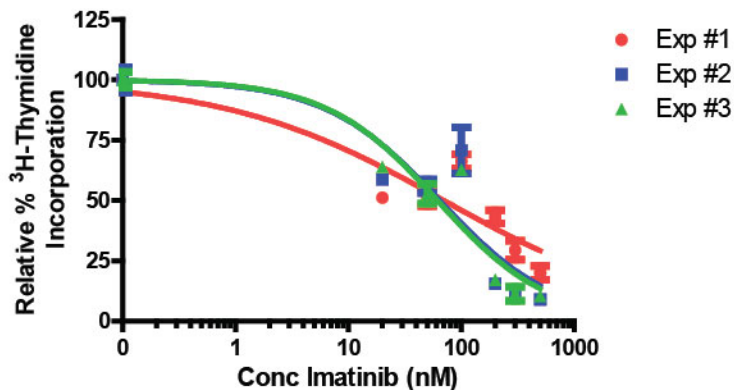
	Exp #1	Exp #2	Exp #3
EC50	10.14	22.20	33.55

Effect of Bafetinib on ³H-Thymidine Incorporation by BV173 Cells



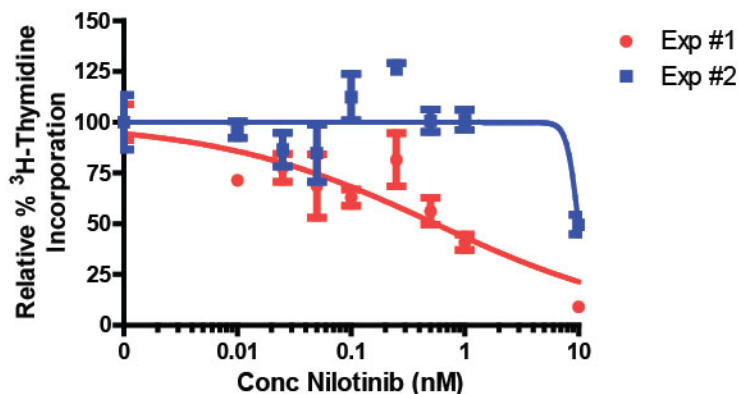
	Exp #1	Exp #2
EC50	1.111	0.1355

Effect of Imatinib on ³H-Thymidine Incorporation by Z119 Cells



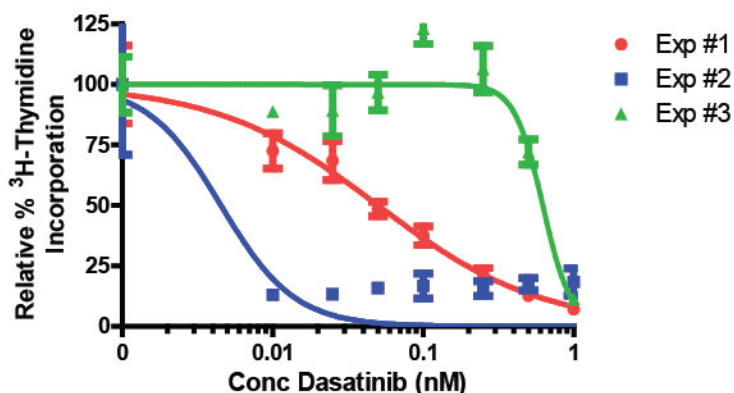
	Exp #1	Exp #2	Exp #3
EC50	69.98	64.23	61.44

Effect of Nilotinib on ³H-Thymidine Incorporation by Z119 Cells



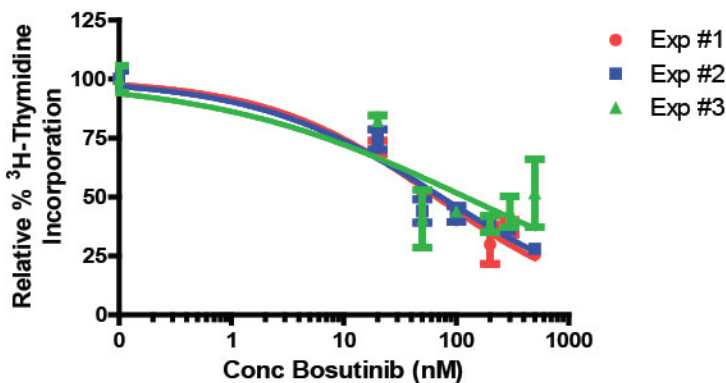
	Exp #1	Exp #2
EC50	0.5506	~9.982

Effect of Dasatinib on ³H-Thymidine Incorporation by Z119 Cells



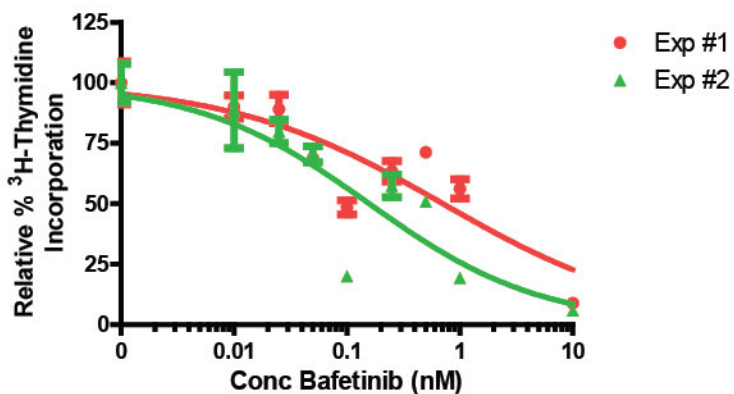
	Exp #1	Exp #2	Exp #3
EC50	0.05004	0.004533	0.6217

Effect of Bosutinib on ³H-Thymidine Incorporation by Z119 Cells



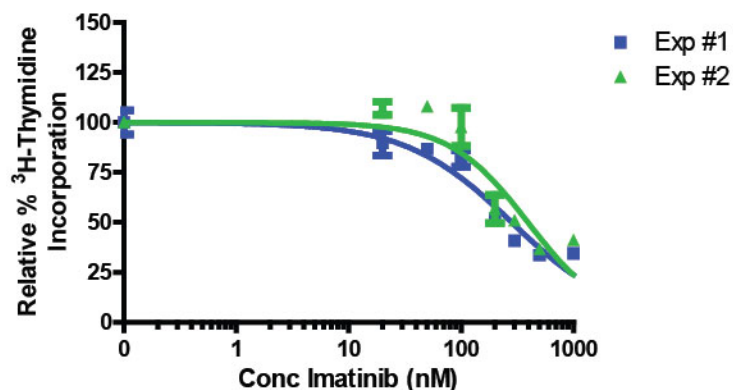
	Exp #1	Exp #2	Exp #3
EC50	66.46	73.47	120.8

