Supporting Information 1

“High-Throughput Synthesis of Azide Libraries Suitable for Direct “Click” Chemistry and in situ Screening

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1. Chemical Synthesis:

1.1. Synthesis of the alkyne warhead (1)

\[ \text{O} \quad \text{O} \quad \text{O} \]
\[ \text{OH} \quad \text{H} \quad \text{Ts} \]
\[ \text{Dibenzo-18-Crown-6} \]
\[ \text{K}_2 \text{CO}_3, \text{CH}_3 \text{CN}, \text{Reflux, } 6 \text{ h} \]

(1) NaOMe

\[ \text{Dimethyloxalate} \quad \text{Reflux, } 12 \text{ h} \]

(2) NH₂OH.HCl

MeOH, Reflux, 3 d

\[ \text{O} \quad \text{O} \quad \text{N} \]
\[ \text{MeOOC} \]
\[ \text{NaOH} \]

MeOH:Water (3:1)

\[ \text{O} \quad \text{O} \quad \text{N} \]
\[ \text{HOOC} \]

1-(4-Fluoro-2-(prop-2-ynyloxy)phenyl)ethanone acid (3):

Potassium carbonate (99 mmol) and benzo-18-crown-6 (3.3 mmol) were added to a solution of propargyl p-toluenesulfonate (66 mmol) and hydroxyl acetophenone 4 (66 mmol) in acetonitrile (100 mL) followed by refluxing for 6 h, after which the organic phase was removed under reduced pressure and taken into dichloromethane layer (80 mL) and extracted with NaHCO₃ (2 x 40 mL), water (2 x 40 mL) and brine (1 x 40 mL). The organic phase was then dried with anhydrous Na₂SO₄, and the solvent was removed in vacuo to afford the crude product, which, upon further purification by flash column chromatography, afforded the pure propargyl phenyl ether 3 as a yellow solid (88% yield).¹H-NMR (300 MHz, CDCl₃) δ 7.85 – 7.79 (m, 1H), 6.82 – 6.72 (m, 2H), 4.80 (d, \( J = 2.46 \) Hz, 2H), 2.61 – 2.59 (m, 4H);¹³C-NMR (75 MHz, CDCl₃) δ 197.6, 167.6, 164.2, 158.5, 132.7 (\( J_{CF} = 10.9 \) Hz), 125.0 (\( J_{CF} = 3.3 \) Hz), 108.6 (\( J_{CF} = 21.3 \) Hz), 101.0 (\( J_{CF} = 26.2 \) Hz), 76.7, 56.5, 31.8; ESI-MS: \( m/z [M-H]^- = 191.2 \).

Methyl 5-(4-fluoro-2-(prop-2-ynyloxy)phenyl)isoxazole-3-carboxylate (2):

To a mixture of alkyne-derivatized acetophenone (53 mmol) and dimethyl oxalate (53 mmol) was added freshly prepared NaOMe (0.5 M in MeOH, 53 mmol). The reaction mixture was refluxed for 12 h before cooled to room temperature. To the same reaction MeOH (80 mL), NH₂OH.HCl (53 mmol) and a catalytic amount of p-TsOH.H₂O were added and the resulting mixture was refluxed continuously for 3 days. Upon cooling to
room temperature, the precipitated compound was collected, washed with water and ice-cold methanol to afford the pure isoxazole-3-carboxylic acid methyl ester 2 as an off white solid (38% yield). $^1$H-NMR (300 MHz, DMSO-$d_6$) $\delta$ 8.02 – 7.99 (m, 1H), 7.27 (dd, $J_1$ = 2.39 Hz, $J_2$ = 11.3 Hz, 1H), 7.15 (s, 1H), 7.09 – 7.03 (m, 1H), 5.12 (d, $J = 2.31$ Hz, 2H), 3.94 (s, 3H), 3.76 (t, $J = 2.22$ Hz, 1H); ESI-MS: $m/z$ [M+H]$^+$ = 274.7.

5-(4-Fluoro-2-(prop-2-ynyloxy)phenyl)isoxazole-3-carboxylic acid (1):
The methyl ester (4 mmol) was suspended in methanol (10 mL) and a NaOH solution (10 mL; 10 M solution) was added slowly and the reaction was stirred for 3 h before the pH was adjusted to ~2 using HCl (2 N solution) in ice-bath. The resulting precipitate was collected, washed with cold water, dried in vacuo to furnish the desired product 1 as a pale brown solid (92% yield). $^1$H-NMR (300 MHz, DMSO-$d_6$) $\delta$ 7.95 (t, $J = 7.65$ Hz, 1H), 7.21 (d, $J = 11.19$ Hz, 1H), 7.08 (s, 1H), 7.00 (t, $J = 8.48$ Hz, 1H), 5.08 (s, 2H), 3.71 (s, 1H); $^{13}$C-NMR (75 MHz, DMSO-$d_6$) $\delta$ 165.8 (d, $J_{CF} = 2.18$ Hz), 166.2, 162.5, 160.9, 157.7, 155.5 (d, $J_{CF} = 10.9$ Hz), 129.0 (d, $J_{CF} = 10.4$ Hz), 112.0 (d, $J_{CF} = 3.3$ Hz), 108.7 (d, $J_{CF} = 21.8$ Hz), 103.2, 102.0 (d, $J_{CF} = 26.2$ Hz), 79.3, 78.1, 56.9; ESI-MS: $m/z$ [M+H]$^+$ = 262.1.

1.2. Synthesis of the azide libraries

1.2.1. Synthesis of linkers

![Scheme S2. Synthesis of linkers.](image)

Linkers 5a, 5b, were prepared from their corresponding acids as reported. Linkers 5c, 5d and 5e were prepared as previously reported. Linkers 6a-b was prepared as reported. 6c-e were prepared from the diazides as reported.

