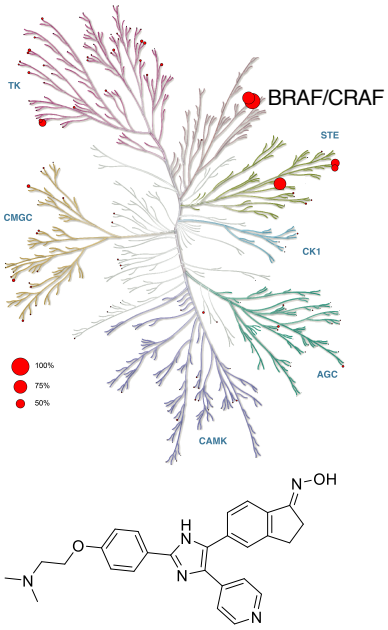
A

UNC10112687



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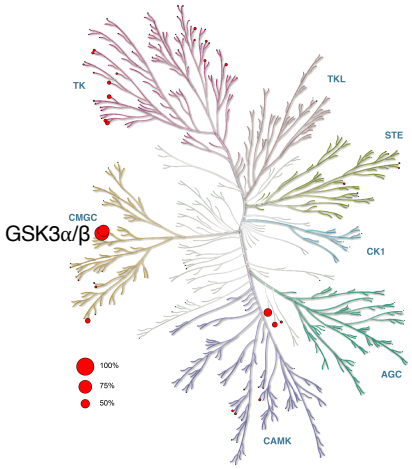

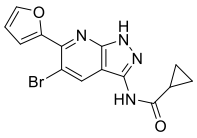

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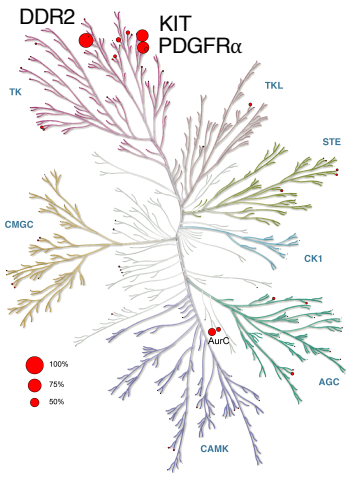
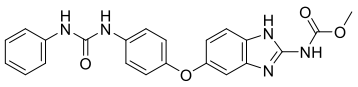
UNC10112731





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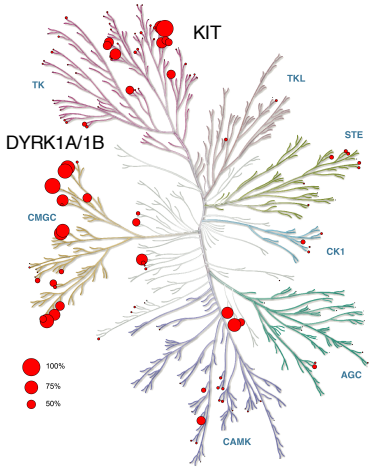
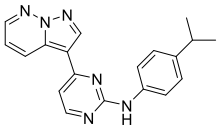
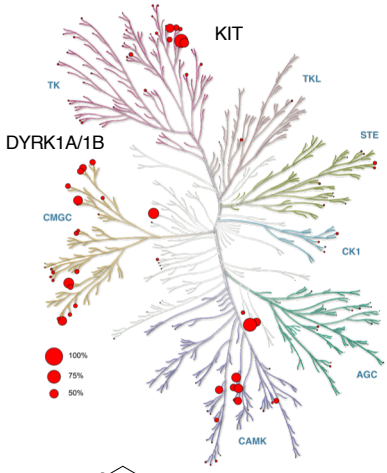
UNC10112785

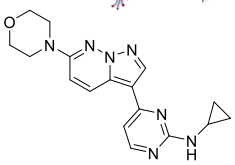




E

UNC10112849





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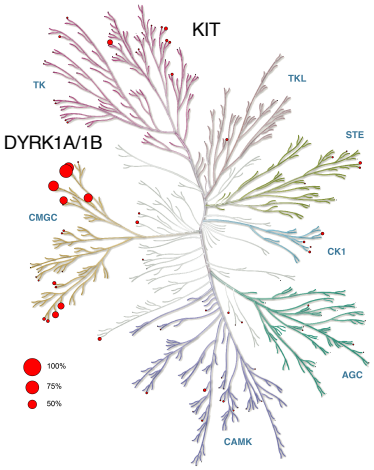
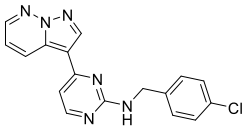