Effect of Bafetinib on ³H-Thymidine Incorporation by Z119 Cells



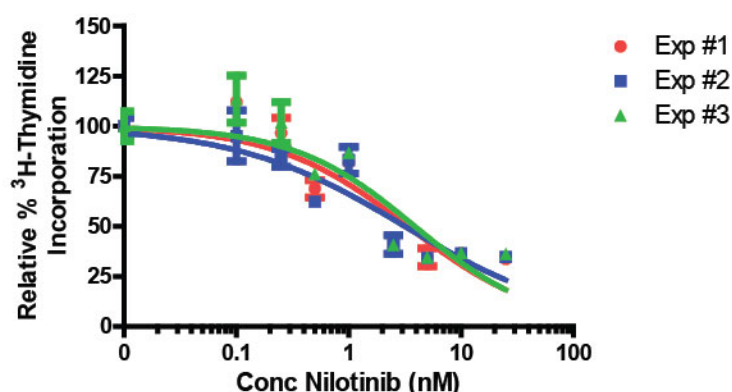
	Exp #1	Exp #2
EC50	0.9293	0.2781

Effect of Imatinib on ³H-Thymidine Incorporation by SUP-B15 Cells



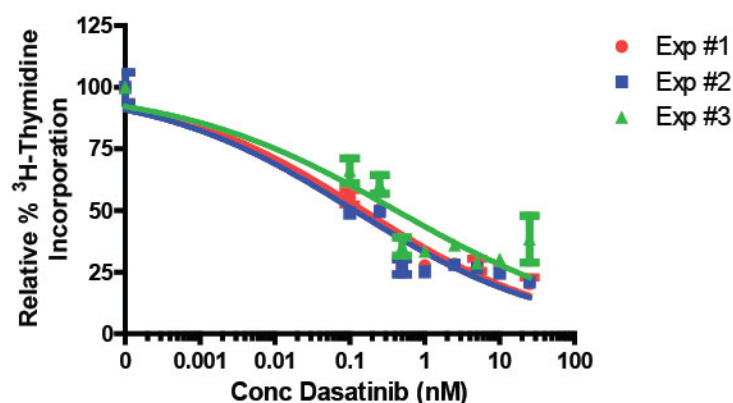
	Exp #1	Exp #2
EC50	282.5	394.2

Effect of Nilotinib on ³H-Thymidine Incorporation by SUP-B15 Cells



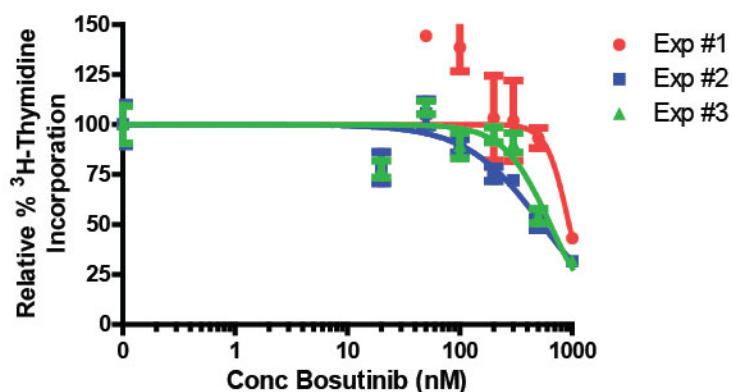
	Exp #1	Exp #2	Exp #3
EC50	3.367	3.193	3.901

Effect of Dasatinib on ³H-Thymidine Incorporation by SUP-B15 Cells



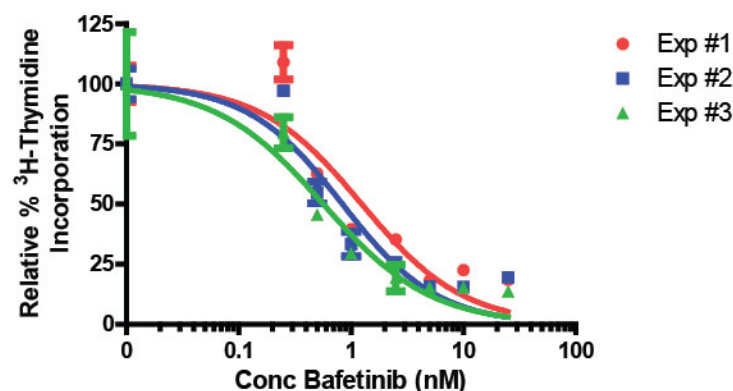
	Exp #1	Exp #2	Exp #3
EC50	0.2619	0.2158	0.5736

Effect of Bosutinib on ³H-Thymidine Incorporation by SUP-B15 Cells



	Exp #1	Exp #2	Exp #3
EC50	939.1	541.5	638.9

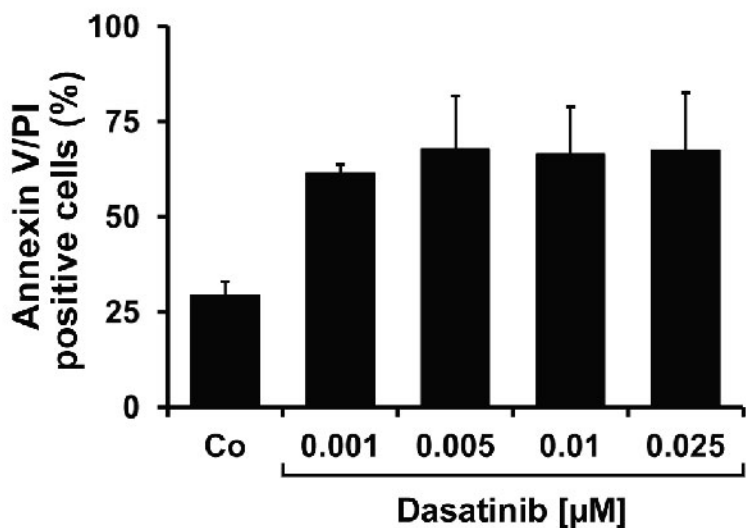
Effect of Bafetinib on ³H-Thymidine Incorporation by SUP-B15 Cells