Scheme for the synthesis of the linker 5a

![Scheme for the synthesis of the linker 5a](image)

Sodium azide (6.95 g, 50 mmol) was dissolved in 30 mL of distilled water and cooled to 0°C. Bromoacetic acid (7.15 g, 100 mmol) was then added over 10 mins and the reaction was allowed to slowly warm to room temperature overnight. The reaction was acidified to pH = 1 and extracted with 5 × 10 mL diethyl ether. The organic layers were
combined, dried over MgSO₄, and concentrated to afford 2-azidoacetic acid as a colorless oil (70% yield). The 2-azidoacetic acid was then dissolved in 50 mL of DCM with two drops of DMF and cooled to 0°C. Oxalyl chloride (3 mL, 35 mmol) was added slowly using a syringe over 15 min. The reaction was allowed to stir for 5 hours and the crude azido chloride 5a (in DCM) as used directly for solid-phase synthesis without further purification.

\[
\text{HO} \quad \text{O} \quad \text{N}_3
\]

\(^1\text{H-NMR}\) (300 MHz, CDCl₃) δ 10.97 (s, 1H), 3.97 (s, 2H). \(^{13}\text{C-NMR}\) (75 MHz, CDCl₃) δ 174.4, 49.9.

Scheme for the synthesis of the linker 5b

3-Bromopropionic acid (25 mmol) was dissolved in acetonitrile (40 mL) and Sodium azide was (50 mmol) added to the solution, the mixture was refluxed for 4 hours after which acetonitrile was removed \textit{in vacuo} and the resulting residue was suspended in ethyl acetate (50 mL) and extracted with 0.1 N HCl (3 x 40mL), water (3 x 40 mL) and brine (1 x 30 mL). The organic layer was dried using anhydrous Na₂SO₄ to afford the 3-azidopropionic acid in 87% yield. 3-Azidopropionic acid (20 mmol) was dissolved in DCM (40 mL) and treated with oxalyl chloride (20 mmol). The reaction was allowed to stir for 6 hours at room temperature to afford 3-azidopropionyl chloride 5b, which was used directly without any further purification.

\[
\text{HO} \quad \text{O} \quad \text{N}_3
\]

\(^1\text{H-NMR}\) (300 MHz, CDCl₃) δ 3.61-3.57 (t, \(J = 6.4\) Hz, 2H), 2.66-2.62 (t, \(J = 6.4\) Hz, 2H). \(^{13}\text{C-NMR}\) (75 MHz, CDCl₃) δ 178.04, 47.01, 34.39

General scheme for the synthesis of the linker 5c-e

\(\text{-Bromoalkynoic acid (40 mmol) was dissolved in MeOH (50 mL) and SOCl}_2\) (120 mmol) or Oxalyl chloride (80 mmol) was added. The resulting solution was allowed to stir for 1 hour at room temperature after which MeOH was removed \textit{in vacuo}, the resulting residue was suspended in ethyl acetate (50 mL) and extracted with NaHCO₃ (3 x 40mL), water (3 x 40 mL) and brine (1 x 30 mL). The organic layer was dried using anhydrous Na₂SO₄ to afford the \(n\)-bromomethyl alkynoate which was used without
further purification. The $n$-bromomethyl alkynoate (30 mmol) was dissolved in DMF (4 mL) and sodium azide (60 mmol) was added, the suspension was heated under microwave irradiation at 80°C for 20 min, after which it was taken to the ethyl acetate (50 mL) and extracted with NaHCO$_3$ (3 x 40mL), water (3 x 40 mL) and brine (1 x 30 mL). The organic layer was dried using anhydrous Na$_2$SO$_4$ to afford the $n$-azidomethyl alkynoate in 84 – 90% yield.

Yield = 84 %. Pale yellow oil. $^1$H-NMR (300 MHz, CDCl$_3$) δ 3.69 (s, 3H), 3.38-3.36 (t, $J$ = 6.6 Hz, 2H), 2.44-2.39 (t, $J$ = 7.23 Hz, 2H), 1.96-1.86 (q, 4H).

Yield = 90 %. Pale yellow oil. $^1$H-NMR (300 MHz, CDCl$_3$) δ 3.67 (s, 3H), 3.39 (t, 2H), 2.38 (m, 2H), 1.91-1.60 (m, 4H).

Yield = 85 %. Pale yellow oil. $^1$H-NMR (300 MHz, CDCl$_3$) δ 3.68 (s, 3H), 3.29-3.25 (t, $J$ = 6.82 Hz, 2H), 2.35-2.30 (t, $J$ = 7.39 Hz, 2H), 1.71-1.57 (m, 4H), 1.46-1.38 (m, 2H).

$n$-Bromomethyl alkynoate (30 mmol) was dissolved in MeOH (30 ml) and LiOH solution (60 mmol in 10 mL water) was added. The suspension was stirred for 4 hours after which MeOH was removed under vacuo, the resulting residue was suspended in ethyl acetate (50 mL) and extracted with 1N HCl (3 x 40mL), water (3 x 40 mL) and brine (1 x 30 mL). The organic layer was dried using anhydrous Na$_2$SO$_4$ to afford the $n$-bromoalkanoic acid in 78 – 85% yield, which was used without further purification. On treatment of the $n$-bromoalkanoic acid (25 mmol) in DCM (50 mL) with oxalyl chloride (50 mmol) and stirring the reaction for 4 hours followed by the removal of the DCM under vacuo afforded 5c-e which was used without further purification.

Yield = 78%. $^1$H-NMR (300 MHz, CDCl$_3$) δ 3.36-3.34(t, $J$ = 6.5 Hz, 2H), 2.50-2.45 (t, $J$ = 7.3 Hz, 2H), 1.95-1.85 (q, 4H).

Yield = 85%. $^1$H-NMR (300 MHz, CDCl$_3$) δ 8.93 (br, 1H), 3.33(t, 2H), 2.39 (t, 2H), 1.75 (m, 4H).

