Chemistry

Melting points were measured using a Mel-Temp 3.0 capillary melting point apparatus which are uncorrected. The progress of chemical reaction was monitored by thin-layer chromatography on silica gel 60-F_{254} aluminum plates acquired from Merck (Darmstadt, Germany) and detected under UV light. ^{1}H and ^{13}C NMR spectra were recorded employing a Bruker 400 spectrometer, and chemical shifts (δ) are in *ppm* relative to TMS as internal standard. Exchangeable protons (NHs) for DB1890, DB1950, DB1852, DB1880 and DB1876 are not reported in ^{1}H NMR data due to deuterium exchange. Mass spectra were recorded on a VG Instruments 70-SE spectrometer. Elemental analyses were obtained from Atlantic Microlab Inc. (Norcross, GA) and are within ±0.4% of the theoretical values. All reagents were commercially available and were used without purification.

General procedure for synthesis of 1-bromo-2-alkoxy-4-nitrobenzene (1a-c)

Potassium *tert*-butoxide (0.6 g, 5.5 mmol) was added to a solution of 2-bromo-5-nitrophenol (1.0 g, 4.6 mmol) in anhydrous THF (10 mL) and anhydrous DMF (2 mL) at 0 ^{o}C in an ice bath. The reaction mixture was stirred at 0 ^{o}C for 15 min. Then, the alkyl iodide (9.2 mmol) was added to the flask dropwise. The mixture was stirred for 30 min at room temperature. Then, a reflux apparatus was attached to the flask and the reaction mixture was allowed to reflux overnight. The solvent was removed under reduced pressure. The red residue was dissolved in ethyl acetate (150 mL) and washed with 5% $NaHCO_3$ (2 × 50 mL). The organic layer was dried over Na_2SO_4, filtered and solvent was removed under reduced pressure to yield a crude solid. The crude material was purified by column chromatography with silica gel, eluting with hexanes/ethyl acetate.

1-Bromo-2-isobutoxy-4-nitrobenzene (1a). Yellow solid, yield 53%, mp 59-60 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (s, 3H), 3.85 (d, *J* = 6.4 Hz, 2H), 2.18 (m, 1H), 1.08 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR ($CDCl_3$) δ 155.9, 147.9, 133.3, 119.9, 116.1, 107.1, 75.8, 28.2, 19.1; ESI-MS: *m/z* calcd. for $C_{10}H_{12}BrNO_3$: 273.0; Found: 272.3 $(M-H)^{+}$. Anal. Calcd. for $C_{10}H_{12}BrNO_3$: C, 43.81; H, 4.41; N, 5.10; Found: C, 43.90; H, 4.35; N, 5.04.

1-Bromo-2-(isopentyloxy)-4-nitrobenzene (1b). White solid, yield 89%, mp 55-56 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.85 (d, *J* = 8.6 Hz, 1H), 7.78 (brs, 1H), 7.71 (d, *J* = 8.6 Hz, 1H), 4.20 (t, *J* = 6.4 Hz, 2H), 3.37 (m, 2H), 1.87-1.80 (m, 1H), 1.12 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (DMSO-d_6) δ 155.8, 148.2, 134, 119.5, 116.8, 106.8, 68.5, 37.5, 25.0, 22.5. Anal. Calcd. for $C_{11}H_{14}BrNO_3$: C, 45.85; H, 4.90; N, 4.86. Found: C, 45.79; H, 4.81; N, 4.83.

