Enabling Synthesis in Fragment-based Drug Discovery (FBDD): Microscale High-throughput Optimisation of the Medicinal Chemist's Toolbox Reactions

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General Experimental Information

Millimolar scale reactions carried out in Analytical Sales 96 well Para-dox® Aluminium Reaction Blocks with 1 mL glass vials containing stirrer bars. Reactions were performed with exclusion of air, unless otherwise stated. This was achieved by using solvent that had been sparged with N_2 for 15 mins and by purging the headspace of the reaction vial with a positive pressure of N_2 and an outlet needle. Commercial solvents and reagents were used without further purification.

Flash column chromatography was performed on a Biotage SP1 system; normal-phase chromatography performed with silica Sfar columns (32−63 µm particle size, KP-Sil, 60 Å pore size) and the stated solvent system (n.b. Petrol refers to Petroleum Ether bp 40–60 ˚C).

MISER Acquisition: Reversed phase HPLC experiments were performed on an Agilent 1290 Infinity II system. The Agilent stack was comprised a G7120A high speed pump, G7167B multisampler, G7116B multicolumn thermostat, G7117B diode array detector and a 6135 Quadrupole LC/MSD XT detector with multimode ionization. The system was controlled by OpenLab CDS Chemstation Edition software, with the FIA mode enabled. Separations were carried out on a 2.0 mm i.d. by 30 mm length, 1.9 µm YMC-Triart C18 column by isocratic elution at a flow rate of 1.5 mL/min. The LC eluents were 16% solvent A (10 mM ammonium acetate in H_2O, pH 6.8) and 84% solvent B (acetonitrile). The column was maintained at a temperature of 40 °C. The MISERgrams were obtained from continuous sample injections (0.5 µL) every 12.5s. The multimode ESI+APCI parameters were fragmentor 60 V, desolvation gas (N2) temperature 350 °C and flow rate 12 L/min, vaporizer temperature 250 °C, the nebulizer was adjusted to 35 psi, the capillary voltage to 3000 V and the corona current to 1µA.

Batch reactions were monitored by LC-MS using an Agilent 1290 Infinity II series UHPLC coupled to an Agilent 6130 single quadrupole mass detector, eluting a gradient of 3-95% (MeCN in H_2O, 0.1% HCO_2H modifier) over 0.93 minutes run on a YMC-Triart C18 50x2.0mm 1.9µm column controlled at 40 °C, or a Shimadzu Nexera UHPLC coupled to a Shimadzu LCMS-2020 single quadrupole mass detector. High resolution mass spectrometry was performed on an Agilent 6550 QTOF mass spectrometer.

NMR spectra were recorded on a Bruker AV400 (Avance 400 MHz) spectrometer. Chemical shifts for ^{1}H and ^{13}C NMR spectra are reported as δ in units of parts per million (ppm) and quoted to the nearest 0.01 ppm relative to the residual protons in $CDCl_3$ (7.26 ppm, 77.16 ppm), d_6-DMSO (2.50 ppm, 39.52 ppm) or CD_3OD (3.31 ppm, 49.00 ppm). Coupling constants (J) are quoted in Hertz (Hz) and are reported to the nearest 0.1 Hz, with multiplicity reported according to the following convention: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad and associated combinations e.g., dd = double of doublets. DEPT 135 and 2-dimensional experiments (COSY, HMBC, HSQC and ROESY) were used to support assignments and are reported where appropriate.

Equipment used in this study

Chronect Quantos, Mettler-Toledo balance and dosing heads

All solid dosing was achieved using the Chronect Quantos platform from Axel Semrau. The platform utilises a Mettler-Toledo balance system coupled with a Universal Robots UR3 cobot, which is a 6-axis robotic arm capable of transporting vials, dosing heads and balance adaptors. Up to 32 solids may be stored in dosing heads which are held in a rack at the back of the platform and all data pertaining to the solids is stored in an RFID tag which can be read by the balance. Finally, the Chronect Quantos is equipped with a three-position deck capable of holding the analytical sales Para-dox aluminium reaction blocks.

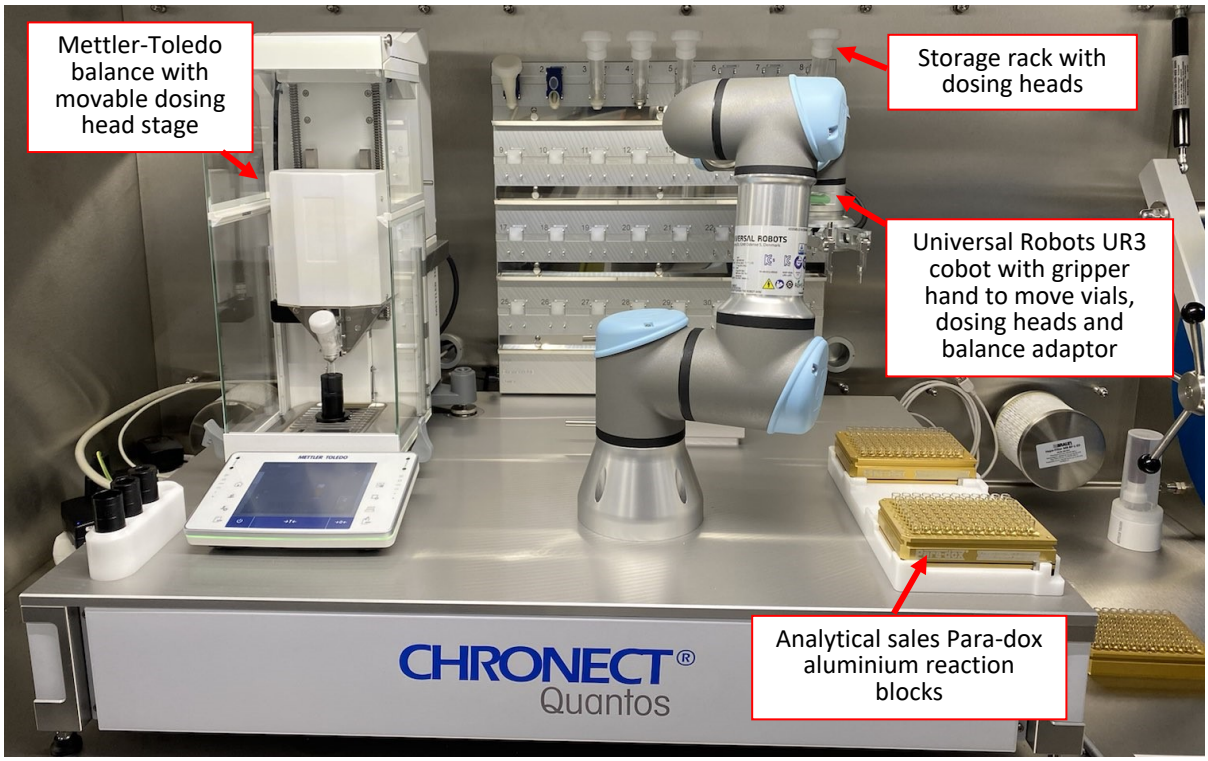


Figure S1: A photograph of our Chronect Quantos platform, with all the components highlighted, featuring a Mettler-Toledo balance, Universal Robots UR3 and analytical sales Para-dox aluminium reaction blocks.

There are several commercially available dosing heads available to purchase through Mettler-Toledo. The three investigated in this work for their combability with our Chronect Quantos and ChemBead selection can be seen below (figure S2). The so called 'normal' dosing head (QH012-LNMW) is a standard dosing head for up to 125 mL of material with a 2.5 mm dosing pin diameter. The antistatic dosing head (QH010-CNMW) is a standard dosing head with a 2.5 mm dosing pin diameter. The final dosing head investigated is a 'Pinocchio' dosing head (QH008-BNMP), so called as it has a 1mm nose which extends into the top of the vial while the substance is dispensed. This dosing head also has a 2.5 mm dosing pin diameter.

Table S1: The components, suppliers and serial numbers required to assemble the screening kits.

Supplier	Component	Serial number
Analytical Sales	96-Well Parallel Synthesis/Optimization Block Assembly	96960
	Replacement PFA Films for 96-Well Blocks	96967
	Replacement Rubber Mats for 96-Well Block Assemblies	96965
	Stackable Tray with 8x30 Shell Vials	884001
	Stir Bars for Photoredox & Parallel Synthesis (gold) Block Systems	13258
Thistle Scientific (formally VP Scientific)	Drop Dispenser, for VP 711 series Tumble Stir Elements	VPS-VP711A-96-AS-1
Sigma-Aldrich	Glass beads, acid-washed, ≤106 µm (−140 U.S. sieve)	G4649
	Glass beads, acid-washed, 150-212 µm (70-100 U.S. sieve)	G1145

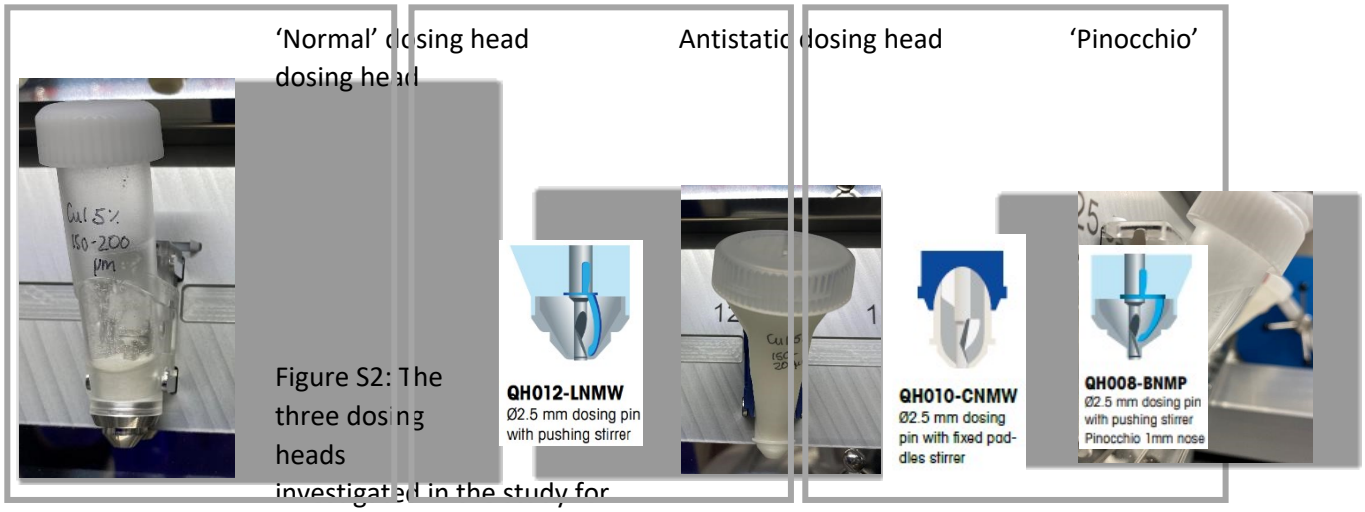


Figure S2: The three dosing heads investigated in the study for their compatibility with our Chronect Quantos and chembead selection. The dosing heads include the 'normal' dosing head (QH012-LNMW), antistatic dosing head (QH010-CNMW) and the 'Pinocchio' dosing head (QH008-BNMP).

Aluminium reaction blocks, glass vials, stir bars and stir bar dispenser

The consumable components for the screening kits can be seen below (figure S3). Analytical sales Para-dox blocks are loaded with 1 mL glass vials (884001). Stir bars (13258) are loaded into every vial using a Drop Dispenser (VPS-VP711A-96-AS-1). Finally, two rubber mats and a new PFA film are added to the lid. A table of the components, suppliers and serial numbers can be found below.

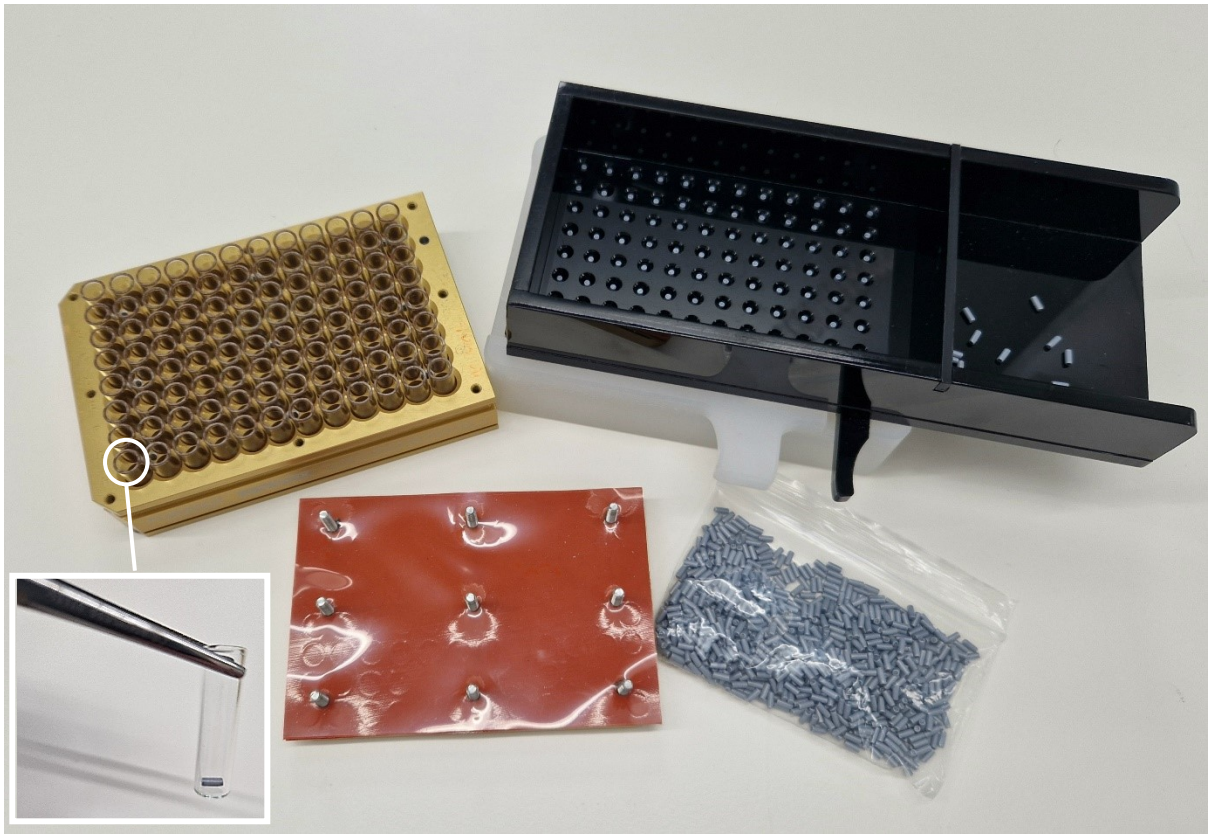


Figure S3: The consumable components used to facilitate the production of the screening kits. An Analytical sales Para-dox plate loaded with 1 mL glass vials containing a stir bar and the lid with a new PFA film in place.

Validation work for screening kits

Selection of glass bead size

Multiple glass bead sizes were available from Sigma, we investigated 150-212 µm (G1145) and ≤106 µm (G4649) in two types of dosing head to start with, the 'normal' dosing head (QH012-LNMW) and the antistatic dosing head (QH010-CNMW). Initially, when coated in a test substrate (Copper Iodide) it appears the smaller glass beads are generally dosed more accurately (figure S4).

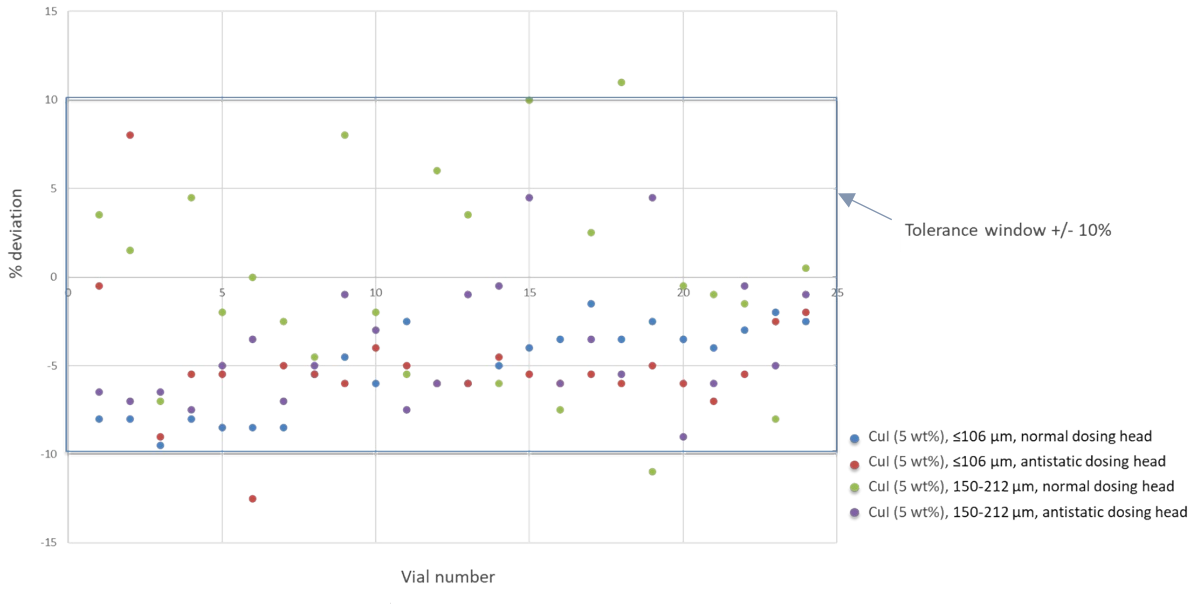


Figure S4: Dosing test to assess the suitability of CuI-ChemBeads, with a 1 mg target weight per dose. Here the percentage deviation (the % over the target dose) is plotted for every vial dosed. Each combination was dosed into 24 (two rows) of glass vials. The blue box denotes the pre-set tolerance window (+/- 10%) on the Chronect Chronos software. Even on a small scale, dosing is constant and largely within the window of +/-10% deviation.

Dosing accuracy inorganic bases

Inorganic bases were milled to a fine powder prior to use in a Resodyn Acoustic Mixer LabRAM1, using stainless steel milling beads [Fisherbrand™ Bulk Beads; 15505809], and the protocol described by Abbvie[1]. Representative pictures of milled bases are shown below, beads were removed afterwards with a PTFE stir bar retriever. Some clumping is observed with hygroscopic bases, prior to use these bases are dried in a heated vacuum desiccator and stored in a glovebox. No visible difference observed between 10 and 20 mins.

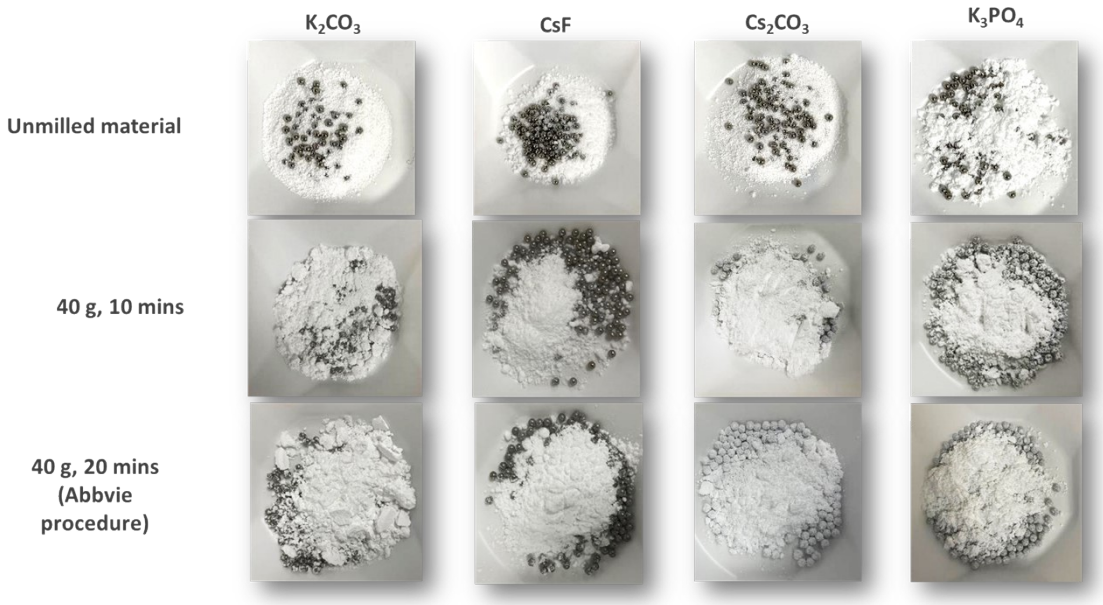


Figure S5: Photograph comparison of four different inorganic bases (K_2CO_3, CsF, Cs_2CO_3 and K_3PO_4) before milling, and after milling at 40 g for 10 mins and 40 g for 20 mins.

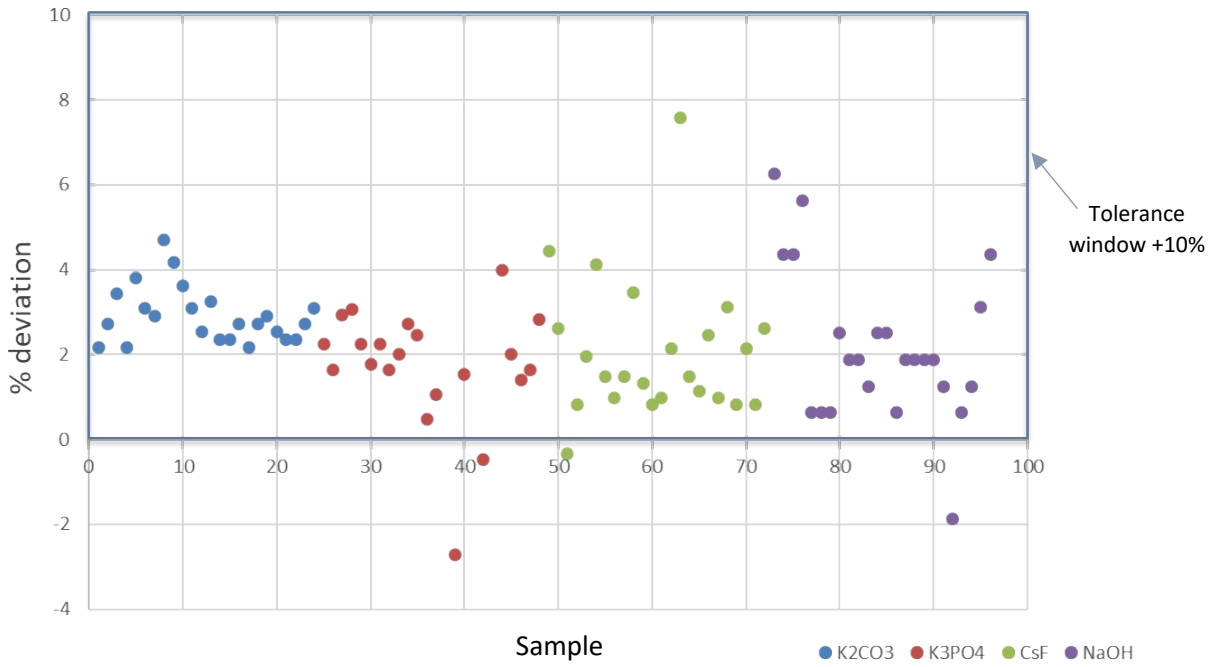


Figure S6: Assessing the dosing accuracy of milled inorganic bases with repeated dosing of K_2CO_3 (2.76 mg), K_3PO_4 (4.25 mg), CsF (3.04 mg). NaOH (0.80 mg). Even on a small scale, dosing is remarkably constant and largely within a window of 10% deviation.

Pd-ChemBead preparation

Palladium catalysts were not milled prior to glass bead coating as milling caused the catalyst powders to adhere to the sides of the glass vials. If catalyst powders are gritty or clumpy, milling beads can be added to the vials during the coating process.

Compared to the procedure reported by AbbVie[1], a modified procedure was used.

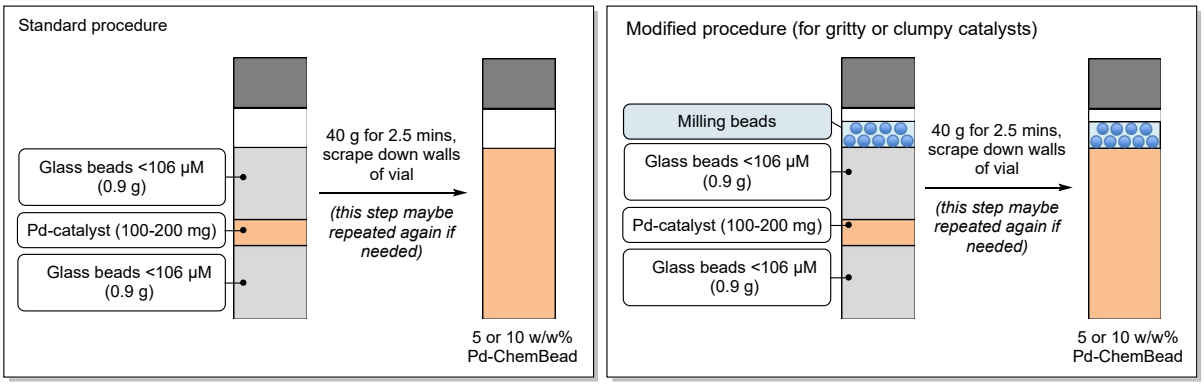


Figure S7: A schematic detailing the procedure used to make the Pd-coated ChemBeads and a photograph of the ChemBeads prepared for the Suzuki-Miyaura screening kit.

[1] Noah P. Tu,Dr. Amanda W. Dombrowski,Dr. Gashaw M. Goshu,Dr. Anil Vasudevan,Dr. Stevan W. Djuric,Dr. Ying Wang, Angew. Chem. Int. Ed. 2019, 7987.

Dosing accuracy Pd-ChemBeads

The repeated dosing accuracy of the Chronect Quantos was tested with all 12 of the Palladium-ChemBeads required for a Suzuki screening plate (figure S8). The target dose for each palladium catalyst can be found in a later section detailing the procedure for kit preparation. Again, the dosing results are remarkably consistent, with only one vial requiring a top up to reach the minimum required amount for the reaction. Typically, we do not correct any doses which exceed the +10% deviation.

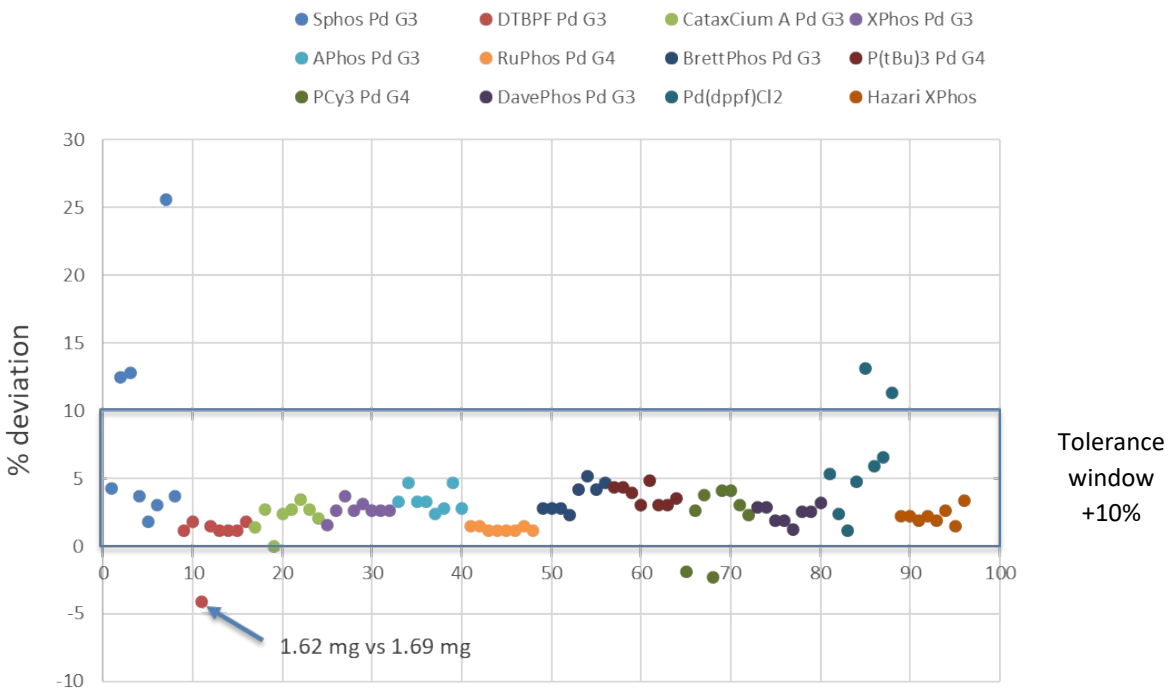


Figure S8: Assessing the dosing accuracy of Pd-ChemBeads with repeated dosing (x8) of 12 different Pd-ChemBeads. Even on a small scale, dosing is constant and largely within a window of +10% deviation. Only one dose failed to reach the minimum amount required [1.62 mg (actual) vs 1.69 mg (required)].

Glass bead spacers

Ideally, we wanted to control when the palladium catalyst and base come into contact to prevent any risk of catalyst decomposition. Cs_2CO_3 and CuI (5 wt%) ChemBeads were used to investigate the weight of glass beads required to keep the two components separate due to the clear colour change when they react. From our investigations it is clear ≥50 mg of glass beads is required to keep the two components separate (Figure S9).

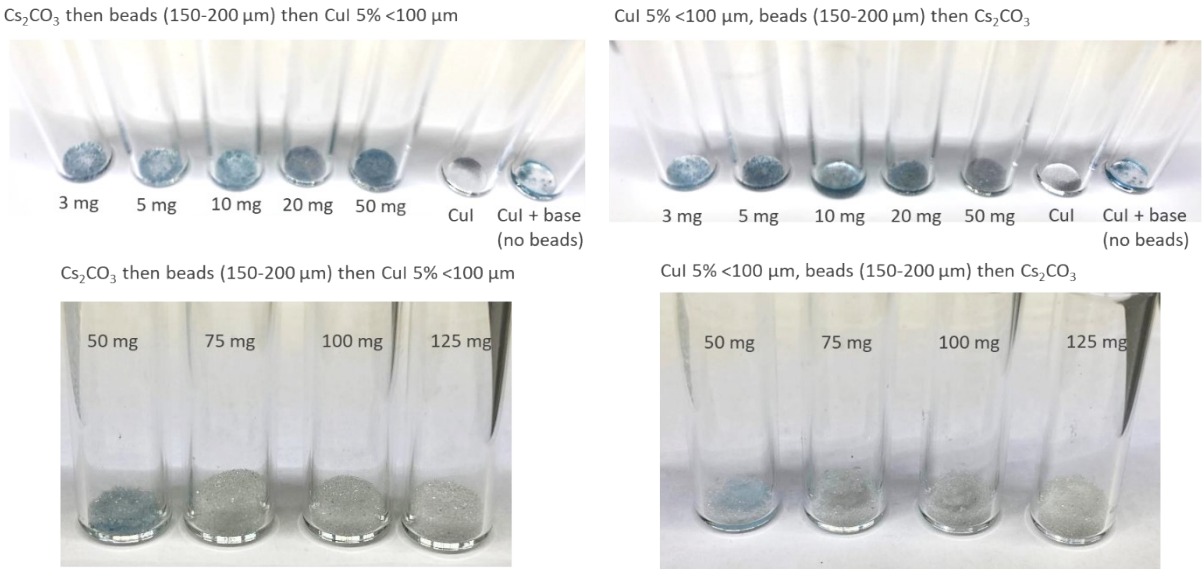


Figure S9: Investigation into the weight of glass beads to act as a spacer to keep Cs_2CO_3 and CuI (5 wt%) ChemBeads apart. A clear colour change can be seen (colourless to blue) when they react.

Reaction solvent evaporation

Despite sealing according to the manufacturer's instructions, solvent evaporation still occurs within the plate. Two representative examples of solvent loss are shown below. Despite being heated *c.a.*20 ˚C below the boiling point of these solvents, evaporation of a number of wells occurs. This is typically less than 10% of reaction vials. In these wells the appropriate solvent (100 µL) is added then then the whole block is stirred again for 5 min to ensure all samples are in solution for the creation of the analytical plates.

