Supporting Information
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Supporting Information

Solid-Phase Parallel Synthesis of 5-Amino and 5-Amido-[1,2,4]Thiadiazoles via Cyclization Reactions of a Carboxamidine

Thiourea Linker

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Experimental procedure

**Reagents and conditions:** (a) 3-methoxy-4-formylphenol, K$_2$CO$_3$, KI, DMF, 60 °C, 16 h; (b) NH$_2$OH·HCl, pyridine, rt, 6 h; (c) LiAlH$_4$, THF, rt, 1 d.

Preparation of AMEBA resin b.

To a suspension of Merrifield resin a (2.0 mmol/g, 10.00 g, 20.0 mmol) in DMF (100 mL) was added potassium carbonate (8.3 g, 60.0 mmol) and potassium iodide (0.03 g, 0.20 mmol), followed by 3-methoxy-4-formylphenol (9.1 g, 60.0 mmol). The mixture was stirred at 60 °C for 16 h, after which time the resin was filtered and washed successively with DMF, MeOH, H$_2$O, MeOH, CH$_2$Cl$_2$ and MeOH. The resin was dried in vacuo. Resin b was white in color (11.58 g).

On bead ATR-FT IR: 3025, 2922, 2582, 1678 (C=O, aldehyde), 1598, 1579, 1493, 1452, 1422, 1396, 1292, 1260, 1198, 1162, 1113, 1027, 1016, 816, 757, 735, 698 cm$^{-1}$.

Preparation of 4-oxime-2-methoxylphenyl resin c.

AMEBA resin b (10.00 g) and hydroxylamine hydrochloride (3.4 g, 48.6 mmol) were suspended in pyridine (100 mL). After agitating for 6 h at room temperature, the resin
was filtered and washed with 1:1 pyridine/ H2O, H2O and several times with MeOH and CH2Cl2. FT-IR indicate analysis indicated complete disappearance of the carbonyl peak at 1678 cm\(^{-1}\). Resin \(c\) was white in color (10.02 g)

On bead ATR-FT IR: 3024, 2920, 1605, 1576, 1506, 1493, 1452, 1419, 1375, 1270, 1196, 1162, 1119, 1029, 1017, 948, 821, 757, 678 cm\(^{-1}\).

**Preparation of BOMBA resin \(d\) (1).**

To a suspension of oxime resin \(c\) (10.00 g) in THF (100 mL) was added lithium aluminum hydride (1.2 g, 31.2 mmol). The mixture was stirred at room temperature for 1 day, after which time the reaction mixture was cooled to 0 °C, the excess lithium aluminum hydride slowly quenched with EtOH, and the aluminum salt byproducts were dissolved with a 10% HCl. Once dissolved, the resin was filtered and washed H2O then several times with MeOH and CH2Cl2, followed by washing with 10% triethylamine in CH2Cl2 to neutralize the amine. Following the final wash with MeOH, the resin was dried in vacuum oven. Resin \(d\) was dark yellow in color (9.65 g).

On bead ATR-FT IR: 3415, 3025, 2920, 2850, 1602, 1504, 1493, 1451, 1373, 1285, 1253, 1195, 1156, 1128, 1029, 907, 819, 748, 696 cm\(^{-1}\). (Loading of resin, determined by FMOC deprotection, was 1.2 mmol/g).
<Loading Level determination>

**Loading**: To an ice cold slurry of BOMBA resin (0.20 g) and N, N-Diisopropylethylamine (0.42 mL, 2.4 mmol) was added a solution of 9-Fluorenylmethoxycarbonyl chloride (0.41 g, 1.6 mmol) in CH$_2$Cl$_2$ (5.0 mL). The slurry was incubated for 3 h at room temperature. Then the resin was removed by filtration and sequentially washed with H$_2$O, MeOH and CH$_2$Cl$_2$, following final wash with MeOH, the resin was dried in vacuum oven. Fmoc-amino resin was obtained as a light yellow solid (0.28 g).

On bead ATR-FT IR: 3025, 2922, 1708 (amide), 1612, 1589, 1493, 1450, 1421, 1245, 1197, 1159, 1130, 1029, 1019, 823, 758, 736, 699 cm$^{-1}$.

**Deloading**: A suspension of the Fmoc amino resin (0.28 g) and piperidine (1.0 mL) in CH$_2$Cl$_2$ (4.0 mL) was stirred at room temperature for 2 h. Then the resin was filtered and washed with CH$_2$Cl$_2$ (2 × 50.0 mL). The filtrate was concentrated in vacuo giving a residue which was subjected to silica gel column chromatography (n-hexane-EtOAc, 10:1, v/v) to afford 9-Methylene-9H-fluorene (43 mg, BOMBA resin loading capacity ~ 0.2 mmol).

$^1$H NMR (500MHz, CDCl$_3$) δ 6.09 (s, 2H), 7.30-7.33 (td, 2H, $J = 7.5, 1.1$ Hz), 7.37-
7.40 (td, 2H, $J = 7.5$, 1.1 Hz), 7.70-7.71 (dt, 2H, $J = 7.5$, 0.9 Hz), 7.74-7.76 (dt, 2H, $J = 7.5$, 0.9 Hz).
IR data of Intermediate Resin 1~7

Resin 1

Resin 2
$^1$H, $^{13}$C NMR, LC-Mass data of compound 8a–8v
$^{1}H$, $^{13}C$ NMR, LC-Mass data of compound 9a-9l