Yield = 82%. $^1$H-NMR (300 MHz, CDCl$_3$) δ 11.15 (br, 1H), 3.30-3.26 (t, $J$ = 6.81 Hz, 2H), 2.40-2.35 (t, $J$ = 7.3 Hz, 2H), 1.72-1.57 (m, 4H), 1.46-1.38(m, 2H).
General scheme for the synthesis of the linkers 6a-b

\[
\begin{align*}
&\text{Br} \underbrace{\text{NH}_3\text{Br}}_{n} \xrightarrow{1. \text{NaN}_3/\text{H}_2\text{O}, 80^\circ\text{C}, 12\text{h}} \xrightarrow{2. \text{Aq. KOH}} \text{N}_3 \underbrace{\text{NH}_2}_{n}=1, \ \text{6a} \quad n=2, \ \text{6b}
\end{align*}
\]

\(n\)-bromoalkylammonium bromide (15 mmol) was suspended in water (10 mL) followed by the addition of NaN\(_3\) (50 mmol) in 15 mL of water. The mixture was heated 80 \(^\circ\)C for 12 hrs followed by the removal of 2/3 of the water in vacuum. The resulting mixture was cooled in an ice bath and diethyl ether (50 mL) and KOH pellets (4 g) were added while keeping the temperature <10 \(^\circ\)C. The organic layer was separated and the aqueous phase was extracted with diethyl ether (2 x 30 mL). The combined organic layers were dried over K\(_2\)CO\(_3\) and concentrated to give the pure products.

**Yield 79%, colourless oil**

\(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 1.24 (s, 2H), 2.83 (t, \(J = 5.7\) Hz, 2H), 3.31 (t, \(J = 5.7\) Hz, 2H).

**Yield 84%, clear yellow oil**

\(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 1.13 (s, 2H), 1.70 (m, 2H), 2.77 (t, \(J = 7.0\) Hz, 2H), 3.34 (t, \(J = 6.6\) Hz, 2H).

General scheme for the synthesis of the linkers 6c-e

\[
\begin{align*}
&\text{Br} \underbrace{\text{Br}}_{n} \xrightarrow{\text{NaN}_3/\text{DMF}, 80^\circ\text{C}, 12\text{h}} \xrightarrow{\text{PPh}_3, \text{EA}:\text{Ether}} \text{N}_3 \underbrace{\text{N}_3}_{n}=1, \ \text{6c} \quad n=2, \ \text{6d} \quad n=3, \ \text{6e}
\end{align*}
\]

General procedure for the synthesis of the diazides

\(\text{NaN}_3\) (50.0 mmol) was added to a solution of the dibromoalkyl compound (50.0 mmol) in DMF (50.0 mL). The mixture was stirred at 60\(^\circ\)C for 12 hrs, at which point water (200 mL) was added and the product was extracted with ether (3 x 20 mL). The organic layer was washed three times with water (3 x 20 mL), the solvent was evaporated, and the compound was purified by chromatography on silica gel (hexane as eluent solvent) to give the pure products.

**Yield 91%, colourless oil**

\(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 1.68 (p, \(J = 7.0\) Hz, 6H), 3.32 (t, \(J = 5.7\) Hz, 4H).
Yield 93%, colourless oil
$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 1.41 (m, 2H), 1.68 (m, 4H), 3.28 (t, $J = 6.8$ Hz, 4H).

Yield 94%, colourless oil
$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 1.40 (m, 4H), 1.61 (m, 4H), 3.27 (t, $J = 6.9$ Hz, 4H).

General scheme for the synthesis of the linkers 5c-e
To a solution of diazidoalkane (40.0 mmol) in Et$_2$O (25 mL):EtOAc (25 mL) and 5% HCl (40 mL) was added triphenylphosphine (39.0 mmol) in small portions for 1 h at 0°C and then the mixture was stirred for 24 h at room temperature. The organic layer was discarded and the aqueous layer was washed twice with DCM (50 mL). The resulting aqueous phase was carefully basified with NaOH and then extracted with DCM (3 x 50 mL). The combined extracts were dried with Na$_2$SO$_4$ and evaporated to give the pure products.

Yield 88%, clear yellow oil
$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 1.12 (s, 2H), 1.50 (m, 2H), 1.62 (m, 2H), 2.70 (m, 2H), 3.27 (t, $J = 11.1$ Hz, 2H).

Yield 84%, clear yellow oil
$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 1.17 (s, 2H), 1.39 (m, 4H), 1.56 (p, $J = 14.5$ Hz, 2H), 2.65 (t, $J = 6.9$ Hz, 2H), 3.22 (t, $J = 6.9$ Hz, 2H).

Yield 72%, clear yellow oil
$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 1.10 (s, 2H), 1.38 (m, 6H), 1.57 (m, 2H), 2.66 (t, $J = 6.7$ Hz, 2H), 3.23 (t, $J = 6.9$ Hz, 2H).
1.2.2. Synthesis of azides using amine building blocks

Scheme S3. Synthesis of azides from amine building blocks.

See maintext for details.
1.2.3. Synthesis of azides using acid building blocks

![Scheme S4. Synthesis of azides from acid building blocks.]

**Acid building blocks**

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**Synthesis of the reductive aminated resin (10a-e):**

Pre-swelled PL-FMP resin (34 x 150 mg, 0.9 mmol/g) was taken in to 5 sets (x 34) MacroKan™ reactors each containing a RF tag. The reactors were taken into a 250 ml bottle containing 2% acetic acid in 1,2-dichloroethane (150 mL), DIEA (8 eq) and the amine 6a-e (4 eq). After incubating for about 2 hours, Sodium triacetoxyborohydride (5 eq) was added. After shaken for another 4 hours, the solution was decanted and the microreactors were washed with DCM (200 mL x 5), MeOH (200 mL x 2) and THF (200 mL x 3) and dried to afford the N-acylated resins 10a-e (5 sets, each contains 34 identical reactors).
Synthesis of N-acylated resin (12):

To the first set of the reductive aminated resin 10a (34 x 150 mg) was taken into 34 different bottles (10 mL). A solution (5 mL) of PyBOP (4 eq), HOAt (4 eq) and DIEA (6 eq) in DMF was added followed by the addition of acid building blocks E1-G10 (4 eq), so that each bottle had a unique acid. After shaken for 12 hours the microreactors were decanted, then combined and washed with DCM (200 mL x 5), MeOH (200 mL x 2) and THF (200 mL x 3) and dried to afford the resin 12.

