Supporting Information

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General Remarks

All reagents and solvents were purchased from Fisher Scientific, Alfa Aesar, Sigma-Aldrich, and VWR and were used without further purification. NMR spectra were recorded on a Bruker spectrospin 300 Instrument (300MHz and 75MHz for ¹H and ¹³C, respectively), an Agilent (400MHz and 100 MHz for ¹H and 13C, respectively), a Bruker Avance 300 (300MHz and 75MHz for ¹H and ¹³C, respectively), or a Bruker AvanceIII 500 (500MHz and 125MHz for ¹H and ¹³C, respectively) and were calibrated with the solvent (CDCl₃: 7.26ppm for ¹H NMR and 77.16 for ¹³C NMR). The abbreviations s, t, m signify singlet, triplet, multiplet respectively. NMR spectra were analyzed by using the software MNova.

The LC samples were analyzed by HPLC/MS conducted on an Agilent 1200 HPLC with the following configuration:

Agilent G1379B degasser, G1312A binary pump, G1316A thermal column compartment, diode array detector and 6120 single quad mass spectrometer.

Analytical setting for the detectors are:

DAD - 200 - 400 nm collected at 20 Hz storing all spectra for offline analysis. Peak area for quantification varies depending on the experiment, see calibration curves for details

ESI-MSD – positive mode scan for m/Z 110 – 1500 running at 0.8sec/cycle. drying gas = 7.0 l/min, nebulizer pressure = 20 psi, gas temperature = 300 °C, capillary voltage = 4000 V

HPLC column and mobile phase method include one of the following conditions (see individual experiment for details):

(1) Poroshell 120 Phenylhexyl-C18, 2.1 x 50 mm, 2.7-Micron Column; Temperature = 25 °C;

Solvent A = water, 0.05 % trifluoroacetic acid; Solvent B = acetonitrile, 0.05 % trifluoroacetic acid; Flow Rate = 0.625 mL/min; Starting Conditions = 90 % A, 10 % B; 0.0-4.0 min linear gradient to 20% A, 80 % B.

(2) Poroshell 120 EC-C18, 2.1 x 30 mm, 2.7-Micron Column; Temperature = 25 °C;

Solvent A = water, 0.05 % trifluoroacetic acid; Solvent B = acetonitrile, 0.05 % trifluoroacetic acid; Flow Rate = 0.75 mL/min; Starting Conditions = 35 % A, 65 % B; 0.0-3.0 min linear gradient to 20% A, 80 % B.

(3) Poroshell 120 EC-C18, 2.1 x 30 mm, 2.7-Micron Column; Temperature = $25 \,^{\circ}$ C; Solvent A = water, 0.05 % trifluoroacetic acid; Solvent B = acetonitrile, 0.05 % trifluoroacetic acid; Flow Rate = 0.625 mL/min; Starting Conditions = $65 \,^{\circ}$ A, $35 \,^{\circ}$ B; 0.0-3.0 min linear

gradient to 30% A, 70 % B.

Synthetic Procedures and Characterization Data

(Azidomethyl)benzene (2)



Compound **2** was synthesized using a literature procedure and characterization data was consistent with that of the literature. ^[1] ¹H NMR (400 MHz, CDCl₃) δ 7.50 – 7.37 (m, 5H), 4.38 (s, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 135.4, 128.8, 128.2, 128.2, 54.7.

1-Benzyl-4-phenyl-1H-1,2,3-triazole (3)



To a 16 mL glass vial equipped with PTFE-silicon septum, open-top screw cap, and magnetic stir bar was added 9.5 mL of acetonitrile, (azidomethyl)benzene (0.067 g, 0.50 mmol), and phenylacetylene (0.051 g, 0.50 mmol). CuI (4.8 mg, 0.025 mmol) and TCPTA (12 mg, 0.025 mmol) dissolved in 0.5 mL of acetonitrile was injected via syringe. The reaction was stirred for 3 hours and then quenched with saturated aqueous NaHCO₃ solution and extracted with dichloromethane. The combined organic layers were dried over MgSO₄, filtered, and then concentrated *in vacuo*. The crude material was recrystallized from petroleum ether:ethyl acetate to afford 1-benzyl-4-phenyl-1H-1,2,3-triazole (0.0716 g. 0.305 mmol, 61% yield) as colourless crystals. ¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 7.3 Hz, 2H), 7.66 (s, 1H), 7.43 – 7.29 (m, 10H), 5.57 (s, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 148.3, 134.8, 130.7, 129.3, 128.9, 128.89, 128.3, 128.2, 125.8, 119.6, 54.3; MS ESI+ (calc. for $C_{15}H_{13}N_3$, 235.11): m/z = 236.2 [M+H]⁺, 258.2 [M+Na]⁺.