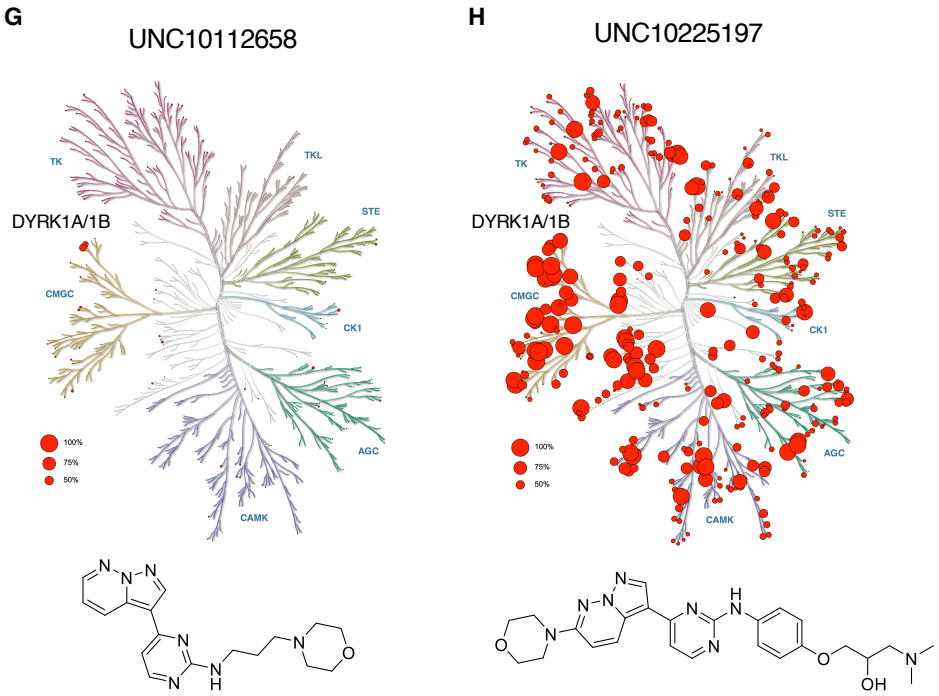
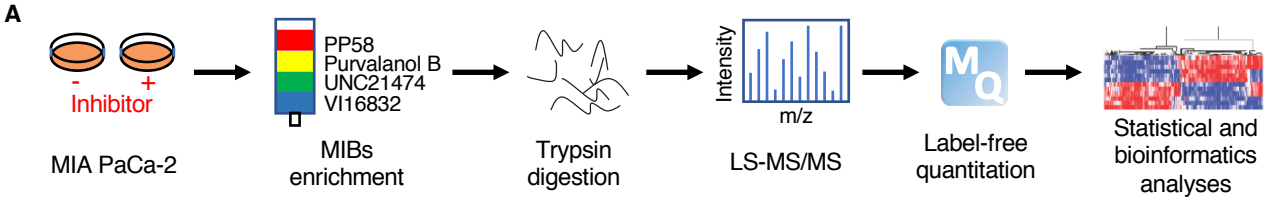
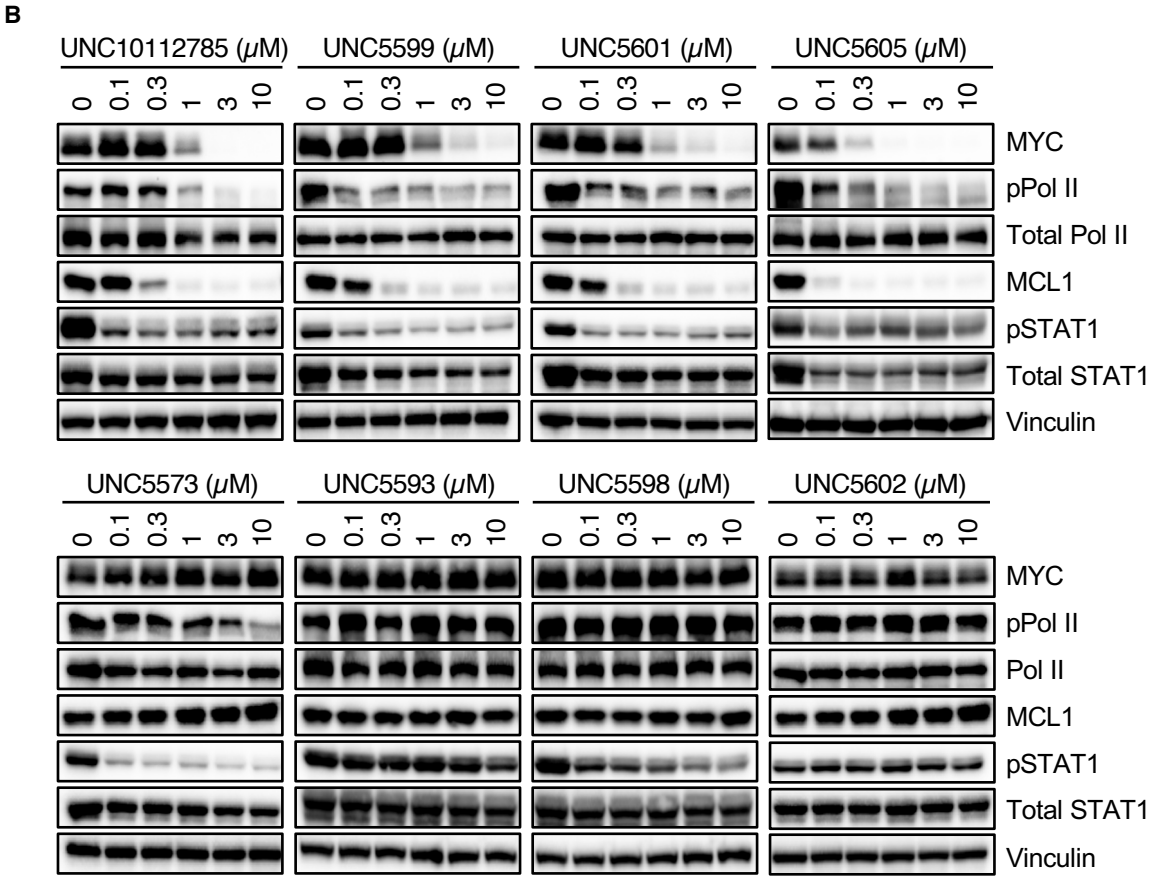
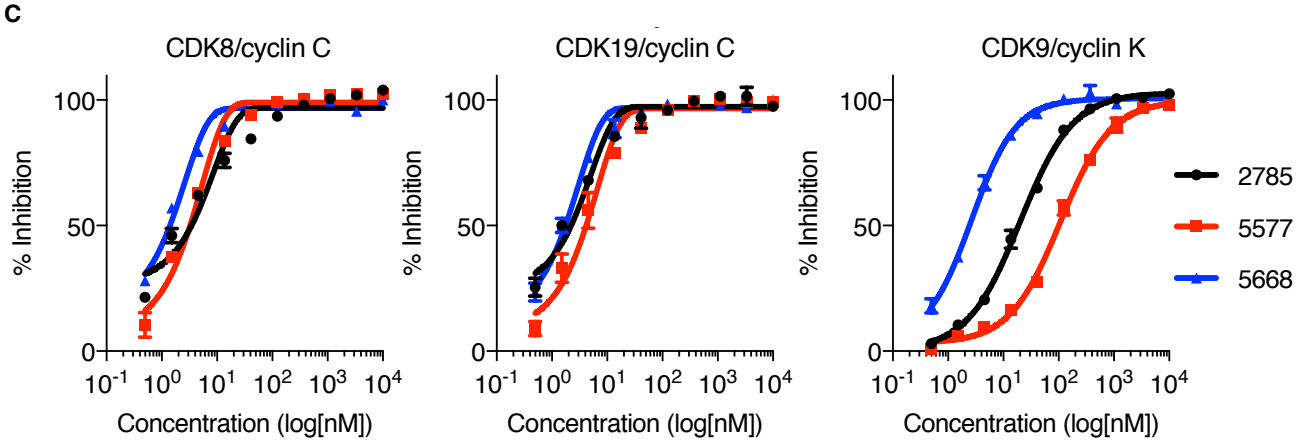