1-Bromo-2-cyclopentyloxy-4-nitro-benzene (1c). White solid, yield 67%, mp 46-47 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72-7.70 (m, 1H), 7.67-7.65 (m, 2H), 4.91 (m, 1H), 1.99-1.66 (m, 8H). ^{13}C NMR ($CDCl_3$): δ 154.9, 147.8, 133.4, 120.7, 115.8, 108.3, 81.6, 32.6, 23.9. ESI-MS: *m/z* Calcd.for $C_{11}H_{12}BrNO_3$: 286.1; Found: 286.1 $(M)^{+}$. Anal. Calcd. For $C_{11}H_{12}BrNO_3$: C, 46.17; H, 4.22; N, 4.89; Found: C, 46.15; H, 4.25; N, 4.77

***tert*-Butyl 4-(2-bromo-5-nitrophenoxy)piperidine-1-carboxylate (1d)** (i) 4-Hydroxypiperidine (10 g, 98.9 mmol) was dissolved in dichloromethane (100 mL) and the solution cooled to 0 ^{o}C. Triethylamine (16.5 mL, 118.6 mmol) was then added to the solution followed by di-*tert*-butyl dicarbonate (25.9 g, 118.6 mmol). After the addition, the solution was allowed to warm to room temperature over a period of 2 h. The reaction mixture was then quenched by the addition of water and acidified by the addition of aqueous 1N HCl. The organic layer was extracted with dichloromethane and washed with a saturated solution of aqueous $NaHCO_3$. The combined organic phase was washed with brine, dried over $MgSO_4$, filtered and concentrated to afford *tert*-butyl 4-hydroxypiperidine-1-carboxylate as a white solid (17.5 g, 88%) which was sufficiently pure for further use. mp 66-68 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.82-3.84 (m, 3H), 3.02 (t, J = 10 Hz, 2H), 2.69 (brs, 1H), 1.83-1.86 (m, 2H), 1.42-1.49 (m, 11H), ^{13}C NMR ($CDCl_3$): δ 154.9, 79.7, 67.6, 41.5, 34.2, 28.5. LRMS ESI: *m/z* Calcd.for $C_{10}H_{19}NO_3$: 201.1, Found: 202.2 $(M+H)^+$. Anal. Calcd. for $C_{10}H_{19}NO_3$: C, 59.68; H, 9.52; N, 6.96. Found: C, 59.47; H, 9.53; N: 6.98. (ii) 2-bromo-5-nitro-phenol (3.3 g, 15 mmol) was dissolved in anhydrous tetrahydrofuran (50 mL) followed by *tert*-butyl 4-hydroxypiperidine-1-carboxylate (3.8 g, 18.7 mmol) and triphenylphosphine (4.93 g, 18.8 mmol) at room temperature. Diisopropyl azodicarboxylate (3.7 mL, 18.9 mmol) was added to the mixture dropwise and after the addition the solution was heated at 55 ^{o}C overnight. The reaction mixture was then cooled and quenched by the addition of aqueous 1N HCl and the organic layers were extracted with dichloromethane. The combined organic layers were dried over $MgSO_4$, filtered and concentrated to yield the crude title compound. This was then purified by column chromatography over silica gel by gradient elution with a mixture of ethylacetate-hexane to give a pale yellow solid (3.9 g, 65%). mp 115-116 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (s, 3H), 4.70-4.74 (m, 1H), 3.57-3.62 (m, 4H), 1.89-1.95 (m, 4H), 1.48 (s, 9H). ^{13}C NMR ($CDCl_3$): δ 154.9, 154.4, 148.2, 134.1, 121.6, 116.9, 109.2, 80.0, 74.2, 40.3, 30.2, 28.6. LRMS ESI: *m/z* Calcd. for $C_{16}H_{21}BrN_2O_5$: 400.1 & 402.1, Found: 401.2 & 403.2 $(M+H)^+$. Anal. Calcd. for $C_{16}H_{21}BrN_2O_5$: C, 47.89; H, 5.28; N, 6.98. Found: C, 47.71; H, 5.34; N, 6.95.