Tris((1-cyclopentyl-1H-1,2,3-triazol-4-yl)methyl)amine (TCPTA)



This compound was prepared through adaptation of a previous report.^[2]

¹H NMR (400 MHz, CDCl₃) δ 7.77 (s, 3H), 4.90 (p, *J* = 7.0 Hz, 3H), 3.74 (s, 6H), 2.29 – 2.16 (m, 6H), 2.08 – 1.97 (m, 6H), 1.94 – 1.82 (m, 6H), 1.78 – 1.65 (m, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 143.5, 122.4, 61.73, 47.1, 33.4, 24.1; MS ESI+ (calc. for C₂₄H₃₆N₁₀, 464.31): m/z = 465.2 [M+H]⁺, 487.2 [M+Na]⁺.

(*E*)-1,2-Dichlorovinyl phenyl ketone (5)



The synthetic procedure described by Jonczyk et al. for **2** did not give complete conversion.^[3] However, another procedure from the same laboratory for methyl 2-formylphenylacetate gave full conversion and was used for the synthesis of $2^{[4]}$ The ¹H chemical shifts we observed for 2 were not consistent with those reported by Jonczyk et al. but we confirmed that we had indeed made 2by subsequent chemistry. The *E*-stereochemistry of compound 2 was validated by synthesizing its *Z* isomer and comparing their ${}^{3}J_{C,H}$ values. Compound 5 was isolated as a yellow oil in 85% yield. ¹H NMR (500 MHz, CDCl₃) δ 6.69 (s, 1H), 7.51-7.54 (m, 2H), 7.64-7.67 (m, 1H), 7.96-7.97 (m, 2H) ppm; ¹³C NMR (125 MHz, CDCl₃) δ 118.9, 127.7, 129.0, 129.8, 133.5, 134.7, 188.2 ppm; HRMS: Calculated for C₉H₆OCl₂: 199.9796, Found: 199.9798

(E)-2-chloro-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (6)



Compound **6** was synthesized using a literature procedure and was isolated as a yellow solid in 78% yield. characterization data was consistent with that of the literature^{[5] 1}H NMR (500 MHz, CDCl₃) δ 3.72 (s, 3H), 6.69-6.72 (m, 2H), 7.09-7.12 (m, 2H), 7.14 (s, 1H), 7.40-7.44 (m, 2H), 7.53-7.57 (m, 1H), 7.96-7.98 (m, 2H) ppm; ¹³C NMR (125 MHz, CDCl₃) δ 55.2, 114.0, 124.8, 126.0, 128.8, 129.9, 130.0, 132.5, 134.1, 134.2, 159.8, 191.8 ppm; HRMS: Calculated for C₁₆H₁₃O₂Cl: 272.0604, Found: 272.0605

(Z)-2-chloro-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (7)



Compound **X** was synthesized using a literature procedure and was isolated as a white solid in 78% yield.^{[5] 1}H NMR (500 MHz, CD₃OD) δ 3.85 (s, 3H), 7.00-7.02 (m, 2H), 7.50 (s, 1H), 7.51-7.55 (m, 2H), 7.61-7.64 (m, 1H), 7.72.7.74 (m, 2H), 7.88-7.90 (m, 2H) ppm; ¹³C NMR (125 MHz, CD₃OD) δ 54.5, 113.8, 125.2, 127.6, 128.2, 128.9, 132.1, 132.7, 137.3, 140.6, 161.8, 191.8 ppm; HRMS: Calculated for C₁₆H₁₃O₂Cl: 272.0604, Found: 272.0604

1-(furan-2-yl)ethanol (8)