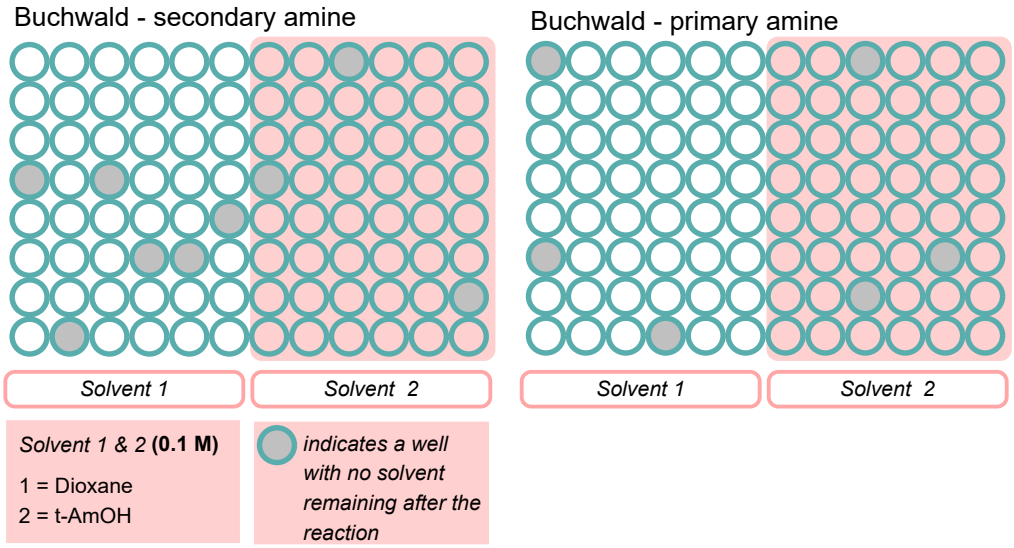
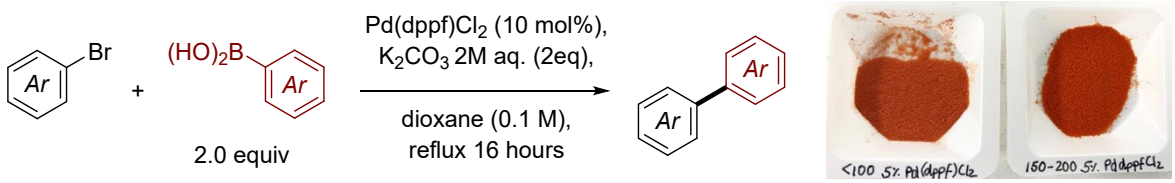
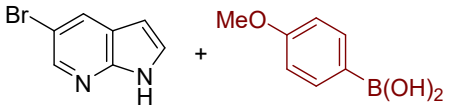


Figure S10: Schematic detailing the solvent evaporation observed from two screening kits. Less than 10% of the wells had no solvent left in them.

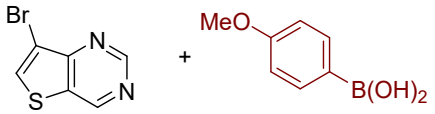
Comparing Pd-ChemBeads to pure Pd-catalysts

Before their use in a screening kit, we wanted to ensure the Pd-ChemBeads were comparable to commercially available, powdered catalyst. The Pd(dppf)Cl_2 ChemBeads (two bed sizes) and powdered catalyst were compared heat-to-head in two test reactions and can be seen below (figure S11). In each case the Chembeads and powdered catalysts proved equivalent, with the same conversion achieved in each test reaction.





Entry	Catalyst	Conversion*
1	Pd(dppf)Cl_2 (powdered catalyst)	>95%
2	Pd(dppf)Cl_2 (5 w/w%, <100 μM)	>95%
3	Pd(dppf)Cl_2 (5 w/w%, 150-200 μM)	>95%



Entry	Catalyst	Conversion*
4	Pd(dppf)Cl_2 (powdered catalyst)	>90%
5	Pd(dppf)Cl_2 (5 w/w%, <100 μM)	>90%
6	Pd(dppf)Cl_2 (5 w/w%, 150-200 μM)	>90%

*Based on LCAP

Reactions 5 and 6 were repeated again in quadruplicate (8 reactions in total) and >95% conversion was observed by LCAP in each case.

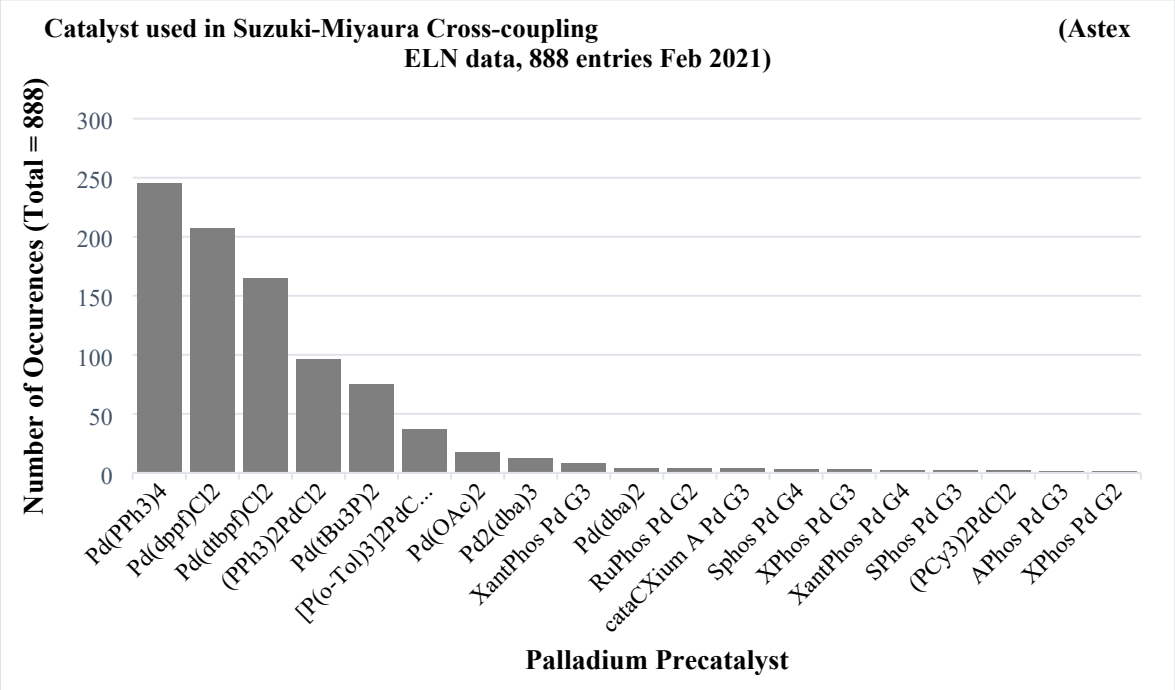
Figure S11: Comparison between powdered catalyst and the manufactured ChemBeads (two bead sizes). In all cases the ChemBeads and powdered catalysts performed equally.

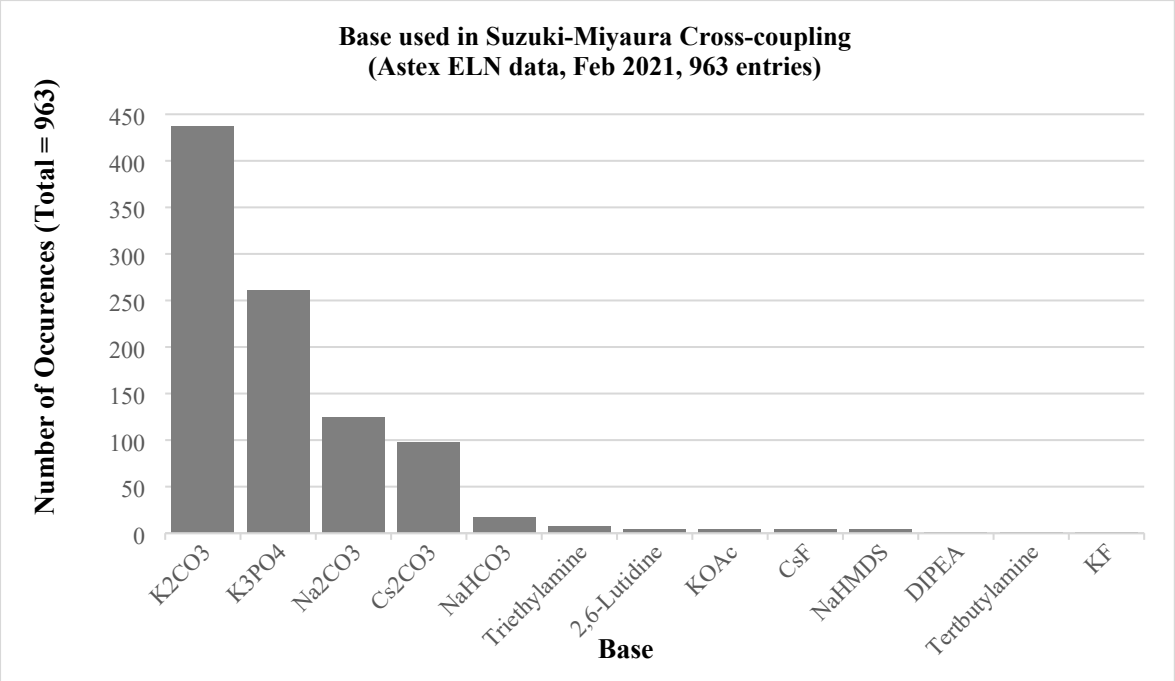
Astex preferred reaction conditions from electronic lab notebook (ELN)

The most common experimental conditions (catalyst, base, and solvent) have been extracted from Astex's electronic lab notebook for the cross-coupling reactions investigated by the screening plates.

Suzuki-Miyaura cross-coupling

The ELN data was extracted in Feb 2021 with only successful reactions were included in this analysis. 888 entries were found for catalysts for the Suzuki-Miyaura reaction, 963 entries relating to bases and 942 entries relating to solvent systems. From the extracted ELN data the most commonly used catalyst, base and solvent system is as follows; $Pd(PPh_3)_4$, K_2CO_3 and dioxane–water.





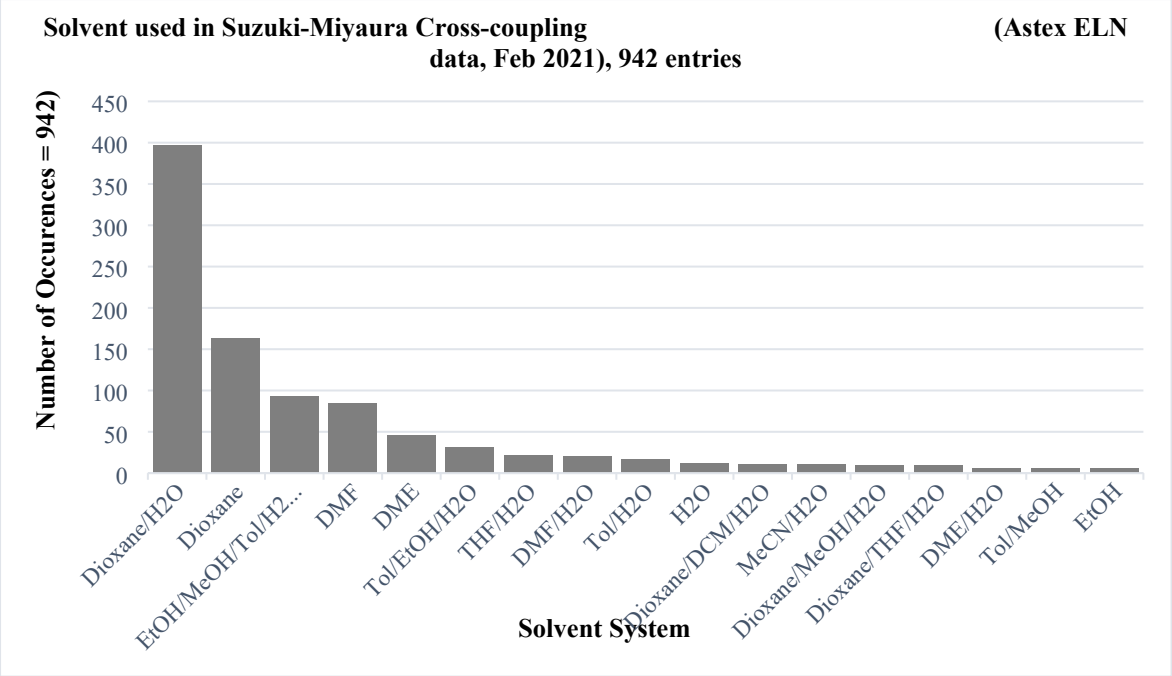
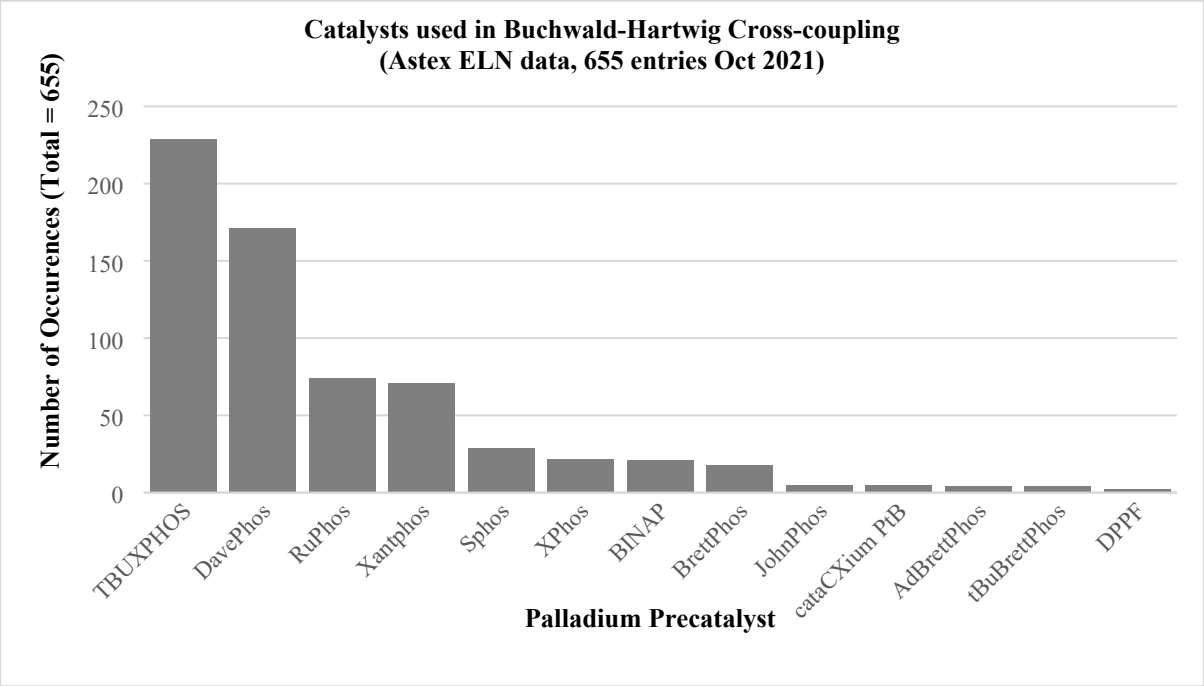
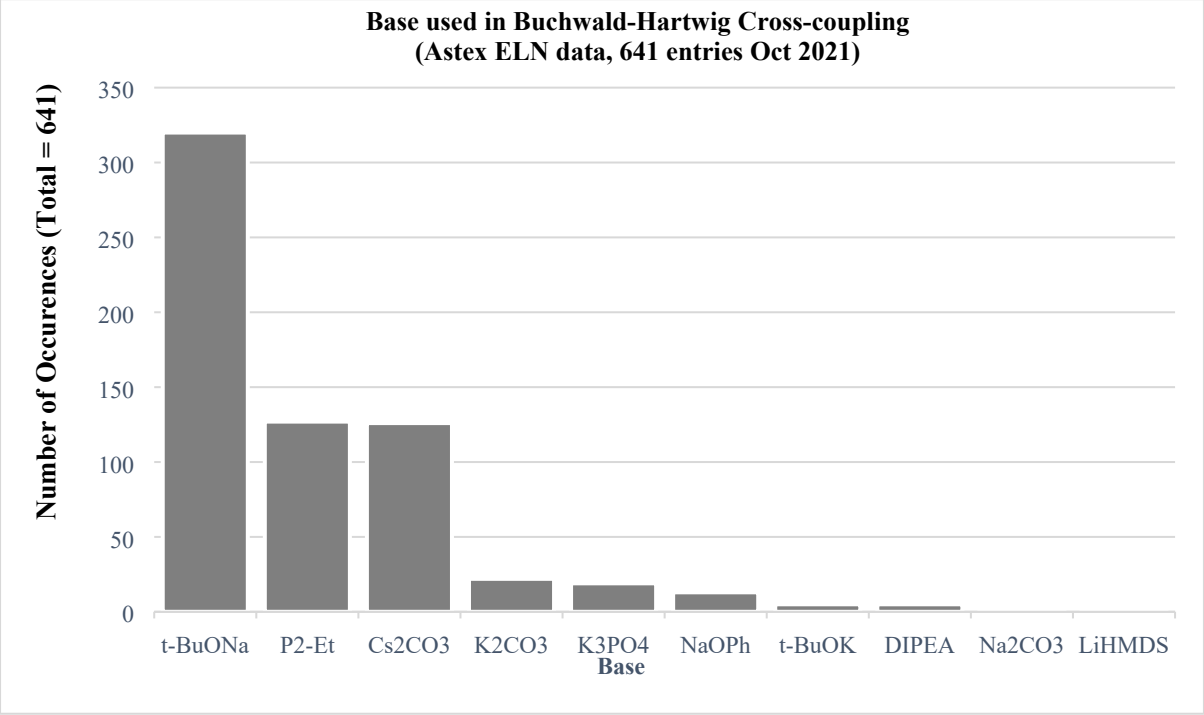


Figure S12: The most commonly used experimental conditions within the ELN for the Suzuki-Miyaura cross coupling reaction. A - the most commonly used catalyst, B - the most commonly used bases and C - the most commonly used solvent systems.

Buchwald-Hartwig Amination

The ELN data was extracted in Oct 2021 with only successful reactions were included in this analysis. 655 entries were found for catalysts for the Suzuki-Miyaura reaction, 641 entries relating to bases and 764 entries relating to solvent systems. From the extracted ELN data the most commonly used catalyst, base and solvent system is as follows; ^{t}BuXPhos, t-BuONa and dioxane.





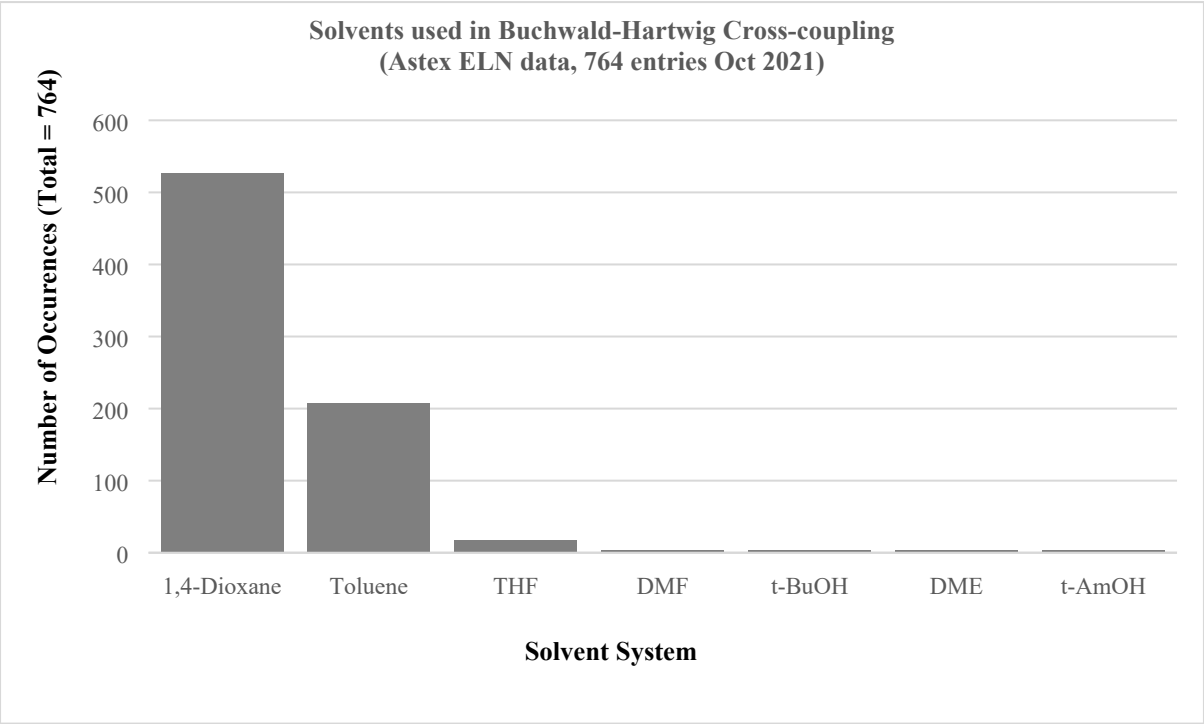


Figure S13: The most commonly used experimental conditions within the ELN for the Buchwald-Hartwig cross coupling reaction. A - the most commonly used catalyst, B - the most commonly used bases and C - the most commonly used solvent systems.

SNAr

The ELN data was extracted in Oct 2022, with only successful reactions were included in this analysis. 1092 entries were found for additives for successful nucleophilic aromatic substitution reactions, 1092 entries relating to bases and additives, and 816 entries relating to solvent systems. From the extracted ELN data the most commonly used additive and solvent system is as follows; DIPEA and DMSO.

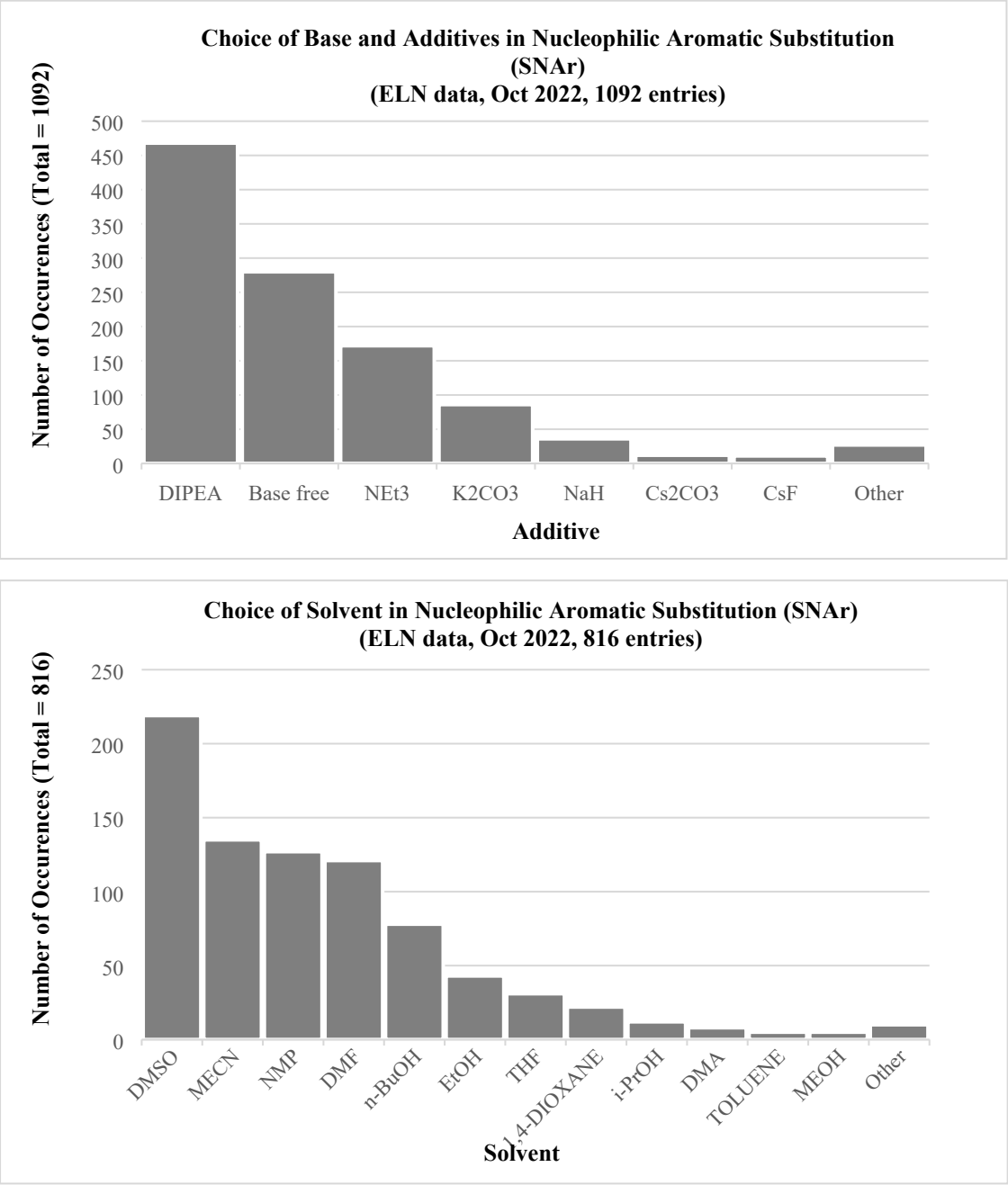


Figure S14: The most commonly used experimental conditions within the ELN for the Nucleophilic Aromatic Substitution (S_NAr) reaction. A - the most commonly used base/additive, B - the most commonly used solvent systems.

Screening plate information

Kit prep

The consumable components for the screening kits are assembled before they are placed on the Chronect Quantos platform for dosing. The analytical sales Para-dox blocks are loaded with 1 mL glass vials (884001). Quick loading of the vials is achieved by inverting the vials into an empty stackable tray (vials are now up-side down and this is repeated into the Para-dox block. Stirrer bars (13258) are loaded into every vial using a Drop Dispenser (VPS-VP711A-96-AS-1). Finally, two rubber mats and a new PFA film are added to the lid.

On completion of the solid dosing, the vials contain a stir bar, base, glass bead spacer and Pd-catalyst with the order depicted below (with the exception of the S_NAr plate). The plates are sealed as per the manufacturer's instructions, then stored in Mylar bags (34 cm × 24 cm) with a 300cc oxygen absorber (both purchased from mylarbags.com). They can then be stored in the freezer until required.

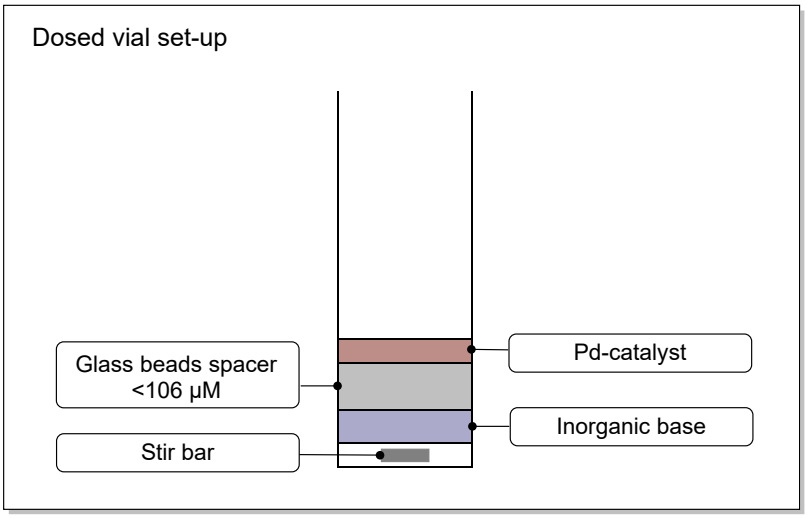
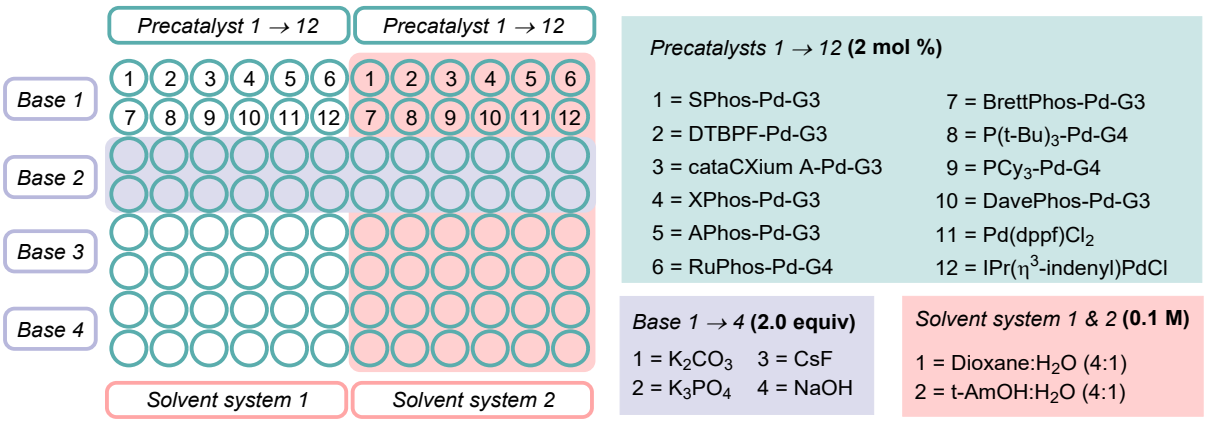


Figure S15: A schematic showing the components in the vials upon completion of solid dosing.

When the kit is required, it can be removed from the freezer and allowed to warm up to room temperature before the mylar bag is opened. Liquid reagents and starting material stock solutions can then be added to the plate using the procedure detailed below.

Suzuki-Miyaura screening kit

The plate design for the Suzuki-Miyaura screening plate can be seen below. An Analytical Sales 96 well Para-dox® Aluminium Reaction Block was dosed with all solid reagents using the Chronect Quantos (Axel Semrau, Germany). The order of addition was as follows; solid base, glass bead spacer and ChemBeads (glass beads coated in palladium pre-catalyst, 10 wt% unless otherwise stated). The addition of the coupling partners follows the procedure listed below.

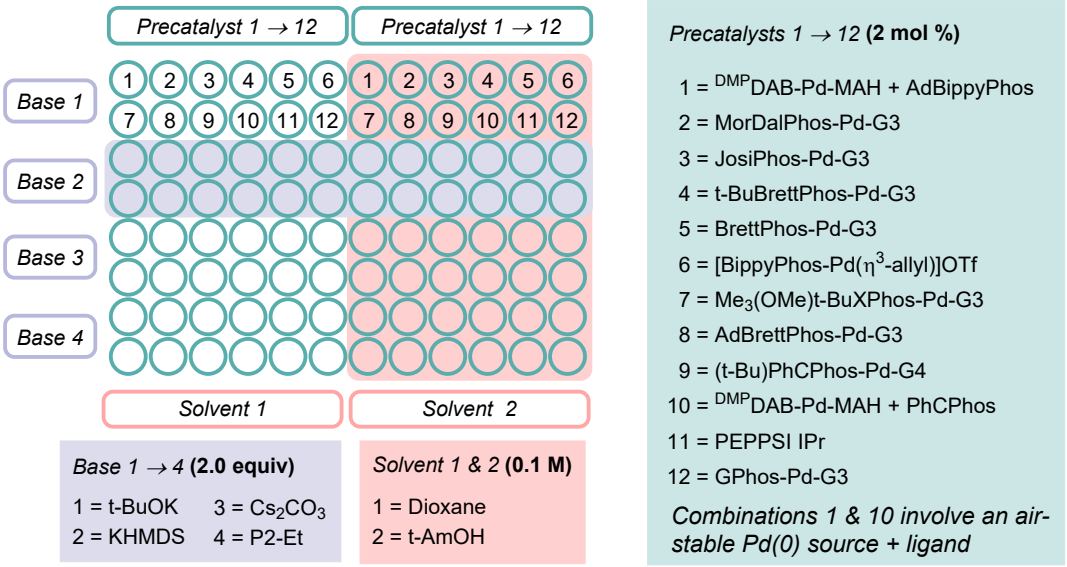


Reagent	FW ($gmol^{-1}$)	Loading (equiv)	Mass (mg)	ChemBead loading	Mass (mg)
SPhos-Pd-G3	780.33	0.02	0.156	10.0%	1.56
DTBPF-Pd-G3	844.24	0.02	0.169	10.0%	1.69
cataCXium A-Pd-G3	728.35	0.02	0.146	10.0%	1.46
XPhos-Pd-G3	846.54	0.02	0.169	10.0%	1.69
APhos-Pd-G3	635.17	0.02	0.127	5.0%	2.54
RuPhos-Pd-G4	850.4	0.02	0.170	10.0%	1.70
BrettPhos-Pd-G3	906.6	0.02	0.181	10.0%	1.81
$P(t\text{-}Bu)_3$-Pd-G4	568.08	0.02	0.114	10.0%	1.14
PCy_3-Pd-G4	664.26	0.02	0.133	10.0%	1.33
DavePhos-Pd-G3	763.35	0.02	0.153	5.0%	3.05
$Pd(dppf)Cl_2$	731.73	0.02	0.146	5.0%	2.93
IPr(η^3-indenyl)PdCl	702.81	0.02	0.141	10.0%	1.34
K_2CO_3	138.21	2.0	2.76	n/a	n/a
K_3PO_4	212.27	2.0	4.25	n/a	n/a
CsF	151.91	2.0	3.04	n/a	n/a
NaOH	18.02	2.0	0.80	n/a	n/a

Figure S16: The plate design and the target dose for each component for the Suzuki-Miyaura screening plate.