4-(2-Bromo-5-nitrophenoxy)-1-isopropylpiperidine (1e) *(i)* **1d** (3 g, 7.5 mmol) was dissolved in dichloromethane (30 mL) and trifluoroacetic acid (5 mL) was added to it. The solution immediately turned deep red in color and was left to stir for 2 h after which the solvent was reduced and diethyl ether added to produce a white precipitate of the trifluoroacetate salt of the title compound. The salt was filtered and washed with ether and dissolved in water. The water solution of the salt was basified with an aqueous solution of K_2CO_3 and the aqueous layer was extracted with dichloromethane. The combined organic layers were dried over $MgSO_4$, filtered and concentrated to yield the title compound in sufficient purity as an yellow-orange solid (2.2 g, 98%). mp 220 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71-7.74 (m, 3H), 4.60-4.63 (m, 1H), 3.16-3.22 (m, 2H), 2.77-2.83 (m, 2H), 2.01-2.06 (m, 2H), 1.79-1.85 (m, 2H), 1.65 (brs, 1H). ^{13}C NMR (DMSO-d_6): δ 153.6, 147.9, 134.0, 120.4, 116.9, 109.6, 72.9, 41.2, 28.6. LRMS ESI: *m/z* Calc. for $C_{11}H_{13}BrN_2O_3$: 300.0 & 302.0, Found: 301.1 & 303.1 $(M+H)^+$. Anal.: Calcd. for $C_{11}H_{13}BrN_2O_3$: C, 43.87; H, 4.35; N, 9.30. Found: C, 43.77; H, 4.26; N, 9.19. (ii) 4-(2-bromo-5-nitro phenoxy)piperidine (2 g, 6.7 mmol) was dissolved in dimethylformamide (10 mL) and anhydrous K_2CO_3 (1.8 g, 13.3 mmol) was added to it. After 30 min. 2-iodopropane (0.7 mL, 6.7 mmol) was added to the mixture dropwise and left to stir overnight at room temperature. The reaction was then quenched by the addition of water, and the organic layer was extracted with dichloromethane. The combined organic layers were dried over $MgSO_4$,

filtered and concentrated to yield the crude alkylated compound. This was then purified by column chromatography over silica gel by gradient elution with a mixture of ethylacetate- hexane to give a pale yellow solid (1.6 g, 70%). mp 163-165 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70-7.72 (m, 3H), 4.53-4.57 (m, 1H), 2.74-2.81 (m, 3H), 2.46-2.51 (m, 2H), 1.95-2.04 (m, 4H), 1.07 (d, *J* = 6.4 Hz, 6H), ^{13}C NMR ($CDCl_3$): δ 154.7, 148.2, 134.0, 121.6, 116.6, 109.3, 75.1, 54.7, 45.3, 30.9, 18.6 LRMS ESI: *m/z* Calcd. for $C_{14}H_{19}BrN_2O_3$: 342.1 & 344.1, Found: 343.1 & 345.1 $(M+H)^+$. Anal. Calcd. for $C_{14}H_{19}BrN_2O_3$: C, 48.99; H, 5.58; N, 8.16. Found: C, 48.74; H, 5.34; N, 7.95.

General procedure for synthesis of 2,5-bis-(2-alkoxy-4-nitrophenyl)-furan (2a-e)

2,5-Bis(trimethylstannyl)furan (1.5 mmol) was injected into a **s**olution of 1-bromo-2-alkoxy-4-nitro-benzene **1a-e** (3.1 mmol) and tetrakis(triphenylphosphine)palladium(0) (0.04 mmol) in anhydrous 1,4-dioxane (10 mL) at room temperature under nitrogen gas. The mixture was allowed to reflux under nitrogen overnight. The orange colored suspension was diluted with hexanes (8 mL) and cooled to room temperature. The residue was filtered and washed with hexanes. The orange fluffy residue was recrystallized from toluene.