Cleavage and release of azides (E1-2C-G10-2C):

The above General protocol for cleavage and release of azides, to afford the E1-2C to G10-2C. All azides synthesized from the above protocols are of high purity (90-95%; see SI_2 for detailed structures, ID and characterizations). Representative compounds were further characterizations, without any purification, by LCMS, \(^1\)H and \(^{13}\)C NMR.

\((G1-3C)\) N-(2-Azido-ethyl)-benzamide. \(^1\)H-NMR (500 MHz, CDCl₃) \(\delta\) 7.79-7.77 (d, \(J = 12.20\) Hz, 2H), 7.54-7.41 (m, 4H), 3.64-3.56 (m, 4H). \(^{13}\)C-NMR (125 MHz, CDCl₃) 132.65, 132.29, 129.21, 127.53, 51.50, 40.00. ESI-MS(ToF): \(m/z\) 191.092 [M + H]^+.

\((G2-3C)\) N-(2-Azido-ethyl)-3-fluoro-benzamide. \(^1\)H-NMR (500 MHz, CDCl₃) \(\delta\) 7.57-7.51 (m, 2H), 7.43-7.36 (q, 4H), 7.22-7.17 (m, 1H), 3.62-3.55 (m, 4H). \(^{13}\)C-NMR (125 MHz, CDCl₃) 167.19, 136.92, 136.92, 130.84(d), 123.12(d), 119.32(d), 119.32(d), 115.13(d), 51.22, 40.08. ESI-MS(ToF): \(m/z\) 209.081 [M + H]^+.

\((G3-3C)\) N-(2-Azido-ethyl)-3,4-difluoro-benzamide. \(^1\)H-NMR (500 MHz, CDCl₃) \(\delta\) 7.73-7.66 (m, 2H), 7.58-7.55 (m, 1H), 7.28-7.17 (m, 1H), 3.62-3.55 (m, 4H). \(^{13}\)C-NMR (125 MHz, CDCl₃) 154.19, 151.98, 131.17, 123.17(m), 117.61(m), 51.10, 40.85. ESI-MS(ToF): \(m/z\) 227.073 [M + H]^+.

\((G4-3C)\) N-(2-Azido-ethyl)-2,4-difluoro-benzamide. \(^1\)H-NMR (500 MHz, CDCl₃) \(\delta\) 8.12-8.10 (d, \(J = 8.95\) Hz, 1H), 3.61-3.56 (m, 4H). \(^{13}\)C-NMR (125 MHz, CDCl₃) 166.09, 164.0, 161, 133.77(d), 127.26, 117.94(d), 51.13, 40.20. ESI-MS(ToF): \(m/z\) 227.072 [M + H]^+.

\((G5-3C)\) N-(2-Azido-ethyl)-4-fluoro-3-trifluoromethyl-benzamide. \(^1\)H-NMR (500 MHz, CDCl₃) \(\delta\) 8.14-8.10 (m, 1H), 7.02-6.86 (m, 1H), 3.67-3.63 (m, 2H), 3.58-3.55 (t, \(J = 5.67\) Hz, 2H). \(^{13}\)C-NMR (125 MHz, CDCl₃) 166.49, 163.24(d), 134.44(m), 117.70(d), 113.10(m), 105.12(m), 51.31, 39.97. ESI-MS(ToF): \(m/z\) 227.068 [M + H]^+.

\((G6-3C)\) N-(2-Azido-ethyl)-4-fluoro-3-methyl-benzamide. \(^1\)H-NMR (500 MHz, CDCl₃) \(\delta\) 7.66 (m, 1H), 7.59-7.57 (m, 1H), 7.04-7.00 (t, \(J = 10\) Hz , 1H), 3.62-3.58 (m, 2H), 3.55-3.53 (t, \(J = 5\) Hz, 2H), 2.40 (s, 3H). \(^{13}\)C-NMR (125 MHz, CDCl₃) 167.60, 164.94, 162.94, 131.35, 51.42, 40.03, 15.04.
(G7-3C) N-(2-Azido-ethyl)-2,3,4-trifluoro-benzamide. $^1$H-NMR (500 MHz, CDCl$_3$) $\delta$ 7.87-7.82 (m, 1H), 7.12-7.07 (m, 1H), 3.67-3.64 (m, 2H), 3.59-3.56 (t, $J = 5.67$ Hz, 2H). ESI-MS(ToF): $m/z$ 245.060 [M + H]$^+$. 

(G8-3C) N-(2-Azido-ethyl)-2-fluoro-benzamide. $^1$H-NMR (500 MHz, CDCl$_3$) 8.09-8.06 (m, 1H), 7.50-7.46 (m, 1H), 7.25 (m, 1H), 7.15-7.11 (m, 1H), 3.68-3.64 (m, 2H), 3.58-3.56 (t, $J = 5.67$, 2H). $^{13}$C-NMR (125 MHz, CDCl$_3$) $\delta$ 164.22, 160.26, 134.16 (d), 132.56 (d), 125.43 (d), 121.22, 116.74 (d), 51.33, 39.94. ESI-MS(ToF): $m/z$ 209.081 [M + H]$^+$. 

(G10-3C) N-(2-Azido-ethyl)-4-ethyl-benzamide. $^1$H-NMR (500 MHz, CDCl$_3$) $\delta$ 7.72-7.69 (d, $J = 13.9$ Hz, 2H), 7.25-7.22 (d, $J = 13.9$ Hz, 2H), 3.63-3.50 (m, 4H), 2.72-2.64 (q, 2H), 1.26-1.21 (t, $J = 12.7$ Hz, 3H). $^{13}$C-NMR (125 MHz, CDCl$_3$) $\delta$ 168.43, 148.94, 131.94, 128.61, 127.62, 51.42, 39.93, 29.28, 15.79. ESI-MS(ToF): $m/z$ 304.983 [M + H]$^+$. 