Buchwald Primary amine screening kit

The plate design for the primary amine Buchwald screening plate can be seen below An Analytical Sales 96 well Para-dox® Aluminium Reaction Block was dosed with all solid inorganic bases using the Chronect Quantos (Axel Semrau, Germany). The organic bases were added as neat solutions using the procedure listed below and the addition of the coupling partners follows the procedure listed below.

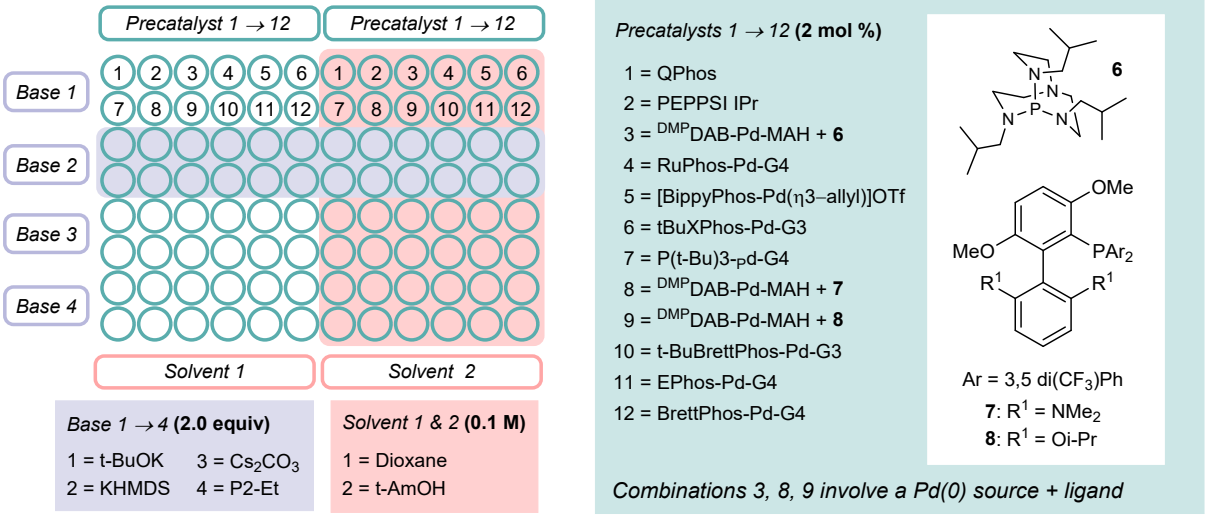


Reagent	FW ($gmol^{-1}$)	Loading (equiv)	Mass (mg)	ChemBead loading	Mass (mg)
^{DMP}DAB Pd-MAH	468.84	0.02	0.094	10.0%	0.94
Ad-BippyPhos	662.84	0.02	0.133	10.0%	1.33
MorDal-Phos-Pd-G4	847.48	0.02	0.169	10.0%	1.69
JosiPhos-Pd-G3	926.40	0.02	0.185	10.0%	1.85
t-BuBrettPhos-Pd-G3	856.54	0.02	0.171	10.0%	1.71
BrettPhos-Pd-G4	906.60	0.02	0.181	10.0%	1.81
[BippyPhos-Pd(η^3-allyl)]OTf	803.19	0.02	0.161	10.0%	1.61
Me_3(OMe)t-BuXPhos-Pd-G3	822.52	0.02	0.165	10.0%	1.65
AdBrettPhos-Pd-G3	1010.76	0.02	0.202	10.0%	2.02
(t-Bu)PhCPhos-Pd-G4	788.36	0.02	0.158	10.0%	1.58
PhCPhos	424.56	0.02	0.085	5.0%	1.70
PEPPSI IPr	681.54	0.02	0.136	10.0%	1.36
GPhos-Pd-G3	906.50	0.02	0.181	10.0%	1.81
t-BuOK	112.23	2.0	2.24	n/a	n/a
KHMDS	199.53	2.0	3.99	n/a	n/a
Cs_2CO_3	325.83	2.0	6.52	n/a	n/a
P2-Et	339.48	2.0	6.79	n/a	n/a

Figure S17: The plate design and the target dose for each component for the Buchwald-Hartwig primary amine screening plate.

Buchwald Secondary amine and aniline screening kit

The plate design for the secondary amine Buchwald screening plate can be seen below An Analytical Sales 96 well Para-dox® Aluminium Reaction Block was dosed with all solid inorganic bases using the Chronect Quantos (Axel Semrau, Germany). The organic bases were added as neat solutions using the procedure listed below and the addition of the coupling partners follows the procedure listed below.

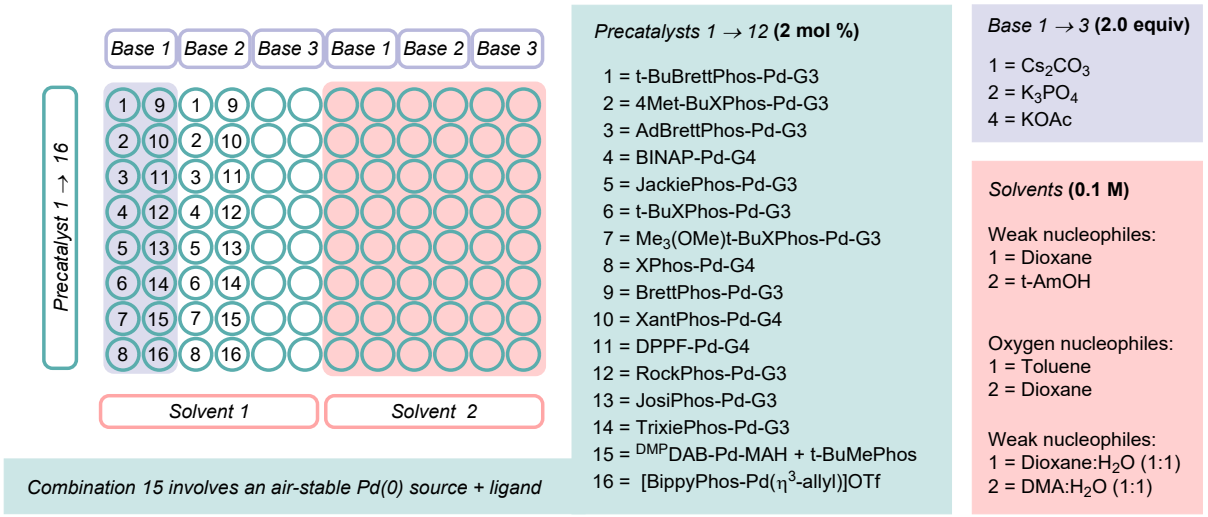


Reagent	FW ($gmol^{-1}$)	Loading (equiv)	Mass (mg)	ChemBead loading	Mass (mg)
DMPDAB-Pd-MAH	468.84	0.02	0.094	10.0%	0.94
QPhos-Pd-G3	1080.44	0.02	0.216	10.0%	2.16
PEPPSI IPr	681.54	0.02	0.136	10.0%	1.36
Triisobutylphosphatrane (**6**)	342.58	0.02	0.137‡		
RuPhos-Pd-G4	850.40	0.02	0.170	10.0%	1.70
[BippyPhos-Pd(η^3-allyl)]OTf	803.19	0.02	0.161	10.0%	1.61
t-BuXPhos-Pd-G3	794.46	0.02	0.159	10.0%	1.59
P(t-Bu)$_3$-Pd-G4	568.08	0.02	0.114	10.0%	1.14
JackieiPhos/CPhos hybrid (**7**)	786.64	0.02	0.157	10.0%	1.57
JackieiPhos/RuPhos hybrid (**8**)	756.62	0.02	0.151	10.0%	1.51
t-BuBrettPhos-Pd-G3	856.54	0.02	0.171	10.0%	1.71
EPhos-Pd-G4	919.67	0.02	0.184	10.0%	1.84
BrettPhos-Pd-G4	906.60	0.02	0.181	10.0%	1.81
t-BuOK	112.23	2.0	2.24	n/a	n/a
KHMDS	199.53	2.0	3.99	n/a	n/a
Cs_2CO_3	325.83	2.0	6.52	n/a	n/a
P2-Et	339.48	2.0	6.79	n/a	n/a

Figure S18: The plate design and the target dose for each component for the Buchwald-Hartwig secondary amine and aniline screening plate. ‡Dosed as stock solution in THF.

Buchwald amide and oxygen screening kit

The plate design for the amide, oxygen and CN Buchwald screening plate can be seen below An Analytical Sales 96 well Para-dox® Aluminium Reaction Block was dosed with all solid inorganic bases using the Chronect Quantos (Axel Semrau, Germany). The addition of the coupling partners follows the procedure listed below.

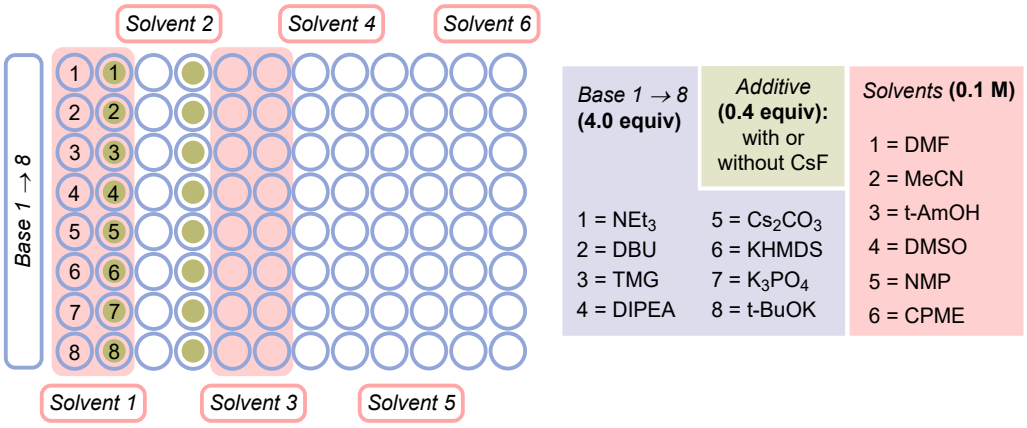


Reagent	FW ($gmol^{-1}$)	Loading (equiv)	Mass (mg)	ChemBead loading	Mass (mg)
^{DMP}DAB-Pd-MAH	468.84	0.02	0.094	10.0%	0.94
t-BuBrettPhos-Pd-G3	856.54	0.02	0.171	10.0%	1.71
4Met-BuXPhos-Pd-G3	850.58	0.02	0.170	10.0%	1.70
AdBrettPhos-Pd-G3	1010.76	0.02	0.202	10.0%	2.02
BINAP-Pd-G4	1006.43	0.02	0.201	10.0%	2.01
JackieiPhos-Pd-G3	1166.48	0.02	0.233	10.0%	2.33
t-BuXPhos-Pd-G3	794.46	0.02	0.159	10.0%	1.59
Me_3(OMe)t-BuXPhos-Pd-G3	822.52	0.02	0.165	10.0%	1.65
XPhos-Pd-G4	859.56	0.02	0.172	10.0%	1.72
BrettPhos-Pd-G3	920.63	0.02	0.184	10.0%	1.84
XantPhos-Pd-G4	962.43	0.02	0.192	10.0%	1.92
DPPF-Pd-G4	925.17	0.02	0.185	7.5%	2.47
RockPhos-Pd-G3	838.52	0.02	0.168	10.0%	1.68
JosiPhos-Pd-G3	926.4	0.02	0.185	10.0%	1.85
TrixiePhos-Pd-G3	768.31	0.02	0.154	10.0%	1.54
t-BuMePhos	312.47	0.02	0.062	5.0%	1.25
[BippyPhos-Pd(η^3-allyl)]OTf	803.19	0.02	0.161	10.0%	1.61
Cs_2CO_3	325.83	2.0	6.52	n/a	n/a
K_3PO_4	212.27	2.0	4.25	n/a	n/a
KOAc	98.15	2.0	1.96	n/a	n/a

Figure S19: The plate design and the target dose for each component for the Buchwald-Hartwig amide and oxygen screening plate.

S_NAr screening kit

The plate design for the S_NAr screening plate can be seen below An Analytical Sales 96 well Para-dox® Aluminium Reaction Block was dosed with all solid inorganic bases using the Chronect Quantos (Axel Semrau, Germany). The organic bases were added as neat solutions using the procedure listed below and the addition of the coupling partners follows the procedure listed below.



Reagent	FW ($gmol^{-1}$)	Loading (equiv)	Mass (mg)
NEt_3	101.22	4	4.05
DBU	152.27	4	6.09
TMG	115.21	4	4.61
DIPEA	129.28	4	5.17
Cs_2CO_3	325.83	4	13.03
KHMDS	199.53	4	7.98
K_3PO_4	212.27	4	8.49
t-BuOK	112.23	4	4.49
CsF	151.91	0.4	0.61

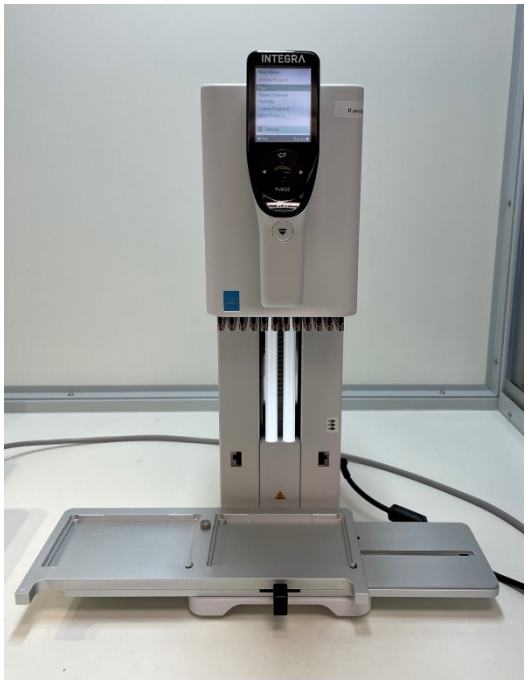
Figure S20: The plate design and the target dose for each component for the S_NAr screening plate.

Setting up the screening kits

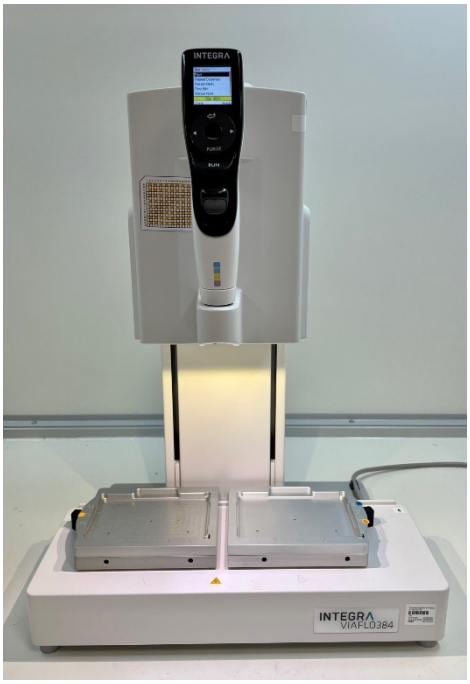
The total amount of solid reagent was aliquoted into the number of solvents required for the screening plate and weighed into an appropriate vial (7 mL screw cap for Suzuki and S_NAr and 10-20 mL vial Biotage, 354833 for Buchwald-Hartwig), both coupling partners were added to the same vial and the vial was degassed if necessary. The appropriate solvent was then added, and the mixture was sonicated until all solid had dissolved. Liquid handling of reagents and stock solutions was performed by Andrew+ liquid handler Andrew Alliance, Switzerland) equipped with Sartorius Picus® electronic pipettes or by hand using Sartorius Picus® electronic pipettes. If liquid reagents are required then these were added first, followed by the addition of the stock solutions. The plate was then sealed according to the manufacturers sealing guide and heated to an appropriate temperature overnight.

Creation of the analytical plates for MISER

Analytical plates with a 1-400-fold dilution were created using the Integra Mini 96 and the Viaflo 96 / 384. t-AmOH (95 µL) was added into all the coloured wells (figure S18) using the Integra Mini 96. Crude reaction mixture (5 µL) was added into wells coloured in light blue (figure S18), mixed five times, then an aliquot (5 µL) of the light blue well was transferred into the dark blue wells and mixed five times. The plate was sealed with a Thermo Scientific™ Easy Pierce Heat Sealing Foil (AB-1720).



Integra Mini 96



Integra Viaflo 96 / 384

Figure S21: The Integra liquid handlers (Mini 96 and Viaflo 96 / 384) utilised in the production of the analytical plates.

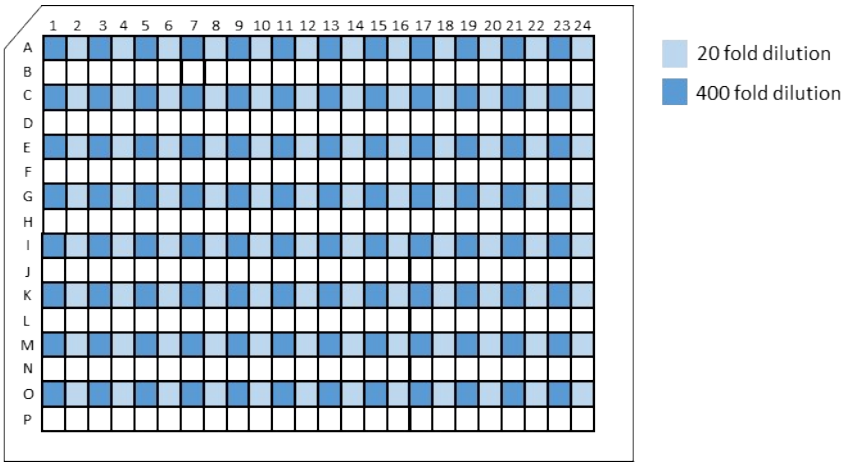
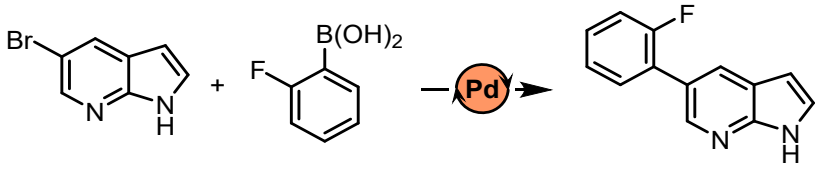


Figure S22: The plate layout for the 1-400-fold dilution required in the preparation of the screening plate.

Screening kit analysis – MISER analysis

Suzuki-Miyaura Cross-coupling screening plate; 5-bromo-1H-pyrrolo[2,3-b]pyridine and (2-fluorophenyl)boronic acid



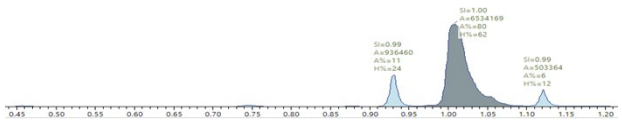
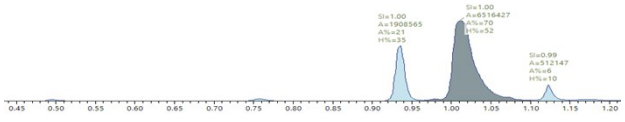
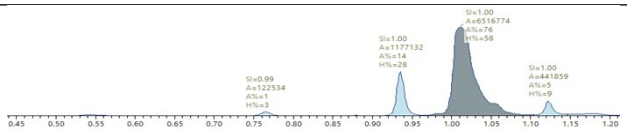
MISER Analysis: 5-(2-fluorophenyl)-1H-pyrrolo[2,3-b]pyridine (Desired Product)

Max response: 464370.25

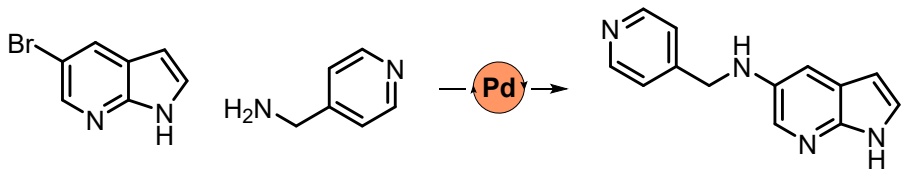
m/z: 213

	1	2	3	4	5	6	7	8	9	10	11	12
A	1.81	39.06	54.70	6.32	44.10	10.05	5.98	91.10	44.49	5.51	76.17	17.29
B	6.56	16.40	25.86	1.76	5.59	13.91	19.20	8.84	68.14	15.26	19.90	1.60
C	4.69	24.15	27.73	0.77	24.56	10.52	2.89	10.74	48.30	58.30	67.42	9.04
D	8.09	7.72	50.41	7.94	8.02	26.70	3.40	15.37	66.73	6.03	15.83	45.28
E	2.67	22.47	48.89	7.64	78.95	9.13	13.12	16.97	22.44	26.57	100.00	40.04
F	15.70	7.80	47.67	5.21	11.37	24.74	26.35	9.13	62.82	36.25	44.81	39.78
G	2.86	13.13	6.91	1.34	11.32	5.14	3.17	29.69	5.69	5.54	40.67	8.47
H	21.08	12.99	5.85	1.56	7.08	30.28	7.74	30.93	2.48	3.88	22.58	19.10

Legend
66.7% ≤ val <100.0%
33.3% ≤ val <66.7%
0.0% ≤ val <33.3%

Well	MISER result (%)	LCAP (%)	LCMS spectra
E11	**100.00**	**80.0**	
A8	91.10	70.0	
E5	78.95	76.0	

Buchwald primary amine screening plate (unhindered primary amine); 5-bromo-1H-pyrrolo[2,3-b]pyridine and 1-(pyridin-4-yl)methanamine



MISER Analysis: N-[(pyridin-4-yl)methyl]-1H-pyrrolo[2,3-b]pyridin-5-amine (Desired Product)

Max response: 393248.44

m/z: 225

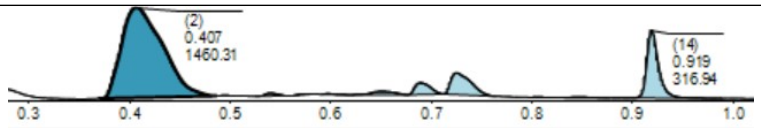
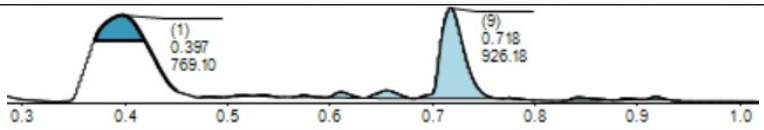
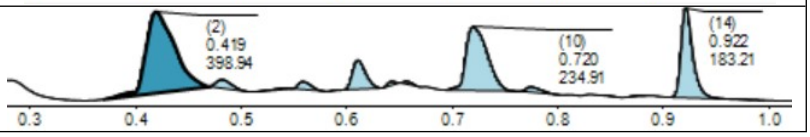
	1	2	3	4	5	6	7	8	9	10	11	12
A	0.00	0.00	0.50	3.63	0.57	10.53	5.35	0.00	0.00	68.87	2.54	14.94
B	47.00	100.00	0.00	2.40	0.59	56.23	42.03	22.66	6.38	0.37	0.00	16.56
C	8.69	1.30	0.36	58.03	0.46	1.04	77.94	0.00	0.00	63.90	2.51	34.14
D	0.48	64.31	0.47	0.37	0.00	1.04	0.00	0.42	1.02	0.00	0.00	22.40
E	0.00	0.00	0.00	0.29	0.00	0.00	9.26	0.00	0.00	6.89	0.00	0.55
F	1.58	10.08	0.00	0.00	0.00	0.56	5.13	1.42	0.00	0.00	0.00	0.00
G	2.46	0.00	0.00	0.72	0.00	0.00	0.35	0.00	0.00	3.70	0.00	0.00
H	2.10	4.08	0.00	0.00	0.00	1.27	0.34	11.18	0.00	0.00	0.00	0.00

Legend

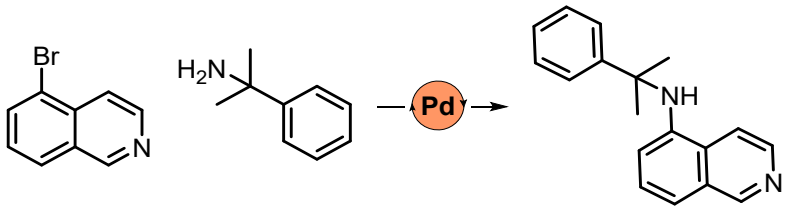
66.7% ≤ val <100.0%

33.3% ≤ val <66.7%

0.0% ≤ val <33.3%

Well	MISER result (%)	LCAP (%)	LCMS spectra
B2	**100.00**	**68.7**	
C7	77.94	40.4	
A10	68.87	41.3	

Buchwald primary amine screening plate (hindered primary amine); 5-bromoisoquinoline and 2-phenylpropan-2-amine



MISER Analysis: N-(2-phenylpropan-2-yl)quinolin-4-amine (Desired Product)

Max response: 988515.56

m/z: 263

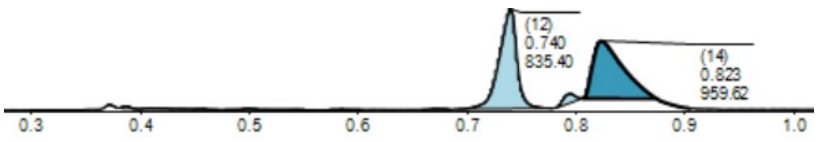
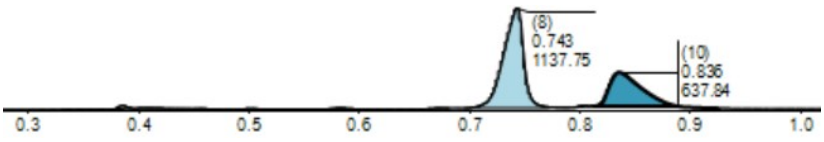
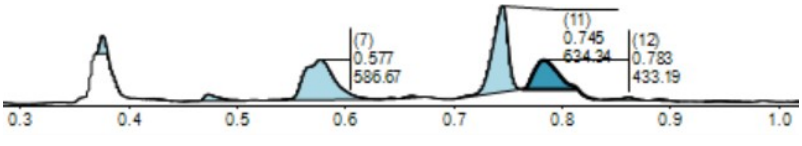
	1	2	3	4	5	6	7	8	9	10	11	12
A	2.80	2.13	0.00	0.00	0.00	0.00	0.00	0.00	2.58	0.00	0.00	7.38
B	1.27	0.00	14.54	2.16	2.27	3.59	0.00	0.00	100.00	51.09	0.00	2.56
C	0.00	0.00	2.93	0.00	4.29	43.62	0.00	0.00	0.00	0.00	0.00	9.07
D	45.35	31.57	0.00	0.00	38.58	41.40	0.00	0.00	8.40	0.00	13.59	0.00
E	3.69	1.22	0.00	0.00	0.00	6.42	13.36	0.00	3.07	0.00	0.00	21.42
F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	14.12	3.30	0.00	1.47
G	1.12	0.00	0.00	0.00	0.00	0.00	1.47	0.00	0.00	0.00	0.00	1.79
H	0.00	0.00	1.62	0.00	0.00	0.00	0.00	0.00	1.36	0.00	0.00	3.66

Legend

66.7% ≤ val <100.0%

33.3% ≤ val <66.7%

0.0% ≤ val <33.3%

Well	MISER result desired product (%)	LCAP (%)	LCMS spectra
B9	**100.00**	**49.4**	
B10	51.09	34.6	
D1	45.35	22.7	

Buchwald secondary amine / aniline screening plate (secondary amine); 5-bromo-1H-pyrrolo[2,3-b]pyridine and tert-butyl piperazine-1-carboxylate

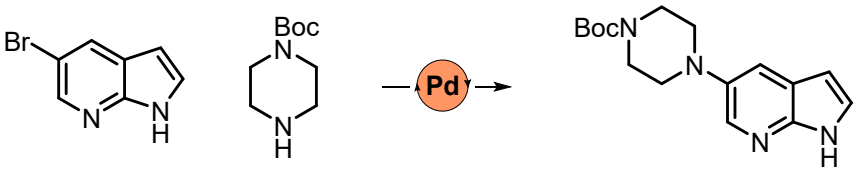
MISER Analysis: tert-butyl 4-{1H-pyrrolo[2,3-b]pyridin-5-yl}piperazine-1-carboxylate (Desired Product)

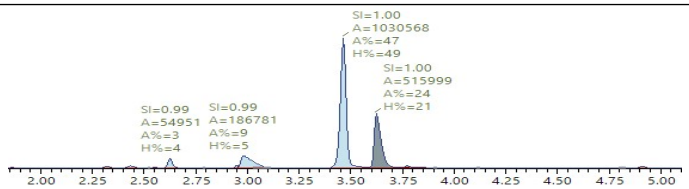
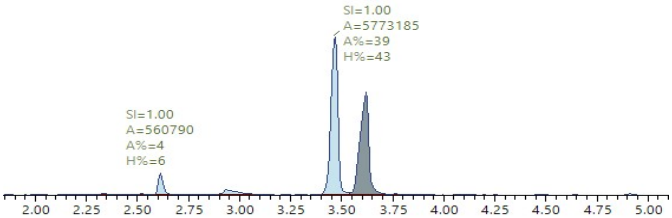
Max response: 375059.47

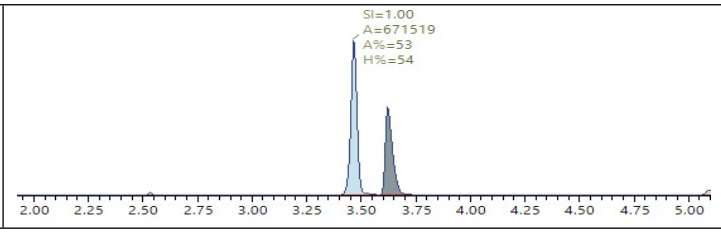
m/z: 303

	1	2	3	4	5	6	7	8	9	10	11	12
A	41.12	0.00	0.00	3.52	45.10	9.54	82.72	0.00	0.00	0.00	25.69	35.57
B	38.87	6.48	0.00	3.55	0.00	10.46	20.50	0.00	24.84	17.04	0.00	59.47
C	70.66	54.67	100.00	83.17	88.80	73.81	68.42	0.00	0.00	53.91	17.01	31.18
D	53.58	70.06	73.61	65.26	51.66	47.18	0.00	0.00	22.17	18.04	0.00	53.54
E	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
G	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

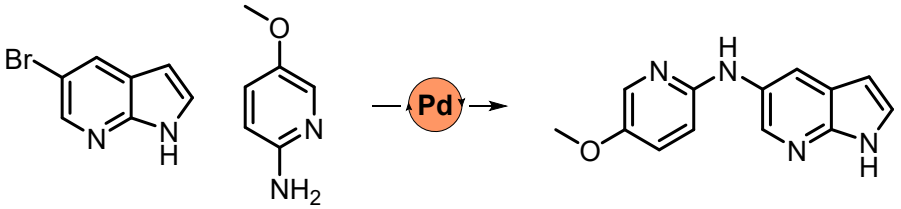
Legend
66.7% ≤ val <100.0%
33.3% ≤ val <66.7%
0.0% ≤ val <33.3%



Well	MISER result desired product (%)	LCAP (%)	LCMS spectra	0.25 mmol scale up LCAP (%)
C3	100.00	24.0		26.0
C5	**88.80**	**28.0**		**60.0**

C4	83.17	28.0		33.0

Buchwald secondary amine / aniline screening plate (aniline); 5-bromo-1H-pyrrolo[2,3-b]pyridine and 5-methoxypyridin-2-amine



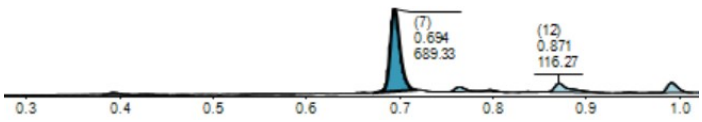
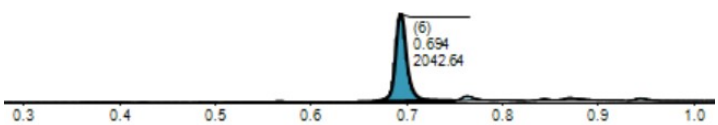
MISER Analysis: 5-methoxy-N-{1H-pyrrolo[2,3-b]pyridin-5-yl}pyridin-2-amine (Desired Product)