1-(furan-2-yl)ethanone (4.536 g, 41.2 mmol) was added to methanol (100 ml) and cooled to 0 °C. Sodium borohydride (1.870 g, 49.4 mmol) was then added in batches. After the borohydride addition was complete, the reaction was warmed to room temperature and stirred for one additional hour. The reaction mixture was quenched with water and extracted with dichloromethane. The combined organic layers were dried over MgSO₄, filtered, and then concentrated *in vacuo* to afford 1-(furan-2-yl)ethanol (3.933 g, 35.1 mmol, 85 % yield) as a light yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.36 (m, 1H), 6.33 (dd, *J* = 3.1, 1.7 Hz, 1H), 6.23 (dd, *J* = 3.2, 0.6 Hz, 1H), 4.88 (p, *J* = 6.4 Hz, 1H), 1.97 – 1.94 (m, 1H), 1.54 (d, *J* = 6.6 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ

135.4, 128.9, 128.3, 128.2, 54.8, 30.9; MS ESI+ (calc. for C₆H₈O₂, 112.05): m/z = 95.2 [M-H2O+H]⁺

N-(1-(furan-2-yl)ethyl)aniline (10a)



1-(furan-2-yl)ethanol (187 mg, 1.67 mmol) and aniline (157 mg, 1.67 mmol) were treated with $Dy(OTf)_3$ (51 mg, 0.083 mmol) in acetonitrile (10 mL). The resulting reaction mixture was heated to 65 °C for 2 hours. The reaction mixture was then quenched with saturated aqueous NaHCO₃ solution and extracted with dichloromethane. The combined organic layers were dried over MgSO₄, filtered, and then concentrated *in vacuo*. The residue was purified on silica gel (petroleum ether/ethyl acetate 19:1) to afford N-(1-(furan-2-yl)ethyl)aniline (74 mg, 0.395 mmol, 23.7 % yield) as an oil. ¹H NMR (400 MHz, CDCl₃) δ 7.34 (dd, *J* = 1.7, 0.7 Hz, 1H), 7.19 – 7.13 (m, 2H), 6.74 – 6.68 (m, 1H), 6.63 (dd, *J* = 8.5, 0.9 Hz, 2H), 6.29 (dd, *J* = 3.2, 1.8 Hz, 1H), 6.16 (d, *J* = 3.2 Hz, 1H), 4.64 (q, *J* = 6.3 Hz, 1H), 3.87 (s, 1H), 1.56 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 157.4, 147.1, 141.6, 129.3, 117.9, 113.6, 110.2, 105.2, 47.4, 21.0. MS ESI+ (calc. for C₁₂H₁₃NO, 187.10): m/z = 95.2 [M-C₆H₇N+H]⁺

N-(1-(furan-2-yl)ethyl)-4-nitroaniline (10b)



1-(furan-2-yl)ethanol (193 mg, 1.721 mmol) and 4-nitroaniline (238 mg, 1.721 mmol) were treated with Dy(OTf)₃ (52.5 mg, 0.086 mmol in acetonitrile (10 mL). The resulting reaction mixture was heated to 65 °C for 20 minutes. The reaction mixture was quenched with saturated aqueous NaHCO₃ solution and extracted with dichloromethane. The combined organic layers were dried over MgSO₄, filtered, and then concentrated *in vacuo*. The residue was purified on silica gel (petroleum ether/ethyl acetate, 4:1) to afford N-(1-(furan-2-yl)ethyl)-4-nitroaniline (364 mg, 1.567 mmol, 91 % yield) as a yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 8.09 – 8.04 (m, 2H), 7.35 (dd, J = 1.7, 0.7 Hz, 1H), 6.60 – 6.54 (m, 2H), 6.31 (dd, J = 3.2, 1.9 Hz, 1H), 6.18 (d, J = 3.2 Hz, 1H), 4.79 – 4.68 (m, 2H), 1.61 (d, J = 6.5 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 155.3, 152.2, 142.2, 138.4, 126.4, 111.8, 110.4, 105.9, 47.0, 20.5; MS ESI+ (calc. for C₁₂H₁₂N₂O₃, 232.08): m/z = 233.2 [M+H]⁺, 255.2 [M+Na]⁺.