Fig. S1. Kinase specificity of compounds identified in the GPS-MYC screen. (A-H) Tree diagrams showing specificity and potency of compounds were generated by KinMap (*1*) utilizing published specificity data (*2,3*). Structures of compounds are shown.

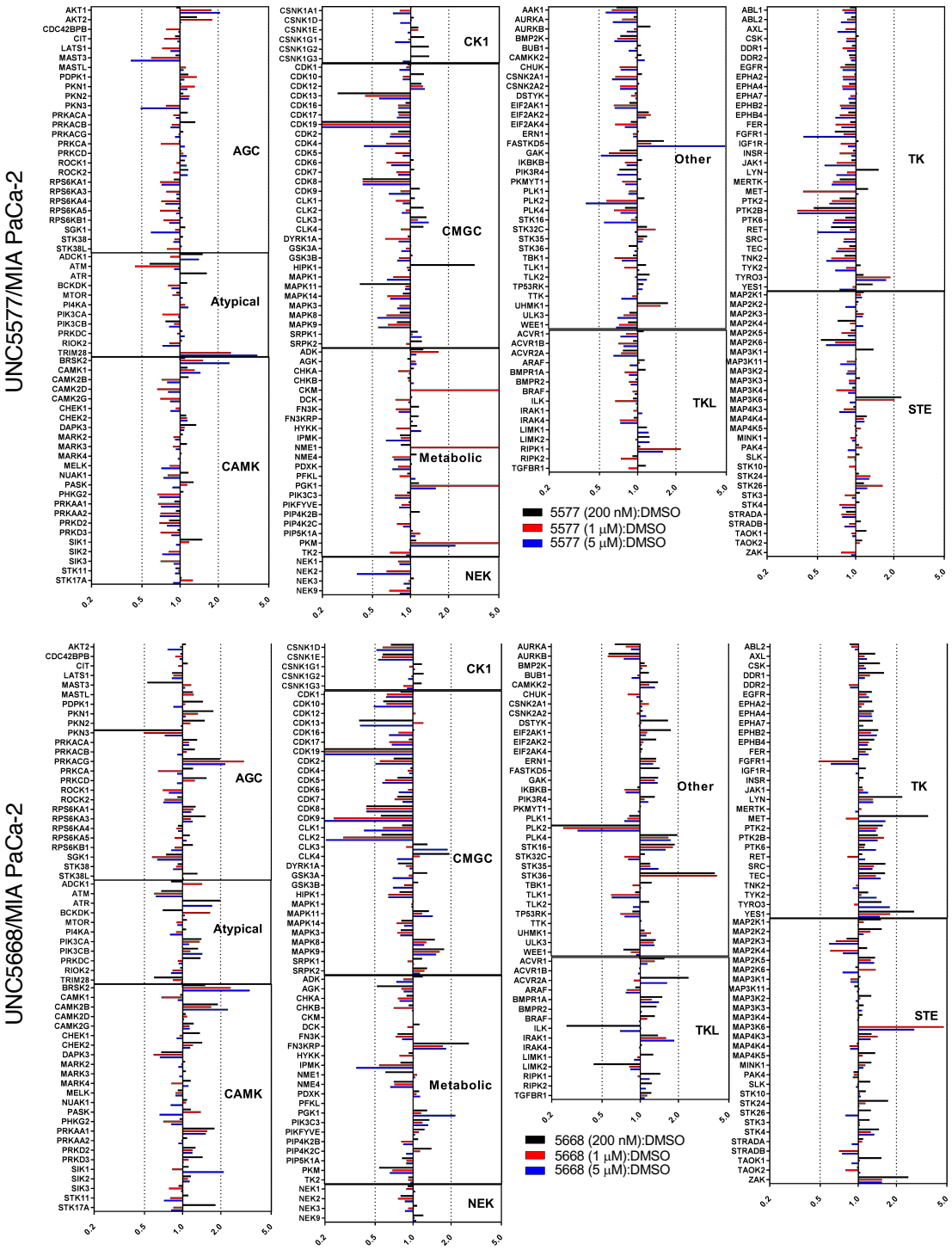






IC_{50} (nM)	UNC10112785	UNC5577	UNC5668
CDK8/cyclin C	2.67	2.89	0.793
CDK19/cyclin C	1.05	2.32	1.33
CDK9/cyclin K	19.9	105	2.65

D


UNC5577/MIA PaCa-2
UNC5668/MIA PaCa-2
AGC
Atypical
CAMK
CK1
CMGC
Metabolic
NEK
Other
TKL
TK
STE
5577 (200 nM):DMSO
5577 (1 μM):DMSO
5577 (5 μM):DMSO
5668 (200 nM):DMSO
5668 (1 μM):DMSO
5668 (5 μM):DMSO