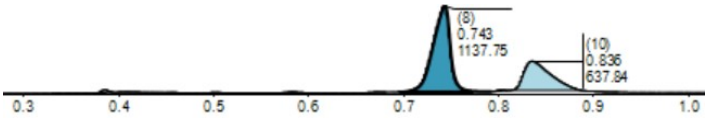
Max response: 328926.25

m/z: 241

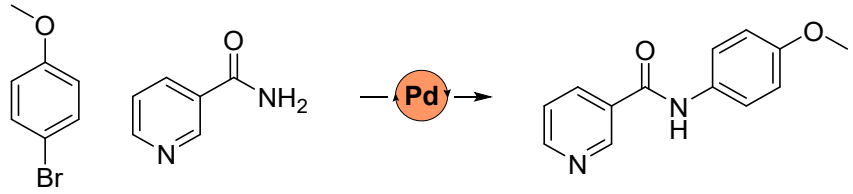
	1	2	3	4	5	6	7	8	9	10	11	12
A	49.71	0.00	0.00	4.16	10.62	0.00	0.00	0.00	0.00	0.00	3.95	25.74
B	22.86	0.00	0.00	75.29	0.00	100.00	4.31	0.00	0.00	81.60	0.00	44.81
C	0.00	0.00	0.00	23.89	0.00	0.00	0.00	0.00	0.00	0.00	84.74	33.48
D	0.00	0.00	0.00	18.23	0.00	0.00	0.00	0.00	0.00	4.22	0.00	0.00
E	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.26	27.75
F	0.00	0.00	0.00	8.28	0.00	0.00	0.00	0.00	0.00	0.00	0.00	13.76
G	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Legend
66.7% ≤ val <100.0%
33.3% ≤ val <66.7%
0.0% ≤ val <33.3%

Well	MISER result desired product (%)	LCAP (%)	LCMS spectra
B6	**100.00**	**73.3**	
C11	84.74	72.2	

B10	81.60	61.8	

Buchwald amide and oxygen screening kit (amide); 1-bromo-4-methoxybenzene and pyridine-3-carboxamide



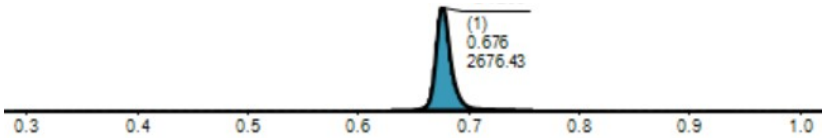
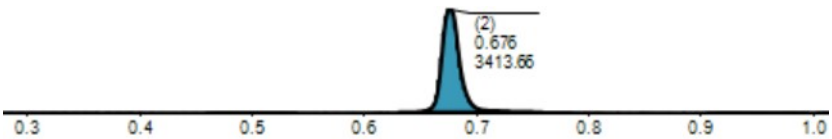
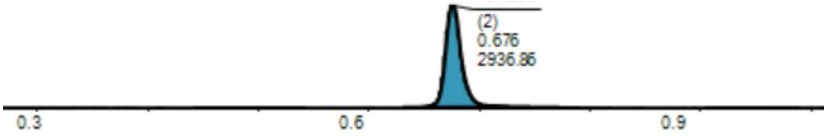
MISER Analysis: N-(4-methoxyphenyl)pyridine-3-carboxamide (Desired Product)

Max response: 1890096.00

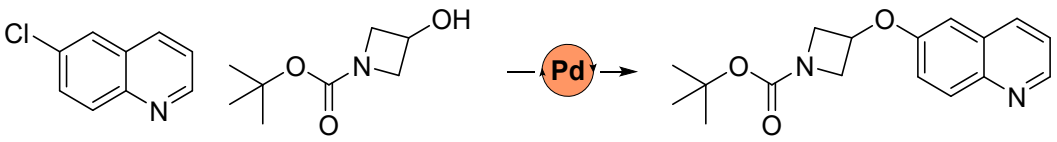
m/z: 229

	1	2	3	4	5	6	7	8	9	10	11	12
A	48.33	27.09	2.26	11.11	12.91	0.00	6.35	60.16	13.41	3.99	18.08	0.00
B	0.80	1.54	0.00	0.00	0.00	0.00	21.42	29.27	2.24	0.00	0.00	0.00
C	6.20	22.39	1.66	0.00	0.00	0.00	100.00	76.43	8.12	0.00	0.00	0.00
D	0.00	0.00	0.00	23.96	53.43	1.27	0.00	0.00	0.00	76.86	61.11	6.00
E	0.00	0.00	0.00	2.74	1.32	0.00	0.00	0.56	0.00	0.00	0.00	0.00
F	1.29	1.58	1.08	1.17	1.48	0.00	30.31	16.39	0.00	14.54	7.38	1.64
G	4.64	1.77	0.00	0.65	0.00	0.00	1.53	48.00	3.28	5.18	2.05	0.00
H	0.00	0.00	0.00	1.61	2.04	0.00	0.00	0.62	0.00	0.00	2.72	0.97

Legend
66.7% ≤ val <100.0%
33.3% ≤ val <66.7%
0.0% ≤ val <33.3%

Well	MISER result desired product (%)	LCAP (%)	LCMS spectra
C7	**100.00**	**98.5**	
D10	76.86	98.1	
C8	81.60	97.8	

Buchwald amide and oxygen screening kit (oxygen); 6-chloroquinoline and tert-butyl 3-hydroxyazetidine-1-carboxylate



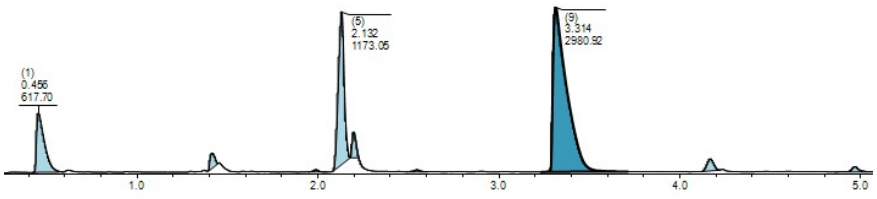
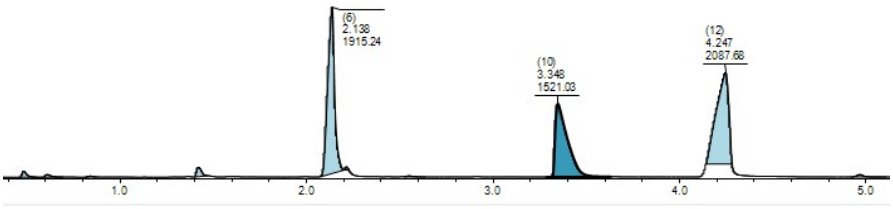
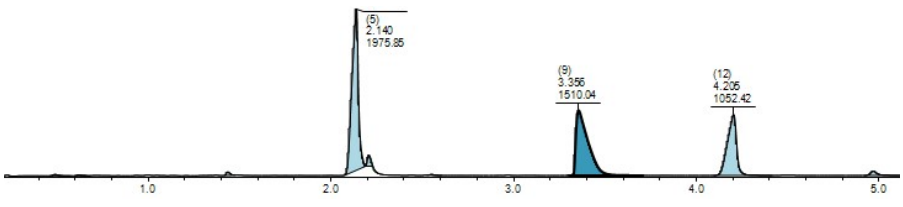
MISER Analysis: tert-butyl 3-(quinolin-6-yloxy)azetidine-1-carboxylate (Desired Product)

Max response: 730117.75

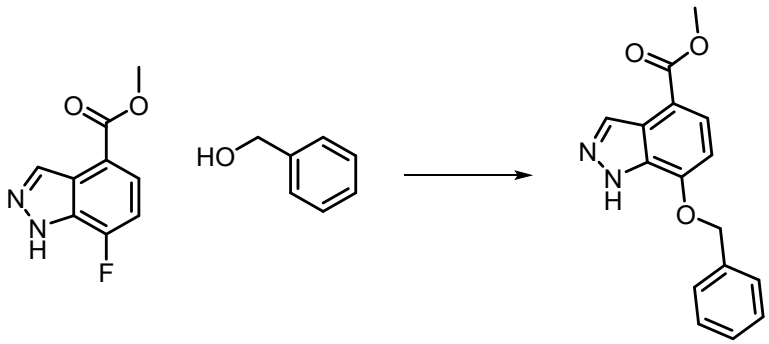
m/z: 301

	1	2	3	4	5	6	7	8	9	10	11	12
A	74.79	62.43	2.12	34.18	6.38	2.02	14.09	2.64	0.00	0.00	0.00	0.00
B	91.17	1.90	0.00	0.00	0.00	0.00	13.95	1.92	0.00	0.00	0.00	0.00
C	19.63	31.07	0.00	0.00	0.00	0.00	2.68	2.90	0.00	0.00	0.00	0.00
D	1.45	0.00	0.00	1.85	65.13	0.00	0.00	0.00	0.00	0.00	13.16	1.98
E	29.38	8.17	0.00	0.00	6.93	0.00	0.00	0.00	0.00	11.82	0.00	0.00
F	31.84	3.96	0.00	8.81	0.00	0.00	3.10	0.00	0.00	44.99	0.00	0.00
G	100.00	2.77	0.00	1.95	0.00	0.00	0.00	14.02	0.00	1.44	1.92	0.00
H	5.27	0.00	0.00	3.40	49.59	0.00	0.00	0.00	0.00	0.00	18.69	0.00

Legend
66.7% ≤ val <100.0%
33.3% ≤ val <66.7%
0.0% ≤ val <33.3%

Well	MISER result desired product (%)	LCAP (%)	LCMS spectra
C1	**100.00**	**56.7**	
F1	79.74	26.5	
A1	67.33	31.7	

SNAr screening plate:



MISER Analysis: methyl 7-(benzyloxy)-1H-indazole-4-carboxylate (Desired Product)

Max response: 365728.12

m/z: 281

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
B	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
D	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
E	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
F	59.54	3.93	0.00	0.00	0.00	0.00	1.38	0.00	5.63	100.00	0.00	0.00
G	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H	1.94	1.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Legend
66.7% ≤ val <100.0%
33.3% ≤ val <66.7%
0.0% ≤ val <33.3%

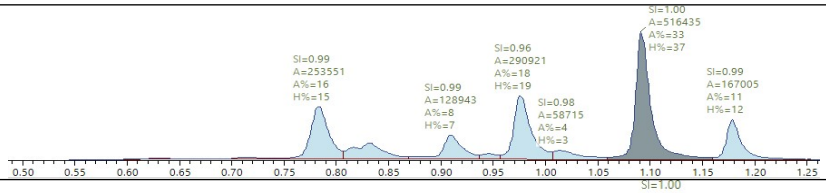
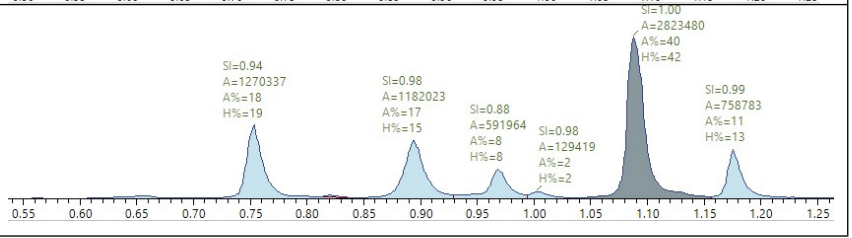
MISER Analysis: 1H-INDAZOLE-4-CARBOXYLIC ACID, 7-FLUORO-, METHYL ESTER (BT301412,FRIDGE F) (Reactant)

Max response: 429213.84

m/z: 193

	1	2	3	4	5	6	7	8	9	10	11	12
A	100.00	15.56	11.85	7.28	73.52	46.35	48.12	26.24	74.50	27.72	90.52	48.05
B	8.13	11.65	7.10	5.73	34.54	25.16	5.27	5.72	24.94	7.01	35.35	41.44
C	7.21	1.80	5.44	6.64	51.14	19.78	6.08	4.58	10.91	3.72	32.31	6.17
D	50.69	21.84	25.80	6.78	34.01	29.41	23.00	38.42	47.48	26.08	34.54	34.17
E	33.77	42.28	3.02	4.09	6.22	7.57	47.25	25.87	42.39	67.12	0.00	6.04
F	0.00	4.65	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.31	1.28	0.00
G	50.40	54.16	1.40	5.03	5.56	0.00	70.33	41.70	66.47	42.58	4.56	2.03
H	0.00	2.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

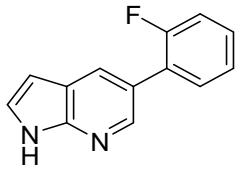
Legend
0.0% ≤ val <33.3%
33.3% ≤ val <66.7%
66.7% ≤ val <100.0%

Well	MISER result (%)	LCAP (%)	LCMS spectra
F10	**100.00**	**33.0**	
F1	59.54	40.0	

The peak with a retention time of 1.17 min represents the trans esterified product (m/z 359.4), where the desired product has reacted with excess benzyl alcohol to give the benzylated ester.

Batch scale-up reactions and characterization data

5-(2-fluorophenyl)-1H-pyrrolo[2,3-b]pyridine (**3**)



Conditions identified on the plate: 5-bromo-1H-pyrrolo[2,3-b]pyridine (49.3 mg, 0.25 mmol), (2-fluorophenyl)boronic acid (52.5 mg, 0.38 mmol), APhos-Pd-G3 (3.90 mg, 0.005 mmol, 2 mol%) and CsF (76.0 mg, 0.50 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar. t-AmOH:water (4:1, 2.50 mL, 0.1 M) was added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 86%. The crude product was purified (10g Sfar cartridge, 0–100% EtOAc/Petrol v/v) to afford the title compound as a yellow solid (47.2 mg, 89% yield).

Closest literature conditions[1]: 5-bromo-1H-pyrrolo[2,3-b]pyridine (49.3 mg, 0.25 mmol), (2-fluorophenyl)boronic acid (52.5 mg, 0.38 mmol), $Pd(dppf)Cl_2$ (3.66 mg, 0.005 mmol, 2 mol%) and K_2CO_3 (69.2 mg, 0.50 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar. Dioxane–water (4:1, 2.50 mL, 0.1 M) was added to the vial, which was then heated to 120 ˚C for 12 h. Crude reaction LCAP for desired product = 10%. The crude product was purified (10g Sfar cartridge, 0–100% EtOAc/Petrol v/v) to afford the title compound as a cream solid (3.0 mg, 6% yield).

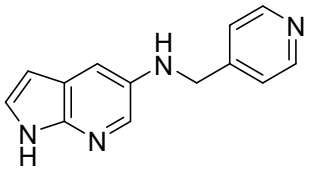
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.77 (s, 1H), 8.37 (d, J = 2.1 Hz, 1H), 8.11 (dd, J = 2.2, 0.8 Hz, 1H), 7.59 (dd, J = 7.6, 1.9 Hz, 1H), 7.53 (dd, J = 3.5, 2.5 Hz, 1H), 7.42 (ddd, J = 8.6, 7.0, 1.8 Hz, 1H), 7.32 (ddd, J = 8.7, 7.3, 1.4 Hz, 2H), 6.52 (dd, J = 3.5, 1.8 Hz, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 159.2 (d, *J* = 245.0 Hz), 147.9, 142.7 (d, *J* = 3.3 Hz), 131.2 (d, *J* = 3.3 Hz), 129.2 (d, *J* = 8.2 Hz), 128.2 (d, *J* = 2.8 Hz), 127.0, 126.9 (d, *J* = 13.7 Hz), 125.0 (d, *J* = 3.4 Hz), 122.8, 119.9, 116.0 (d, *J* = 22.7 Hz), 100.2.

^{19}F NMR (376 MHz, DMSO-d_6) δ -118.66.

HRMS (ESI-QTOF): m/z $[M+H]^+$ Calcd for $C_{13}H_9FN_2$ 213.0822; Found 213.0827. Δ = 2.24 ppm

N-[(pyridin-4-yl)methyl]-1H-pyrrolo[2,3-b]pyridin-5-amine (**4**)



Conditions identified on the plate: 5-bromo-1H-pyrrolo[2,3-b]pyridine (49.3 mg, 0.25 mmol), 4-picolylamine (25.4 µL, 0.38 mmol), AdBrettPhos-Pd-G3 (5.06 mg, 0.005 mmol, 2 mol%) and t-BuOK (56.2 mg, 0.50 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous dioxane (2.50 mL, 0.1 M) was added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 92%. The crude material was purified (11g KPNH Sfar cartridge, 0–100% EtOAc/Petrol v/v then 0–20% MeOH/EtOAc v/v) to afford the title compound as a pale-yellow oil (51.7 mg, 92% yield).

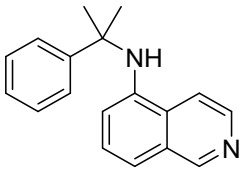
Closest literature conditions[2]: 5-bromo-1H-pyrrolo[2,3-b]pyridine (49.3 mg, 0.25 mmol), tert-butyl piperazine-1-carboxylate (69.9 mg, 0.38 mmol) and BrettPhos-Pd-G3 (2.27 mg, 0.005 mmol, 2 mol%) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous THF (2.0 mL, 0.1 M) and LiHMDS (1 M in THF, 0.5 mL, 0.50 mmol) were added to the vial, which was then heated to 80 ˚C for 16 h. LCMS indicated that no reaction had taken place, therefore no more was done with this sample.

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.13 (s, 1H), 8.53 – 8.46 (m, 2H), 7.81 (d, J = 2.6 Hz, 1H), 7.42 – 7.36 (m, 2H), 7.24 (t, J = 2.9 Hz, 1H), 6.98 – 6.92 (m, 1H), 6.15 (dd, J = 3.3, 1.9 Hz, 1H), 6.06 (t, J = 6.3 Hz, 1H), 4.35 (d, J = 6.2 Hz, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 149.8, 149.5, 142.7, 138.9, 132.3, 125.6, 122.4, 119.6, 108.9, 98.5, 46.3.

HRMS (ESI-QTOF): m/z $[M+H]^+$ Calcd for $C_{13}H_{12}N_4$ 225.1135; Found 225.1143. Δ = 3.65 ppm

N-(2-phenylpropan-2-yl)isoquinolin-5-amine (**5**)



Conditions identified on the plate: 5-bromoisoquinoline (52.0 mg, 0.25 mmol), cumylamine (50.7 mg, 0.38 mmol), ^{t}BuPhCPhos-Pd-G4 (3.94 mg, 0.005 mmol, 2 mol%) and t-BuOK (56.2 mg, 0.50 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous t-AmOH (2.50 mL, 0.1 M) was added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 76%. The crude material was purified (10g Sfar cartridge, 0–100% EtOAc/Petrol v/v then 0–20% MeOH/EtOAc v/v) to afford the title compound as a pale-yellow oil (27.1 mg, 41.3% yield).

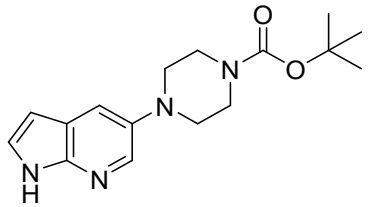
Closest literature conditions[3]: 5-bromoisoquinoline (52.0 mg, 0.25 mmol), cumylamine (50.7 mg, 0.38 mmol), ^{t}BuPhCPhos-Pd-G4 (3.94 mg, 0.005 mmol, 2 mol%) and t-BuOK (56.2 mg, 0.50 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous dioxane (2.0 mL, 0.1 M) were added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 7%. The crude product was purified (10g Sfar cartridge, 0–100% EtOAc/Petrol v/v then 0–20% MeOH/EtOAc v/v) but no material was successfully isolated.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.09 (d, J = 0.9 Hz, 1H), 8.43 (d, J = 6.0 Hz, 1H), 8.27 (d, J = 6.0 Hz, 1H), 7.49 – 7.44 (m, 2H), 7.31 (dd, J = 8.4, 7.0 Hz, 2H), 7.19 (ddt, J = 15.1, 8.6, 1.1 Hz, 2H), 7.11 (t, J = 7.9 Hz, 1H), 6.31 (s, 1H), 6.07 (dd, J = 7.7, 1.1 Hz, 1H), 1.72 (s, 6H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 152.0, 147.1, 141.0, 140.4, 129.2, 128.5, 127.4, 126.4, 126.2, 125.2, 115.4, 114.3, 110.7, 55.7, 29.8.

HRMS (ESI-QTOF): m/z $[M+H]^+$ Calcd for $C_{18}H_{18}N_2$ 263.1543; Found 263.1549. Δ = 2.43 ppm

tert-Butyl 4-{1H-pyrrolo[2,3-b]pyridin-5-yl}piperazine-1-carboxylate (**9**)



Conditions identified on the plate: 5-bromo-1H-pyrrolo[2,3-b]pyridine (49.3 mg, 0.25 mmol), tert-butyl piperazine-1-carboxylate (69.9 mg, 0.38 mmol), [BippyPhos Pd(allyl)]OTf (4.02 mg, 0.005 mmol, 2 mol%) and KHMDS (99.8 mg, 0.50 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous dioxane (2.50 mL, 0.1 M) was added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 60%. The crude product was purified (10g Sfar cartridge, 0–100% EtOAc/Petrol v/v) to afford the title compound as a colourless solid (46.3 mg, 61% yield).

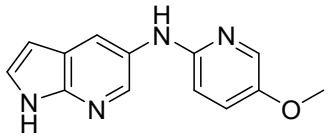
Closest literature conditions[2]: 5-bromo-1H-pyrrolo[2,3-b]pyridine (49.3 mg, 0.25 mmol), tert-butyl piperazine-1-carboxylate (69.9 mg, 0.38 mmol) and RuPhos-Pd-G4 (4.54 mg, 0.005 mmol, 2 mol%) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous THF (2.0 mL, 0.1 M) and LiHMDS (1 M in THF, 0.5 mL, 0.50 mmol) were added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 37%. The crude product was purified (10g Sfar cartridge, 0–100% EtOAc/Petrol v/v) to afford the title compound as a colourless solid (31.0 mg, 41% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.38 (s, 1H), 8.07 (d, *J* = 2.6 Hz, 1H), 7.52 (dd, *J* = 2.7, 0.7 Hz, 1H), 7.38 (dd, *J* = 3.4, 2.5 Hz, 1H), 6.33 (dd, *J* = 3.4, 1.9 Hz, 1H), 3.50 (t, *J* = 5.1 Hz, 4H), 3.06 – 2.99 (m, 4H), 1.44 (s, 9H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 154.3, 144.8, 142.6, 137.0, 126.8, 119.9, 116.4, 99.8, 79.4, 51.6, 28.6.

HRMS (ESI-QTOF): m/z $[M+H]^+$ Calcd for $C_{16}H_{22}N_4O_2$ 303.1812; Found 303.182. Δ = 2.65 ppm

5-methoxy-N-{1H-pyrrolo[2,3-b]pyridin-5-yl}pyridin-2-amine (**10**)



Conditions identified on the plate: 5-bromo-1H-pyrrolo[2,3-b]pyridine (49.3 mg, 0.25 mmol), 5-methoxypyridin-2-amine (46.6 mg, 0.38 mmol), BrettPhos-Pd-G4 (4.54 mg, 0.005 mmol, 2 mol%) and t-BuOK (56.2 mg, 0.50 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous dioxane (2.50 mL, 0.1 M) was added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 76%. The crude product was purified (10g Sfar cartridge, 0–100% EtOAc/Petrol v/v) to afford the title compound as a beige solid (52.0 mg, 86% yield).

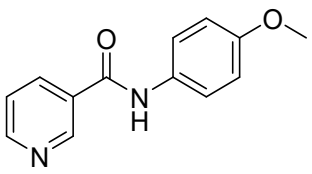
Closest literature conditions[2]: 5-bromo-1H-pyrrolo[2,3-b]pyridine (49.3 mg, 0.25 mmol), 5-methoxypyridin-2-amine (46.6 mg, 0.38 mmol) and BrettPhos-Pd-G3 (4.54 mg, 0.005 mmol, 2 mol%) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous dioxane (2.50 mL, 0.1 M) and LiHMDS (1 M in THF, 0.5 mL, 0.50 mmol) were added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 46%. The crude product was purified (10g Sfar cartridge, 0–100% EtOAc/Petrol v/v) to afford the title compound as a beige solid (30.2 mg, 50% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.35 (s, 1H), 8.62 (s, 1H), 8.32 (dd, *J* = 2.4, 0.7 Hz, 1H), 8.25 (d, *J* = 2.4 Hz, 1H), 7.87 (dd, *J* = 3.1, 0.7 Hz, 1H), 7.37 (dd, *J* = 3.4, 2.5 Hz, 1H), 7.28 (dd, *J* = 9.0, 3.1 Hz, 1H), 6.78 (dd, *J* = 9.0, 0.7 Hz, 1H), 6.36 (dd, *J* = 3.4, 1.9 Hz, 1H), 3.75 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 151.4, 148.8, 144.2, 136.1, 132.3, 132.2, 126.2, 125.4, 119.3, 117.1, 110.6, 99.4, 56.0.

HRMS (ESI-QTOF): m/z $[M+H]^+$ Calcd for $C_{13}H_{12}N_4O$ 241.1085; Found 241.1086. Δ = 0.24 ppm.

N-(4-methoxyphenyl)pyridine-3-carboxamide (**11**)



Conditions identified on the plate: 1-bromo-4-methoxybenzene (46.8 mg, 0.25 mmol), nitcotinamide (45.8 mg, 0.38 mmol), AdBrettPhos-Pd-G3 (5.06 mg, 0.005 mmol, 2 mol%) and Cs_2CO_3 (163.0 mg, 0.50 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous t-AmOH (2.50 mL, 0.1 M) was added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 92%. The crude material was dissolved in the minimum amount of EtOAc and a precipitate formed, which was collected under vacuum, washed with EtOAc, giving the title compound[5] as a cream solid (49.8 mg, 87% yield).

Exact literature conditions [4]: 1-bromo-4-methoxybenzene (46.8 mg, 0.25 mmol), nitcotinamide (45.8 mg, 0.38 mmol), ^{t}BuBrettPhos-Pd-G3 (5.06 mg, 0.005 mmol, 2 mol%) and K_3PO_4 (74.4 mg, 0.35 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). t-BuOH (0.5 mL, 0.5 M) was added to the vial, which was then heated to 110 ˚C for 6 h. Crude reaction LCAP for desired product = 86%. The crude material was dissolved in the minimum amount of EtOAc and a precipitate formed, which was collected under vacuum, washed with EtOAc, giving the title compound[5] as a cream solid (47.1 mg, 82% yield).

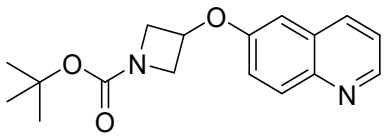
Characterization data matches the literature[4]

^{1}H NMR (400 MHz, MeOD) δ 9.07 (dd, *J* = 2.3, 0.9 Hz, 1H), 8.71 (dd, *J* = 4.9, 1.6 Hz, 1H), 8.34 (ddd, *J* = 8.0, 2.3, 1.6 Hz, 1H), 7.63 – 7.54 (m, 3H), 6.98 – 6.90 (m, 2H), 3.81 (s, 3H).

^{13}C NMR (101 MHz, MeOD) δ 166.2, 158.5, 152.7, 149.3, 137.2, 132.8, 132.4, 125.1, 124.0, 115.0, 55.9.

HRMS (ESI-QTOF): m/z $[M+H]^+$ Calcd for $C_{13}H_{12}N_2O_2$ 229.0971; Found 229.0975. Δ = 1.66 ppm

tert-butyl 3-(quinolin-6-yloxy)azetidine-1-carboxylate (**12**)



Conditions identified on the plate: 6-Chloroquinoline (40.9 mg, 0.25 mmol), 1-Boc-3-(hydroxy)azetidine (65.0 mg, 0.38 mmol), $Me_3(OMe)^tBuXPhos$ Pd G3 (4.11 mg, 0.005 mmol, 2 mol%) and Cs_2CO_3 (163.0 mg, 0.50 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar which was degassed by N_2 sparging (5–10 mins). Anhydrous toluene (2.50 mL, 0.1 M) was added to the vial, which was then heated to 80 ˚C for 16 h. Crude reaction LCAP for desired product = 89%. The crude product was purified by achiral SFC (20:80 MeOH:CO_2; 60mL/min) to afford the title compound as a sticky pale-yellow oil (63.0 mg, 84% yield).

Exact literature conditions[5]: The literature method uses AdCyBrettPhos-Pd-G3, which is not commercially available and thus would need to be synthesised, this is prohibitive, so this method cannot be repeated.

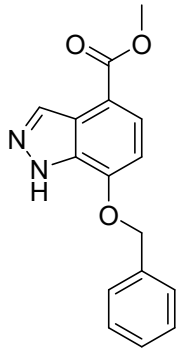
Characterization data matches the literature[5]

^{1}H NMR (400 MHz, MeOD) δ 8.70 (dd, J = 4.4, 1.7 Hz, 1H), 8.27 (ddd, J = 8.2, 1.7, 0.8 Hz, 1H), 8.00 – 7.93 (m, 1H), 7.47 (ddd, J = 20.5, 8.8, 3.5 Hz, 2H), 7.09 (d, J = 2.8 Hz, 1H), 5.14 (tt, J = 6.4, 3.9 Hz, 1H), 4.49 – 4.40 (m, 2H), 3.99 (dd, J = 10.4, 3.6 Hz, 2H), 1.46 (s, 9H).

^{13}C NMR (101 MHz, MeOD) δ 158.1, 156.4, 149.1, 145.1, 137.3, 131.0, 130.9, 123.9, 122.9, 107.9, 81.4, 67.5, 28.6.

HRMS (ESI-QTOF): m/z $[M+H]^+$ Calcd for $C_{17}H_{20}N_2O_3$ 301.1547; Found 301.1551. Δ = 1.45 ppm

methyl 7-(benzyloxy)-1H-indazole-4-carboxylate (**15**)



Conditions identified on the plate: Methyl 7-fluoro-1H-indazole-4-caroxylate (48.5 mg, 0.25 mmol), benzyl alcohol (40.5 mg, 0.38 mmol), KHMDS (199.0 mg, 0.5 mmol) and CsF (15.2 mg, 0.01 mmol) were weighed into a crimp top glass vial (2–5 mL vial Biotage, 354833) equipped with a magnetic stir bar. NMP (2.50 mL, 0.1 M) was added to the vial, which was then heated to 80 ˚C for 16 h. Again, in the LCMS of the crude reaction the trans esterified product was observed therefore MeOH (1 mL) was added, and the reaction was heated to 60 ˚C for 3 h. Crude reaction LCAP for desired product = 61%. The crude product was purified (10g Sfar cartridge, 0–100% EtOAc/Petrol v/v) to afford the title compound as a colourless oil (59.9 mg, 85% yield).

Closest literature conditions: There are no exact or similar reactions on SciFinder^n for this heterocycle.

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.74 – 13.69 (m, 1H), 8.37 – 8.33 (m, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.62 – 7.55 (m, 2H), 7.48 – 7.32 (m, 3H), 7.06 (d, *J* = 8.1 Hz, 1H), 5.41 (s, 2H), 3.89 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 165.9, 148.4, 136.2, 134.1, 132.1, 128.5, 128.1, 127.8, 126.3, 122.9, 114.0, 105.6, 69.9, 51.7.