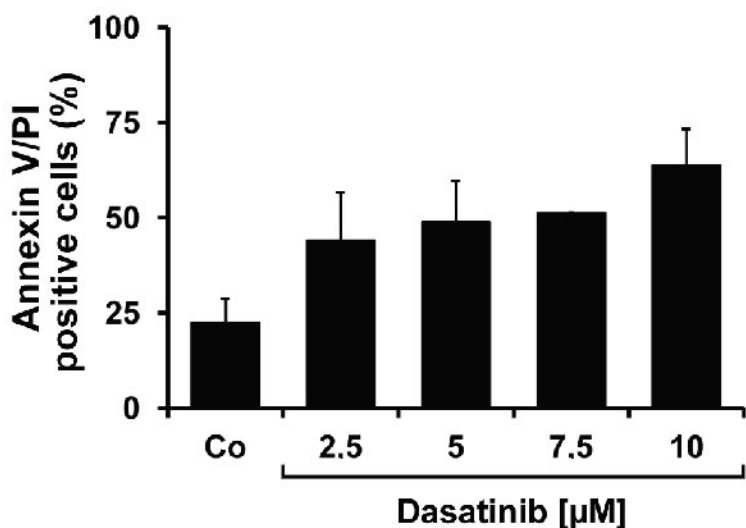
	Exp #1	Exp #2	Exp #3
EC50	1.246	0.8384	0.5664

Rix et al., Figure S7

A BV173



B Z119



C

ED ₅₀	BV173	Z119
Imatinib	0.1 μM	>10 μM
Nilotinib	0.005 μM	>10 μM
Dasatinib	<0.001 μM	7.5 μM
Bosutinib	0.1 μM	2.5 μM

Patient	Gender	Age (y)	Diagnosis	BCR-ABL	WBC (G/L)	Hb (g/dL)	Plt (G/L)	Cytogenetics
1	m	73	pre-B-ALL	y	140	10	19	46, XY, t(9;22)(q34;q11)
2	m	39	c-ALL	y	61.6	9.4	56	46, XY, t(9;22)(q34;q11)
3	f	35	c-ALL	y	24.72	13.1	177	complex
4	f	56	pre-B-ALL	y	2.3	7.4	86	46, XX, t(9;22)(q34;q11)
5	f	55	c-ALL	y	71.3	13.7	73	46, XX, t(9;22)(q34;q11)
6	f	37	pre-B-ALL	y	4.4	7.6	3	46, XX

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11. Declaration of Interest
12. Funding Source
13. Data Availability Statement

14. Ethics Statement
15. Conflicts of Interest

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41. Social Responsibility

42. Environmental Impact
43. Community Engagement

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45. Employee Well-being

46. Safety and Security
47. Risk Management

48. Compliance
49. Regulatory Updates

50. Industry Trends
51. Market Analysis

52. Competitive Landscape
53. Strategic Initiatives

54. Innovation and R&D
55. Intellectual Property

56. Patent Applications
57. Trademark Registrations

Drug	Kinase	IC₅₀ [nM]
Bosutinib	MAP2K1 (MEK1)	2480
Bosutinib	MAP2K2 (MEK2)	143
Bosutinib	MAP3K2 (MEKK2)	68
Nilotinib	MAPK9 (JNK2)	12900

1. **Introduction**
This document provides a comprehensive overview of the project's objectives, scope, and the methodology employed for data analysis. The primary goal is to evaluate the effectiveness of the proposed system in enhancing operational efficiency and reducing costs. The scope of the study is limited to the core processes of the organization, excluding peripheral activities. The methodology involves a combination of qualitative and quantitative techniques, including interviews, surveys, and data mining, to gather and analyze relevant information.

2. **Methodology**
The research methodology is designed to ensure the reliability and validity of the findings. It consists of several key components: **2.1. Data Collection:** Data is collected through a series of structured interviews with key stakeholders and a survey of employees. **2.2. Data Analysis:** The collected data is analyzed using statistical software to identify trends and correlations. **2.3. Validation:** The results are validated through a series of focus groups and expert reviews to ensure accuracy and relevance.

3. **Results**
The analysis reveals several significant findings. First, there is a clear correlation between the implementation of the proposed system and an increase in productivity. Second, the system has effectively reduced operational costs, particularly in the areas of resource allocation and waste management. These results suggest that the proposed system is a viable and beneficial solution for the organization.

4. **Conclusion**
In conclusion, the study demonstrates that the proposed system is highly effective in achieving its intended goals. The findings provide a strong basis for the implementation of the system on a larger scale. Further research is recommended to explore the long-term impacts and potential challenges associated with the system's adoption.

5. **References**
The following references are cited in this document to provide context and support for the research findings.

6. **Appendix A**
Appendix A contains supplementary information, including detailed data tables and additional charts that support the main findings of the report.

7. **Appendix B**
Appendix B provides a detailed breakdown of the system's architecture and the specific components that facilitate its operation.

8. **Appendix C**
Appendix C includes a list of the interviewees and survey participants, along with their respective roles within the organization.

9. **Appendix D**
Appendix D contains a glossary of key terms and definitions used throughout the document to ensure clarity and consistency.

10. **Appendix E**
Appendix E provides a detailed timeline of the project's progress, from the initial planning stages to the final implementation and evaluation.

11. **Appendix F**
Appendix F includes a list of the software tools and technologies used in the development and analysis of the system.

12. **Appendix G**
Appendix G contains a list of the organizations and institutions that have provided support and resources for the project.

13. **Appendix H**
Appendix H includes a list of the authors and their affiliations, along with their contact information for further inquiries.

14. **Appendix I**
Appendix I contains a list of the organizations and institutions that have provided support and resources for the project.