2,5-Bis(2-isobutoxy-4-nitrophenyl)furan (2a) Yellow fluffy solid, yield 72%, mp 230-232 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.6 Hz, 2H), 7.94 (d, *J* = 8.6 Hz, 2H), 7.82 (s, 2H), 7.36 (s, 2H), 4.01 (d, *J* = 6 Hz, 4H), 2.35-2.28 (m, 2H), 1.16 (d, *J* = 6.8 Hz, 12H); ^{13}C NMR ($CDCl_3$): δ 155.1, 148.9, 147.1, 125.9, 124.9, 116.2, 116.1, 106.9, 75.8, 28.3, 19.5. ESI-MS: *m/z* Calcd. for: $C_{24}H_{26}N_2O_7$: 454.1; Found: 455.2 $(M+H)^+$. Anal. Calcd. for $C_{24}H_{26}N_2O_7$-0.7H_2O: C, 61.71; H, 5.91; N, 5.99; Found: C, 61.61; H, 5.65; N, 5.59.

2,5-Bis-(2-*iso*pentyloxy-4-nitrophenyl)furan (2b) Yellow solid, yield 52%, mp 221-222 ^{o}C; ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.8 Hz, 2H), 7.98 (dd, *J* = 8.8, 2 Hz, 2H), 7.71 (d, *J* = 2 Hz, 2H), 7.35 (s, 2H), 4.29(t, *J* = 6.4 Hz, 4H), 1.87-1.80 (m, 2H), 1.58 (brs, 4H), 1.06 (d, *J* = 6 Hz, 12H); ^{13}C NMR ($CDCl_3$) δ 155, 148.8, 147.1, 125.8, 125, 116.3, 116.2, 106.9, 67.9, 37.8, 25.3, 22.6; ESI-MS: *m/z* Calcd. for $C_{26}H_{30}N_2O_7$: 482.53, Found: 483.3 $(M+H)^+$. Anal. Calcd. for $C_{26}H_{30}N_2O_7$: C, 64.72; H, 6.27; N, 5.81. Found: C, 64.7; H, 6.17; N, 5.82.

2,5-Bis-(2-cyclopentyloxy-4-nitrophenyl)-furan (2c). Yellow fluffy solid, yield 74%, mp 271-273 ^{o}C. ^{1}H NMR ($CDCl_3$): δ 8.08 (d, *J* = 8.9 Hz, 2H), 7.91 (dd, *J* = 8.9, 2.0 Hz, 2H), 7.27 (d, *J* = 2.0 Hz, 2H), 7.29 (s, 2H), 5.08-5.04 (m, 2H), 2.12-1.74 (m, 16H), ^{13}C NMR ($CDCl_3$): δ 153.9, 148.9, 147.0, 125.9, 125.5, 116.1, 115.8, 107.9, 80.9, 32.9, 24.1; ESI-MS: *m/z* Calcd.for $C_{26}H_{26}N_2O_7$: 478.1; Found: 479.0 $(M+H)^+$. Anal. Calcd. for $C_{26}H_{26}N_2O_7$: C, 65.2; H, 5.47; N, 5.85; Found: C, 64.9; H, 5,76; N, 5.85.

2,5-Bis(2-(*tert*-butyl 4-hydroxypiperidine-1-carboxylate)-4-nitrophenyl)furan (2d) Yellow solid, yield 59%, mp 226-228 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.8 Hz, 2H), 7.94 (m, 2H), 7.84 (m, 2H), 7.32 (s, 2H), 4.79-4.83 (m, 2H), 3.82-3.84 (m, 4H), 3.39-3.45 (m, 4H), 2.10-2.16 (m, 4H), 1.90-1.96 (m, 4H), 1.49 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.8, 153.4, 149.0, 147.3, 126.6, 125.9, 116.5, 108.2, 80.2, 74.3, 41.1, 30.7, 28.6. LRMS ESI: *m/z* Calcd. for

$C_{36}H_{44}N_4O_{11}$: 708.3, Found: 709.5 $(M+H)^+$. Anal. Calcd. for $C_{36}H_{44}N_4O_{11}$: C, 61.01; H, 6.26; N, 7.90. Found: C, 60.94; H, 6.14; N, 7.78.