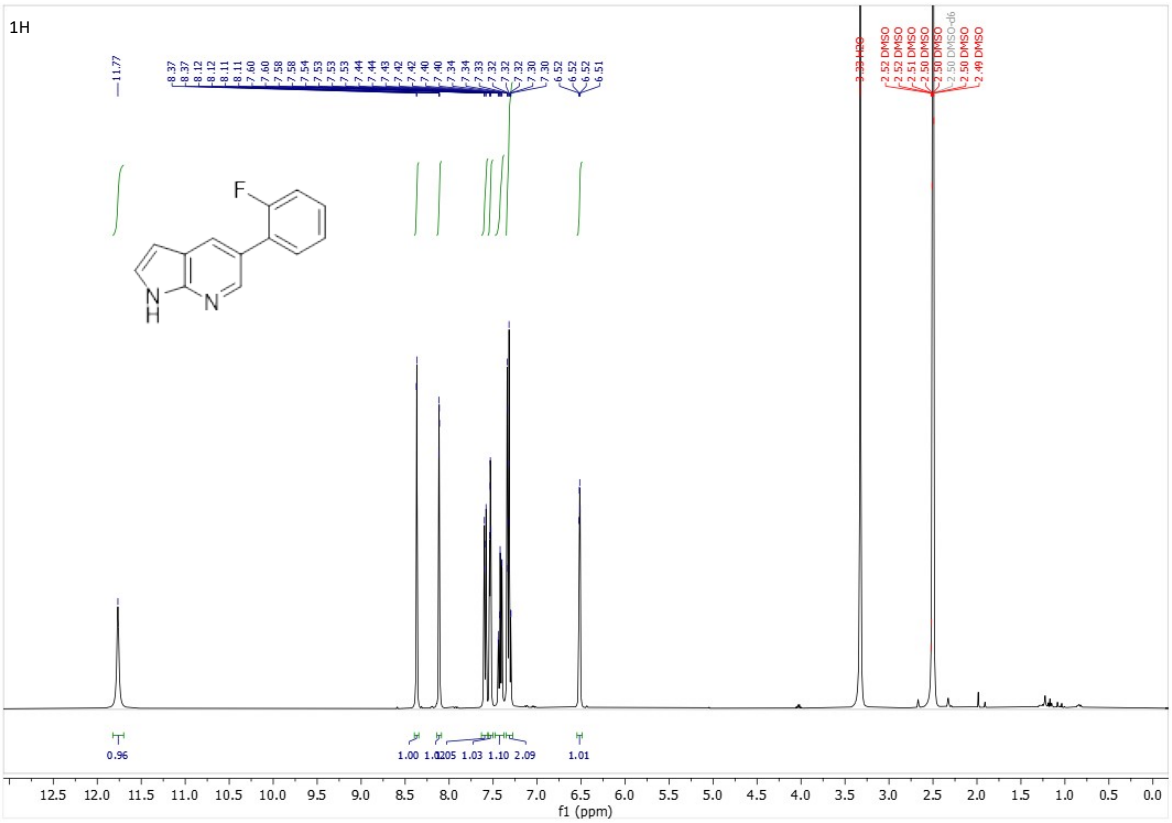
HRMS (ESI-QTOF): m/z $[M+H]^+$ Calcd for $C_{16}H_{14}N_2O_3$ 283.1076; Found 283.1079. Δ = 0.93 ppm

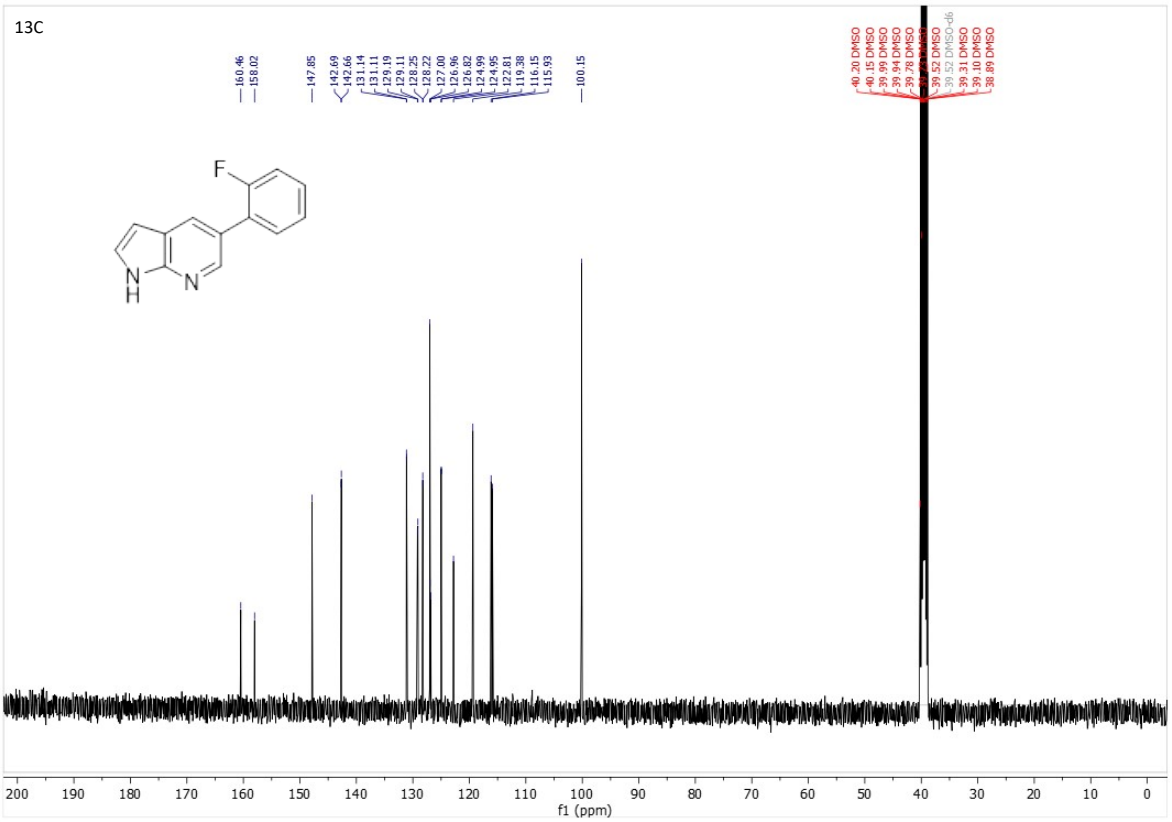
Experimental References

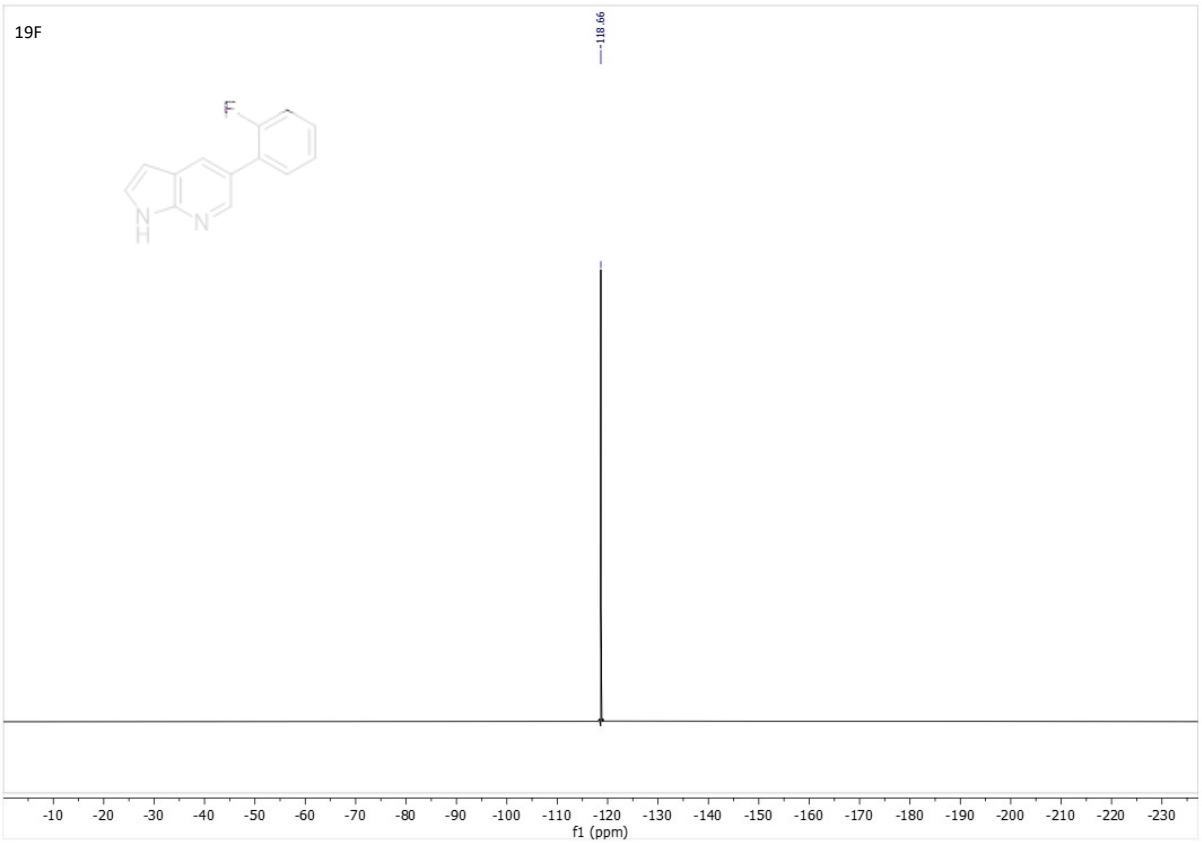
1. Kaneko, Takushi; et al. World Intellectual Property Organization, WO2021062316 A1 2021-04-01
2. Henderson, J. L. McDermott, S. M. Buchwald, S. L. *Org. Lett.*, **12**, 4438-4441 (2010).
3. Ruiz-Castillo, P. Blackmond, D. G. Buchwald, S. L. J. Am. Chem. Socs., **137**, 3085-3092 (2015).
4. Fors, B. P. Dooleweerdt, K. Zeng, Q. Buchwald, S. L. *Tetrahedron*, **65**, 6576–6583 (2009).
5. Zhang, H. Ruiz-Castillo, P. Schuppe, A. W., Buchwald, S. L. *Org. Lett.*, **22**, 14, 5369–5374 (2020).

NMR spectra

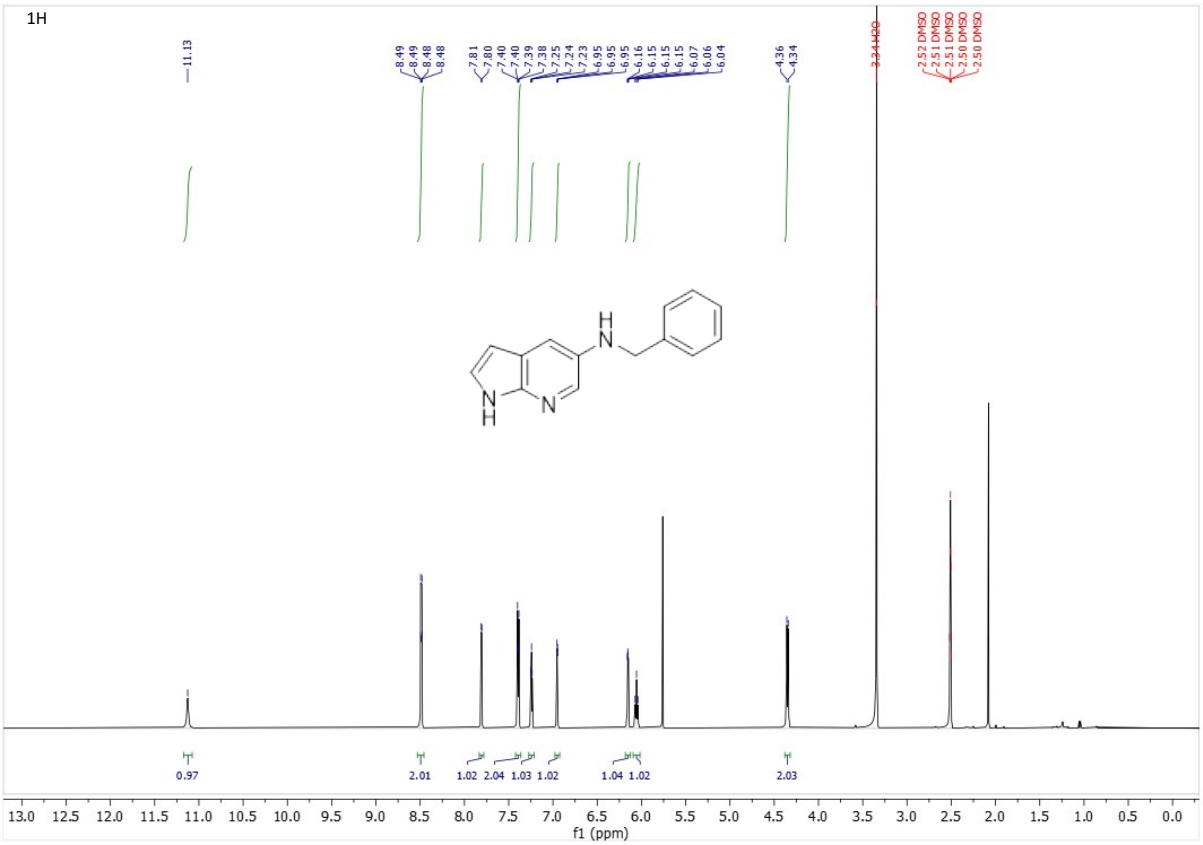
5-(2-fluorophenyl)-1H-pyrrolo[2,3-b]pyridine (3)

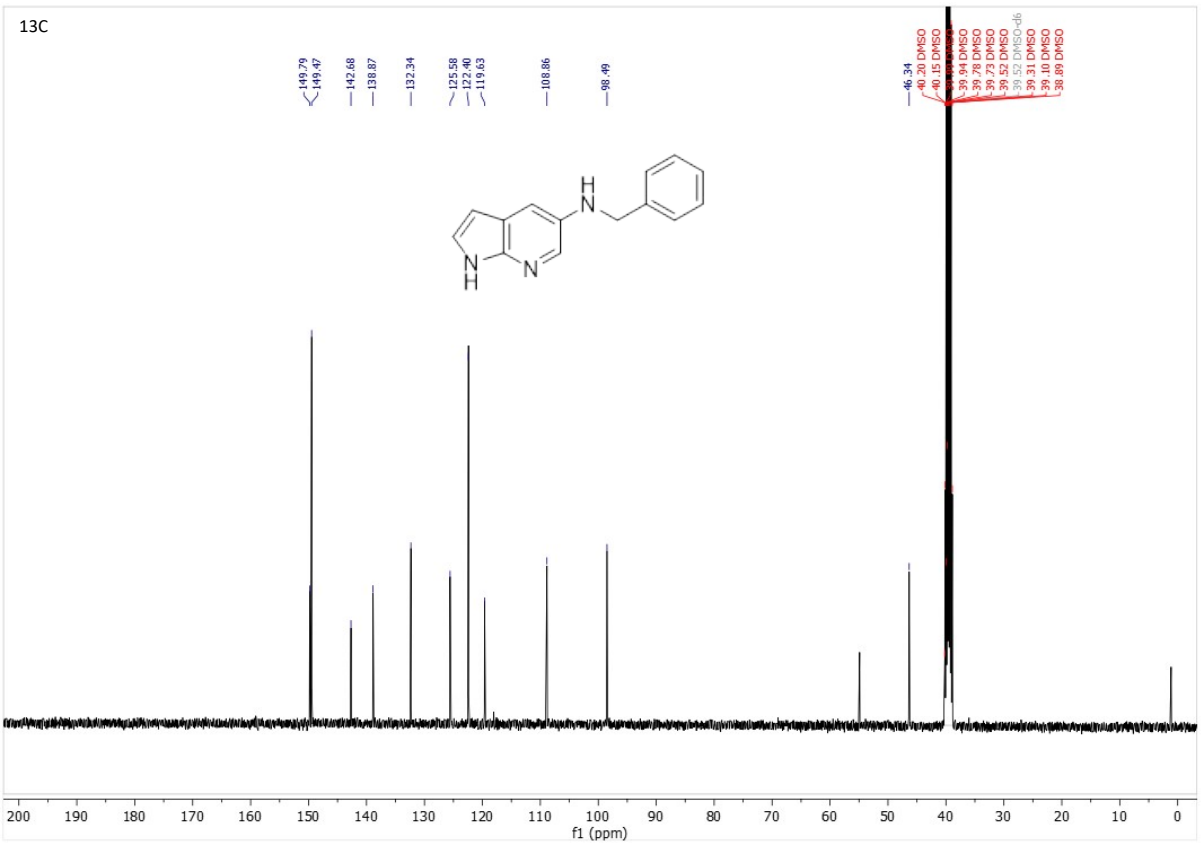




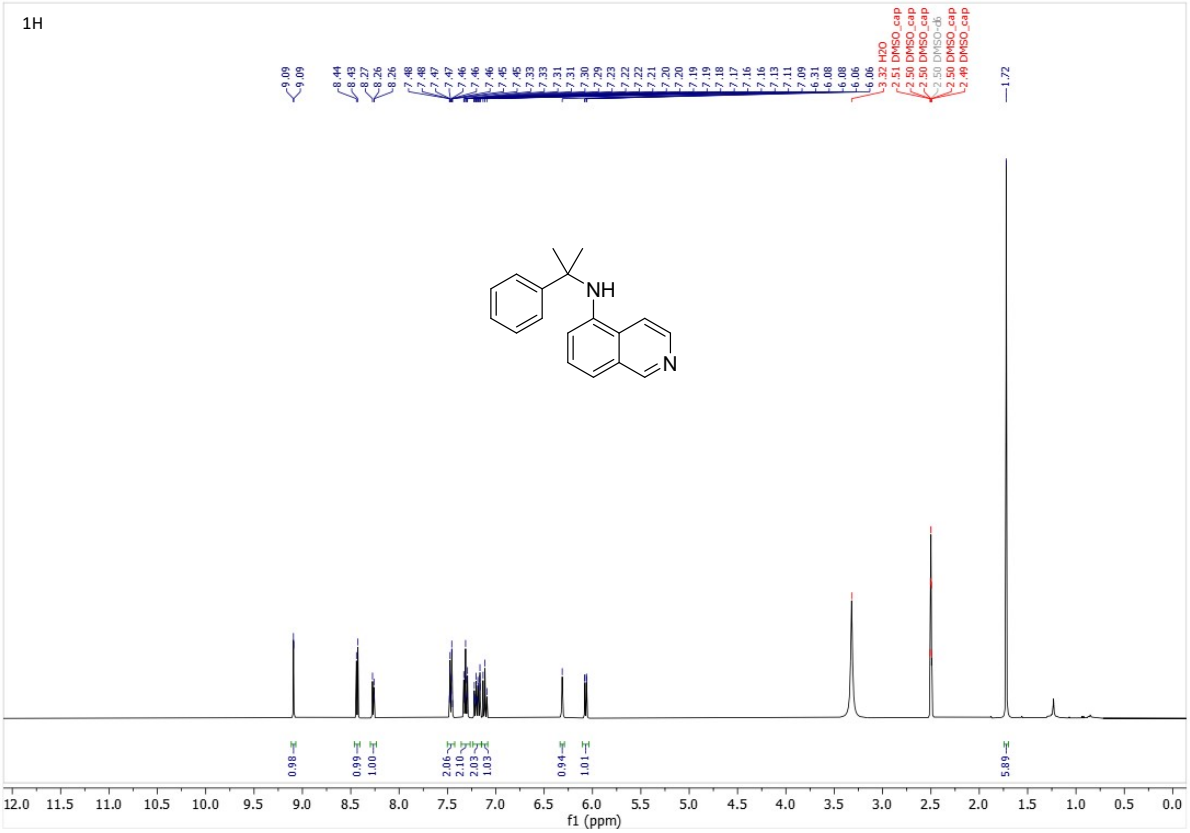

19F
-118.66
F
N
H
N
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230
f1 (ppm)

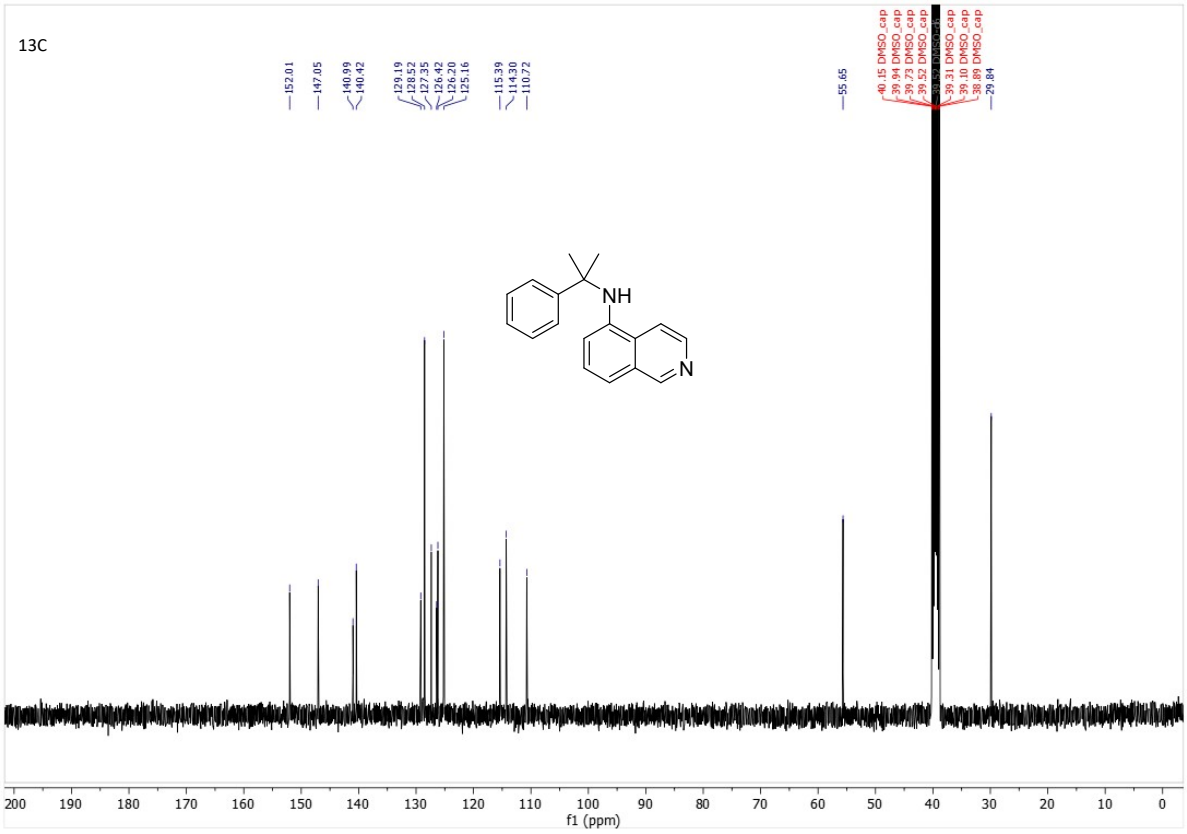
***N*-[(pyridin-4-yl)methyl]-1H-pyrrolo[2,3-b]pyridin-5-amine (4)**



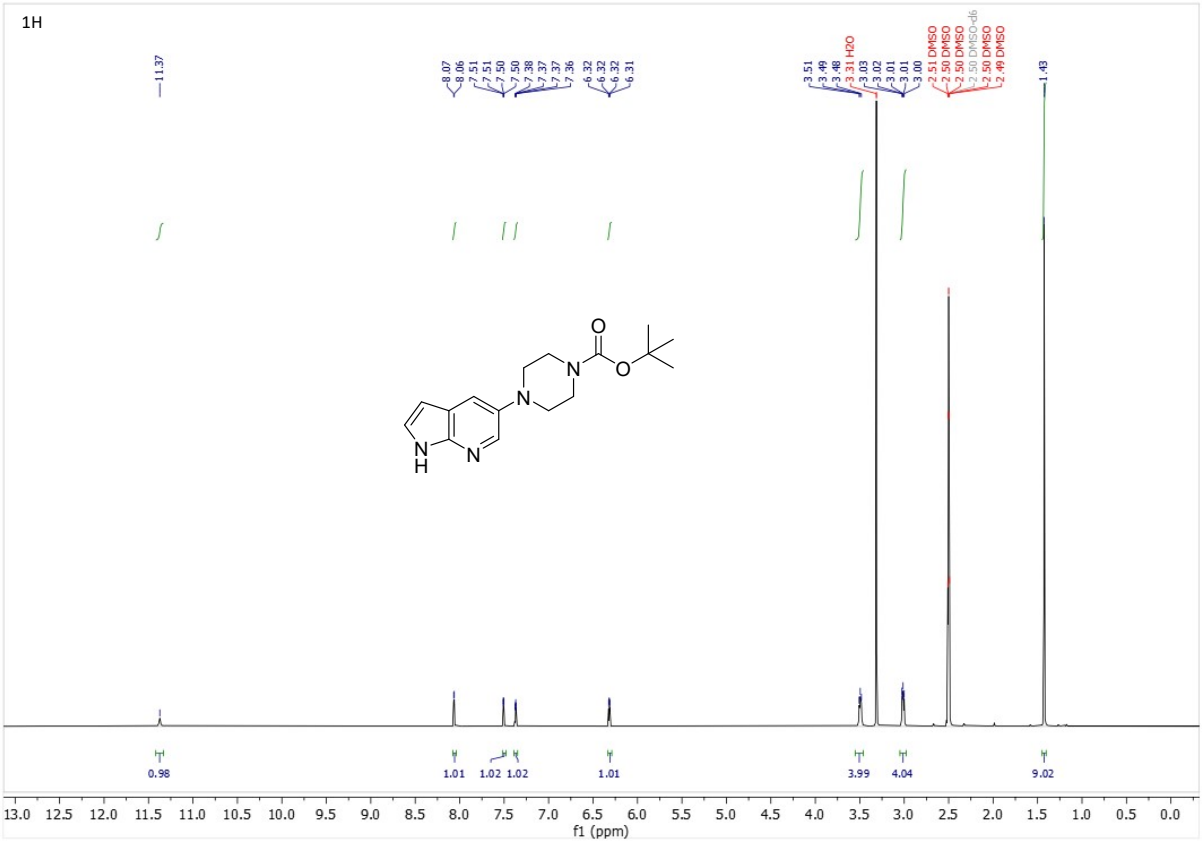


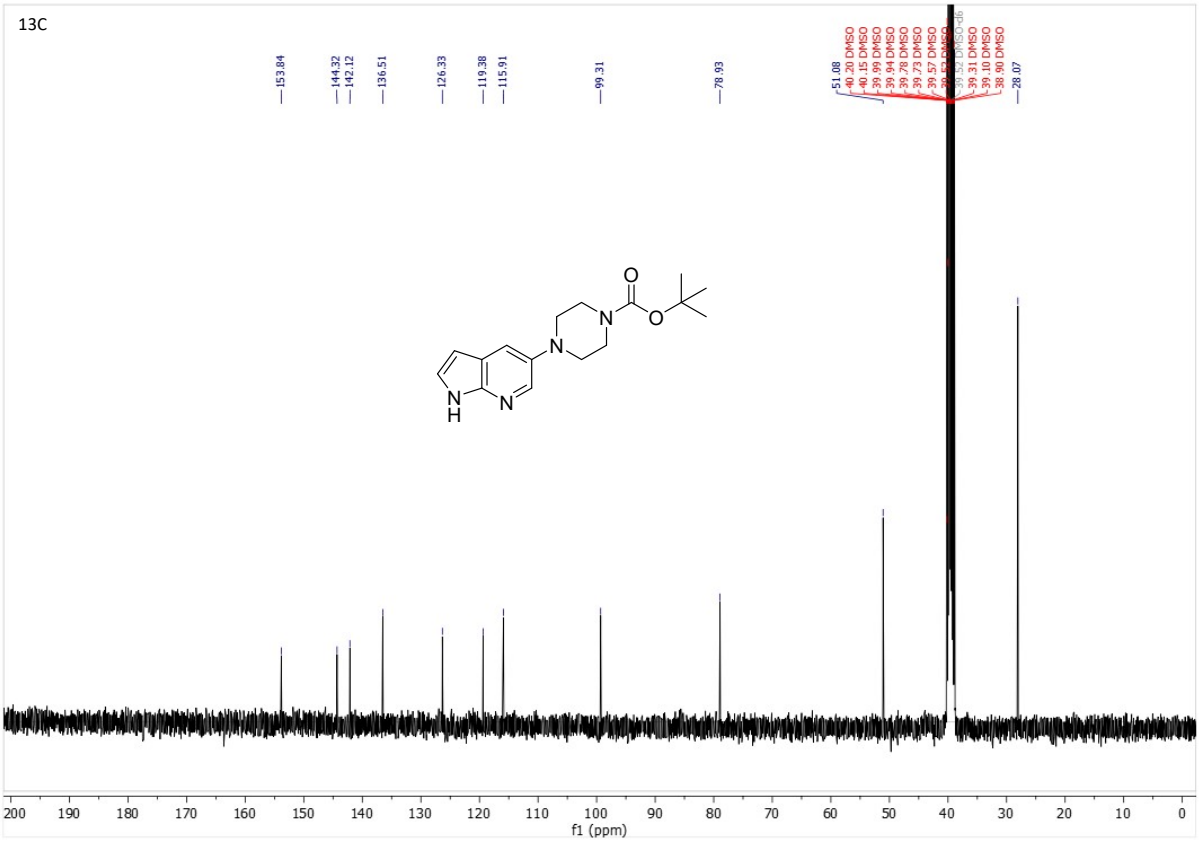
N-(2-phenylpropan-2-yl)isoquinolin-5-amine (5)



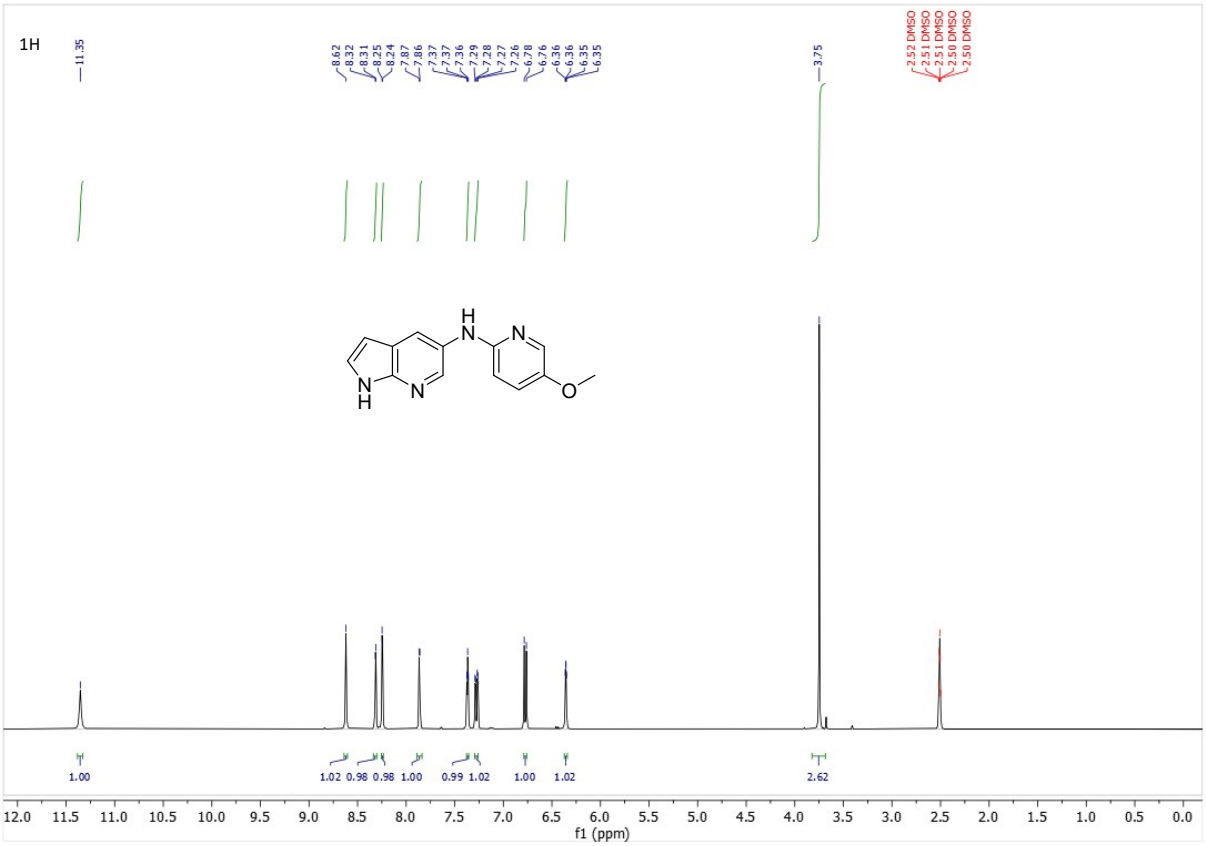


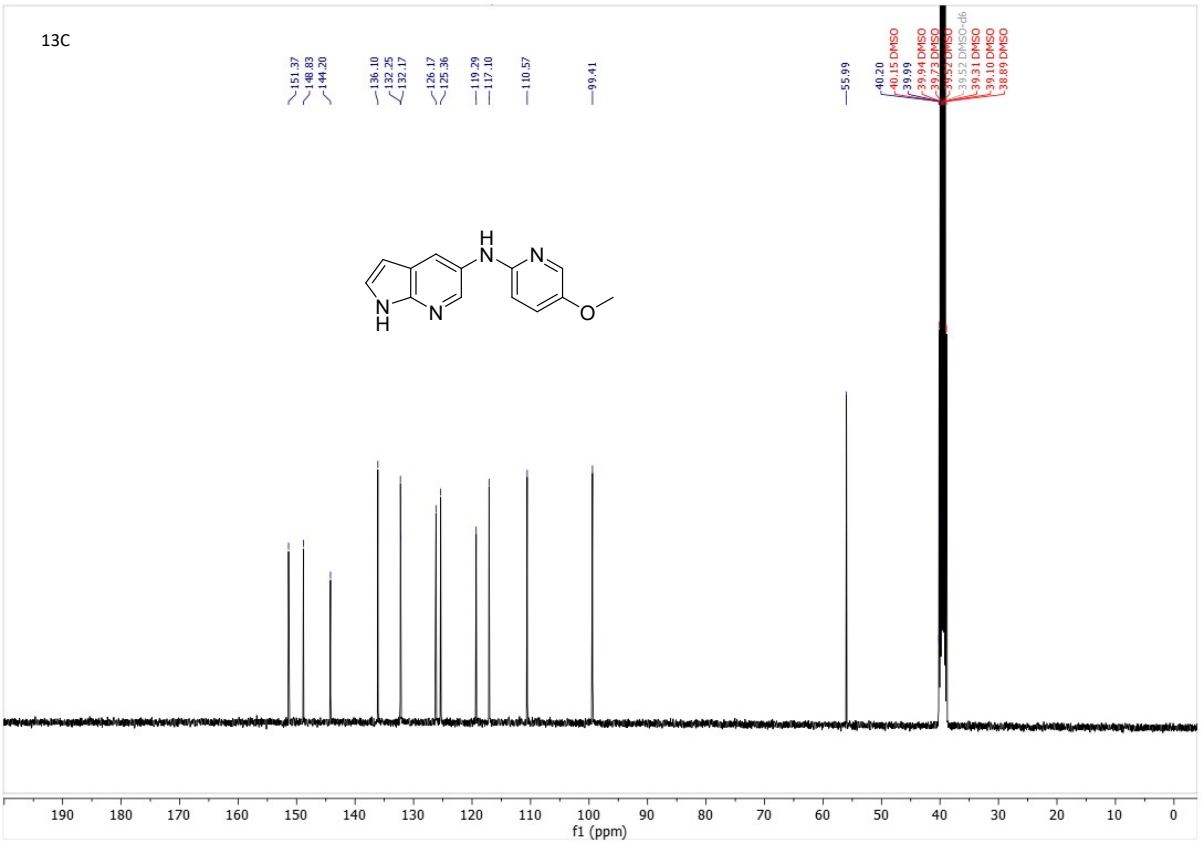
***tert*-Butyl 4-{1H-pyrrolo[2,3-b]pyridin-5-yl}piperazine-1-carboxylate (9)**