15. **Appendix J**
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16. **Appendix K**
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17. **Appendix L**
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18. **Appendix M**
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19. **Appendix N**
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22. **Appendix Q**
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23. **Appendix R**
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24. **Appendix S**
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25. **Appendix T**
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Item	Value	Item	Value
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83	0.00	183	0.00
84	0.00	184	0.00
85	0.00	185	0.00
86	0.00	186	0.00
87	0.00	187	0.00
88	0.00	188	0.00
89	0.00	189	0.00
90	0.00	190	0.00
91	0.00	191	0.00
92	0.00	192	0.00
93	0.00	193	0.00
94	0.00	194	0.00
95	0.00	195	0.00
96	0.00	196	0.00
97	0.00	197	0.00
98	0.00	198	0.00
99	0.00	199	0.00

AC	ID	Gene_symbol	Descr	Dasatinib score	Bosutinib score	Bafetinib score	Nilotinib score
Q2M2I8	AAK1_HUMAN	AAK1	AP2-associated protein kinase 1	0	49.8325	0	0
Q8I2P0-1	ABI1_HUMAN	ABI1	Abi interactor 1	0.9425	0.45	0	0
P00519-1	ABL1_HUMAN	ABL1	Tyrosine-protein kinase ABL1	68.46	37.125	10.75	0.1725
P42684-1	ABL2_HUMAN	ABL2	Tyrosine-protein kinase ABL2	22.4025	10.1325	5.16	0
P60709	ACTB_HUMAN	ACTB	Actin, cytoplasmic 1	0.525	9.45	0.7875	1.35
P55263-1	ADK_HUMAN	ADK	Adenosine kinase	23.54	0.0525	0	0
O95782-1	AP2A1_HUMAN	AP2A1	AP-2 complex subunit alpha-1	0	5.1975	0	0
Q96CW1-1	AP2M1_HUMAN	AP2M1	AP-2 complex subunit mu	0.105	0.09	0	0
bcra1	bcra1	BCR-ABL	BCR-ABL fusion protein	135.975	79.975	24.4375	0.27
P51451	BLK_HUMAN	BLK	Tyrosine-protein kinase Blk	23.1275	7.395	0.405	0
Q9NSY1-1	BMP2K_HUMAN	BMP2K	BMP-2-inducible protein kinase	0	16.64	0	0
Q06187	BTX_HUMAN	BTX	Tyrosine-protein kinase BTX	488.895	393.7375	4.37	11.7075
Q8WUW1-1	BRK1_HUMAN	C3orf10	Probable protein BRK1	1.5725	0.5625	0	0
Q8N60-1	ADC3_HUMAN	CABC1	Chaperone activity of bc1 complex-like, mitochondrial	4.9875	0	0	0
Q13554-3	KCC2B_HUMAN	CAMK2B	Calcium/calmodulin-dependent protein kinase type II subunit beta	0	40.235	0	0.09
Q13557-1	KCC2D_HUMAN	CAMK2D	Calcium/calmodulin-dependent protein kinase type II subunit delta	0	223.02	0	0.5775
Q13555-3	KCC2G_HUMAN	CAMK2G	Calcium/calmodulin-dependent protein kinase type II subunit gamma	0	78.435	0	0.09
Q14004-1	CDK13_HUMAN	CDK13	Cell division protein kinase 13	0.44	0	0	0
Q00535	CDK5_HUMAN	CDK5	Cell division protein kinase 5	0	0	0	0.0525
P50750-1	CDK9_HUMAN	CDK9	Cell division protein kinase 9	0	0	0	1.65
O96017-1	CHK2_HUMAN	CHEK2	Serine/threonine-protein kinase Chk2	0	1.3	0	0
P41240	CSK_HUMAN	CSK	Tyrosine-protein kinase CSK	152.2625	50.43	5.0625	21.3125
P68400	CSK21_HUMAN	CSNK2A1	Casein kinase II subunit alpha	2.325	0.8925	0.025	0
P19784	CSK22_HUMAN	CSNK2A2	Casein kinase II subunit alpha'	0.4275	0.36	0	0
P67870	CSK2B_HUMAN	CSNK2B	Casein kinase II subunit beta	0.225	0.27	0.1125	0
Q96F07-1	CYFP2_HUMAN	CYFIP2	Cytosolic FMR1-interacting protein 2	0.54	0.06	0	0
P06733-1	ENO4_HUMAN	ENO1	Alpha-enolase	0	1.485	0	0.2275
P13929-1	ENO8_HUMAN	ENO3	Beta-enolase	0	0.21	0	0.04
P54753	EPHB3_HUMAN	EPHB3	Ephrin type-B receptor 3	7.8	4.44	0	0
P54760	EPHB4_HUMAN	EPHB4	Ephrin type-B receptor 4	38.88	49.9625	0	0
P22830	HEMH_HUMAN	FECH	Ferrochelatase, mitochondrial	0	0	0	3.3
P16591	FER_HUMAN	FER	Tyrosine-protein kinase Fer	0	7.14	0	0