Reaction Progress Curves

Copper Catalyzed Azide-Alkyne Cycloaddition Reaction



To a 16 mL glass vial equipped with PTFE-silicon septum, open-top screw cap, and magnetic stir bar was added 9.5 mL of acetonitrile, (azidomethyl)benzene (0.067 g, 0.50 mmol), and phenylacetylene (0.051 g, 0.50 mmol). CuI (4.8 mg, 0.025 mmol) and TCPTA (12 mg, 0.025 mmol) dissolved in 0.5 mL of acetonitrile was injected via syringe to initiate the reaction. For HPLC/MS analysis, sampling of the reaction began immediately after injection of the catalyst. A

total of 40 samples were collected at a rate of one sample every five minutes. An aliquot of 50 μ L was taken during each sampling event at a rate of 2.0 mL/min. A dilution volume of 500 μ L of methanol was used to deliver the aliquot to the second sample loop. HPLC analysis was performed using HPLC method (1).



Figure S1: Reaction progress curves for the CuAAC reaction to form the triazole product 3.

Suzuki Cross-Coupling Reaction

The compound **5** (100.525 mg, 0.5mmol, 1 eq), p-MeOPhB(OH)₂ (75.98 mg, 0.5 mmol, 1 eq), Pd₂(dba)₃ (1.145 mg, 0.00125 mmol, .0025 eq). and Cs₂CO₃ (488.73 mg, 1.5 mmol, 3 eq) were placed in a thick glass tube with a screw cap. Anhydrous dioxane (5 ml, 0.1M with respect to **2**) was added to the glass tube. The stirred solution was heated at 40 °C. For HPLC/MS analysis, sampling of the reaction began immediately after addition of the dioxane. An aliquot of 50 μ L was taken during each sampling event (1 per five minutes) at a rate of 2.0 mL/min. A dilution volume

of 500 μ L of methanol was used to deliver the aliquot to the second sample loop. HPLC analysis was performed using HPLC method (2).



Figure S2: Reaction progress curve for the Suzuki cross-coupling reaction

Carbinol Substitution Competition Reaction



To a 16 mL glass vial equipped with PTFE-silicon septum, open-top screw cap, and magnetic stir bar was added 4.75 mL of acetonitrile, 1-(furan-2-yl)ethanol (0.056 g, 0.5 mmol), 4-nitroaniline (0.035 g, 0.250 mmol), and aniline (0.023 g, 0.250 mmol) and heated to 65v°C. Dy(OTf)₃ (15 mg, 0.025 mmol) dissolved in 0.5 mL of acetonitrile at 65 °C was injected via syringe

to initiate the reaction. For HPLC/MS analysis, sampling of the reaction began immediately after injection of the catalyst. A total of 40 samples were collected at a rate of one sample every seven minutes. An aliquot of 50 μ L was taken during each sampling event at a rate of 2.0 mL/min. A dilution volume of 500 μ L of methanol was used to deliver the aliquot to the second sample loop. HPLC analysis was performed using HPLC method (3).



Figure S3: Reaction progress curves for the substitution competition reaction; A) Reaction curves of isolated and calibrated sampled; B) Total speciation observed in the reaction including numerous Frield-Crafts products (not isolated)

Calibration Curves



Figure S4: Calibration curves for components involved in the CuAAC reaction to form the triazole product **3**. Integration of the UV peaks for phenylacetylene (**1**) and benzylazide (**2**) were taken at 210 nm. Integration of the UV peaks for triazole (**3**) were taken at 230 nm.



Figure S5: Calibration curves for components involved in the substitution competition reaction. Integration of the UV peaks for carbinol (8). aniline (9a), exoproduct (10a), and cyclopentenone (11a) were taken at 210 nm. Integration of the UV peaks for 4-nitroaniline (9b) and exoproduct (10b) were taken at 310 nm.

Hardware and Instrumentation

Photos of the Device



Figure S6: Closeup photo of the device. A is the syringe pump, B is the mixing block, C is the EasyMax sample container, D is the first Rheodyne 6-port 2-position valve.



Figure S7: Alternative angle close-up of device



Figure S8: Zoomed out photo of the device



Figure S9: Photo of the second Rheodyne 6-port 2-position valve and HPLC column.