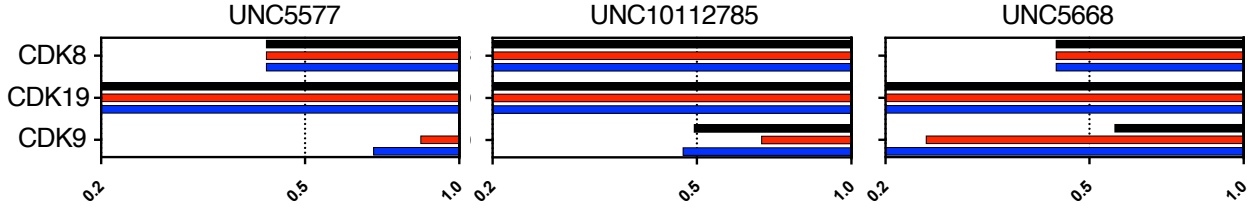

UNC5577
UNC10112785
UNC5668
CDK8
CDK19
CDK9

Fig. S2. CDK9 inhibition and not CDK8/19 inhibition is responsible for MYC loss caused by UNC10112785A. (A) Workflow of MIB-MS analysis to profile the substrate specificity of protein kinase inhibitors. Total cell lysates were prepared from MIA PaCa-2 cells were treated with vehicle control or the indicated compound for 1 hour, then subjected to affinity capture of endogenous kinases, followed by quantitative mass spectrometry to measure kinome activity profiles. (B) MIA PaCa-2 cells were treated with the indicated compounds for 6 h and CDK8/19 and CDK9 inhibition was measured by pSTAT1 and pPol II, respectively. Immunoblot from cells treated with UNC10112785 are from Figure 5D. All blots are representative of at least three independent experiments. (C) In vitro kinase activity (LanthaScreen) assays were performed using recombinant the indicated kinases and compounds and IC_{50} values were calculated (lower panel). Data were calculated from at least three independent experiments. (D) Boxplots of MIB/MS analysis data (log2 LFQ) for MIA PaCa-2 cells treated with UNC5577 (upper panel) or UNC5668 (middle panel), with enlargement of data for CDK8/19 and CDK9 indicated in lower panel. Data is from one experiment. Data for UNC10112785 are from Fig. 5A.

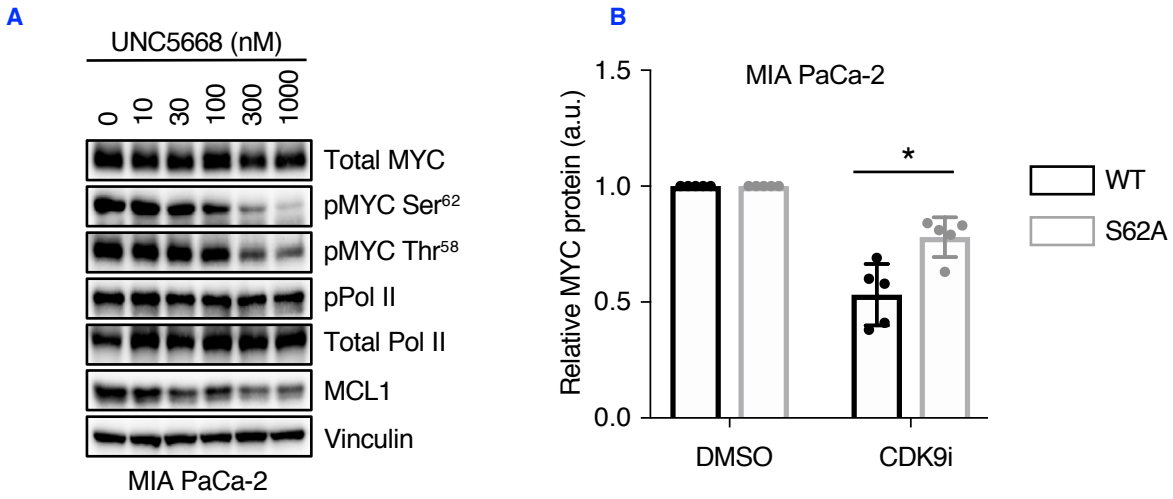
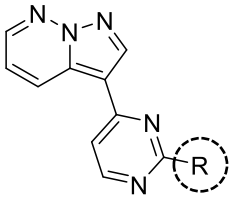
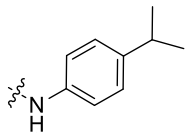
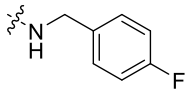
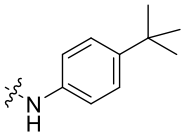
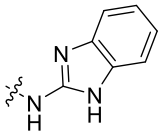
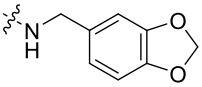
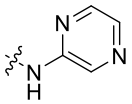
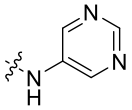
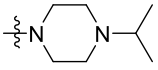
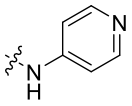
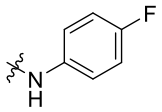


Fig. S3. UNC5668 regulation of MYC expression involves Ser[62] (A) MIA PaCa2 cells were treated with UNC5668 for 30 minutes and protein levels were measured by immunoblotting for the indicated proteins. Blots are representative of two independent experiments. (B) MIA PaCa2 cells stably expressing MYC proteins were treated with UNC5668 (CDK9i) for 2 hours and MYC levels were measured by immunoblotting for the indicated proteins (Fig. 6F). HA-MYC levels were measured by densitometry and normalized to vinculin levels. Blots are representative of five independent experiments.

REFERENCES

1. S. Eid, S. Turk, A. Volkamer, F. Rippmann, S. Fulle, KinMap: a web-based tool for interactive navigation through human kinome data. *BMC Bioinformatics* **18**, 16 (2017).
2. J. M. Elkins *et al.*, Comprehensive characterization of the Published Kinase Inhibitor Set. *Nat Biotechnol* **34**, 95-103 (2016).
3. D. H. Drewry, T. M. Willson, W. J. Zuercher, Seeding collaborations to advance kinase science with the GSK Published Kinase Inhibitor Set (PKIS). *Curr Top Med Chem* **14**, 340-342 (2014).