Q8NFF5-1	FAD1_HUMAN	FLAD1	FAD synthase	0	0	18.655	0
P42685	FRK_HUMAN	FRK	Tyrosine-protein kinase FRK	1.3575	0.6675	0	0
P06241-2	FYN_HUMAN	FYN	Tyrosine-protein kinase Fyn	21.75	18.6875	0.24	0
Q14976	GAK_HUMAN	GAK	Cyclin-G-associated kinase	8.625	54.1125	0	0
P04406	G3P_HUMAN	GAPDH	Glyceraldehyde-3-phosphate dehydrogenase	0.045	0.42	0	0.99
P14136-1	GFAP_HUMAN	GFAP	Glial fibrillary acidic protein	0.16	0.18	0.27	0.97
Q13588	GRAP_HUMAN	GRAP	GRB2-related adapter protein	4.4	4.2	0.375	0
P62993-1	GRB2_HUMAN	GRB2	Growth factor receptor-bound protein 2	44.01	46.44	19.875	0.09
P08631-1	HCK_HUMAN	HCK	Tyrosine-protein kinase HCK	11.72	16.905	0.405	0.1725
P10412	H14_HUMAN	HIST1H1E	Histone H1.4	0.1125	0.0675	0.77	0.7975
O60814	H2B1K_HUMAN	HIST1H2BK	Histone H2B type 1-K	0	1.575	1.8375	4.64
P08107	HSP71_HUMAN	HSPA1B	Heat shock 70 kDa protein 1A/1B	0.6475	1.785	0.2975	0.6625
P34931	HSP71L_HUMAN	HSPA1L	Heat shock 70 kDa protein 1-like	1	1.55	0.8	1.5
P17066	HSP76_HUMAN	HSPA6	Heat shock 70 kDa protein 6	0.6475	1.44	0.2975	0.6625
P04792	HSPB1_HUMAN	HSPB1	Heat shock protein beta-1	0.9775	2.535	0.715	1.0075
Q14164	IKKE_HUMAN	IKBK	Inhibitor of nuclear factor kappa-B kinase subunit epsilon	0	2.2425	0	0
Q13418	ILK_HUMAN	ILK	Integrin-linked protein kinase	40.32	0.15	0	0
O15357-1	SHIP2_HUMAN	INPPL1	Phosphatidylinositol-3,4,5-trisphosphate 5-phosphatase 2	0.49	0.48	0	0
Q9NWZ3	IRAK4_HUMAN	IRAK4	Interleukin-1 receptor-associated kinase 4	0.0375	3.12	0	0
P06239-1	LCK_HUMAN	LCK	Tyrosine-protein kinase Lck	76.0225	54.795	21.06	0.715
P07195	LDHB_HUMAN	LDHB	L-lactate dehydrogenase B chain	0	1.24	0.03	0
P53671-1	LIMK2_HUMAN	LIMK2	LIM domain kinase 2	0.945	0	0	0
P48059	LIMS1_HUMAN	LIMS1	LIM and senescent cell antigen-like-containing domain protein 1	28.8	0.04	0	0
Q72417-1	LIMS2_HUMAN	LIMS2	LIM and senescent cell antigen-like-containing domain protein 2	5.875	0	0	0
P07948-2	LYN_HUMAN	LYN	Tyrosine-protein kinase Lyn	212.3875	182.8575	25.0575	3.7525
Q02750	MAP2K1_HUMAN	MAP2K1	Dual specificity mitogen-activated protein kinase kinase 1	0	59.5725	0	0
P36507	MAP2K2_HUMAN	MAP2K2	Dual specificity mitogen-activated protein kinase kinase 2	0	78.21	0	0
Q13163-1	MAP2K5_HUMAN	MAP2K5	Dual specificity mitogen-activated protein kinase kinase 5	0	0.9425	0	0
Q13223	MAP3K1_HUMAN	MAP3K1	Mitogen-activated protein kinase kinase kinase 1	0	1.38	0	0
Q9Y2U5	MAP3K2_HUMAN	MAP3K2	Mitogen-activated protein kinase kinase kinase 2	0.7	19.955	0	0
Q99759-1	MAP3K3_HUMAN	MAP3K3	Mitogen-activated protein kinase kinase kinase 3	0.45	6.76	0	0
Q92918	MAP4K1_HUMAN	MAP4K1	Mitogen-activated protein kinase kinase kinase kinase 1	0	4.68	0	0
Q12851	MAP4K2_HUMAN	MAP4K2	Mitogen-activated protein kinase kinase kinase kinase 2	0	24.5	0	0
Q8IVH8-1	MAP4K3_HUMAN	MAP4K3	Mitogen-activated protein kinase kinase kinase kinase 3	0	0.1	0	0
O95819-1	MAP4K4_HUMAN	MAP4K4	Mitogen-activated protein kinase kinase kinase kinase 4	0	0.35	0	0
Q9Y4K4	MAP4K5_HUMAN	MAP4K5	Mitogen-activated protein kinase kinase kinase kinase 5	4	31.7625	0	0
P53779-1	MAPK10_HUMAN	MAPK10	Mitogen-activated protein kinase 10	0	0	3.29	13.5
Q16539-1	MAPK14_HUMAN	MAPK14	Mitogen-activated protein kinase 14	37.56	0	78.6675	76.8
P45983-3	MAPK8_HUMAN	MAPK8	Mitogen-activated protein kinase 8	0	0	5.58	55.3
P45984-1	MAPK9_HUMAN	MAPK9	Mitogen-activated protein kinase 9	0	0	13.98	45.6875
P49137-1	MAPK2_HUMAN	MAPKAP2	MAP kinase-activated protein kinase 2	0	0	0.06	0