2,5-Bis(2-(1-isopropylpiperidin-4-yloxy)-4-nitrophenyl)furan (2e): Red solid, yield 77%, mp 195-197 ^oC. ^1H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, *J* = 8.4 Hz, 2H), 7.90 (m, 2H), 7.81 (s, 2H), 7.36 (s, 2H), 4.60-4.64 (m, 2H), 2.80-2.90 (m, 6H), 2.50 (m, 4H), 2.18-2.23 (m, 4H), 1.95-2.02 (m, 4H), 1.11 (d, *J* = 6.8 Hz, 12H). ^{13}C NMR ($CDCl_3$): δ 153.7, 149.0, 147.2, 126.3, 126.0, 116.6, 116.2, 108.2, 75.2, 67.3, 54.7, 46.2, 31.4, 18.6. LRMS ESI: *m/z* Calcd. for $C_{32}H_{40}N_4O_7$: 592.3, Found: $(M+H^+)$: 592.2. Anal. Calcd. for $C_{32}H_{40}N_4O_7$: C, 64.85; H, 6.80; N, 9.45. Found: C, 64.68; H, 6.70; N, 9.22.

General procedure for synthesis of 2,5-Bis(2-alkoxy-4-aminophenyl)furan (3a-e)

Pd/C (0.5 g, 10%) was added to a suspension of 2,5-bis(2-alkoxy-4-nitrophenyl) furan **2a-e** (5.2 mmol) in a mixture of ethyl acetate (50 mL) and anhydrous ethanol (20 mL). The suspension was bubbled with dry nitrogen for 15 min. and hydrogenated overnight on a Parr apparatus with a starting pressure of 50 psi. The consumption of hydrogen gave a clear solution. The solution was filtrated over well-packed celite, and the filtrate was removed under reduced pressure.

2,5-Bis(2-isobutyloxy-4-aminophenyl)furan (3a) Light orange-solid, yield 76%, mp 91-92 ^oC. ^1H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 2H), 6.88 (s, 2H), 6.38 (d, *J* = 8.0 Hz, 2H), 6.29 (s, 2H), 3.82 (d, *J* = 6 Hz, 4H), 3.71(brs, 4H), 2.26-2.24 (m, 2H), 1.14 (d, *J* = 6.8 Hz, 12H); ^{13}C NMR ($CDCl_3$): δ 156.1, 148.3, 146.3, 126.8, 111.7, 109.4, 107.2, 99.1, 74.7, 28.4, 19.6. ESI-MS: *m/z* calcd. for $C_{24}H_{30}N_2O_3$: 394.2; Found: 395.2 $(M+H)^+$. Anal. Calcd. for $C_{24}H_{30}N_2O_3$: C, 73.07; H, 7.66; N, 7.10; Found: C, 73.29; H, 7.92; N, 7.07.

2,5-Bis-(2-*iso*pentyloxy-4-aminophenyl)furan (3b) Yellowish white solid, yield 80%, mp 110-111 ^oC; ^{1}HNMR (400 MHz, DMSO-d_6) δ 7.77(d, 2H, *J* = 8.4Hz), 6.82 (s, 2H), 6.39-6.36 (m, 2H), 6.23 (br s, 2H), 4.09 (t, 4H, *J* = 6.4 Hz), 3.73 (s, 4H), 1.99-1.97 (m, 2H), 1.86-1.82 (m, 4H), 1.25-1.10 (m, 12H); ^{13}CNMR (DMSO-d_6) δ 156.0, 149.6, 148.3, 126.3, 108.6, 108.3, 106.8, 98.3, 66.3, 38.1, 25.3, 23.0; ESI-MS: *m/z* calcd. for $C_{26}H_{34}N_2O_3$: 422.56, Found: 423.4 $(M+H)^+$. This compound was used in the next step without further characterization.