Table S2. Structure and cellular activity of UNC10112785 analogs

Compound		Cellular activity (MIA PaCa-2)[a]		
		MYC	CDK8/19 (pSTAT1)	CDK9 (pPol II)
UNC10112785		+	++	++
UNC5573		–	++	+
UNC5577		–	++	–
UNC5593		–	+	–
UNC5598		–	++	–
UNC5599		++	++	++
UNC5601		++	++	++
UNC5602		–	–	–
UNC5605		++	++	++
UNC5668		++	++	++

[a] – No activity; + > 1 μM; ++ < 1 μM

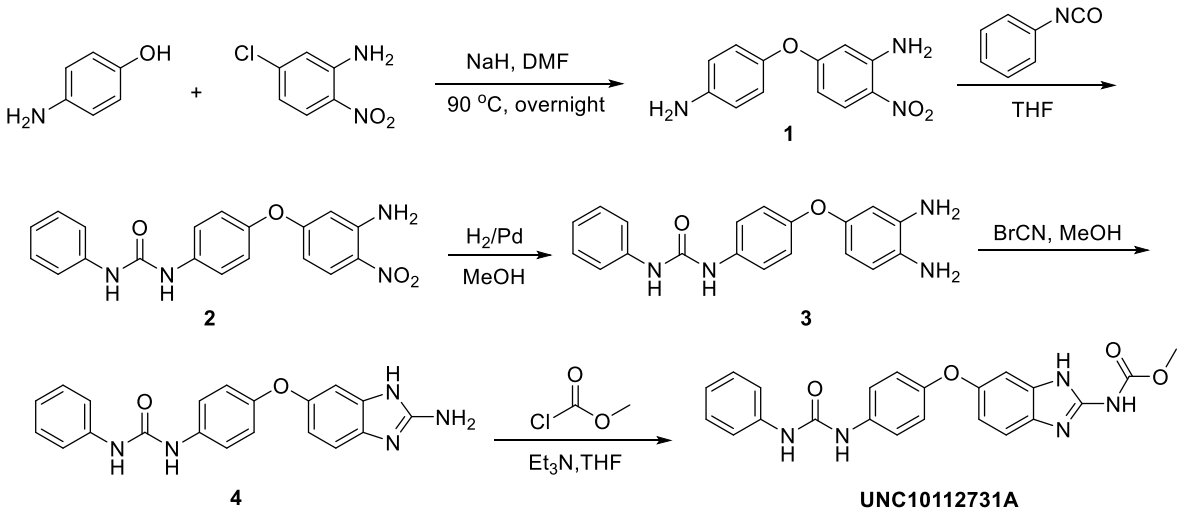
Synthesis of Analogues

Experimental:

All solvents and reagents were purchased from commercial suppliers and used without any further purification, unless stated otherwise. All dry reactions were carried out under nitrogen in oven-dried glassware with magnetic stirring using standard gaslight syringes, cannula and septa. Flash chromatography was carried out with pre-packed silica gel disposable columns. Preparative HPLC was performed with the UV detection at 220 or 254 nm. Samples were injected onto a 75 x 30 mm, 5 μM, C18(2) column at room temperature. The flow rate was 30 mL/min. Various linear gradients were used with A being H_2O + 0.1% TFA and B being CH_3CN. Analytical thin-layer chromatography (TLC) was performed with silica gel 60 F_{254}, 0.25 mm pre-coated TLC plates. TLC plates were visualized using UV_{254} and iodine. Microwave reaction was carried out using a CEM Discover-S reactor with a vertically-focused IR external temperature sensor and an Explorer 72 auto-sampler. The dynamic mode was used to set up the desired temperature and hold time with the following fixed parameters: Pre Stirring, 1 min; Pressure, 200 psi; Power, 200 W; PowerMax, off; Stirring, high. All ^1H NMR spectra were obtained with a 400 MHz spectrometer using $CDCl_3$ (7.26 ppm), DMSO-d_6 (2.50 ppm), or CD_3OD (2.05 ppm) as an internal reference. Signals are reported as m (multiplet), s (singlet), d (doublet), t (triplet), q (quartet), and brs (broad singlet); and coupling constants are reported in Hertz (Hz). LC-MS was performed using an analytical instrument with the UV detector set to 220 nm, 254 nm, and 280 nm, and a single quadrupole mass spectrometer using electrospray ionization (ESI) source. Samples were injected (2 μL) onto a 4.6 x 50 mm, 1.8 μM, C18 column

at room temperature. A linear gradient from 10% to 100% B (MeOH + 0.1% Acetic Acid) in 5.0 min was followed by pumping 100% B for another 2 or 4 minutes with A being H_2O + 0.1% acetic acid. The flow rate was 1.0 mL/min.

Synthesis of UNC10112731



5-(4-Aminophenoxy)-2-nitroaniline (**1**) A solution of 4-aminophenol (2.0 g, 18.0 mmol) in DMF (20 mL) was slowly added NaH (60% in mineral oil, 0.80 g, 20.0 mmol), followed by 5-chloro-2-nitroaniline (3.5 g, 20.0 mmol). The mixture was stirred at 90 °C overnight. The reaction mixture was poured into a saturated NH_4Cl solution. The formed solid was collected by filtration, washed with hexane, and dried to provide the title compound **1** (4.1 g, 92%) as a yellow solid.