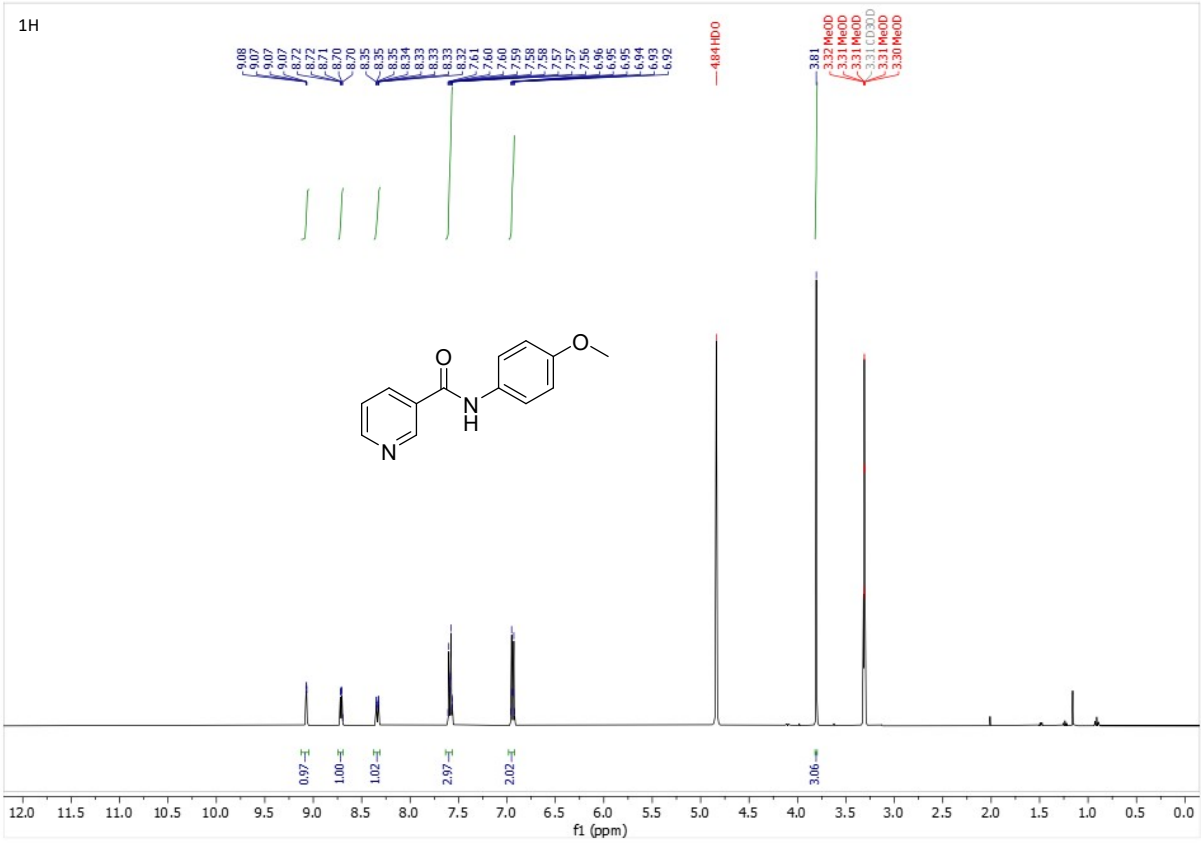


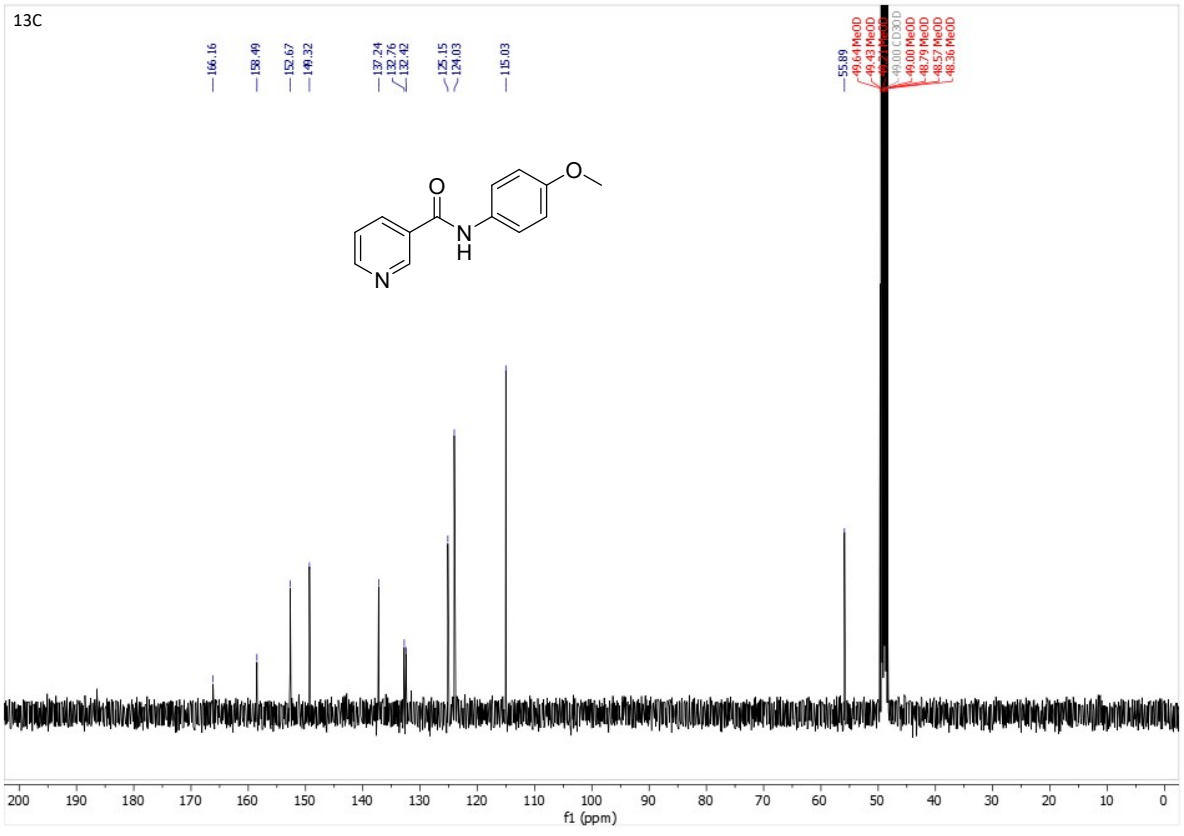
5-methoxy-N-{1H-pyrrolo[2,3-b]pyridin-5-yl}pyridin-2-amine (10)



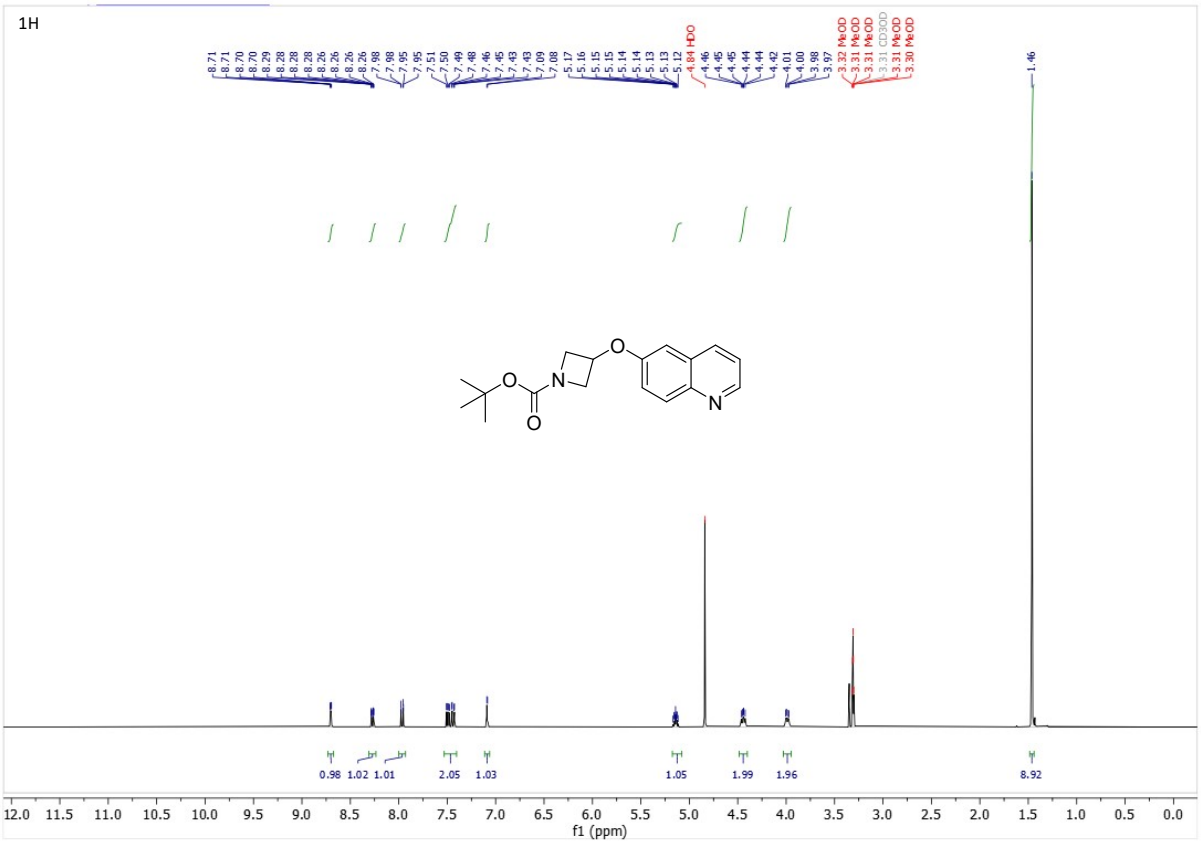


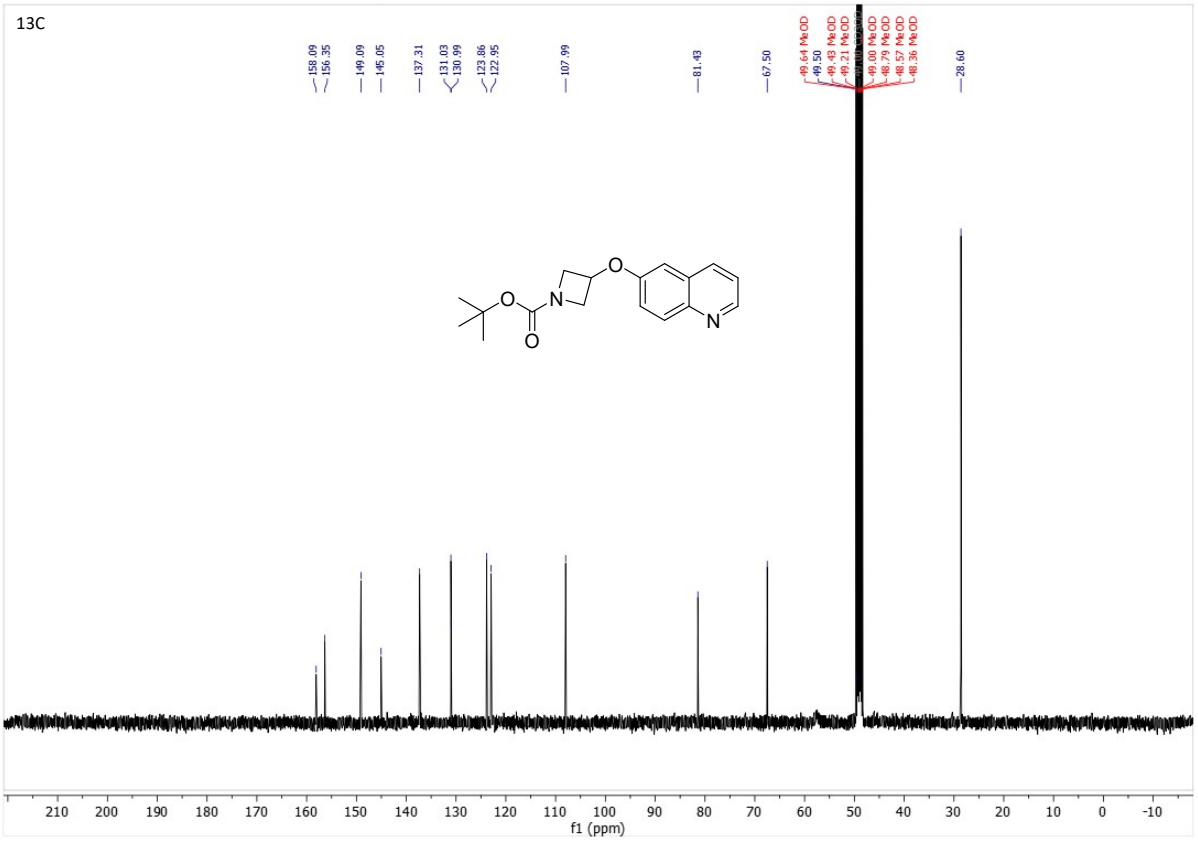
***N*-(4-methoxyphenyl)pyridine-3-carboxamide (11)**[4]



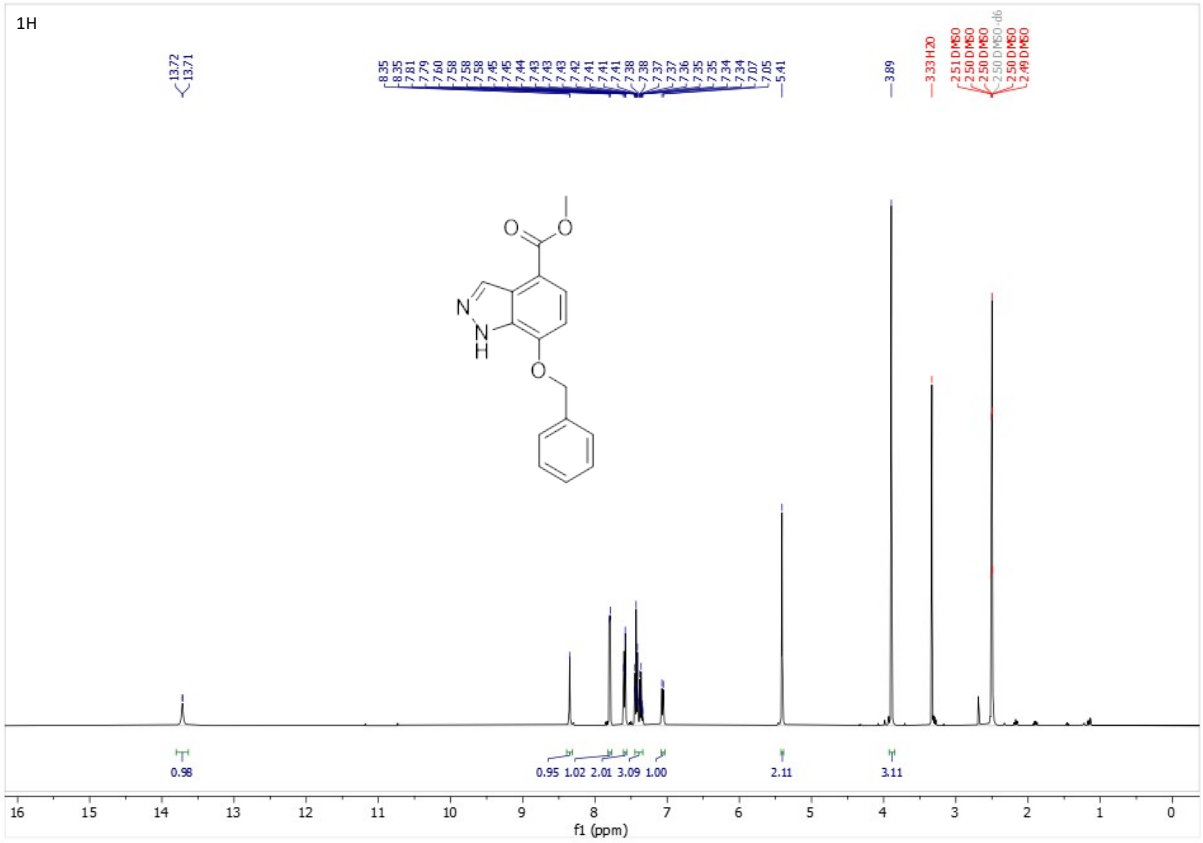


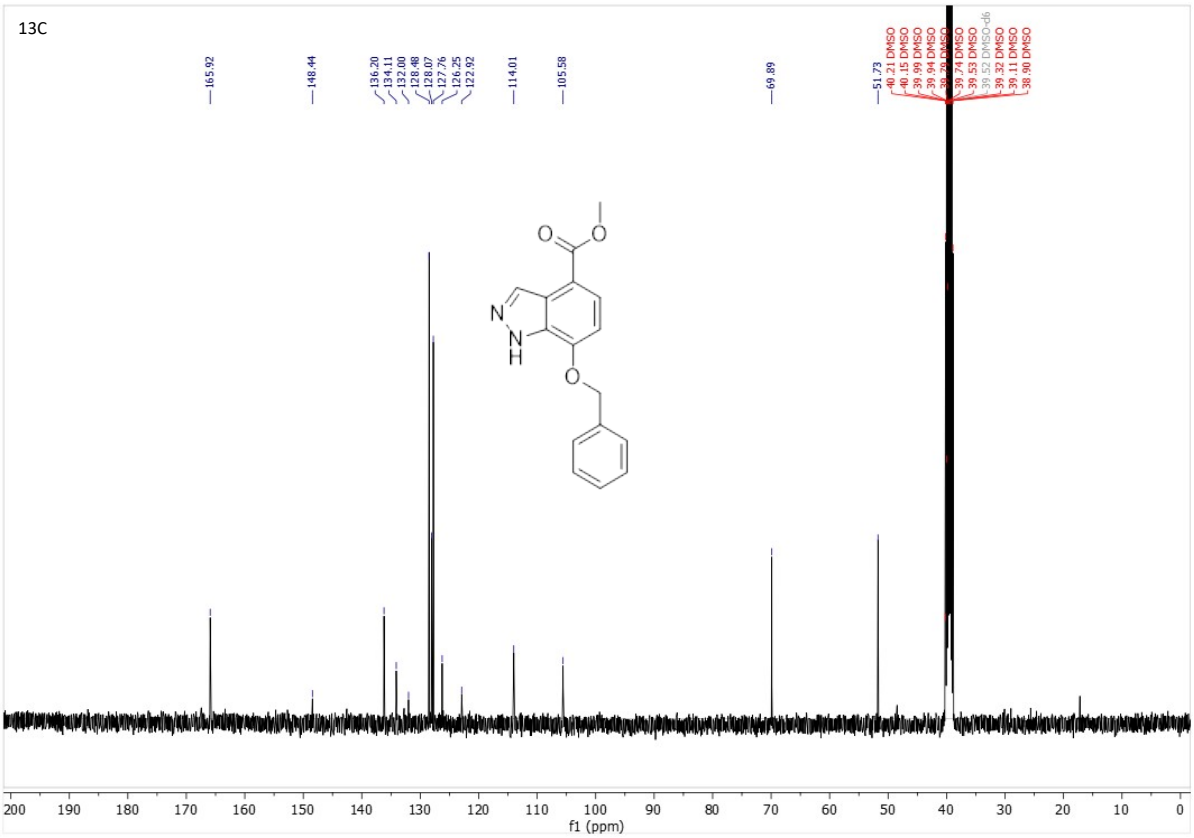
***tert*-butyl 3-(quinolin-6-yloxy)azetidine-1-carboxylate (12)**[5]





methyl 7-(benzyloxy)-1H-indazole-4-carboxylate





Tabulated MISER data:

Suzuki-Miyaura screening kit

Cell ID	Desired Product (%) 5-(2-fluorophenyl-1H-pyrrolo[2,3-b]pyridine Max Resp:464370.2 m/z:213	Reactant (%) 5-bromo-1H-pyrrolo[2,3-b]pyridine Max Resp:67047.5 m/z:197	Components
E11	100.00	9.84	APhos-Pd-G3: 0.13 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
A8	91.10	23.10	DTBPF-Pd-G3: 0.17 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
E5	78.95	9.23	APhos-Pd-G3: 0.13 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
A11	76.17	5.08	APhos-Pd-G3: 0.13 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
B9	68.14	11.65	PCy3-Pd-G4: 0.13 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
C11	67.42	17.60	APhos-Pd-G3: 0.13 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
D9	66.73	20.29	PCy3-Pd-G4: 0.13 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
F9	62.82	15.12	PCy3-Pd-G4: 0.13 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
C10	58.30	100.00	XPhos-Pd-G3: 0.17 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
A3	54.70	8.36	cataCXium A-Pd-G3: 0.15 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
D3	50.41	18.28	PCy3-Pd-G4: 0.13 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
E3	48.89	50.28	cataCXium A-Pd-G3: 0.15 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
C9	48.30	28.66	cataCXium A-Pd-G3: 0.15 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
F3	47.67	12.69	PCy3-Pd-G4: 0.13 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
D12	45.28	31.62	IPr(h3-indenyl)PdCl: 0.14 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL

F11	44.81	28.59	Pd(dppf)Cl2: 0.13 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
A9	44.49	0.00	cataCXium A-Pd-G3: 0.15 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
A5	44.10	27.51	APhos-Pd-G3: 0.13 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
G11	40.67	17.83	APhos-Pd-G3: 0.13 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
E12	40.04	26.33	RuPhos-Pd-G4: 0.17 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
F12	39.78	30.50	IPr(h3-indenyl)PdCl: 0.14 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
A2	39.06	7.54	DTBPF-Pd-G3: 0.17 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
F10	36.25	18.51	DavePhos-Pd-G3: 0.15 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
H8	30.93	35.02	P(t-Bu)3-Pd-G4: 0.11 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
H6	30.28	27.37	IPr(h3-indenyl)PdCl: 0.14 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
G8	29.69	38.02	DTBPF-Pd-G3: 0.17 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
C3	27.73	61.67	cataCXium A-Pd-G3: 0.15 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
D6	26.70	0.00	IPr(h3-indenyl)PdCl: 0.14 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
E10	26.57	31.48	XPhos-Pd-G3: 0.17 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
F7	26.35	32.54	BrettPhos-Pd-G3: 0.18 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
B3	25.86	9.86	PCy3-Pd-G4: 0.13 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
F6	24.74	9.48	IPr(h3-indenyl)PdCl: 0.14 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
C5	24.56	8.35	APhos-Pd-G3: 0.13 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
C2	24.15	58.05	DTBPF-Pd-G3: 0.17 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
H11	22.58	53.75	Pd(dppf)Cl2: 0.13 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
E2	22.47	0.00	DTBPF-Pd-G3: 0.17 mg CsF: 3.04 mg dioxane:

			80.00 uL H2O: 20.00 uL
E9	22.44	0.00	cataCXium A-Pd-G3: 0.15 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
H1	21.08	50.65	BrettPhos-Pd-G3: 0.18 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
B11	19.90	44.60	Pd(dppf)Cl2: 0.13 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
B7	19.20	53.62	BrettPhos-Pd-G3: 0.18 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
H12	19.10	48.89	IPr(h3-indenyl)PdCl: 0.14 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
A12	17.29	52.22	RuPhos-Pd-G4: 0.17 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
E8	16.97	0.00	DTBPF-Pd-G3: 0.17 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
B2	16.40	38.03	P(t-Bu)3-Pd-G4: 0.11 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
D11	15.83	33.94	Pd(dppf)Cl2: 0.13 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
F1	15.70	55.43	BrettPhos-Pd-G3: 0.18 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
D8	15.37	7.19	P(t-Bu)3-Pd-G4: 0.11 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
B10	15.26	56.55	DavePhos-Pd-G3: 0.15 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
B6	13.91	49.46	IPr(h3-indenyl)PdCl: 0.14 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
G2	13.13	14.96	DTBPF-Pd-G3: 0.17 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
E7	13.12	12.13	SPhos-Pd-G3: 0.16 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
H2	12.99	33.61	P(t-Bu)3-Pd-G4: 0.11 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
F5	11.37	46.61	Pd(dppf)Cl2: 0.13 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
G5	11.32	11.57	APhos-Pd-G3: 0.13 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
C8	10.74	0.00	DTBPF-Pd-G3: 0.17 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
C6	10.52	33.38	RuPhos-Pd-G4: 0.17 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL

A6	10.05	58.15	RuPhos-Pd-G4: 0.17 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
F8	9.13	5.27	P(t-Bu)3-Pd-G4: 0.11 mg CsF: 3.04 mg t-AmOH: 80.00 uL H2O: 20.00 uL
E6	9.13	0.00	RuPhos-Pd-G4: 0.17 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
C12	9.04	32.99	RuPhos-Pd-G4: 0.17 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
B8	8.84	5.77	P(t-Bu)3-Pd-G4: 0.11 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
G12	8.47	35.19	RuPhos-Pd-G4: 0.17 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
D1	8.09	54.89	BrettPhos-Pd-G3: 0.18 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
D5	8.02	33.17	Pd(dppf)Cl2: 0.13 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
D4	7.94	38.07	DavePhos-Pd-G3: 0.15 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
F2	7.80	31.24	P(t-Bu)3-Pd-G4: 0.11 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
H7	7.74	36.12	BrettPhos-Pd-G3: 0.18 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
D2	7.72	22.20	P(t-Bu)3-Pd-G4: 0.11 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
E4	7.64	0.00	XPhos-Pd-G3: 0.17 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
H5	7.08	52.56	Pd(dppf)Cl2: 0.13 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
G3	6.91	44.73	cataCXium A-Pd-G3: 0.15 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
B1	6.56	37.84	BrettPhos-Pd-G3: 0.18 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
A4	6.32	54.62	XPhos-Pd-G3: 0.17 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
D10	6.03	19.06	DavePhos-Pd-G3: 0.15 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
A7	5.98	54.77	SPhos-Pd-G3: 0.16 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
H3	5.85	8.93	PCy3-Pd-G4: 0.13 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
G9	5.69	13.52	cataCXium A-Pd-G3: 0.15 mg NaOH: 0.80

			mg t-AmOH: 80.00 uL H2O: 20.00 uL
B5	5.59	13.34	Pd(dppf)Cl2: 0.13 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
G10	5.54	40.36	XPhos-Pd-G3: 0.17 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
A10	5.51	5.89	XPhos-Pd-G3: 0.17 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
F4	5.21	10.19	DavePhos-Pd-G3: 0.15 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
G6	5.14	35.56	RuPhos-Pd-G4: 0.17 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
C1	4.69	62.39	SPhos-Pd-G3: 0.16 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL
H10	3.88	10.10	DavePhos-Pd-G3: 0.15 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
D7	3.40	5.18	BrettPhos-Pd-G3: 0.18 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
G7	3.17	32.14	SPhos-Pd-G3: 0.16 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
C7	2.89	7.80	SPhos-Pd-G3: 0.16 mg K3PO4: 4.25 mg t-AmOH: 80.00 uL H2O: 20.00 uL
G1	2.86	57.22	SPhos-Pd-G3: 0.16 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
E1	2.67	0.00	SPhos-Pd-G3: 0.16 mg CsF: 3.04 mg dioxane: 80.00 uL H2O: 20.00 uL
H9	2.48	14.51	PCy3-Pd-G4: 0.13 mg NaOH: 0.80 mg t-AmOH: 80.00 uL H2O: 20.00 uL
A1	1.81	65.55	SPhos-Pd-G3: 0.16 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
B4	1.76	6.03	DavePhos-Pd-G3: 0.15 mg K2CO3: 2.76 mg dioxane: 80.00 uL H2O: 20.00 uL
B12	1.60	54.84	IPr(h3-indenyl)PdCl: 0.14 mg K2CO3: 2.76 mg t-AmOH: 80.00 uL H2O: 20.00 uL
H4	1.56	9.77	DavePhos-Pd-G3: 0.15 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
G4	1.34	8.34	XPhos-Pd-G3: 0.17 mg NaOH: 0.80 mg dioxane: 80.00 uL H2O: 20.00 uL
C4	0.77	6.03	XPhos-Pd-G3: 0.17 mg K3PO4: 4.25 mg dioxane: 80.00 uL H2O: 20.00 uL

Buchwald-Hartwig primary amine screening kit (primary amine)

Cell ID	Desired Product (%) N-[(pyridin-4-yl)methyl]-1H-pyrrolo[2,3-b]pyridin-5-amine Max Resp:393248.4 m/z:225	Reactant (%) 5-bromo-1H-pyrrolo[2,3-b]pyridine Max Resp:46931.4 m/z:197	Components
B2	100.00	20.87	AdBrettPhos Pd G3: 0.20 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
C7	77.94	0.00	DMPDAB Pd MAH: 0.09 mg Ad-BippyPhos: 0.13 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
A10	68.87	0.00	tBuBrettPhos Pd G3: 0.17 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
D2	64.31	26.04	AdBrettPhos Pd G3: 0.20 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C10	63.90	0.00	tBuBrettPhos Pd G3: 0.17 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
C4	58.03	26.51	tBuBrettPhos Pd G3: 0.17 mg KHMDS: 3.99 mg dioxane: 100.00 uL
B6	56.23	27.63	Gphos Pd G3: 0.18 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B1	47.00	52.02	Me3(OMe)tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B7	42.03	16.42	Me3(OMe)tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
C12	34.14	16.89	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
B8	22.66	0.00	AdBrettPhos Pd G3: 0.20 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
D12	22.40	19.13	Gphos Pd G3: 0.18 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
B12	16.56	11.76	Gphos Pd G3: 0.18 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A12	14.94	15.05	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
H8	11.18	12.15	P2-Et: 6.66 uL AdBrettPhos Pd G3: 0.20 mg t-AmOH: 100.00 uL