Easy Sampler Actuator Controller – Gilson Interface

Figure S10: Circuit diagram of actuator controller

The actuator is a motor driven scoop, with the CW/CCW motion of the motor the scoop goes DOWN and UP, capturing 20µL of reaction sample from the reactor. The above circuit controls the actuator motion, upon receiving a signal from a remotely located switch, which is the output relay from the Gilson GX-281. The first switch ON/OFF makes the actuator extend down and the second signal makes will retract the sample tip. The control circuit is implemented using a microcontroller (PIC16F690), a comparator (IC2A, LM358), a motor driver (IC1, L6203) and other discrete components such as resistors, capacitors and a transistor as needed. The microcontroller is programmed to accept the input signal from the remote switch and gives out two output signals to the motor driver for CW and CCW rotation. As there are no limit switches

inside the actuator, the extreme ends of the actuator are detected by sensing the current through the motor. When the actuator reaches of the stroke, the motor stops as a result of the armature current going higher than that for the motor in motion. For the specific actuator, we found that the normal operational current is ~ 700 mA; when the stroke limit is reached the current goes to a little over ~1000 mA. A sense resistor (R5) is used to detect the over-at each limit. The voltage divider resistors (R3 and R4) connected to the comparator are chosen such that, when the motor-current is ~800 mA or less the comparator output remains low. Whenever the current goes ~1A or higher the output goes high. A proper logic high and low level for the microcontroller is translated by a MOSFET transistor, Q1. Upon receiving the high current signal the microcontroller stops sending output signal to motor driver. Two power supplies are used, a 5V supply is used to power the microcontroller, comparator and the logic level translator. A 24V supply is used by the motor driver to adequately drive the motor-actuator.

EasySampler Probe Function and Geometry

The sampling head consists of a Hasteloy sampling pocket housed inside a PTFE sleeve. While in the closed position (Figure S10; left) the sampling pocket is housed inside the shaft of the probe head. A linear actuator drives the head into the reaction media allowing the sampling pocket to be exposed to the media (Figure S10; right). This process can be visualized in an animation published on YouTube.

https://www.youtube.com/watch?v=IMVZw3wMhU0



Closed

Open

Figure S11: Cut-away schematic for the EasySampler Probe head. Figure illustrates both the closed (left) and open (right) geometries of the sampler.

References

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NMR Spectra

(Azidomethyl)benzene (2) – ¹H NMR



(Azidomethyl)benzene (2) – ¹³C NMR



1-Benzyl-4-phenyl-1H-1,2,3-triazole (3) - ¹H NMR



1-Benzyl-4-phenyl-1H-1,2,3-triazole (3) – ¹³C NMR





Tris((1-cyclopentyl-1H-1,2,3-triazol-4-yl)methyl)amine (TCPTA) – ¹H NMR



Tris((1-cyclopentyl-1H-1,2,3-triazol-4-yl)methyl)amine (TCPTA) – ¹³C NMR

(*E*)-1,2-Dichlorovinyl phenyl ketone (5) – 1 H NMR



file: D:\nmr 500\NKC_8_65_trans\1\fid expt: <zg30> transmitter freq.: 500.133089 MHz time domain size: 65536 points width: 10000.00 Hz = 19.9947 ppm = 0.152588 Hz/pt number of scans: 16 freq. of 0 ppm: 500.130000 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000

(*E*)-1,2-Dichlorovinyl phenyl ketone (5) – 13 C NMR



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(E)-2-chloro-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (6) – ¹H NMR



file: D:\nmr 500\NKC_8_44_F6-14\1\fid expt: <zg30> transmitter freq.: 500.133089 MHz time domain size: 65536 points width: 10000.00 Hz = 19.9947 ppm = 0.152588 Hz/pt number of scans: 16

freq. of 0 ppm: 500.130002 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000

(E)-2-chloro-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (6) – ¹³C NMR



transmitter freq.: 125.770364 MHz time domain size: 65536 points width: 29761.90 Hz = 236.6369 ppm = 0.454131 Hz/pt number of scans: 1024 freq. of 0 ppm: 125.757789 MHz processed size: 32768 complex points LB: 1.000 GF: 0.0000

(E)-2-chloro-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (6) – ¹³C NMR zoomed



(Z)-2-chloro-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (7) - ¹H NMR



(Z)-2-chloro-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (7) – ¹³C NMR





(Z)-2-chloro-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (7) – ¹³C NMR zoomed

1-(furan-2-yl)ethanol (8) – ¹H NMR



1-(furan-2-yl)ethanol (8) – ¹³C NMR



N-(1-(furan-2-yl)ethyl)aniline (10a) – ¹H NMR



N-(1-(furan-2-yl)ethyl)aniline (10a) – ¹³C NMR







N-(1-(furan-2-yl)ethyl)-4-nitroaniline (10b) – ¹³C NMR