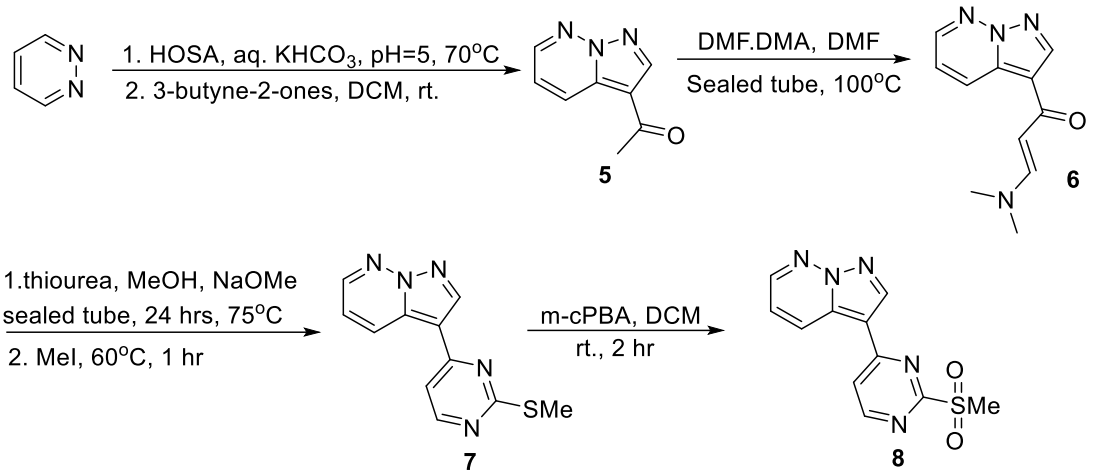
1-(4-(3-Amino-4-nitrophenoxy)phenyl)-3-phenylurea (**2**) A solution of **1** (2.0 g, 8.2 mmol) in THF (20 mL) was slowly added isocyanatobenzene (1.0 g, 8.4 mmol). The reaction mixture was stirred at 25 °C overnight, then was poured into a saturated NH_4Cl solution. The formed solid was collected by filtration, washed with hexane, and dried to provide the title compound **2** (2.64 g, 89%) as a yellow solid.

1-(4-(3,4-Diaminophenoxy)phenyl)-3-phenylurea (**3**) A solution of **2** (2.0 g, 5.5 mmol) in MeOH (60 mL) was added a 10% Pd/C (300 mg, 15 mmol%). The reaction mixture was stirred under hydrogen atmosphere at room temperature overnight, then passed through a pad of celite. The filtrate was concentrated under the reduced pressure. The residue was purified by column chromatography with pre-packed silica gel disposable column to yield the desired product **3** (1.5 g, 84%) as a yellow solid.

1-(4-((2-Amino-1*H*-benzo[d]imidazol-6-yl)oxy)phenyl)-3-phenylurea (**4**) A solution of **3** (1.5 g, 4.5 mmol) in MeOH (20 mL) was added cyanic bromide (0.62 g, 5.8 mmol). The reaction mixture was stirred at room temperature for 1 h and then quenched with a 2.0 M NaOH solution. The crude mixture was extracted with ethyl acetate (20 mL, 3x), dried ($MgSO_4$), and concentrated. The residue was purified by column chromatography with pre-packed silica gel disposable column to yield the desired product **4** (1.2 g, 74%) as a brown solid.

Methyl (6-(4-(3-phenylureido)phenoxy)-1*H*-benzo[d]imidazol-2-yl)carbamate (**UNC10112731**) A solution of **4** (295 mg, 0.82 mmol) in THF (20 mL) was added methyl carbonochloridate (155 mg, 164 mmol) and triethylamine (332 mg, 3.28 mmol). The reaction mixture was stirred at room temperature overnight, quenched with water, and extracted with EtOAc. The organic layer was dried ($MgSO_4$) and concentrated. The residue was purified by recrystallization in MeOH to provide the desired compound **UNC10112731** (247 mg, 72%) as an off-white solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 11.54 (s, 1H), 8.59 (s, 2H), 7.46 – 7.39 (m, 4H), 7.36 (d, J = 8.5 Hz, 1H), 7.30 – 7.24 (m, 2H), 7.02 – 6.88 (m, 5H), 6.78 (dd, J = 8.6, 2.4 Hz, 1H), 3.74 (s, 3H). LC-MS (ESI$^+$) for $[M+H]^+$ found *m/z* 418.10; HPLC: >95% purity.

Synthesis of 3-(2-(methylsulfonyl)pyrimidin-4-yl)pyrazolo[1,5-b]pyridazine



1-(Pyrazolo[1,5-*b*]pyridazin-3-yl)ethan-1-one (**5**) A solution of hydroxylamine-*O*-sulfonic acid (HOSA) (4.2 g, 37.1 mmol) was neutralized with 2.5 M potassium bicarbonate (~15 mL) to pH 5 and then was added pyridazine (4.0 g, 49.9 mmol) at 70 °C. The reaction mixture was stirred at 70 °C for 2 h. After cooling to room temperature, reaction mixture was neutralized to pH 8 using saturated sodium bicarbonate solution and then was added a solution of but-3-yn-2-one (1.0 g, 24.9 mmol) in dichloromethane (50 mL) followed by potassium hydroxide (2.6 g, 46.8 mmol). The reaction mixture was stirred at room temperature overnight and was extracted with dichloromethane (20mL, 3x). The combined organic layers were washed with brine, dried (Na_2SO_4), and concentrated. The residue was purified by column chromatography with pre-packed silica gel disposable column to yield the desired product **5** (1.0 g, 49%) as a brown solid. ^{1}HNMR (400 MHz, DMSO-d_6): 8.77 (s, 1H), 8.69 - 8.62 (m, 2H), 7.60 (m, 1H), 2.54 (s, 3H).

(*E*)-3-(Dimethylamino)-1-(pyrazolo[1,5-*b*]pyridazin-3-yl)prop-2-en-1-one (**6**) A solution of **5** (0.50 g, 3.1 mmol) in DMF (1.0 mL) in a sealed tube was added *N*,*N*-dimethylformamide-dimethyl acetals (DMF-DMA) (1.48 g, 12.4 mmol). The reaction mixture was heated at 100 °C overnight. Then the solvent was removed under vacuum. The residue was added ether and was

filtered. The solid was washed with ether (3x) to provide the title compound **6** (5.5 g, 82%) as a brown solid which was used without further purification.