A6	10.53	34.24	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
F2	10.08	35.30	Cs2CO3: 6.52 mg AdBrettPhos Pd G3: 0.20 mg dioxane: 100.00 uL
E7	9.26	29.65	DMPDAB Pd MAH: 0.09 mg Ad-BippyPhos: 0.13 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
C1	8.69	46.96	DMPDAB Pd MAH: 0.09 mg Ad-BippyPhos: 0.13 mg KHMDS: 3.99 mg dioxane: 100.00 uL
E10	6.89	21.10	Cs2CO3: 6.52 mg tBuBrettPhos Pd G3: 0.17 mg t-AmOH: 100.00 uL
B9	6.38	39.56	(tBu)PhCPhos Pd G4: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A7	5.35	0.00	DMPDAB Pd MAH: 0.09 mg Ad-BippyPhos: 0.13 mg T-BuOK: 2.24 mg t-AmOH: 100.00 uL
F7	5.13	18.45	Cs2CO3: 6.52 mg Me3(OMe)tBuXPhos Pd G3: 0.16 mg t-AmOH: 100.00 uL
H2	4.08	0.00	P2-Et: 6.66 uL AdBrettPhos Pd G3: 0.20 mg dioxane: 100.00 uL
G10	3.70	4.34	P2-Et: 6.66 uL tBuBrettPhos Pd G3: 0.17 mg t-AmOH: 100.00 uL
A4	3.63	39.34	tBuBrettPhos Pd G3: 0.17 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A11	2.54	49.06	BrettPhos Pd G3: 0.18 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
C11	2.51	32.09	BrettPhos Pd G3: 0.18 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
G1	2.46	34.70	P2-Et: 6.66 uL DMPDAB Pd MAH: 0.09 mg Ad-BippyPhos: 0.13 mg dioxane: 100.00 uL
B4	2.40	54.00	DMPDAB Pd MAH: 0.09 mg PhCPhos: 0.08 mg T-BuOK: 2.24 mg dioxane: 100.00 uL
H1	2.10	11.09	P2-Et: 6.66 uL Me3(OMe)tBuXPhos Pd G3: 0.16 mg dioxane: 100.00 uL
F1	1.58	36.01	Cs2CO3: 6.52 mg Me3(OMe)tBuXPhos Pd G3: 0.16 mg dioxane: 100.00 uL
F8	1.42	41.61	Cs2CO3: 6.52 mg AdBrettPhos Pd G3: 0.20 mg t-AmOH: 100.00 uL
C2	1.30	50.36	MorDalPhos Pd G4: 0.17 mg KHMDS: 3.99

			mg dioxane: 100.00 uL
H6	1.27	11.67	P2-Et: 6.66 uL Gphos Pd G3: 0.18 mg dioxane: 100.00 uL
D6	1.04	55.97	Gphos Pd G3: 0.18 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C6	1.04	46.33	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D9	1.02	36.14	(tBu)PhCPhos Pd G4: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
G4	0.72	6.91	P2-Et: 6.66 uL tBuBrettPhos Pd G3: 0.17 mg dioxane: 100.00 uL
B5	0.59	45.62	Pd PEPPSI Ipr: 0.14 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A5	0.57	26.80	BrettPhos Pd G3: 0.18 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
F6	0.56	40.12	Cs2CO3: 6.52 mg Gphos Pd G3: 0.18 mg dioxane: 100.00 uL
E12	0.55	24.71	Cs2CO3: 6.52 mg [Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-AmOH: 100.00 uL
A3	0.50	41.66	JosiPhos Pd G3: 0.19 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
D1	0.48	5.38	Me3(OMe)tBuXPhos Pd G3: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D3	0.47	50.44	(tBu)PhCPhos Pd G4: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C5	0.46	37.28	BrettPhos Pd G3: 0.18 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D8	0.42	49.32	AdBrettPhos Pd G3: 0.20 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
B10	0.37	29.76	DMPDAB Pd MAH: 0.09 mg PhCPhos: 0.08 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
D4	0.37	35.01	DMPDAB Pd MAH: 0.09 mg PhCPhos: 0.08 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C3	0.36	14.20	JosiPhos Pd G3: 0.19 mg KHMDS: 3.99 mg dioxane: 100.00 uL
G7	0.35	7.40	P2-Et: 6.66 uL DMPDAB Pd MAH: 0.09 mg Ad-BippyPhos: 0.13 mg t-AmOH: 100.00 uL

H7	0.34	3.63	P2-Et: 6.66 uL Me3(OMe)tBuXPhos Pd G3: 0.16 mg t-AmOH: 100.00 uL
E4	0.29	50.90	tBuBrettPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
A1	0.00	100.00	DMPDAB Pd MAH: 0.09 mg Ad-BippyPhos: 0.13 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A2	0.00	14.78	MorDalPhos Pd G4: 0.17 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A8	0.00	39.43	MorDalPhos Pd G4: 0.17 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A9	0.00	34.07	JosiPhos Pd G3: 0.19 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
B3	0.00	0.00	(tBu)PhCPhos Pd G4: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B11	0.00	36.60	Pd PEPPSI Ipr: 0.14 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
C8	0.00	54.40	MorDalPhos Pd G4: 0.17 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
C9	0.00	20.27	JosiPhos Pd G3: 0.19 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D5	0.00	41.27	Pd PEPPSI Ipr: 0.14 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D7	0.00	41.11	Me3(OMe)tBuXPhos Pd G3: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D10	0.00	34.10	DMPDAB Pd MAH: 0.09 mg PhCPhos: 0.08 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D11	0.00	32.60	Pd PEPPSI Ipr: 0.14 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
E1	0.00	44.98	DMPDAB Pd MAH: 0.09 mg Ad-BippyPhos: 0.13 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E2	0.00	38.32	MorDalPhos Pd G4: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E3	0.00	46.12	JosiPhos Pd G3: 0.19 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E5	0.00	48.24	BrettPhos Pd G3: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E6	0.00	35.60	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL

E8	0.00	41.10	Cs2CO3: 6.52 mg MorDalPhos Pd G4: 0.17 mg t-AmOH: 100.00 uL
E9	0.00	48.02	Cs2CO3: 6.52 mg JosiPhos Pd G3: 0.19 mg t-AmOH: 100.00 uL
E11	0.00	22.26	Cs2CO3: 6.52 mg BrettPhos Pd G3: 0.18 mg t-AmOH: 100.00 uL
F3	0.00	32.93	Cs2CO3: 6.52 mg (tBu)PhCPhos Pd G4: 0.16 mg dioxane: 100.00 uL
F4	0.00	49.77	Cs2CO3: 6.52 mg DMPDAB Pd MAH: 0.09 mg PhCPhos: 0.08 mg dioxane: 100.00 uL
F5	0.00	39.18	Cs2CO3: 6.52 mg Pd PEPPSI Ipr: 0.14 mg dioxane: 100.00 uL
F9	0.00	37.26	Cs2CO3: 6.52 mg (tBu)PhCPhos Pd G4: 0.16 mg t-AmOH: 100.00 uL
F10	0.00	36.96	Cs2CO3: 6.52 mg DMPDAB Pd MAH: 0.09 mg PhCPhos: 0.08 mg t-AmOH: 100.00 uL
F11	0.00	17.61	Cs2CO3: 6.52 mg Pd PEPPSI Ipr: 0.14 mg t-AmOH: 100.00 uL
F12	0.00	21.22	Cs2CO3: 6.52 mg Gphos Pd G3: 0.18 mg t-AmOH: 100.00 uL
G2	0.00	7.43	P2-Et: 6.66 uL MorDalPhos Pd G4: 0.17 mg dioxane: 100.00 uL
G3	0.00	8.45	P2-Et: 6.66 uL JosiPhos Pd G3: 0.19 mg dioxane: 100.00 uL
G5	0.00	7.49	P2-Et: 6.66 uL BrettPhos Pd G3: 0.18 mg dioxane: 100.00 uL
G6	0.00	8.10	P2-Et: 6.66 uL [Pd(bippyPhos)(allyl)]OTf: 0.16 mg dioxane: 100.00 uL
G8	0.00	15.96	P2-Et: 6.66 uL MorDalPhos Pd G4: 0.17 mg t-AmOH: 100.00 uL
G9	0.00	12.35	P2-Et: 6.66 uL JosiPhos Pd G3: 0.19 mg t-AmOH: 100.00 uL
G11	0.00	0.00	P2-Et: 6.66 uL BrettPhos Pd G3: 0.18 mg t-AmOH: 100.00 uL
G12	0.00	5.50	P2-Et: 6.66 uL [Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-AmOH: 100.00 uL
H3	0.00	7.36	P2-Et: 6.66 uL (tBu)PhCPhos Pd G4: 0.16 mg dioxane: 100.00 uL
H4	0.00	10.81	P2-Et: 6.66 uL DMPDAB Pd MAH: 0.09 mg PhCPhos: 0.08 mg dioxane: 100.00 uL
H5	0.00	3.46	P2-Et: 6.66 uL Pd PEPPSI Ipr: 0.14

			mg dioxane: 100.00 uL
H9	0.00	4.67	P2-Et: 6.66 uL (tBu)PhCPhos Pd G4: 0.16 mg t-AmOH: 100.00 uL
H10	0.00	9.61	P2-Et: 6.66 uL DMPDAB Pd MAH: 0.09 mg PhCPhos: 0.08 mg t-AmOH: 100.00 uL
H11	0.00	6.63	P2-Et: 6.66 uL Pd PEPPSI Ipr: 0.14 mg t-AmOH: 100.00 uL
H12	0.00	3.04	P2-Et: 6.66 uL Gphos Pd G3: 0.18 mg t-AmOH: 100.00 uL

Buchwald-Hartwig primary amine screening plate (sterically hindered primary amine)

Cell ID	Desired Product (%) N-(2-phenylpropan-2-yl)quinolin-4-amine Max Resp:988515.6 m/z:263	Reactant (%) CUMYLAMINE (BT107694,TOXIC C) Max Resp:0.0 m/z:136	Reactant (%) 4-BROMOQUINOLINE (BT117687, B) Max Resp:605374.8 m/z:208	Components
D2	31.57	0.00	0.00	AdBrettPhos Pd G3: 0.20 mg KHMDS: 3.99 mg dioxane: 100.00 uL
B9	100.00	0.00	0.17	(tBu)PhCPhos Pd G4: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
D5	38.58	0.00	0.17	Pd PEPPSI Ipr: 0.14 mg KHMDS: 3.99 mg dioxane: 100.00 uL
B4	2.16	0.00	0.17	PhCPhos: 0.08 mg t-BuOK: 2.24 mg DMPDAB Pd MAH: 0.09 mg dioxane: 100.00 uL
H3	1.62	0.00	0.17	(tBu)PhCPhos Pd G4: 0.16 mg P2-Et: 6.66 uL dioxane: 100.00 uL
E3	0.00	0.00	0.17	JosiPhos Pd G3: 0.19 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
B6	3.59	0.00	0.18	Gphos Pd G3: 0.18 mg t-BuOK: 2.24 mg dioxane:

				100.00 uL
H9	1.36	0.00	0.18	(tBu)PhCPhos Pd G4: 0.16 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H7	0.00	0.00	0.18	Me3(OMe)tBuXPhos Pd G3: 0.16 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
E9	3.07	0.00	0.19	JosiPhos Pd G3: 0.19 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
H6	0.00	0.00	0.19	Gphos Pd G3: 0.18 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G5	0.00	0.00	0.19	BrettPhos Pd G3: 0.18 mg P2-Et: 6.66 uL dioxane: 100.00 uL
E2	1.22	0.00	0.21	Cs2CO3: 6.52 mg MorDalPhos Pd G4: 0.17 mg dioxane: 100.00 uL
B7	0.00	0.00	0.21	Me3(OMe)tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A7	0.00	0.00	0.21	t-BuOK: 2.24 mg Ad-BippyPhos: 0.13 mg DMPDAB Pd MAH: 0.09 mg t-AmOH: 100.00 uL
F11	0.00	0.00	0.22	Pd PEPPSI Ipr: 0.14 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
H4	0.00	0.00	0.23	PhCPhos: 0.08 mg P2-Et: 6.66 uL DMPDAB Pd MAH: 0.09 mg dioxane: 100.00 uL
F5	0.00	0.00	0.23	Pd PEPPSI Ipr: 0.14 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
C5	4.29	0.00	0.26	BrettPhos Pd G3: 0.18 mg KHMDS: 3.99 mg dioxane: 100.00 uL
H2	0.00	0.00	0.27	AdBrettPhos Pd G3: 0.20 mg P2-Et: 6.66 uL dioxane: 100.00 uL
F4	0.00	0.00	0.27	PhCPhos: 0.08 mg Cs2CO3: 6.52 mg DMPDAB Pd MAH: 0.09 mg dioxane: 100.00 uL

B3	14.54	0.00	0.28	(tBu)PhCPhos Pd G4: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
C6	43.62	0.00	0.31	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
G12	1.79	0.00	0.31	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
F2	0.00	0.00	0.34	AdBrettPhos Pd G3: 0.20 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F9	14.12	0.00	0.37	(tBu)PhCPhos Pd G4: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
G3	0.00	0.00	0.60	JosiPhos Pd G3: 0.19 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G4	0.00	0.00	0.82	tBuBrettPhos Pd G3: 0.17 mg P2-Et: 6.66 uL dioxane: 100.00 uL
C10	0.00	0.00	8.76	tBuBrettPhos Pd G3: 0.17 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
F10	3.30	0.00	9.36	PhCPhos: 0.08 mg Cs2CO3: 6.52 mg DMPDAB Pd MAH: 0.09 mg t-AmOH: 100.00 uL
C8	0.00	0.00	9.76	KHMDS: 3.99 mg MorDalPhos Pd G4: 0.17 mg t-AmOH: 100.00 uL
D6	41.40	0.00	15.78	Gphos Pd G3: 0.18 mg KHMDS: 3.99 mg dioxane: 100.00 uL
H5	0.00	0.00	17.00	Pd PEPPSI Ipr: 0.14 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G11	0.00	0.00	18.60	BrettPhos Pd G3: 0.18 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
C7	0.00	0.00	22.40	Ad-BippyPhos: 0.13 mg KHMDS: 3.99 mg DMPDAB Pd MAH: 0.09 mg t-AmOH: 100.00 uL
F12	1.47	0.00	22.48	Gphos Pd G3: 0.18

				mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
H10	0.00	0.00	22.70	PhCPhos: 0.08 mg P2-Et: 6.66 uL DMPDAB Pd MAH: 0.09 mg t-AmOH: 100.00 uL
E10	0.00	0.00	23.06	tBuBrettPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
G9	0.00	0.00	23.60	JosiPhos Pd G3: 0.19 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
D1	45.35	0.00	23.64	Me3(OMe)tBuXPhos Pd G3: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D11	13.59	0.00	26.47	Pd PEPPSI Ipr: 0.14 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
B10	51.09	0.00	27.32	PhCPhos: 0.08 mg t-BuOK: 2.24 mg DMPDAB Pd MAH: 0.09 mg t-AmOH: 100.00 uL
A9	2.58	0.00	28.92	JosiPhos Pd G3: 0.19 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A1	2.80	0.00	29.30	Ad-BippyPhos: 0.13 mg t-BuOK: 2.24 mg DMPDAB Pd MAH: 0.09 mg dioxane: 100.00 uL
C11	0.00	0.00	30.17	BrettPhos Pd G3: 0.18 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
E7	13.36	0.00	31.45	Ad-BippyPhos: 0.13 mg Cs2CO3: 6.52 mg DMPDAB Pd MAH: 0.09 mg t-AmOH: 100.00 uL
G7	1.47	0.00	31.67	Ad-BippyPhos: 0.13 mg P2-Et: 6.66 uL DMPDAB Pd MAH: 0.09 mg t-AmOH: 100.00 uL
A6	0.00	0.00	32.67	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B11	0.00	0.00	35.03	Pd PEPPSI Ipr: 0.14 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL

G8	0.00	0.00	35.83	P2-Et: 6.66 uL MorDalPhos Pd G4: 0.17 mg t-AmOH: 100.00 uL
F7	0.00	0.00	36.48	Me3(OMe)tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
H8	0.00	0.00	37.87	AdBrettPhos Pd G3: 0.20 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
A3	0.00	0.00	37.98	JosiPhos Pd G3: 0.19 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
D8	0.00	0.00	38.22	AdBrettPhos Pd G3: 0.20 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
E12	21.42	0.00	38.44	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
D7	0.00	0.00	39.34	Me3(OMe)tBuXPhos Pd G3: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
A10	0.00	0.00	39.79	tBuBrettPhos Pd G3: 0.17 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
G10	0.00	0.00	40.15	tBuBrettPhos Pd G3: 0.17 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
D9	8.40	0.00	40.26	(tBu)PhCPhos Pd G4: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
A8	0.00	0.00	40.51	t-BuOK: 2.24 mg MorDalPhos Pd G4: 0.17 mg t-AmOH: 100.00 uL
C12	9.07	0.00	41.23	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
B12	2.56	0.00	41.45	Gphos Pd G3: 0.18 mg T-BuOK: 2.24 mg t-AmOH: 100.00 uL
E6	6.42	0.00	41.67	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
D12	0.00	0.00	41.75	Gphos Pd G3: 0.18 mg KHMDS: 3.99 mg t-

				AmOH: 100.00 uL
G6	0.00	0.00	41.98	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H1	0.00	0.00	42.23	Me3(OMe)tBuXPhos Pd G3: 0.16 mg P2-Et: 6.66 uL dioxane: 100.00 uL
E11	0.00	0.00	42.40	BrettPhos Pd G3: 0.18 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
B5	2.27	0.00	42.59	Pd PEPPSI Ipr: 0.14 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
H11	0.00	0.00	42.71	Pd PEPPSI Ipr: 0.14 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
C9	0.00	0.00	44.16	JosiPhos Pd G3: 0.19 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
A12	7.38	0.00	44.62	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
E8	0.00	0.00	45.86	Cs2CO3: 6.52 mg MorDalPhos Pd G4: 0.17 mg t-AmOH: 100.00 uL
H12	3.66	0.00	47.14	Gphos Pd G3: 0.18 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
C1	0.00	0.00	47.69	Ad-BippyPhos: 0.13 mg KHMDS: 3.99 mg DMPDAB Pd MAH: 0.09 mg dioxane: 100.00 uL
B8	0.00	0.00	49.38	AdBrettPhos Pd G3: 0.20 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
E5	0.00	0.00	50.29	BrettPhos Pd G3: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F3	0.00	0.00	51.15	(tBu)PhCPhos Pd G4: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F6	0.00	0.00	51.51	Gphos Pd G3: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL

D4	0.00	0.00	51.79	PhCPhos: 0.08 mg KHMDS: 3.99 mg DMPDAB Pd MAH: 0.09 mg dioxane: 100.00 uL
A11	0.00	0.00	54.00	BrettPhos Pd G3: 0.18 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
E4	0.00	0.00	54.97	tBuBrettPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
B1	1.27	0.00	56.81	Me3(OMe)tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
C3	2.93	0.00	57.81	JosiPhos Pd G3: 0.19 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D3	0.00	0.00	58.08	(tBu)PhCPhos Pd G4: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
F8	0.00	0.00	58.26	AdBrettPhos Pd G3: 0.20 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
G2	0.00	0.00	58.85	P2-Et: 6.66 uL MorDalPhos Pd G4: 0.17 mg dioxane: 100.00 uL
C4	0.00	0.00	59.15	tBuBrettPhos Pd G3: 0.17 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C2	0.00	0.00	61.07	KHMDS: 3.99 mg MorDalPhos Pd G4: 0.17 mg dioxane: 100.00 uL
G1	1.12	0.00	63.25	Ad-BippyPhos: 0.13 mg P2-Et: 6.66 uL DMPDAB Pd MAH: 0.09 mg dioxane: 100.00 uL
D10	0.00	0.00	63.63	PhCPhos: 0.08 mg KHMDS: 3.99 mg DMPDAB Pd MAH: 0.09 mg t-AmOH: 100.00 uL
A4	0.00	0.00	64.65	tBuBrettPhos Pd G3: 0.17 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
E1	3.69	0.00	64.68	Ad-BippyPhos: 0.13 mg Cs2CO3: 6.52 mg DMPDAB Pd MAH: 0.09 mg dioxane: 100.00 uL

A5	0.00	0.00	65.13	BrettPhos Pd G3: 0.18 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B2	0.00	0.00	67.34	AdBrettPhos Pd G3: 0.20 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
F1	0.00	0.00	71.04	Me3(OMe)tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
A2	2.13	0.00	100.00	t-BuOK: 2.24 mg MorDalPhos Pd G4: 0.17 mg dioxane: 100.00 uL

Buchwald-Hartwig secondary amine and aniline screening kit (secondary amine)

Cell ID	Desired Product (%) tert-butyl 4-{1H-pyrrolo[2,3-b]pyridin-5-yl}piperazine-1-carboxylate Max Resp:375059.5 m/z:303	Reactant (%) 5-bromo-1H-pyrrolo[2,3-b]pyridine Max Resp:194346.0 m/z:197	Components
C3	100.00	41.97	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL KHMDS: 3.99 mg dioxane: 100.00 uL
C5	88.80	49.35	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C4	83.17	27.68	RuPhos Pd G4: 0.17 mg KHMDS: 3.99 mg dioxane: 100.00 uL
A7	82.72	27.60	Qphos Pd G3: 0.22 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
C6	73.81	43.75	tBuXPhos Pd G3: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D3	73.61	37.70	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C1	70.66	34.88	Qphos Pd G3: 0.22 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D2	70.06	33.19	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL

C7	68.42	34.29	Qphos Pd G3: 0.22 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D4	65.26	47.87	tBuBrettPhos Pd G3: 0.17 mg KHMDS: 3.99 mg dioxane: 100.00 uL
B12	59.47	30.62	BrettPhos Pd G3: 0.18 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
C2	54.67	55.07	Pd PEPPSI Ipr: 0.14 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C10	53.91	48.63	RuPhos Pd G4: 0.17 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D1	53.58	42.85	P(tBu)3 Pd G4: 0.11 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D12	53.54	29.49	BrettPhos Pd G3: 0.18 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D5	51.66	54.34	Ephos Pd G4: 0.18 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D6	47.18	46.61	BrettPhos Pd G3: 0.18 mg KHMDS: 3.99 mg dioxane: 100.00 uL
A5	45.10	60.25	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A1	41.12	40.94	Qphos Pd G3: 0.22 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B1	38.87	73.90	P(tBu)3 Pd G4: 0.11 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A12	35.57	31.99	tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
C12	31.18	32.08	tBuXPhos Pd G3: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
A11	25.69	41.10	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
B9	24.84	35.14	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
D9	22.17	43.02	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
B7	20.50	43.65	P(tBu)3 Pd G4: 0.11 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
D10	18.04	0.00	tBuBrettPhos Pd G3: 0.17 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
B10	17.04	37.68	tBuBrettPhos Pd G3: 0.17 mg t-BuOK: 2.24

			mg t-AmOH: 100.00 uL
C11	17.01	43.32	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
B6	10.46	38.77	BrettPhos Pd G3: 0.18 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A6	9.54	24.93	tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B2	6.48	100.00	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B4	3.55	74.22	tBuBrettPhos Pd G3: 0.17 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A4	3.52	7.55	RuPhos Pd G4: 0.17 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
G4	0.00	38.35	RuPhos Pd G4: 0.17 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G5	0.00	51.15	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G6	0.00	54.40	tBuXPhos Pd G3: 0.16 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G7	0.00	29.67	Qphos Pd G3: 0.22 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
G8	0.00	35.26	Pd PEPPSI Ipr: 0.14 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
G9	0.00	24.55	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL P2-Et: 6.66 uL t-AmOH: 100.00 uL
G10	0.00	35.56	RuPhos Pd G4: 0.17 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
G11	0.00	30.41	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
G12	0.00	34.17	tBuXPhos Pd G3: 0.16 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H1	0.00	31.56	P(tBu)3 Pd G4: 0.11 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H2	0.00	60.56	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H3	0.00	29.83	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg P2-Et: 6.66 uL dioxane: 100.00 uL

H4	0.00	36.62	tBuBrettPhos Pd G3: 0.17 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H5	0.00	34.23	Ephos Pd G4: 0.18 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H6	0.00	42.34	BrettPhos Pd G3: 0.18 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H7	0.00	37.07	P(tBu)3 Pd G4: 0.11 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H8	0.00	30.38	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H9	0.00	22.05	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H10	0.00	42.85	tBuBrettPhos Pd G3: 0.17 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H11	0.00	39.78	Ephos Pd G4: 0.18 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H12	0.00	25.73	BrettPhos Pd G3: 0.18 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
A2	0.00	31.07	Pd PEPPSI Ipr: 0.14 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A3	0.00	22.80	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL t-BuOK: 2.24 mg dioxane: 100.00 uL
A8	0.00	11.62	Pd PEPPSI Ipr: 0.14 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A9	0.00	8.05	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A10	0.00	5.63	RuPhos Pd G4: 0.17 mg T-BuOK: 2.24 mg t-AmOH: 100.00 uL
B3	0.00	65.03	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B5	0.00	62.86	Ephos Pd G4: 0.18 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B8	0.00	40.15	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
B11	0.00	50.07	Ephos Pd G4: 0.18 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL

C8	0.00	61.45	Pd PEPPSI Ipr: 0.14 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
C9	0.00	45.26	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL KHMDS: 3.99 mg t-AmOH: 100.00 uL
D7	0.00	32.23	P(tBu)3 Pd G4: 0.11 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D8	0.00	15.10	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D11	0.00	0.00	Ephos Pd G4: 0.18 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
E1	0.00	0.00	Qphos Pd G3: 0.22 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E2	0.00	63.51	Pd PEPPSI Ipr: 0.14 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E3	0.00	0.00	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL Cs2CO3: 6.52 mg dioxane: 100.00 uL
E4	0.00	38.07	RuPhos Pd G4: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E5	0.00	59.68	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E6	0.00	53.00	tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E7	0.00	9.39	Qphos Pd G3: 0.22 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E8	0.00	39.45	Pd PEPPSI Ipr: 0.14 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E9	0.00	40.68	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E10	0.00	47.19	RuPhos Pd G4: 0.17 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E11	0.00	48.44	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E12	0.00	43.76	tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F1	0.00	37.48	P(tBu)3 Pd G4: 0.11 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F2	0.00	58.84	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg Cs2CO3:

			6.52 mg dioxane: 100.00 uL
F3	0.00	37.87	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F4	0.00	48.89	tBuBrettPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F5	0.00	50.87	Ephos Pd G4: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F6	0.00	60.68	BrettPhos Pd G3: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F7	0.00	30.67	P(tBu)3 Pd G4: 0.11 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F8	0.00	56.88	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F9	0.00	16.28	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F10	0.00	26.53	tBuBrettPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F11	0.00	15.00	Ephos Pd G4: 0.18 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F12	0.00	34.37	BrettPhos Pd G3: 0.18 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
G1	0.00	49.59	Qphos Pd G3: 0.22 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G2	0.00	52.99	Pd PEPPSI Ipr: 0.14 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G3	0.00	40.54	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL P2-Et: 6.66 uL dioxane: 100.00 uL

Buchwald secondary amine and aniline screening kit (aniline)

Cell ID	Desired Product (%) 5-methoxy-N-{1H-pyrrolo[2,3-b]pyridin-5-yl}pyridin-2-amine Max Resp:328926.2 m/z:241	Reactant (%) 5-bromo-1H-pyrrolo[2,3-b]pyridine Max Resp:58428.6 m/z:197	Components

B6	100.00	0.00	BrettPhos Pd G3: 0.18 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
C11	84.74	0.00	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
B10	81.60	0.00	tBuBrettPhos Pd G3: 0.17 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
B4	75.29	6.97	tBuBrettPhos Pd G3: 0.17 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A1	49.71	28.59	Qphos Pd G3: 0.22 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B12	44.81	3.63	BrettPhos Pd G3: 0.18 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
C12	33.48	27.47	tBuXPhos Pd G3: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
E12	27.75	33.94	tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
A12	25.74	3.65	tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
C4	23.89	37.25	RuPhos Pd G4: 0.17 mg KHMDS: 3.99 mg dioxane: 100.00 uL
B1	22.86	1.96	P(tBu)3 Pd G4: 0.11 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
D4	18.23	35.51	tBuBrettPhos Pd G3: 0.17 mg KHMDS: 3.99 mg dioxane: 100.00 uL
F12	13.76	50.01	BrettPhos Pd G3: 0.18 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
A5	10.62	96.50	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
F4	8.28	49.22	tBuBrettPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
B7	4.31	47.64	P(tBu)3 Pd G4: 0.11 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
E11	4.26	31.42	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
D10	4.22	40.55	tBuBrettPhos Pd G3: 0.17 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
A4	4.16	58.39	RuPhos Pd G4: 0.17 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A11	3.95	64.06	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A2	0.00	59.99	Pd PEPPSI Ipr: 0.14 mg t-BuOK: 2.24

			mg dioxane: 100.00 uL
A3	0.00	39.25	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL t-BuOK: 2.24 mg dioxane: 100.00 uL
A6	0.00	77.72	tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
A7	0.00	29.50	Qphos Pd G3: 0.22 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A8	0.00	55.71	Pd PEPPSI Ipr: 0.14 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A9	0.00	65.64	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL t-BuOK: 2.24 mg t-AmOH: 100.00 uL
A10	0.00	42.06	RuPhos Pd G4: 0.17 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
B2	0.00	34.85	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B3	0.00	38.68	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B5	0.00	61.91	Ephos Pd G4: 0.18 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B8	0.00	51.81	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
B9	0.00	42.28	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg t-BuOK: 2.24 mg t-AmOH: 100.00 uL
B11	0.00	39.82	Ephos Pd G4: 0.18 mg T-BuOK: 2.24 mg t-AmOH: 100.00 uL
C1	0.00	84.76	Qphos Pd G3: 0.22 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C2	0.00	41.75	Pd PEPPSI Ipr: 0.14 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C3	0.00	42.96	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL KHMDS: 3.99 mg dioxane: 100.00 uL
C5	0.00	68.80	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
C6	0.00	41.57	tBuXPhos Pd G3: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL

C7	0.00	52.30	Qphos Pd G3: 0.22 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
C8	0.00	65.56	Pd PEPPSI Ipr: 0.14 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
C9	0.00	47.51	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL KHMDS: 3.99 mg t-AmOH: 100.00 uL
C10	0.00	58.86	RuPhos Pd G4: 0.17 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D1	0.00	48.75	P(tBu)3 Pd G4: 0.11 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D2	0.00	44.05	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D3	0.00	38.24	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D5	0.00	27.77	Ephos Pd G4: 0.18 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D6	0.00	56.81	BrettPhos Pd G3: 0.18 mg KHMDS: 3.99 mg dioxane: 100.00 uL
D7	0.00	41.96	P(tBu)3 Pd G4: 0.11 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D8	0.00	33.70	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D9	0.00	52.31	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D11	0.00	65.17	Ephos Pd G4: 0.18 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
D12	0.00	0.00	BrettPhos Pd G3: 0.18 mg KHMDS: 3.99 mg t-AmOH: 100.00 uL
E1	0.00	54.63	Qphos Pd G3: 0.22 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E2	0.00	31.24	Pd PEPPSI Ipr: 0.14 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E3	0.00	40.30	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL Cs2CO3: 6.52 mg dioxane: 100.00 uL
E4	0.00	41.19	RuPhos Pd G4: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL

E5	0.00	34.23	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E6	0.00	52.27	tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E7	0.00	46.44	Qphos Pd G3: 0.22 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E8	0.00	30.78	Pd PEPPSI Ipr: 0.14 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E9	0.00	30.61	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E10	0.00	42.64	RuPhos Pd G4: 0.17 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F1	0.00	97.00	P(tBu)3 Pd G4: 0.11 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F2	0.00	97.91	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F3	0.00	39.56	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F5	0.00	48.86	Ephos Pd G4: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F6	0.00	71.74	BrettPhos Pd G3: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F7	0.00	39.51	P(tBu)3 Pd G4: 0.11 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F8	0.00	33.56	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F9	0.00	19.25	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F10	0.00	48.38	tBuBrettPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F11	0.00	100.00	Ephos Pd G4: 0.18 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
G1	0.00	40.68	Qphos Pd G3: 0.22 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G2	0.00	45.31	Pd PEPPSI Ipr: 0.14 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G3	0.00	60.02	DMPDAB Pd MAH: 0.09

			mg Triisobutylphosphatrane: 0.07 uL P2-Et: 6.66 uL dioxane: 100.00 uL
G4	0.00	69.49	RuPhos Pd G4: 0.17 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G5	0.00	28.81	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G6	0.00	34.06	tBuXPhos Pd G3: 0.16 mg P2-Et: 6.66 uL dioxane: 100.00 uL
G7	0.00	30.20	Qphos Pd G3: 0.22 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
G8	0.00	28.83	Pd PEPPSI Ipr: 0.14 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
G9	0.00	57.23	DMPDAB Pd MAH: 0.09 mg Triisobutylphosphatrane: 0.07 uL P2-Et: 6.66 uL t-AmOH: 100.00 uL
G10	0.00	37.03	RuPhos Pd G4: 0.17 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
G11	0.00	8.94	[Pd(bippyPhos)(allyl)]OTf: 0.16 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
G12	0.00	25.50	tBuXPhos Pd G3: 0.16 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H1	0.00	34.66	P(tBu)3 Pd G4: 0.11 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H2	0.00	43.98	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H3	0.00	52.60	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H4	0.00	67.22	tBuBrettPhos Pd G3: 0.17 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H5	0.00	17.49	Ephos Pd G4: 0.18 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H6	0.00	32.09	BrettPhos Pd G3: 0.18 mg P2-Et: 6.66 uL dioxane: 100.00 uL
H7	0.00	49.79	P(tBu)3 Pd G4: 0.11 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H8	0.00	32.74	DMPDAB Pd MAH: 0.09 mg Brett/Ru/JackiePhos: 0.16 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H9	0.00	34.61	DMPDAB Pd MAH: 0.09 mg Brett/C/JackiePhos: 0.15 mg P2-Et: 6.66

			uL t-AmOH: 100.00 uL
H10	0.00	13.34	tBuBrettPhos Pd G3: 0.17 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H11	0.00	44.97	Ephos Pd G4: 0.18 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL
H12	0.00	55.14	BrettPhos Pd G3: 0.18 mg P2-Et: 6.66 uL t-AmOH: 100.00 uL