Q16644	MAPK3_HUMAN	MAPKAP3	MAP kinase-activated protein kinase 3	0	0	3.3925	0.275
Q9NYL2-2	MLTK_HUMAN	MLTK	Mitogen-activated protein kinase kinase kinase MLT	18.81	20.8	36.9075	21.6
Q9P289	MST4_HUMAN	MST4	Serine/threonine-protein kinase MST4	0	2.55	0	0
P60660-1	MYL6_HUMAN	MYL6	Myosin light polypeptide 6	0	0	0.45	0.15
P16083	NQO2_HUMAN	NQO2	Ribosylidihydroxynicotinamide dehydrogenase [quinone]	0	0	1.0625	0
Q9UKK9	NUDT5_HUMAN	NUDT5	ADP-sugar pyrophosphatase	3.2625	0	0	0
Q9NWQ8	PAG1_HUMAN	PAG1	Phosphoprotein associated with glycosphingolipid-enriched microdomains 1	2.405	0.22	0	0
Q9HBI0-1	PARVG_HUMAN	PARVG	Gamma-parvin	51.92	1.3175	0	0
Q9BUL8	PDC10_HUMAN	PDCD10	Programmed cell death protein 10	0	0.6875	0	0
P09619	PGFRB_HUMAN	PDGFRB	Beta-type platelet-derived growth factor receptor	8.04	0	0	0
Q99640	PMY1_HUMAN	PKMYT1	Membrane-associated tyrosine- and threonine-specific cdc2-inhibitory kinase	4.03	5.58	0	0
Q06203	PURI_HUMAN	PPAT	Amidophosphoribosyltransferase	16.96	0	0	0
P23284	PPIB_HUMAN	PPIB	Peptidyl-prolyl cis-trans isomerase B	0.045	0.405	1.35	0.69
Q13131-1	PRKA1_HUMAN	PRKA1	5'-AMP-activated protein kinase catalytic subunit alpha-1	0	4.23	0	0
Q05397-1	FAK1_HUMAN	PTK2	Focal adhesion kinase 1	0	8.4575	0	0
Q14289-2	FAK2_HUMAN	PTK2B	Protein-tyrosine kinase 2-beta	0	6.93	16.125	1.82
O43353-1	RIPK2_HUMAN	RIPK2	Receptor-interacting serine/threonine-protein kinase 2	29.785	0	0	0
Q15404	RSU1_HUMAN	RSU1	Ras suppressor protein 1	54.52	0.5625	0	0
P31947-1	1433S_HUMAN	SFN	14-3-3 protein sigma	1.7775	1.62	0.495	0.03
Q86V5	SG223_HUMAN	SGK223	Tyrosine-protein kinase Sgk223	1.7875	0.2975	0	0
Q9H0K1	SIK2_HUMAN	SIK2	Serine/threonine-protein kinase SIK2	1.7625	0.55	0	0
Q9H2G2-1	SLK_HUMAN	SLK	STE20-like serine/threonine-protein kinase	0	5.58	0	0
P12931-1	SRC_HUMAN	SRC	Proto-oncogene tyrosine-protein kinase Src	9.4875	5.985	0	0
O94804	STK10_HUMAN	STK10	Serine/threonine-protein kinase 10	0	30.225	0	0
Q7RTN6-1	STRAA_HUMAN	STRADA	STE20-related kinase adapter protein alpha	0.03	0	0	0
P53999	TCP4_HUMAN	SUB1	Activated RNA polymerase II transcriptional coactivator p15	6.65	3.01	5.67	7.21
Q9UHD2	TBK1_HUMAN	TBK1	Serine/threonine-protein kinase TBK1	0	6.045	0	0
P42680	TEC_HUMAN	TEC	Tyrosine-protein kinase Tec	1.47	0	0	0
Q15569	TESK1_HUMAN	TESK1	Dual specificity testis-specific protein kinase 1	0.42	0	0	0
Q71U36	TBA1A_HUMAN	TUBA1A	Tubulin alpha-1A chain	19.3875	29.07	16.74	21.6975
P68363	TBA1B_HUMAN	TUBA1B	Tubulin alpha-1B chain	21.96	30.4	16.92	24.66
Q9BQE3	TBA1C_HUMAN	TUBA1C	Tubulin alpha-1C chain	19.47	29.26	16.74	23.85
P49411	EFTU_HUMAN	TUFM	Elongation factor Tu, mitochondrial	0	0.675	0	0
P29597	TYK2_HUMAN	TYK2	Non-receptor tyrosine-protein kinase TYK2	0.02	0	0	0
Q8TF42	UB53B_HUMAN	UBASH3B	Ubiquitin-associated and SH3 domain-containing protein B	0.55	0.1575	0	0
Q6PHR2-1	ULK3_HUMAN	ULK3	Serine/threonine-protein kinase ULK3	0	7.9825	0	0
Q13432-1	U119A_HUMAN	UNC119	Protein unc-119 homolog A	1.5	1.92	0.7	0
P07947	YES_HUMAN	YES1	Proto-oncogene tyrosine-protein kinase Yes	22.815	10.3125	0.24	0
P31946-1	1433B_HUMAN	YWHA8	14-3-3 protein beta/alpha	8.4975	10.01	1.75	0.035
P62258	1433E_HUMAN	YWHA8	14-3-3 protein epsilon	10.44	11.7	5.28	0.4375
P61981	1433G_HUMAN	YWHA8	14-3-3 protein gamma	18.815	16.56	5.3475	1.2
Q04917	1433F_HUMAN	YWHA8	14-3-3 protein eta	4.5125	4.4175	2.2875	0.035
P27348	1433T_HUMAN	YWHAQ	14-3-3 protein theta	9.9	9.72	3.78	0.1925
P63104	1433Z_HUMAN	YWHAZ	14-3-3 protein zeta/delta	26.04	29.37	6.545	2.21