1.2.4. Synthesis of azides using acid chloride building block

Scheme S5. Synthesis of azides from acid chloride building block.

Synthesis of N-acylated resin from acid chloride (11a, 11c-e):

The reductive aminated resins 10a, 10c-e (4 x 150 mg) were taken in a bottle (25 ml) containing DCM (15 ml). 2-chlorobenzoyl chloride, H (4 eq) and DIEA (5 eq) were added. After shaken for 6 hours, the solution was decanted and the microreactors were washed with DCM (50 mL x 5), MeOH (50 mL x 2) and THF (50 mL x 3) and dried to afford the N-acylated resin 11a, 11c-e.

Cleavage and release of the azides (H1-2C to H1-6C):

Each dried resin was treated with an 1.5 ml solution containing of TFA (10 %) and DCM (90 %) the mixture was shaken for 1 hour and transferred into 96-well plate, dried in vacuo, then redisolved in DMSO (1 mL) to give 50 mM solutions (assuming 50 % yield). All azides synthesized from the above protocols are of high purity (90-95%; see SI_2 for detailed structures, ID and characterizations). Representative compounds were further characterizations, without any purification, by LCMS, $^1$H and $^{13}$C NMR.
1.2.5. Synthesis of azides using sulfonyl chlorides

**Scheme S6. Synthesis of azides from sulfonyl chloride building blocks.**

**Sulfonyl chloride building blocks**

**Synthesis of the N-sulfonamide resin (13a-e):**

The reductive aminated resin 10a-e (23 x 150 mg) was taken in to 23 different bottles (10 ml) each containing a unique sulfonyl chloride (I1 to J11) and DIEA (5 eq) in DCM (5 ml). After shaken for 6 hours, the solution was decanted and the microreactors were washed with DCM (200 mL x 5), MeOH (200 mL x 2) and THF (200 mL x 3) and dried to afford the N-sulfonylated resin 13(a-e).

Cleavage and release of the sulfonamide-based azides (I1-2C to J11-6C):

Each dried resin was treated with an 1.5 ml solution containing TFA (10 %) and DCM (90 %) the mixture was shaken for 1 hour and transferred into 2 different 96-well plates, dried in vacuo, then redissolved in DMSO (1 mL) to give 50 mM solutions
(assuming 50% yield). All azides synthesized from the above protocols are of high purity (90-95%; see SI_2 for detailed structures, ID and characterizations). Representative compounds were further characterized, without any purification, by LCMS, $^1$H and $^{13}$C-NMR.

(I1-2S) 4-Acetyl-N-(2-azidoethyl)benzenesulfonamide. $^1$H-NMR (300 MHz, DMSO-d$_6$) $\delta$ 2.63 (s, 3H), 2.94-3.00 (m, 2H), 3.33 (t, $J$ = 5.8 Hz, 2H), 7.93 (d, $J$ = 8.4 Hz, 2H), 8.13-8.16 (m, 3H). $^{13}$C-NMR (75 MHz, DMSO- d$_6$) $\delta$ 27.0, 42.1, 50.1, 126.8, 129.0, 139.5, 144.0, 197.3.

(I2-2S) N-(2-azidoethyl)biphenyl-4-sulfonamide. $^1$H-NMR (300 MHz, DMSO-d$_6$) $\delta$ 2.95-3.00 (m, 2H), 3.33 (t, $J$ = 5.8 Hz, 2H), 7.44-7.54 (m, 3H), 7.74 (d, $J$ = 7.0 Hz, 2H), 7.89 (m, 4H), 7.99 (t, $J$ = 5.9 Hz, 2H). $^{13}$C-NMR (75 MHz, DMSO- d$_6$) $\delta$ 42.2, 50.1, 127.0, 127.4, 128.5, 129.1, 132.3, 138.5, 139.1, 144.0.

(J6-2S) N-(2-azidoethyl)naphthalene-2-sulfonamide. $^1$H-NMR (300 MHz, DMSO-d$_6$) $\delta$ 2.95-3.01 (m, 2H), 3.33 (t, $J$ = 5.8 Hz, 2H), 7.64-7.72 (m, 2H), 7.82 (d, $J$ = 1.7 Hz, 2H), 8.02-8.17 (m, 4H), 8.46 (s, 1H). $^{13}$C-NMR (75 MHz, DMSO- d$_6$) $\delta$ 42.2, 50.1, 122.2, 127.4, 127.8, 128.7, 129.2, 129.4, 131.7, 134.2, 137.3.

(I1-3S) 4-Acetyl-N-(3-azido-propyl)-benzenesulfonamide. $^1$H-NMR (300 MHz, CDCl$_3$) $\delta$ 8.08-8.05 (d, $J$ = 8.37 Hz, 2H), 7.96-7.93 (d, $J$ = 8.37 Hz, 2H), 5.31-5.27 (t, $J$ = 6.09 Hz, 1H), 3.38-3.34 (t, $J$ = 6.43 Hz, 2H), 3.09-3.02 (m, 2H), 2.7 (s, 3H), 1.75-1.71 (m, 2H). $^{13}$C-NMR (300 MHz, CDCl$_3$) $\delta$ 144.38, 140.71, 129.70, 127.96, 49.32, 41.36, 29.49, 27.53.

(I4-3S) 5-Chloro-thiophene-2-sulfonic acid (3-azido-propyl)-amide. $^1$H-NMR (300 MHz, CDCl$_3$) $\delta$ 7.40-7.39 (d, $J$ = 3.54 Hz, 1H), 6.93-6.92 (d, $J$ = 3.84 Hz, 1H), 5.23-5.20 (t, $J$ = 5.86 Hz, 1H), 3.42-3.38 (t, $J$ = 6.43 Hz, 2H), 3.15-3.09 (m, 2H), 1.82-1.74 (m, 2H). $^{13}$C-NMR (300 MHz, CDCl$_3$) $\delta$ 124.88-124.73(m), 119.09, 118.85, 117.81-117.54(d), 49.37, 41.41, 29.47.