3-(2-(Methylthio)pyrimidin-4-yl) pyrazolo[1,5-b]pyridazine (**7**) A solution of **6** (0.55 g, 2.54 mmol) in MeOH (3.0 mL) in a sealed tube was added thiourea (0.23 g 3.0 mmol) and sodium methoxide (0.83 g, 3.8 mmol). The resulting mixture was stirred at 70 ^{o}C for 18 hr. After cooling to room temperature, methyl iodide (0.36 g, 2.5 mmol) was added slowly. The resulting solution was heated at 60 ^{o}C for 1 hr. Then, the precipitate formed in reaction was filtered and washed with MeOH (3x) to provide the title compound **7** (0.60 g, 97%) as a pale yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.93 (s, 1H), 8.90 (dd, J = 9.1, 1.9 Hz, 1H), 8.62 (dd, J = 4.4, 1.9 Hz, 1H), 8.57 (d, J=4.9 Hz, 1H), 7.68 (d, J = 4.6 Hz, 1H), 7.50 (dd, J = 9.1, 4.5 Hz, 1H), 2.60 (s, 3H).

3-(2-(Methylsulfonyl)pyrimidin-4-yl)pyrazolo[1,5-*b*]pyridazine (**8**) A solution of **7** (0.23 g, 0.95 mmol) in CH_2Cl_2 (10 mL) was added meta-chloroperoxybenzoic acid (m-CPBA) (0.41 g 2.36 mmol). The reaction mixture was stirred at room temperature for 2 hr, then quenched with a saturated sodium sulfite solution (10 mL), extracted with CH_2Cl_2. The organic layer was washed with a saturated NaOH solution (10 mL) and brine, dried (Na_2SO_4), and concentrated to provide the title compound **8** (0.19 g, 73%) as a light yellow solid which was used without further purification.

***N*-(4-Isopropylphenyl)-4-(pyrazolo[1,5-*b*]pyridazin-3-yl)pyrimidin-2-amine** (**UNC10112785**) (General procedure A) A mixture of **8** (110 mg, 0.40 mmol) and 4-isopropylaniline (540 mg, 4.0 mmol, 10 equiv.) was heated at 120 °C for 30 minutes under microwave irradiation. After cooling to room temperature, methanol was added. The resulting solid was filtered and washed with methanol (3x) to afford the title compound **UNC10112785** (16 mg, 12%) as a yellow solid. ^{1}H NMR (400 MHz, CD_3OD) δ 8.88 (d, J = 8.4 Hz, 1H), 8.82 (s,

1H), 8.55 (dd, J = 4.5, 1.9 Hz, 1H), 8.22 (d, J = 6.1 Hz, 1H), 7.46 (d, J = 8.4 Hz, 2H), 7.43 – 7.31 (m, 4H), 3.05 – 2.92 (m, 1H), 1.31 (d, J = 6.9 Hz, 6H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 331.2; t_R = 5.845 min, LC-MS: >95% purity.

***N*-(4-Fluorobenzyl)-4-(pyrazolo[1,5-*b*]pyridazin-3-yl)pyrimidin-2-amine** (**UNC5573**) The title compound **UNC5573** (40 mg, 69%) was prepared as a white solid according to general procedure A from (4-fluorophenyl)methanamine (140 mg, 1.8 mmol, 10 equiv.) at 150 °C. ^{1}H NMR (400 MHz, CD_3OD) δ 8.88 (s, 1H), 8.60 (d, J=4.9 Hz, 2H), 8.22 (d, J=4.5 Hz, 1H), 7.50-7.45 (m, 4H), 7.12 (t, J=8.0 Hz, 2H), 4.85 (s, 2H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 322.0; t_R = 4.988 min, LC-MS: >95% purity.

***N*-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-4-(pyrazolo[1,5-*b*]pyridazin-3-yl)pyrimidin-2-amine** (**UNC5598**) The title compound **UNC5598** (10 mg, 16%) was prepared as a pale yellow solid according to general procedure A from benzo[*d*][1,3]dioxol-5-ylmethanamine (270 mg, 1.8 mmol) at 150 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.78 (s, 1H), 8.54 (d, J = 2.4 Hz, 1H), 8.28 (d, J=4.9 Hz, 1H), 7.70 (t, J = 6.2 Hz, 1H), 7.33 (brs, 1H), 7.12 (d, J= 7.9 Hz, 1H), 6.93 (s, 1H), 6.84 (s, 2H), 5.94 (s, 2H), 4.47 (d, J = 5.4 Hz, 2H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 347.0; t_R = 4.773 min, LC-MS: >95% purity.

***N*-(4-(Pyrazolo[1,5-*b*]pyridazin-3-yl)pyrimidin-2-yl)-1*H*-benzo[*d*]imidazol-2-amine (UNC5593)** The title compound **UNC5593** (13 mg, 22%) was prepared as a white solid according to general procedure A at 170 °C in *N*,*N*-dimethylacetamide (5.0 mL) from 1*H*-benzo[*d*]imidazol-2-amine (120 mg, 0.91 mmol). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.35 (s, 2H), 9.09 (s, 1H), 8.96 (d, *J* = 5.4 Hz, 1H), 8.88 (dd, *J* = 9.1, 1.8 Hz, 1H), 8.69 (dd, *J* = 4.5, 1.8 Hz, 1H), 8.27 (d, *J* = 7.9 Hz, 1H), 8.11 (d, *J* = 5.5 Hz, 1H), 7.55 (dd, *J* = 9.1, 4.5 Hz, 1H), 7.49 (d, *J*

= 7.5 Hz, 1H), 7.36 (dt, *J* = 21.1, 6.9 Hz, 2H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 329.2; t_R = 2.835 min, LC-MS: >95% purity.