Buchwald amide and oxygen screening kit (amide)

Cell ID	Desired Product (%) N-(4-methoxyphenyl)pyridine-3-carboxamide Max Resp:1890096.0 m/z:229	Reactant (%) NICOTINAMIDE (BT1703, N) Max Resp:462573.8 m/z:123	Components
C7	100.00	5.95	AdBrettPhos-Pd-G3: 0.20 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
D10	76.86	5.68	RockPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
C8	76.43	5.97	AdBrettPhos-Pd-G3: 0.20 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
D11	61.11	11.95	RockPhos Pd G3: 0.17 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
A8	60.16	9.04	K3PO4: 4.25 mg tBuBrettPhos Pd G3: 0.17 mg t-AmOH: 100.00 uL
D5	53.43	40.87	RockPhos Pd G3: 0.17 mg K3PO4: 4.25 mg dioxane: 100.00 uL
A1	48.33	28.33	Cs2CO3: 6.52 mg tBuBrettPhos Pd G3: 0.17 mg dioxane: 100.00 uL
G8	48.00	41.05	Me3(Ome)tBuXPhos Pd G3: 0.16 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
F7	30.31	50.45	tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
B8	29.27	64.04	K3PO4: 4.25 mg 4MetBuXPhos Pd G3: 0.17 mg t-AmOH: 100.00 uL
A2	27.09	23.07	K3PO4: 4.25 mg tBuBrettPhos Pd G3: 0.17 mg dioxane: 100.00 uL
D4	23.96	23.35	RockPhos Pd G3: 0.17 mg Cs2CO3:

			6.52 mg dioxane: 100.00 uL
C2	22.39	22.84	AdBrettPhos-Pd-G3: 0.20 mg K3PO4: 4.25 mg dioxane: 100.00 uL
B7	21.42	40.13	Cs2CO3: 6.52 mg 4MetBuXPhos Pd G3: 0.17 mg t-AmOH: 100.00 uL
A11	18.08	74.14	BrettPhos Pd G4: 0.18 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
F8	16.39	36.04	tBuXPhos Pd G3: 0.16 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
F10	14.54	98.04	TrixiePhos Pd G3: 0.15 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
A9	13.41	63.75	KOAc: 1.96 mg tBuBrettPhos Pd G3: 0.17 mg t-AmOH: 100.00 uL
A5	12.91	52.13	BrettPhos Pd G4: 0.18 mg K3PO4: 4.25 mg dioxane: 100.00 uL
A4	11.11	33.31	BrettPhos Pd G4: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
C9	8.12	58.23	AdBrettPhos-Pd-G3: 0.20 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
F11	7.38	46.62	TrixiePhos Pd G3: 0.15 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
A7	6.35	77.36	Cs2CO3: 6.52 mg tBuBrettPhos Pd G3: 0.17 mg t-AmOH: 100.00 uL
C1	6.20	21.60	AdBrettPhos-Pd-G3: 0.20 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
D12	6.00	52.77	RockPhos Pd G3: 0.17 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
G10	5.18	65.15	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
G1	4.64	22.05	Me3(Ome)tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
A10	3.99	34.45	BrettPhos Pd G4: 0.18 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
G9	3.28	77.64	Me3(Ome)tBuXPhos Pd G3: 0.16 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
E4	2.74	38.26	JosiPhos Pd G3: 0.19 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
H11	2.72	36.80	Pd(allyl)Otf-BippyPhos: 0.16 mg K3PO4: 4.25 mg t-AmOH: 100.00

			uL
A3	2.26	41.67	KOAc: 1.96 mg tBuBrettPhos Pd G3: 0.17 mg dioxane: 100.00 uL
B9	2.24	60.71	KOAc: 1.96 mg 4MetBuXPhos Pd G3: 0.17 mg t-AmOH: 100.00 uL
G11	2.05	48.82	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
H5	2.04	29.59	Pd(allyl)Otf-BippyPhos: 0.16 mg K3PO4: 4.25 mg dioxane: 100.00 uL
G2	1.77	28.00	Me3(Ome)tBuXPhos Pd G3: 0.16 mg K3PO4: 4.25 mg dioxane: 100.00 uL
C3	1.66	36.73	AdBrettPhos-Pd-G3: 0.20 mg KOAc: 1.96 mg dioxane: 100.00 uL
F12	1.64	44.28	TrixiePhos Pd G3: 0.15 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
H4	1.61	57.46	Pd(allyl)Otf-BippyPhos: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F2	1.58	22.13	tBuXPhos Pd G3: 0.16 mg K3PO4: 4.25 mg dioxane: 100.00 uL
B2	1.54	36.46	K3PO4: 4.25 mg 4MetBuXPhos Pd G3: 0.17 mg dioxane: 100.00 uL
G7	1.53	36.06	Me3(Ome)tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
F5	1.48	67.22	TrixiePhos Pd G3: 0.15 mg K3PO4: 4.25 mg dioxane: 100.00 uL
E5	1.32	42.46	JosiPhos Pd G3: 0.19 mg K3PO4: 4.25 mg dioxane: 100.00 uL
F1	1.29	26.48	tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
D6	1.27	65.55	RockPhos Pd G3: 0.17 mg KOAc: 1.96 mg dioxane: 100.00 uL
F4	1.17	54.49	TrixiePhos Pd G3: 0.15 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F3	1.08	46.13	tBuXPhos Pd G3: 0.16 mg KOAc: 1.96 mg dioxane: 100.00 uL
H12	0.97	54.09	Pd(allyl)Otf-BippyPhos: 0.16 mg KOAc: 1.96 mg t-AmOH: 100.00 uL

B1	0.80	29.59	Cs2CO3: 6.52 mg 4MetBuXPhos Pd G3: 0.17 mg dioxane: 100.00 uL
G4	0.65	53.49	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
H8	0.62	45.69	Xphos Pd G4: 0.17 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
E8	0.56	43.70	JackiePhos Pd G3: 0.23 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
A6	0.00	48.88	BrettPhos Pd G4: 0.18 mg KOAc: 1.96 mg dioxane: 100.00 uL
A12	0.00	62.08	BrettPhos Pd G4: 0.18 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
B3	0.00	46.65	KOAc: 1.96 mg 4MetBuXPhos Pd G3: 0.17 mg dioxane: 100.00 uL
B4	0.00	63.09	XantPhos Pd G4: 0.19 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
B5	0.00	53.48	XantPhos Pd G4: 0.19 mg K3PO4: 4.25 mg dioxane: 100.00 uL
B6	0.00	56.24	XantPhos Pd G4: 0.19 mg KOAc: 1.96 mg dioxane: 100.00 uL
B10	0.00	74.00	XantPhos Pd G4: 0.19 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
B11	0.00	45.87	XantPhos Pd G4: 0.19 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
B12	0.00	57.90	XantPhos Pd G4: 0.19 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
C4	0.00	66.57	DPPF Pd G3: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
C5	0.00	58.17	DPPF Pd G3: 0.18 mg K3PO4: 4.25 mg dioxane: 100.00 uL
C6	0.00	66.79	DPPF Pd G3: 0.18 mg KOAc: 1.96 mg dioxane: 100.00 uL
C10	0.00	45.56	DPPF Pd G3: 0.18 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
C11	0.00	43.68	DPPF Pd G3: 0.18 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
C12	0.00	49.35	DPPF Pd G3: 0.18 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
D1	0.00	23.74	rac-BINAP Pd G4: 0.20 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL

D2	0.00	32.29	rac-BINAP Pd G4: 0.20 mg K3PO4: 4.25 mg dioxane: 100.00 uL
D3	0.00	43.94	rac-BINAP Pd G4: 0.20 mg KOAc: 1.96 mg dioxane: 100.00 uL
D7	0.00	96.62	rac-BINAP Pd G4: 0.20 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
D8	0.00	47.65	rac-BINAP Pd G4: 0.20 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
D9	0.00	71.27	rac-BINAP Pd G4: 0.20 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
E1	0.00	61.27	JackiePhos Pd G3: 0.23 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E2	0.00	25.26	JackiePhos Pd G3: 0.23 mg K3PO4: 4.25 mg dioxane: 100.00 uL
E3	0.00	35.17	JackiePhos Pd G3: 0.23 mg KOAc: 1.96 mg dioxane: 100.00 uL
E6	0.00	56.99	JosiPhos Pd G3: 0.19 mg KOAc: 1.96 mg dioxane: 100.00 uL
E7	0.00	75.57	JackiePhos Pd G3: 0.23 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E9	0.00	74.46	JackiePhos Pd G3: 0.23 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
E10	0.00	72.04	JosiPhos Pd G3: 0.19 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
E11	0.00	53.16	JosiPhos Pd G3: 0.19 mg K3PO4: 4.25 mg t-AmOH: 100.00 uL
E12	0.00	66.35	JosiPhos Pd G3: 0.19 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
F6	0.00	54.66	TrixiePhos Pd G3: 0.15 mg KOAc: 1.96 mg dioxane: 100.00 uL
F9	0.00	0.00	tBuXPhos Pd G3: 0.16 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
G3	0.00	27.29	Me3(Ome)tBuXPhos Pd G3: 0.16 mg KOAc: 1.96 mg dioxane: 100.00 uL
G5	0.00	64.45	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg K3PO4: 4.25 mg dioxane: 100.00 uL
G6	0.00	38.86	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg KOAc: 1.96 mg dioxane: 100.00 uL
G12	0.00	51.31	DMPDAB-Pd-MAH: 0.09

			mg tBuMePhos: 0.06 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
H1	0.00	22.23	Xphos Pd G4: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
H2	0.00	33.75	Xphos Pd G4: 0.17 mg K3PO4: 4.25 mg dioxane: 100.00 uL
H3	0.00	40.40	Xphos Pd G4: 0.17 mg KOAc: 1.96 mg dioxane: 100.00 uL
H6	0.00	42.53	Pd(allyl)Otf-BippyPhos: 0.16 mg KOAc: 1.96 mg dioxane: 100.00 uL
H7	0.00	37.87	Xphos Pd G4: 0.17 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL
H9	0.00	68.48	Xphos Pd G4: 0.17 mg KOAc: 1.96 mg t-AmOH: 100.00 uL
H10	0.00	100.00	Pd(allyl)Otf-BippyPhos: 0.16 mg Cs2CO3: 6.52 mg t-AmOH: 100.00 uL

Buchwald amide and oxygen screening kit (oxygen)

Cell ID	Desired Product (%) tert-butyl 3-(quinolin-6-yloxy)azetidine-1-carboxylate Max Resp:730117.8 m/z:301	Reactant (%) tert-butyl 3-hydroxyazetidine-1-carboxylate Max Resp:0.0 m/z:174	Components
G1	100.00	0.00	Me3(Ome)tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
B1	91.17	0.00	Cs2CO3: 6.52 mg 4MetBuXPhos Pd G3: 0.17 mg toluene: 100.00 uL
A1	74.79	0.00	Cs2CO3: 6.52 mg tBuBrettPhos Pd G3: 0.17 mg toluene: 100.00 uL
D5	65.13	0.00	RockPhos Pd G3: 0.17 mg K3PO4: 4.25 mg toluene: 100.00 uL
A2	62.43	0.00	K3PO4: 4.25 mg tBuBrettPhos Pd G3: 0.17 mg toluene: 100.00 uL
H5	49.59	0.00	Pd(allyl)Otf-BippyPhos: 0.16 mg K3PO4: 4.25 mg toluene: 100.00

			uL
F10	44.99	0.00	TrixiePhos Pd G3: 0.15 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
A4	34.18	0.00	BrettPhos Pd G4: 0.18 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
F1	31.84	0.00	tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
C2	31.07	0.00	AdBrettPhos-Pd-G3: 0.20 mg K3PO4: 4.25 mg toluene: 100.00 uL
E1	29.38	0.00	JackiePhos Pd G3: 0.23 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
C1	19.63	0.00	AdBrettPhos-Pd-G3: 0.20 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
H11	18.69	0.00	Pd(allyl)Otf-BippyPhos: 0.16 mg K3PO4: 4.25 mg dioxane: 100.00 uL
A7	14.09	0.00	Cs2CO3: 6.52 mg tBuBrettPhos Pd G3: 0.17 mg dioxane: 100.00 uL
G8	14.02	0.00	Me3(Ome)tBuXPhos Pd G3: 0.16 mg K3PO4: 4.25 mg dioxane: 100.00 uL
B7	13.95	0.00	Cs2CO3: 6.52 mg 4MetBuXPhos Pd G3: 0.17 mg dioxane: 100.00 uL
D11	13.16	0.00	RockPhos Pd G3: 0.17 mg K3PO4: 4.25 mg dioxane: 100.00 uL
E10	11.82	0.00	JosiPhos Pd G3: 0.19 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
F4	8.81	0.00	TrixiePhos Pd G3: 0.15 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
E2	8.17	0.00	JackiePhos Pd G3: 0.23 mg K3PO4: 4.25 mg toluene: 100.00 uL
E5	6.93	0.00	JosiPhos Pd G3: 0.19 mg K3PO4: 4.25 mg toluene: 100.00 uL
A5	6.38	0.00	BrettPhos Pd G4: 0.18 mg K3PO4: 4.25 mg toluene: 100.00 uL
H1	5.27	0.00	Xphos Pd G4: 0.17 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
F2	3.96	0.00	tBuXPhos Pd G3: 0.16 mg K3PO4: 4.25 mg toluene: 100.00 uL
H4	3.40	0.00	Pd(allyl)Otf-BippyPhos: 0.16

			mg Cs2CO3: 6.52 mg toluene: 100.00 uL
F7	3.10	0.00	tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
C8	2.90	0.00	AdBrettPhos-Pd-G3: 0.20 mg K3PO4: 4.25 mg dioxane: 100.00 uL
G2	2.77	0.00	Me3(Ome)tBuXPhos Pd G3: 0.16 mg K3PO4: 4.25 mg toluene: 100.00 uL
C7	2.68	0.00	AdBrettPhos-Pd-G3: 0.20 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
A8	2.64	0.00	K3PO4: 4.25 mg tBuBrettPhos Pd G3: 0.17 mg dioxane: 100.00 uL
A3	2.12	0.00	t-BuOK: 2.24 mg tBuBrettPhos Pd G3: 0.17 mg toluene: 100.00 uL
A6	2.02	0.00	BrettPhos Pd G4: 0.18 mg t-BuOK: 2.24 mg toluene: 100.00 uL
D12	1.98	0.00	RockPhos Pd G3: 0.17 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
G4	1.95	0.00	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
G11	1.92	0.00	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg K3PO4: 4.25 mg dioxane: 100.00 uL
B8	1.92	0.00	K3PO4: 4.25 mg 4MetBuXPhos Pd G3: 0.17 mg dioxane: 100.00 uL
B2	1.90	0.00	K3PO4: 4.25 mg 4MetBuXPhos Pd G3: 0.17 mg toluene: 100.00 uL
D4	1.85	0.00	RockPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
D1	1.45	0.00	rac-BINAP Pd G4: 0.20 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
G10	1.44	0.00	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
A9	0.00	0.00	t-BuOK: 2.24 mg tBuBrettPhos Pd G3: 0.17 mg dioxane: 100.00 uL
A10	0.00	0.00	BrettPhos Pd G4: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
A11	0.00	0.00	BrettPhos Pd G4: 0.18 mg K3PO4:

			4.25 mg dioxane: 100.00 uL
A12	0.00	0.00	BrettPhos Pd G4: 0.18 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
B3	0.00	0.00	t-BuOK: 2.24 mg 4MetBuXPhos Pd G3: 0.17 mg toluene: 100.00 uL
B4	0.00	0.00	XantPhos Pd G4: 0.19 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
B5	0.00	0.00	XantPhos Pd G4: 0.19 mg K3PO4: 4.25 mg toluene: 100.00 uL
B6	0.00	0.00	XantPhos Pd G4: 0.19 mg t-BuOK: 2.24 mg toluene: 100.00 uL
B9	0.00	0.00	T-BuOK: 2.24 mg 4MetBuXPhos Pd G3: 0.17 mg dioxane: 100.00 uL
B10	0.00	0.00	XantPhos Pd G4: 0.19 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
B11	0.00	0.00	XantPhos Pd G4: 0.19 mg K3PO4: 4.25 mg dioxane: 100.00 uL
B12	0.00	0.00	XantPhos Pd G4: 0.19 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
C3	0.00	0.00	AdBrettPhos-Pd-G3: 0.20 mg t-BuOK: 2.24 mg toluene: 100.00 uL
C4	0.00	0.00	DPPF Pd G3: 0.18 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
C5	0.00	0.00	DPPF Pd G3: 0.18 mg K3PO4: 4.25 mg toluene: 100.00 uL
C6	0.00	0.00	DPPF Pd G3: 0.18 mg t-BuOK: 2.24 mg toluene: 100.00 uL
C9	0.00	0.00	AdBrettPhos-Pd-G3: 0.20 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
C10	0.00	0.00	DPPF Pd G3: 0.18 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
C11	0.00	0.00	DPPF Pd G3: 0.18 mg K3PO4: 4.25 mg dioxane: 100.00 uL
C12	0.00	0.00	DPPF Pd G3: 0.18 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
D2	0.00	0.00	rac-BINAP Pd G4: 0.20 mg K3PO4: 4.25 mg toluene: 100.00 uL
D3	0.00	0.00	rac-BINAP Pd G4: 0.20 mg t-BuOK: 2.24 mg toluene: 100.00 uL
D6	0.00	0.00	RockPhos Pd G3: 0.17 mg t-BuOK: 2.24 mg toluene: 100.00 uL

D7	0.00	0.00	rac-BINAP Pd G4: 0.20 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
D8	0.00	0.00	rac-BINAP Pd G4: 0.20 mg K3PO4: 4.25 mg dioxane: 100.00 uL
D9	0.00	0.00	rac-BINAP Pd G4: 0.20 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
D10	0.00	0.00	RockPhos Pd G3: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E3	0.00	0.00	JackiePhos Pd G3: 0.23 mg t-BuOK: 2.24 mg toluene: 100.00 uL
E4	0.00	0.00	JosiPhos Pd G3: 0.19 mg Cs2CO3: 6.52 mg toluene: 100.00 uL
E6	0.00	0.00	JosiPhos Pd G3: 0.19 mg t-BuOK: 2.24 mg toluene: 100.00 uL
E7	0.00	0.00	JackiePhos Pd G3: 0.23 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
E8	0.00	0.00	JackiePhos Pd G3: 0.23 mg K3PO4: 4.25 mg dioxane: 100.00 uL
E9	0.00	0.00	JackiePhos Pd G3: 0.23 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
E11	0.00	0.00	JosiPhos Pd G3: 0.19 mg K3PO4: 4.25 mg dioxane: 100.00 uL
E12	0.00	0.00	JosiPhos Pd G3: 0.19 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
F3	0.00	0.00	tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg toluene: 100.00 uL
F5	0.00	0.00	TrixiePhos Pd G3: 0.15 mg K3PO4: 4.25 mg toluene: 100.00 uL
F6	0.00	0.00	TrixiePhos Pd G3: 0.15 mg t-BuOK: 2.24 mg toluene: 100.00 uL
F8	0.00	0.00	tBuXPhos Pd G3: 0.16 mg K3PO4: 4.25 mg dioxane: 100.00 uL
F9	0.00	0.00	tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
F11	0.00	0.00	TrixiePhos Pd G3: 0.15 mg K3PO4: 4.25 mg dioxane: 100.00 uL
F12	0.00	0.00	TrixiePhos Pd G3: 0.15 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
G3	0.00	0.00	Me3(Ome)tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg toluene: 100.00 uL

G5	0.00	0.00	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg K3PO4: 4.25 mg toluene: 100.00 uL
G6	0.00	0.00	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg t-BuOK: 2.24 mg toluene: 100.00 uL
G7	0.00	0.00	Me3(Ome)tBuXPhos Pd G3: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
G9	0.00	0.00	Me3(Ome)tBuXPhos Pd G3: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
G12	0.00	0.00	DMPDAB-Pd-MAH: 0.09 mg tBuMePhos: 0.06 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
H2	0.00	0.00	Xphos Pd G4: 0.17 mg K3PO4: 4.25 mg toluene: 100.00 uL
H3	0.00	0.00	Xphos Pd G4: 0.17 mg t-BuOK: 2.24 mg toluene: 100.00 uL
H6	0.00	0.00	Pd(allyl)Otf-BippyPhos: 0.16 mg t-BuOK: 2.24 mg toluene: 100.00 uL
H7	0.00	0.00	Xphos Pd G4: 0.17 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
H8	0.00	0.00	Xphos Pd G4: 0.17 mg K3PO4: 4.25 mg dioxane: 100.00 uL
H9	0.00	0.00	Xphos Pd G4: 0.17 mg t-BuOK: 2.24 mg dioxane: 100.00 uL
H10	0.00	0.00	Pd(allyl)Otf-BippyPhos: 0.16 mg Cs2CO3: 6.52 mg dioxane: 100.00 uL
H12	0.00	0.00	Pd(allyl)Otf-BippyPhos: 0.16 mg t-BuOK: 2.24 mg dioxane: 100.00 uL

S_NAr screening kit

Cell ID	Desired Product (%)	Reactant (%)	Components
	methyl 7-(benzyloxy)-1H-indazole-4-carboxylate	1H-INDAZOLE-4-CARBOXYLIC ACID, 7-FLUORO-, METHYL ESTER (BT301412,FRIDGE F)	
	Max Resp:365728.1	Max Resp:429213.8	

	m/z:281	m/z:193	
F10	100.00	1.31	CsF: 0.60 mg KHMDS: 7.98 mg NMP: 100.00 uL
F1	59.54	0.00	No ligand: 0.00 mg KHMDS: 7.98 mg DMF: 100.00 uL
F9	5.63	0.00	No ligand: 0.00 mg KHMDS: 7.98 mg NMP: 100.00 uL
F2	3.93	4.65	CsF: 0.60 mg KHMDS: 7.98 mg DMF: 100.00 uL
H1	1.94	0.00	No ligand: 0.00 mg T-BuOK: 4.49 mg DMF: 100.00 uL
F7	1.38	0.00	No ligand: 0.00 mg KHMDS: 7.98 mg DMSO: 100.00 uL
H2	1.01	2.09	CsF: 0.60 mg T-BuOK: 4.49 mg DMF: 100.00 uL
A1	0.00	100.00	No ligand: 0.00 mg NEt3: 5.56 uL DMF: 100.00 uL
A10	0.00	27.72	CsF: 0.60 mg NEt3: 5.56 uL NMP: 100.00 uL
A11	0.00	90.52	No ligand: 0.00 mg NEt3: 5.56 uL CPME: 100.00 uL
A12	0.00	48.05	CsF: 0.60 mg NEt3: 5.56 uL CPME: 100.00 uL
A2	0.00	15.56	CsF: 0.60 mg NEt3: 5.56 uL DMF: 100.00 uL
A3	0.00	11.85	No ligand: 0.00 mg NEt3: 5.56 uL MeCN: 100.00 uL
A4	0.00	7.28	CsF: 0.60 mg NEt3: 5.56 uL MeCN: 100.00 uL
A5	0.00	73.52	No ligand: 0.00 mg NEt3: 5.56 uL t-AmOH: 100.00 uL
A6	0.00	46.35	CsF: 0.60 mg NEt3: 5.56 uL t-AmOH: 100.00 uL
A7	0.00	48.12	No ligand: 0.00 mg NEt3: 5.56 uL DMSO: 100.00 uL

A8	0.00	26.24	CsF: 0.60 mg NEt3: 5.56 uL DMSO: 100.00 uL
A9	0.00	74.50	No ligand: 0.00 mg NEt3: 5.56 uL NMP: 100.00 uL
B1	0.00	8.13	No ligand: 0.00 mg DBU: 5.97 uL DMF: 100.00 uL
B10	0.00	7.01	CsF: 0.60 mg DBU: 5.97 uL NMP: 100.00 uL
B11	0.00	35.35	No ligand: 0.00 mg DBU: 5.97 uL CPME: 100.00 uL
B12	0.00	41.44	CsF: 0.60 mg DBU: 5.97 uL CPME: 100.00 uL
B2	0.00	11.65	CsF: 0.60 mg DBU: 5.97 uL DMF: 100.00 uL
B3	0.00	7.10	No ligand: 0.00 mg DBU: 5.97 uL MeCN: 100.00 uL
B4	0.00	5.73	CsF: 0.60 mg DBU: 5.97 uL MeCN: 100.00 uL
B5	0.00	34.54	No ligand: 0.00 mg DBU: 5.97 uL t-AmOH: 100.00 uL
B6	0.00	25.16	CsF: 0.60 mg DBU: 5.97 uL t-AmOH: 100.00 uL
B7	0.00	5.27	No ligand: 0.00 mg DBU: 5.97 uL DMSO: 100.00 uL
B8	0.00	5.72	CsF: 0.60 mg DBU: 5.97 uL DMSO: 100.00 uL
B9	0.00	24.94	No ligand: 0.00 mg DBU: 5.97 uL NMP: 100.00 uL
C1	0.00	7.21	No ligand: 0.00 mg TMG: 5.02 uL DMF: 100.00 uL
C10	0.00	3.72	CsF: 0.60 mg TMG: 5.02 uL NMP: 100.00 uL
C11	0.00	32.31	No ligand: 0.00 mg TMG: 5.02 uL CPME: 100.00 uL
C12	0.00	6.17	CsF: 0.60 mg TMG: 5.02 uL CPME: 100.00 uL
C2	0.00	1.80	CsF: 0.60 mg TMG: 5.02 uL DMF: 100.00 uL
C3	0.00	5.44	No ligand: 0.00 mg TMG: 5.02 uL MeCN: 100.00 uL
C4	0.00	6.64	CsF: 0.60 mg TMG: 5.02

			uL MeCN: 100.00 uL
C5	0.00	51.14	No ligand: 0.00 mg TMG: 5.02 uL t-AmOH: 100.00 uL
C6	0.00	19.78	CsF: 0.60 mg TMG: 5.02 uL t-AmOH: 100.00 uL
C7	0.00	6.08	No ligand: 0.00 mg TMG: 5.02 uL DMSO: 100.00 uL
C8	0.00	4.58	CsF: 0.60 mg TMG: 5.02 uL DMSO: 100.00 uL
C9	0.00	10.91	No ligand: 0.00 mg TMG: 5.02 uL NMP: 100.00 uL
D1	0.00	50.69	No ligand: 0.00 mg DIPEA: 6.97 uL DMF: 100.00 uL
D10	0.00	26.08	CsF: 0.60 mg DIPEA: 6.97 uL NMP: 100.00 uL
D11	0.00	34.54	No ligand: 0.00 mg DIPEA: 6.97 uL CPME: 100.00 uL
D12	0.00	34.17	CsF: 0.60 mg DIPEA: 6.97 uL CPME: 100.00 uL
D2	0.00	21.84	CsF: 0.60 mg DIPEA: 6.97 uL DMF: 100.00 uL
D3	0.00	25.80	No ligand: 0.00 mg DIPEA: 6.97 uL MeCN: 100.00 uL
D4	0.00	6.78	CsF: 0.60 mg DIPEA: 6.97 uL MeCN: 100.00 uL
D5	0.00	34.01	No ligand: 0.00 mg DIPEA: 6.97 uL t-AmOH: 100.00 uL
D6	0.00	29.41	CsF: 0.60 mg DIPEA: 6.97 uL t-AmOH: 100.00 uL
D7	0.00	23.00	No ligand: 0.00 mg DIPEA: 6.97 uL DMSO: 100.00 uL
D8	0.00	38.42	CsF: 0.60 mg DIPEA: 6.97 uL DMSO: 100.00 uL
D9	0.00	47.48	No ligand: 0.00 mg DIPEA: 6.97 uL NMP: 100.00 uL
E1	0.00	33.77	No ligand: 0.00 mg Cs2CO3: 13.03 mg DMF: 100.00 uL
E10	0.00	67.12	CsF: 0.60 mg Cs2CO3: 13.03 mg NMP: 100.00 uL
E11	0.00	0.00	No ligand: 0.00 mg Cs2CO3: 13.03 mg CPME: 100.00 uL

E12	0.00	6.04	CsF: 0.60 mg Cs2CO3: 13.03 mg CPME: 100.00 uL
E2	0.00	42.28	CsF: 0.60 mg Cs2CO3: 13.03 mg DMF: 100.00 uL
E3	0.00	3.02	No ligand: 0.00 mg Cs2CO3: 13.03 mg MeCN: 100.00 uL
E4	0.00	4.09	CsF: 0.60 mg Cs2CO3: 13.03 mg MeCN: 100.00 uL
E5	0.00	6.22	No ligand: 0.00 mg Cs2CO3: 13.03 mg t-AmOH: 100.00 uL
E6	0.00	7.57	CsF: 0.60 mg Cs2CO3: 13.03 mg t-AmOH: 100.00 uL
E7	0.00	47.25	No ligand: 0.00 mg Cs2CO3: 13.03 mg DMSO: 100.00 uL
E8	0.00	25.87	CsF: 0.60 mg Cs2CO3: 13.03 mg DMSO: 100.00 uL
E9	0.00	42.39	No ligand: 0.00 mg Cs2CO3: 13.03 mg NMP: 100.00 uL
F11	0.00	1.28	No ligand: 0.00 mg KHMDS: 7.98 mg CPME: 100.00 uL
F12	0.00	0.00	CsF: 0.60 mg KHMDS: 7.98 mg CPME: 100.00 uL
F3	0.00	0.00	No ligand: 0.00 mg KHMDS: 7.98 mg MeCN: 100.00 uL
F4	0.00	0.00	CsF: 0.60 mg KHMDS: 7.98 mg MeCN: 100.00 uL
F5	0.00	0.00	No ligand: 0.00 mg KHMDS: 7.98 mg t-AmOH: 100.00 uL
F6	0.00	0.00	CsF: 0.60 mg KHMDS: 7.98 mg t-AmOH: 100.00 uL
F8	0.00	0.00	CsF: 0.60 mg KHMDS: 7.98 mg DMSO: 100.00 uL
G1	0.00	50.40	No ligand: 0.00 mg K3PO4: 8.49 mg DMF: 100.00 uL
G10	0.00	42.58	CsF: 0.60 mg K3PO4: 8.49 mg NMP: 100.00 uL
G11	0.00	4.56	No ligand: 0.00 mg K3PO4: 8.49 mg CPME: 100.00 uL
G12	0.00	2.03	CsF: 0.60 mg K3PO4: 8.49 mg CPME: 100.00 uL
G2	0.00	54.16	CsF: 0.60 mg K3PO4: 8.49

			mg DMF: 100.00 uL
G3	0.00	1.40	No ligand: 0.00 mg K3PO4: 8.49 mg MeCN: 100.00 uL
G4	0.00	5.03	CsF: 0.60 mg K3PO4: 8.49 mg MeCN: 100.00 uL
G5	0.00	5.56	No ligand: 0.00 mg K3PO4: 8.49 mg t-AmOH: 100.00 uL
G6	0.00	0.00	CsF: 0.60 mg K3PO4: 8.49 mg t-AmOH: 100.00 uL
G7	0.00	70.33	No ligand: 0.00 mg K3PO4: 8.49 mg DMSO: 100.00 uL
G8	0.00	41.70	CsF: 0.60 mg K3PO4: 8.49 mg DMSO: 100.00 uL
G9	0.00	66.47	No ligand: 0.00 mg K3PO4: 8.49 mg NMP: 100.00 uL
H10	0.00	0.00	CsF: 0.60 mg T-BuOK: 4.49 mg NMP: 100.00 uL
H11	0.00	0.00	No ligand: 0.00 mg T-BuOK: 4.49 mg CPME: 100.00 uL
H12	0.00	0.00	CsF: 0.60 mg T-BuOK: 4.49 mg CPME: 100.00 uL
H3	0.00	0.00	No ligand: 0.00 mg T-BuOK: 4.49 mg MeCN: 100.00 uL
H4	0.00	0.00	CsF: 0.60 mg T-BuOK: 4.49 mg MeCN: 100.00 uL
H5	0.00	0.00	No ligand: 0.00 mg T-BuOK: 4.49 mg t-AmOH: 100.00 uL
H6	0.00	0.00	CsF: 0.60 mg T-BuOK: 4.49 mg t-AmOH: 100.00 uL
H7	0.00	0.00	No ligand: 0.00 mg T-BuOK: 4.49 mg DMSO: 100.00 uL
H8	0.00	0.00	CsF: 0.60 mg T-BuOK: 4.49 mg DMSO: 100.00 uL
H9	0.00	0.00	No ligand: 0.00 mg T-BuOK: 4.49 mg NMP: 100.00 uL