(17-3S) N-(3-Azido-propyl)-3,4-difluoro-benzenesulfonamide. $^1$H-NMR (300 MHz, CDCl$_3$) $\delta$ 7.74-7.63 (m, 2H), 7.36-7.26 (m, 1H), 5.22-5.18 (t, $J$ = 5.92 Hz, 1H), 3.40-3.36 (t, $J$ = 6.43 Hz, 2H), 3.08-3.02 (m, 2H), 1.79-1.71 (m, 2H). $^{13}$C-NMR (300 MHz, CDCl$_3$) $\delta$ 124.88-124.73(m), 119.09(d), 117.81(d), 49.37, 41.41, 29.47.

(J6-3S) Naphthalene-2-sulfonic acid (3-azido-propyl)-amide. $^1$H-NMR (300 MHz, CDCl$_3$) $\delta$ 8.45 (s, 1H), 7.98-7.82 (m, 4H), 7.67-7.58 (m, 2H), 5.25-5.21 (t, $J$ = 6.01 Hz, 1H), 3.37-3.33 (t, $J$ = 6.45 Hz, 2H), 3.10-3.05 (m, 2H), 1.78-1.69 (m, 2H). $^{13}$C-NMR (300 MHz, CDCl$_3$) $\delta$ 130.30-128.29(m), 122.81, 49.39, 41.35, 29.51.
(I1-4S) 4-Acetyl-N-(4-azidobutyl)benzenesulfonamide. $^1$H-NMR (300 MHz, DMSO-$d_6$) \(\delta 1.37-1.53\) (m, 4H), 2.63 (s, 3H), 2.76-2.82 (m, 2H), 3.26 (t, $J = 5.6$ Hz, 2H), 7.83 (t, $J = 5.7$ Hz, 1H), 7.92 (d, $J = 8.3$ Hz, 2H), 8.13 (d, $J = 8.3$ Hz, 2H). $^{13}$C-NMR (75 MHz, DMSO-$d_6$) \(\delta 25.4, 26.3, 27.0, 42.0, 50.1, 126.8, 129.0, 139.4, 144.3, 197.3\).

(II-4S) N-(4-azidobutyl)biphenyl-4-sulfonamide. $^1$H-NMR (300 MHz, DMSO-$d_6$) \(\delta 1.32-1.44\) (m, 4H), 2.77-2.83 (m, 2H), 3.26 (t, $J = 6.4$ Hz, 2H), 7.61-7.74 (m, 3H), 7.96-8.23 (m, 4H), 8.67 (d, $J = 8.4$ Hz, 1H). $^{13}$C-NMR (75 MHz, DMSO-$d_6$) \(\delta 25.5, 26.3, 42.0, 50.2, 127.0, 127.4, 127.8, 128.4, 129.1, 132.3, 138.6, 139.3, 143.8\).

(J5-4S) N-(4-azidobutyl)naphthalene-1-sulfonamide. $^1$H-NMR (300 MHz, DMSO-$d_6$) \(\delta 1.32-1.44\) (m, 4H), 2.77-2.83 (m, 2H), 3.26 (t, $J = 6.3$ Hz, 2H), 7.63-7.84 (m, 4H), 8.02-8.17 (m, 3H), 8.44 (s, 1H). $^{13}$C-NMR (75 MHz, DMSO-$d_6$) \(\delta 23.2, 27.7, 28.5, 42.3, 50.5, 122.2, 127.5, 127.8, 128.6, 129.1, 131.7, 134.1, 137.6\).

(II-5S) 4-Acetyl-N-(5-azidopentyl)benzenesulfonamide. $^1$H-NMR (300 MHz, DMSO-$d_6$) \(\delta 1.22-1.49\) (m, 6H), 2.63 (s, 3H), 2.73-2.79 (m, 2H), 3.25 (t, $J = 6.8$ Hz, 2H), 7.79 (t, $J = 5.7$ Hz, 1H), 7.92 (d, $J = 8.0$ Hz, 2H), 8.13 (d, $J = 8.0$ Hz, 2H). $^{13}$C-NMR (75 MHz, DMSO-$d_6$) \(\delta 23.2, 27.0, 27.7, 28.5, 42.3, 50.5, 126.8, 129.0, 139.3, 144.3, 197.3\).

(J6-5S) N-(5-azidopentyl)naphthalene-2-sulfonamide. $^1$H-NMR (300 MHz, DMSO-$d_6$) \(\delta 1.22-1.45\) (m, 6H), 2.74-2.80 (m, 2H), 3.20 (t, $J = 6.8$ Hz, 2H), 7.63-7.84 (m, 4H), 8.02-8.17 (m, 3H), 8.43 (s, 1H). $^{13}$C-NMR (75 MHz, DMSO-$d_6$) \(\delta 23.2, 27.0, 27.7, 28.5, 42.3, 50.5, 122.2, 127.5, 127.8, 128.6, 129.1, 131.7, 134.1, 137.6\).

(J7-5S) N-(5-azidopentyl)-3-nitrobenzenesulfonamide. $^1$H-NMR (300 MHz, DMSO-$d_6$) \(\delta 1.23-1.45\) (m, 6H), 2.74-2.80 (m, 2H), 3.20 (t, $J = 6.8$ Hz, 2H), 7.63-7.84 (m, 4H), 8.01-8.17 (m, 3H), 8.43 (s, 1H). $^{13}$C-NMR (75 MHz, DMSO-$d_6$) \(\delta 23.2, 27.0, 27.7, 28.5, 42.3, 50.5, 122.3, 127.2, 127.5, 127.8, 128.6, 129.1, 131.7, 134.1, 137.6\).