AC	ID	Gene_symbol	Descr	Dasatinib score	Bosutinib score	Bafetinib score	Nilotinib score
Q2M2I8	AAK1_HUMAN	AAK1	AP2-associated protein kinase 1	0	42.352	0	0
P42684-1	ABL2_HUMAN	ABL2	Tyrosine-protein kinase ABL2	4.424	1.0242	0.11	0
P60709	ACTB_HUMAN	ACTB	Actin, cytoplasmic 1	5.1875	3.024	3.08	3.3
P68032	ACTC_HUMAN	ACTC1	Actin, alpha cardiac muscle 1	2.655	1.3325	1.182	1.54
P55263-1	ADK_HUMAN	ADK	Adenosine kinase	12.69	1.405	0	0
O95782-1	AP2A1_HUMAN	AP2A1	AP-2 complex subunit alpha-1	0	4.0964	0	0
O94973-1	AP2A2_HUMAN	AP2A2	AP-2 complex subunit alpha-2	0	0.46	0	0
P63010-1	AP2B1_HUMAN	AP2B1	AP-2 complex subunit beta	0	0.9408	0	0
Q96CW1-1	AP2M1_HUMAN	AP2M1	AP-2 complex subunit mu	0	0.3094	0	0
P53680-1	AP2S1_HUMAN	AP2S1	AP-2 complex subunit sigma	0	0.3406	0	0
bcrabl	bcrabl	BCR-ABL	BCR-ABL fusion protein	2.6	1.262	0.025	0
P51451	BLK_HUMAN	BLK	Tyrosine-protein kinase Blk	6.215	0.63	0	0
Q9NSY1-1	BMP2K_HUMAN	BMP2K	BMP-2-inducible protein kinase	0	9.6912	0	0
Q06187	BTK_HUMAN	BTK	Tyrosine-protein kinase BTK	256.725	151.335	0	0.15
Q8N160-1	ADCK3_HUMAN	CABC1	Chaperone activity of bc1 complex-like, mitochondrial	0.1908	0	0	0
Q13555-1	KCC2G_HUMAN	CAMK2G	Calcium/calmodulin-dependent protein kinase type II subunit gamma	0	8.025	0	0
Q14004-1	CDK13_HUMAN	CDK13	Cell division protein kinase 13	0.0262	0	0	0
Q07002-1	CDK18_HUMAN	CDK18	Cell division protein kinase 18	0.119	0	0	0
P50750-1	CDK9_HUMAN	CDK9	Cell division protein kinase 9	0	0	0	0.0434
O96017-1	CHK2_HUMAN	CHEK2	Serine/threonine-protein kinase Chk2	0	0.6048	0	0
Q16630-1	CPSF6_HUMAN	CPSF6	Cleavage and polyadenylation specificity factor subunit 6	1.032	0.7828	2.2	1.76
Q8N684-1	CPSF7_HUMAN	CPSF7	Cleavage and polyadenylation specificity factor subunit 7	0.35	0.05	0.04	0.212
P41240	CSK_HUMAN	CSK	Tyrosine-protein kinase CSK	21.115	5.1852	0	0.843
P27707	DCK_HUMAN	DCK	Deoxycytidine kinase	0	2.925	0	0
P59665	DEF1_HUMAN	DEFA1B	Neutrophil defensin 1	0	0.38	0	0
P54760	EPHB4_HUMAN	EPHB4	Ephrin type-B receptor 4	38.34	27.114	0	0
P22830	HEMH_HUMAN	FECH	Ferrochelatase, mitochondrial	2.0688	2.2475	0	8.3232
P16591	FER_HUMAN	FER	Tyrosine-protein kinase Fer	0	0.455	0	0
P07332	FES_HUMAN	FES	Tyrosine-protein kinase Fes/Fps	0	0.0186	0	0
Q8NFF5-1	FAD1_HUMAN	FLAD1	FAD synthase	0	0	0.4192	0
P36888	FLT3_HUMAN	FLT3	FL cytokine receptor	0.0424	0	0	0
P42685	FRK_HUMAN	FRK	Tyrosine-protein kinase FRK	0.225	0.0486	0	0
P06241-2	FYN_HUMAN	FYN	Tyrosine-protein kinase Fyn	10.295	5.076	0	0
O14976	GAK_HUMAN	GAK	Cyclin-G-associated kinase	2.38	15.0016	0	0
P14136-1	GFAP_HUMAN	GFAP	Glial fibrillary acidic protein	0.0648	0.4352	0.1448	0.12
P62993-1	GRB2_HUMAN	GRB2	Growth factor receptor-bound protein 2	0.98	0.9802	0	0
P08631-1	HCK_HUMAN	HCK	Tyrosine-protein kinase HCK	1.98	2.4408	0.1386	0
P08107	HSP71_HUMAN	HSPA1B	Heat shock 70 kDa protein 1A/1B	0.225	1.4625	0.194	0.5625
P34931	HSP71L_HUMAN	HSPA1L	Heat shock 70 kDa protein 1-like	0.6096	1.238	0.52	0.495
P17066	HSP76_HUMAN	HSPA6	Heat shock 70 kDa protein 6	0.225	0.9792	0.194	0.2925
Q14164	IKKE_HUMAN	IKBKE	Inhibitor of nuclear factor kappa-B kinase subunit epsilon	0	0.0375	0	0
Q13418	ILK_HUMAN	ILK	Integrin-linked protein kinase	23.679	0	0	0
Q9Y616	IRAK3_HUMAN	IRAK3	Interleukin-1 receptor-associated kinase 3	0.0434	0	0	0
Q9NWZ3	IRAK4_HUMAN	IRAK4	Interleukin-1 receptor-associated kinase 4	0.18	2.3184	0	0
P35968	VGFR2_HUMAN	KDR	Vascular endothelial growth factor receptor 2	0.0038	0	0	0
P06239-1	LCK_HUMAN	LCK	Tyrosine-protein kinase Lck	18.1368	13.28	0.72	0
P07195	LDHB_HUMAN	LDHB	L-lactate dehydrogenase B chain	0	0.1696	0	0
Q32P28-1	P3H1_HUMAN	LEPRE1	Prolyl 3-hydroxylase 1	0.3504	0.06	0.5742	0.3696
P53671-1	LIMK2_HUMAN	LIMK2	LIM domain kinase 2	0.0228	0	0	0
P48059	LIMS1_HUMAN	LIMS1	LIM and senescent cell antigen-like-containing domain protein 1	7.7128	0	0	0
Q9Y383-1	LC7L2_HUMAN	LUC7L2	Putative RNA-binding protein Luc7-like 2	1.05	0.9792	1	1.35
P07948-2	LYN_HUMAN	LYN	Tyrosine-protein kinase Lyn	107.328	83.3625	5.8146	0.0152
Q02750	MP2K1_HUMAN	MAP2K1	Dual specificity mitogen-activated protein kinase kinase 1	0	27.935	0	0
P36507	MP2K2_HUMAN	MAP2K2	Dual specificity mitogen-activated protein kinase kinase 2	0	38.6952	0	0
Q13163-1	MP2K5_HUMAN	MAP2K5	Dual specificity mitogen-activated protein kinase kinase 5	0	0.0228	0	0
Q13233	M3K1_HUMAN	MAP3K1	Mitogen-activated protein kinase kinase kinase 1	0	0.131	0	0
Q9Y2U5	M3K2_HUMAN	MAP3K2	Mitogen-activated protein kinase kinase kinase 2	0.21	8.8088	0	0
Q99759-1	M3K3_HUMAN	MAP3K3	Mitogen-activated protein kinase kinase kinase 3	0.0636	2.8125	0	0
Q92918	M4K1_HUMAN	MAP4K1	Mitogen-activated protein kinase kinase kinase kinase 1	0	0.9256	0	0