***N*-(4-(*tert*-Butyl)phenyl)-4-(pyrazolo[1,5-*b*]pyridazin-3-yl)pyrimidin-2-amine** (**UNC5577**) The title compound **UNC5577** (72 mg, 29%) was prepared as a yellow solid according to general procedure A at 170 °C from 4-(*tert*-butyl)aniline (41 mg, 0.27 mmol). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.73 (s, 1H), 9.09 (d, *J* = 6.6 Hz, 1H), 8.93 (s, 1H), 8.63 (dd, *J* = 4.5, 1.9 Hz, 1H), 8.44 (d, *J* = 5.5 Hz, 1H), 7.61 (d, *J* = 8.6 Hz, 2H), 7.44 (dd, *J* = 9.0, 4.5 Hz, 1H), 7.39 (dt, *J* = 1.8, 1.4 Hz, 3H), 1.31 (s, 9H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 345.2; t_R = 5.558 min, LC-MS: >95% purity.

***N*-(4-Fluorophenyl)-4-(pyrazolo[1,5-*b*]pyridazin-3-yl)pyrimidin-2-amine** (**UNC5668**) (General procedure B) A solution of 4-fluoroaniline (30 mg, 0.27 mmol) in THF (10 mL) was added a 1.0 M solution of lithium bis(trimethylsilyl)amide (LiHMDS) in THF (0.73 mL, 4.0 equiv.) at -70 °C followed by slow addition of **8** (50 mg, 0.18 mmol). The reaction mixture was stirred at -70 °C. After complete conversion of **8**, the reaction mixture was quenched with water (10 mL), extracted with EtOAc, dried (Na_2SO_4), and concentrated. The residue was purified by an ISCO silica gel column to provide the title compound **UNC5668** (9.0 mg, 12%) as a light yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.71 (s, 1H), 9.08 (d, *J* = 9.0 Hz, 1H), 8.91 (s, 1H), 8.61 (d, *J* = 4.4 Hz, 1H), 8.44 (d, *J* = 5.3 Hz, 1H), 7.76–7.68 (m, 2H), 7.47 (dd, *J* = 9.1, 4.5 Hz, 1H), 7.38 (d, *J* = 5.4 Hz, 1H), 7.18 (t, *J* = 8.8 Hz, 2H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 307.1; t_R = 4.461 min, LC-MS: >95% purity.

***N*-(Pyrazin-2-yl)-4-(pyrazolo[1,5-*b*]pyridazin-3-yl)pyrimidin-2-amine** (**UNC5599**) The title compound **UNC5599** (8.0 mg, 13%) was prepared as a yellow solid according to general procedure B from pyrazin-2-amine (31 mg, 0.33 mmol). ^{1}H NMR (400 MHz, CD_3OD) δ 9.32 (d,

J= 8.0 Hz, 1H), 8.96 (s, 1H), 8.89 (s, 1H), 8.67 (dd, J = 4.5, 1.9 Hz, 1H), 8.53 (d, J= 8.1 Hz, 1H), 8.46-8.42 (m, 2H), 7.79 (d, J=8.3 Hz, 1H), 7.61 (dd, J = 9.1, 4.5 Hz, 1H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 291.0; t_R = 4.449 min, LC-MS: >95% purity.

4-(Pyrazolo[1,5-*b*]pyridazin-3-yl)-*N*-(pyrimidin-5-yl)pyrimidin-2-amine (**UNC5601**) The title compound **UNC5601** (7.0 mg, 13%) was prepared as a light yellow solid according to general procedure B from pyrimidin-5-amine (27 mg, 0.27 mmol). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.98 (s, 1H), 9.19 (s, 2H), 9.11 (d, *J* = 9.0 Hz, 1H), 8.91 (s, 1H), 8.80 (s, 1H), 8.64–8.60 (m, 1H), 8.53 (d, *J* = 5.3 Hz, 1H), 7.51–7.45 (m, 2H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 291.2; t_R = 3.049 min, LC-MS: >95% purity.

4-(Pyrazolo[1,5-*b*]pyridazin-3-yl)-*N*-(pyridin-4-yl)pyrimidin-2-amine (**UNC5605**) The title compound **UNC5605** (12 mg, 18%) was prepared as a yellow solid according to general procedure A from pyridin-4-amine (169 mg, 1.80 mmol). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.77 (s, 1H), 8.52 (s, 1H), 8.27 (d, J = 5.2 Hz, 1H), 7.77 (t, J = 6.2 Hz, 1H), 7.36 (d, J = 7.4 Hz, 1H), 7.30 (t, J = 7.6 Hz, 1H), 7.20 (t, J = 7.2 Hz, 1H), 7.11 (d, J = 5.2 Hz, 1H), 4.57 (d, J = 5.8 Hz, 2H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 290.0; t_R = 3.333 min, LC-MS: >95% purity.

3-(2-(4-Isopropylpiperazin-1-yl)pyrimidin-4-yl)pyrazolo[1,5-*b*]pyridazine (**UNC5602**) The title compound **UNC5602** (16 mg, 27%) was prepared as a yellow solid according to general procedure A from 1-isopropylpiperazine (246 mg, 1.8 mmol). ^{1}H NMR (400 MHz, CD_3OD) δ 8.94 (d, J=7.9 Hz, 1H), 8.79 (s, 1H), 8.56 (dd, J = 4.5, 1.9 Hz, 1H), 8.40 (d, J=8.4 Hz, 1H), 7.46 (dd, J = 9.1, 4.5 Hz, 1H), 7.36 (d, J=7.6 Hz, 1H), 5.01 (d, J=14.1 Hz, 2H), 3.70-3.62 (m, 4H), 3.53-3.46 (m, 2H), 3.28-3.26 (m, 1H), 1.44 (d, J = 6.7 Hz, 6H). LC-MS (ESI+) for $[M+H]^+$ found *m/z* 324.0; t_R = 3.143 min, LC-MS: >95% purity.