(I1-6S) 4-Acetyl-N-(6-azidoheptyl)benzenesulfonamide. $^1$H-NMR (300 MHz, DMSO-$d_6$) \(\delta 1.21-1.45\) (m, 6H), 2.74-2.80 (m, 2H), 3.20 (t, $J = 6.8$ Hz, 2H), 7.88-7.98 (m, 2H), 8.21 (d, $J = 7.7$ Hz, 1H), 8.46-8.52 (m, 2H). $^{13}$C-NMR (75 MHz, DMSO-$d_6$) \(\delta 23.2, 27.7, 28.5, 42.3, 50.5, 121.2, 126.9, 131.3, 132.5, 142.3, 147.9\).

S1-13
(I2-6S) \(N\)-(6-azidohexyl)biphenyl-4-sulfonamide. \(^1\)H-NMR (300 MHz, DMSO-\(d_6\)) \(\delta\) 1.22-1.46 (m, 8H), 2.73-2.80 (m, 2H), 3.25 (t, \(J = 6.8\) Hz, 2H), 7.40-7.53 (m, 3H), 7.60-7.74 (m, 3H), 7.87 (m, 4H). \(^{13}\)C-NMR (75 MHz, DMSO-\(d_6\)) \(\delta\) 25.5, 25.6, 28.0, 28.8, 42.4, 50.5, 127.0, 127.1, 127.3, 128.4, 128.5, 129.1, 132.2, 138.6, 139.4, 143.8.

(J6-6S) \(N\)-(6-azidohexyl)naphthalene-2-sulfonamide. \(^1\)H-NMR (300 MHz, DMSO-\(d_6\)) \(\delta\) 1.17-1.40 (m, 8H), 2.73-2.80 (m, 2H), 3.19 (t, \(J = 7.0\) Hz, 2H), 7.63-7.84 (m, 4H), 8.01-8.17 (m, 3H), 8.43 (s, 1H). \(^{13}\)C-NMR (75 MHz, DMSO-\(d_6\)) \(\delta\) 25.4, 25.6, 28.0, 28.8, 42.4, 50.4, 122.3, 127.2, 127.5, 127.8, 128.6, 129.1, 129.3, 131.7, 134.1, 137.6.

(J7-6S) \(N\)-(6-azidohexyl)-3-nitrobenzenesulfonamide. \(^1\)H-NMR (300 MHz, DMSO-\(d_6\)) \(\delta\) 1.22-1.47 (m, 8H), 2.76-2.81 (m, 2H), 3.26 (t, \(J = 6.8\) Hz, 2H), 7.88-7.96 (m, 2H), 8.21 (d, \(J = 8.0\) Hz, 1H), 8.46-8.52 (m, 2H). \(^{13}\)C-NMR (75 MHz, DMSO-\(d_6\)) \(\delta\) 26.5, 26.6, 29.1, 29.8, 30.0, 43.4, 51.5, 122.3, 128.0, 132.3, 133.6, 143.4, 149.0.

1.2.6. Synthesis of azides using chloroformate building block

![Scheme S7. Synthesis of azides from chloroformate building block.](image_url)

Synthesis of carbamate resin (14):

The reductive aminated resins 10a, 10d-e (3 x 150 mg) were taken in a bottle (25 ml) containing DCM (15 ml). Benzylchloro formate and DIEA (5 eq) were added. After shaken for 6 hours, the solution was decanted and the microreactors were washed with DCM (50 mL x 5), MeOH (50 mL x 2) and THF (50 mL x 3) and dried to afford the carbamate resin 14a, 14d-e.

Cleavage and release of the azides (L1-2C to L1-6C):

Each dried resin was treated with an 1.5 ml solution containing of TFA (10 %) and DCM (90 %) the mixture was shaken for 1 hour and transferred into 96-well plate, dried in vacuo, then redissolved in DMSO (1 mL) to give 50 mM solutions (assuming 50 % yield). All azides synthesized from the above protocols are of high purity (90-95%; see SI 2 for detailed structures, ID and characterizations). Representative compounds were further characterizations, without any purification, by LCMS, \(^1\)H and \(^{13}\)C-NMR.

S1-14
2. Click Chemistry:

![Click Chemistry Diagram]

2.1. Optimization of Click Chemistry:

For detailed protocols, see the maintext. In summary, a number of different click chemistry conditions (Table S1) were tried, and the most suitable conditions (highlighted) were chosen for all subsequent large-scale assembly of the 325-member click products.

### Table S1: Optimization of the Click reaction

<table>
<thead>
<tr>
<th>No.</th>
<th>Catalyst</th>
<th>Additive</th>
<th>Solvent (1:1)</th>
<th>Yield</th>
<th>Purity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CuSO$_4$.5H$_2$O</td>
<td>Sodium ascorbate</td>
<td>t-BuOH: H$_2$O</td>
<td>~100</td>
<td>&gt;95</td>
</tr>
<tr>
<td>2</td>
<td>CuSO$_4$.5H$_2$O</td>
<td>Sodium ascorbate</td>
<td>DMSO: H$_2$O</td>
<td>&gt;95</td>
<td>&gt;95</td>
</tr>
<tr>
<td>3</td>
<td>CuSO$_4$.5H$_2$O</td>
<td>Sodium ascorbate</td>
<td>DCM: H$_2$O</td>
<td>~100</td>
<td>~100</td>
</tr>
<tr>
<td>4</td>
<td>CuSO$_4$.5H$_2$O</td>
<td>Sodium ascorbate</td>
<td>DCE: H$_2$O</td>
<td>~100</td>
<td>~100</td>
</tr>
<tr>
<td>5</td>
<td>CuI</td>
<td>Acetonitrile, Pyridine</td>
<td>t-BuOH: H$_2$O</td>
<td>&gt;90</td>
<td>80</td>
</tr>
<tr>
<td>6</td>
<td>CuI</td>
<td>Acetonitrile, Pyridine</td>
<td>DMSO: H$_2$O</td>
<td>&gt;95</td>
<td>90</td>
</tr>
</tbody>
</table>

a Based on % conversion of the starting material (i.e. alkyne)
b Most suitable reaction conditions in 384-well plate, due to high conversion/purity and easy-to-handle properties.
c Easily evaporated from the 384-well reaction plate, thus needs regular top-up of the solvent.