Q12851	M4K2_HUMAN	MAP4K2	Mitogen-activated protein kinase kinase kinase kinase 2	0	1.5808	0	0
O95819-1	M4K4_HUMAN	MAP4K4	Mitogen-activated protein kinase kinase kinase kinase 4	0	0.0375	0	0
Q9Y4K4	M4K5_HUMAN	MAP4K5	Mitogen-activated protein kinase kinase kinase kinase 5	2.1375	9.035	0	0
Q16539-1	MK14_HUMAN	MAPK14	Mitogen-activated protein kinase 14	33.8432	0.1504	29.9934	19.3704
P45983-3	MK08_HUMAN	MAPK8	Mitogen-activated protein kinase 8	0	0	0.2	13.0708
P45984-1	MK09_HUMAN	MAPK9	Mitogen-activated protein kinase 9	0	0	2.3544	11.767
Q16644	MAPK3_HUMAN	MAPKAP3	MAP kinase-activated protein kinase 3	0	0	0.0125	0
Q9NYL2-2	MLTK_HUMAN	MLTK	Mitogen-activated protein kinase kinase kinase MLT	13.6648	8.8776	12.5425	5.25
Q9P289	MST4_HUMAN	MST4	Serine/threonine-protein kinase MST4	0	0.9775	0	0
P35579-1	MYH9_HUMAN	MYH9	Myosin-9	2.2232	1.3325	3.5784	1.9125
O14950	ML12B_HUMAN	MYL12B	Myosin regulatory light chain 12B	0.48	0.78	1.38	0.57
Q6Z5R9	YJ005_HUMAN	NA	Uncharacterized protein FL45252	0	15.77	0	0
P16083	NQO2_HUMAN	NQO2	Ribosylidihydroxycotinamide dehydrogenase [quinone]	0	0	4.7275	2.5978
O43809	CPSF5_HUMAN	NUDT21	Cleavage and polyadenylation specificity factor subunit 5	44.928	47.203	55.497	46.41
Q9UKK9	NUDT5_HUMAN	NUDT5	ADP-sugar pyrophosphatase	7.0744	0	0	0
P13674-1	P4HA1_HUMAN	P4HA1	Prolyl 4-hydroxylase subunit alpha-1	1.55	1.52	3.915	2.6325
Q9HB10-1	PARVG_HUMAN	PARVG	Gamma-parvin	23.4866	1.5912	0	0
Q9BUL8	PDC10_HUMAN	PDCD10	Programmed cell death protein 10	0	0.855	0	0
P09619	PGFRB_HUMAN	PDGFRB	Beta-type platelet-derived growth factor receptor	19.845	0	0	0
Q99623	PHB2_HUMAN	PHB2	Prohibitin-2	4.0968	16.7024	5.1675	5.679
Q99640	PMYT1_HUMAN	PKMYT1	Membrane-associated tyrosine- and threonine-specific cdc2-inhibitory kinase	0.1932	1.6675	0	0
ASA3E0	POTEF_HUMAN	POTEF	POTE ankyrin domain family member F	0.51	0.3048	0.26	0.2048
Q06203	PUR1_HUMAN	PPAT	Amidophosphoribosyltransferase	16.314	0	0	0
Q13131-1	AAPK1_HUMAN	PRKAA1	5'-AMP-activated protein kinase catalytic subunit alpha-1	0	2.0688	0	0
Q05397-1	FAK1_HUMAN	PTK2	Focal adhesion kinase 1	0	0.36	0	0
Q14289-2	FAK2_HUMAN	PTK2B	Protein-tyrosine kinase 2-beta	0	5.265	4.7725	0.069
Q96D71-1	REPS1_HUMAN	REPS1	RalBP1-associated Eps domain-containing protein 1	0	0.4268	0	0
O43353-1	RIPK2_HUMAN	RIPK2	Receptor-interacting serine/threonine-protein kinase 2	5.8125	0	0	0
Q15404	RSU1_HUMAN	RSU1	Ras suppressor protein 1	30.535	0.2484	0	0
P31947-1	14335_HUMAN	SFN	14-3-3 protein sigma	0.3708	0.6975	0.0528	0
Q9H0K1	SIK2_HUMAN	SIK2	Serine/threonine-protein kinase SIK2	0.0372	0.005	0	0
Q9Y2K2-1	SIK3_HUMAN	SIK3	Serine/threonine-protein kinase SIK3	0.106	0	0	0
Q9H2G2-1	SLK_HUMAN	SLK	STE20-like serine/threonine-protein kinase	0	2.3856	0	0
P12931-1	SRC_HUMAN	SRC	Proto-oncogene tyrosine-protein kinase Src	4.68	2.3028	0	0
O94804	STK10_HUMAN	STK10	Serine/threonine-protein kinase 10	0	10.6375	0	0
Q9Y6E0-1	STK24_HUMAN	STK24	Serine/threonine-protein kinase 24	0	0.26	0	0
Q9UHD2	TBK1_HUMAN	TBK1	Serine/threonine-protein kinase TBK1	0	3.5088	0	0
P42680	TEC_HUMAN	TEC	Tyrosine-protein kinase Tec	8.7348	0	0	0
Q96553-1	TESK2_HUMAN	TESK2	Dual specificity testis-specific protein kinase 2	0.0828	0	0	0
P49411	EFTU_HUMAN	TUFM	Elongation factor Tu, mitochondrial	0	2.8875	0	0
P26368-1	U2AF2_HUMAN	U2AF2	Splicing factor U2AF 65 kDa subunit	1.36	1.5392	2.8864	2.576
Q6PHR2-1	ULK3_HUMAN	ULK3	Serine/threonine-protein kinase ULK3	0	1.155	0	0
Q13432-1	U119A_HUMAN	UNC119	Protein unc-119 homolog A	0.48	0.64	0	0
P07947	YES_HUMAN	YES1	Proto-oncogene tyrosine-protein kinase Yes	11.1302	4.5684	0	0
P31946-1	1433B_HUMAN	YWHAB	14-3-3 protein beta/alpha	1.05	2.0688	0.0616	0
P62258	1433E_HUMAN	YWHAE	14-3-3 protein epsilon	3.9928	7.6518	0.45	0.0875
P61981	1433G_HUMAN	YWHAG	14-3-3 protein gamma	3.4	5.3992	0.5792	0.1242
Q04917	1433F_HUMAN	YWHAH	14-3-3 protein eta	1.032	1.725	0.0616	0
P27348	1433T_HUMAN	YWHAQ	14-3-3 protein theta	2.2736	3.6828	0.3196	0.06
P63104	1433Z_HUMAN	YWHAZ	14-3-3 protein zeta/delta	4.165	9.5786	0.7875	0.315

Cell Line	IKZF1	CDKN2A	PAX5	C20orf94	RB1	MEF2C	EBF1	BTG1	DLEU2	FHIT	ETV6
BV-173	-5.28	-3.0816	0.1053	-0.047	0.0765	0.012	0.2693	0.0036	0.0765	0.1211	0.0182
Z-119	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
SUP-B15	-0.8345	-2.2783	-0.8556	-4.0348	0.0687	-0.0184	0.0457	-0.9328	0.0687	0.0612	0.0158

mRNA levels relative to ABL

Patient	BTK	LYN	ILK	TEC
1	6.68	3.61	4.40	0.51
2	6.44	1.35	6.77	0.39
3	5.15	1.86	11.67	0.24
4	11.55	6.63	5.48	1.51
5	8.22	1.57	17.98	0.37
6	5.37	3.42	8.83	0.25

mRNA levels relative to ABL

Cell Line	BTK	LYN	ILK	TEC
BV-173	1.57	1.24	0.45	0.01
Z-119	11.52	7.74	2.85	0.42
SUP-B15	3.52	1.03	2.55	0.17