### Table S2: Optimized conditions for click chemistry

<table>
<thead>
<tr>
<th>No.</th>
<th>Component</th>
<th>Equivalent</th>
<th>Concentration (mM)</th>
<th>Volume (μL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Alkyne (in DMSO)</td>
<td>1</td>
<td>25 mM</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>Azide (in DMSO)</td>
<td>1.4</td>
<td>50 mM</td>
<td>7</td>
</tr>
<tr>
<td>3</td>
<td>CuSO$_4$.5 H$_2$O (in Water)</td>
<td>0.2</td>
<td>25 mM</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>Sodium ascorbate (in Water)</td>
<td>0.5</td>
<td>50 mM</td>
<td>5</td>
</tr>
<tr>
<td>5</td>
<td>t-BuOH</td>
<td>-</td>
<td>-</td>
<td>43</td>
</tr>
<tr>
<td>6</td>
<td>Water</td>
<td>-</td>
<td>-</td>
<td>33</td>
</tr>
</tbody>
</table>
For full LC-MS (IT-Tof) spectra and $^1$H-NMR spectra of the click products, see SI_3.
LC condition = 10-100% Acetonitrile in 10 min. 100 % acetonitrile in 10-15 min
3. Biological Screening:

- **A5-2C-W2**: $IC_{50} = 634 \, \mu M$
- **A6-2C-W2**: $IC_{50} = 159 \, \mu M$
- **B7-2C-W2**: $IC_{50} = 35 \, \mu M$
- **B8-2C-W2**: $IC_{50} = 70.8 \, \mu M$
- **B9-2C-W2**: $IC_{50} = 34 \, \mu M$
- **B10-2C-W2**: $IC_{50} = 148 \, \mu M$
- **B11-2C-W2**: $IC_{50} = 11.1 \, \mu M$
- **C8-2C-W2**: $IC_{50} = 24 \, \mu M$
4. References:

A5-2C-W2

*** Current Data Parameters ***
NAME : ag10kka
EXPNO : 9
PROCNO : 1

*** Acquisition Parameters ***
DATE_t : 21:00:36
DATE_d : Aug 08 2007
NS : 13
O1 : 1007.90 Hz
O2 : 1853.43 Hz
O3 : 1853.43 Hz
SFO1 : 300.1310079 MHz
SFO2 : 300.1318534 MHz
SFO3 : 300.1318534 MHz

*** 1D NMR Plot Parameters ***
SR : 1.26 Hz

1H Water suppression
A6-2C-W2

1H Water suppression

*** Current Data Parameters ***
NAME : ag09kka
EXPNO : 15
PROCNO : 1

*** Acquisition Parameters ***
DATE_t : 19:58:48
DATE_d : Aug 08 2007
NS : 20
O1 : 1008.20 Hz
O2 : 1853.43 Hz
SFO1 : 300.1310082 MHz
SFO2 : 300.1318534 MHz
SFO3 : 300.1318534 MHz

*** 1D NMR Plot Parameters ***
SR : 1.08 Hz
**Current Data Parameters***

NAME : ag10kka
EXPNO : 12
PROCNO : 1

*** Acquisition Parameters ***
DATE_t : 21:09:30
DATE_d : Aug 08 2007
NS : 16
O1 : 1002.60 Hz
O2 : 1853.43 Hz
SFO1 : 300.1310026 MHz
SFO2 : 300.1318534 MHz
SFO3 : 300.1318534 MHz

*** 1D NMR Plot Parameters ***
SR : 1.11 Hz
B8-2C-W2

1H normal range AC300, B08-MeOD

*** Current Data Parameters ***
NAME : ag06kka
EXPNO : 1
PROCNO : 1

*** Acquisition Parameters ***
DATE_t : 03:58:43
DATE_d : Aug 07 2007
NS : 32
O1 : 1853.43 Hz
O2 : 1853.43 Hz
O3 : 1853.43 Hz
SFO1 : 300.1318534 MHz
SFO2 : 300.1318534 MHz
SFO3 : 300.1318534 MHz

*** 1D NMR Plot Parameters ***
SR : 4.70 Hz
*** Current Data Parameters ***
NAME : ag10kka
EXPNO : 3
PROCNO : 1

*** Acquisition Parameters ***
DATE_t : 20:41:40
DATE_d : Aug 08 2007
NS : 17
O1 : 1013.50 Hz
O2 : 1853.43 Hz
O3 : 1853.43 Hz
SFO1 : 300.1310135 MHz
SFO2 : 300.1318534 MHz
SFO3 : 300.1318534 MHz

*** 1D NMR Plot Parameters ***
SR : 0.92 Hz
B10-2C-W2

1H Water suppression, B10

*** Current Data Parameters ***
NAME : ag09kka
EXPNO : 12
PROCNO : 1

*** Acquisition Parameters ***
DATE_t : 19:48:25
DATE_d : Aug 08 2007
NS : 20
O1 : 1002.80 Hz
O2 : 1853.43 Hz
SFO1 : 300.1310028 MHz
SFO2 : 300.1318534 MHz
SFO3 : 300.1318534 MHz

*** 1D NMR Plot Parameters ***
SR : 0.80 Hz

S1-24
B11-2C-W2

1H Water suppression

*** Current Data Parameters ***
NAME : ag06kka
EXPNO : 11
PROCNO : 1

*** Acquisition Parameters ***
DATE_t : 04:40:58
DATE_d : Aug 07 2007
NS : 16
O1 : 1016.00 Hz
O2 : 1853.43 Hz
O3 : 1853.43 Hz
SFO1 : 300.1310160 MHz
SFO2 : 300.1318534 MHz
SFO3 : 300.1318534 MHz

*** 1D NMR Plot Parameters ***
SR : 0.75 Hz