2,5-Bis(2-cyclopentyloxy-4-aminophenyl)furan (3c) Light brown fluffy solid, yield 64%, mp 114-116 ^oC. ^1H NMR (400 MHz, DMSO-d_6): δ 7.51 (d, *J* = 8.0 Hz, 2H), 6.60 (brs, 2H), 6.35 (br s, 2H), 6.30 (br s, 2H), 6.23 (s, 2H), 5.40 (b rs, 4H), 4.82-4.79 (m, 2H), 1.97-1.61 (m, 8H), 1.69-1.63 (m, 8 H). ^{13}C NMR (DMSO-d_6): δ 154.3, 148.8, 148.0, 125.9, 108.6, 107.7, 106.2, 99.0, 78.6, 32.5, 23.7. ESI-MS: *m/z* calcd. for $C_{26}H_{30}N_2O_3$: 418.2; Found: 419.1 $(M+H)^+$. Anal. Calcd. for $C_{26}H_{30}N_2O_3$: C, 74.61; H, 7.22; N, 6.69; Found: C, 74.55; H, 7.19; N, 6.99.

2,5-Bis(2-(*tert*-butyl 4-hydroxypiperidine-1-carboxylate)-4-aminophenyl) furan (3d) Brownish-white solid, yield 92%. mp 159-160 ^oC.^1H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 7.8 Hz, 2H), 6.77 (s, 2H), 6.36 (d, *J* = 7.8 Hz, 2H), 6.29 (s, 2H), 4.53-4.56 (m, 2H), 3.73-3.77 (br s, 4H), 3.33-3.39 (m, 8H), 1.96-2.05 (m, 8H), 1.84-1.89 (m, 4H), 1.47 (s, 18H). ^{13}C NMR ($CDCl_3$): δ 191.3, 159.6, 154.9, 153.8, 133.4, 117.7, 107.9, 98.2, 79.9, 73.5, 61.6, 41.1, 30.8, 28.6. LRMS ESI: *m/z*

Calcd. for $C_{36}H_{48}N_4O_7$: 648.4, Found: 649.5 $(M+H)^+$. Anal. Calcd. for $C_{36}H_{48}N_4O_7$: C, 66.64; H, 7.46; N, 8.64. Found: C, 66.25; H, 7.41; N, 8.41.

2,5-Bis(2-(1-*iso*propylpiperidin-4-yloxy)-4-aminophenyl)furan (3e): Brownish white solid, yield 94 %, mp 147-149 ^oC. ^1H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.4 Hz, 2H), 6.83 (s, 2H), 6.35 (m, 2H), 6.30 (br s, 2H), 4.40-4.42 (m, 2H), 3.69 (brs, 4H), 2.73-2.87 (m, 6H), 2.43-2.47 (m, 4H), 2.06-2.12 (m, 4H), 1.92-1.99 (m, 4H),1.07 (d, *J* = 6.8 Hz, 12H). ^{13}C NMR ($CDCl_3$): δ 154.6, 148.5, 146.4, 127.4, 112.9, 109.9, 107.9, 100.9, 73.4, 54.7, 46.0, 31.4,18.6. LRMS ESI: *m/z* Calcd. for $C_{32}H_{44}N_4O_3$: 532.3, Found: 533.5 $(M+H)^+$. Anal. Calcd. for $C_{32}H_{44}N_4O_3$: C, 72.15; H, 8.33; N, 10.52. Found; C, 72.28; H, 8.51; N, 10.60.

General procedure for synthesis of 2,5-Bis[2-alkoxyl-4-(2-pyridylimino) amino-phenyl]-furan hydrochloride salt (4a-e)

(i) Free base preparation: Napthalen-2-ylmethylpyridine-2-carbimidothioate hydrobromide salt (1.0 mmol) was added into a cooled solution of 2,5-bis(2-alkoxy-4-aminophenyl)furan **3a-e** (0.5 mmol) in mixture of dry ethanol (10 mL) and dry acetonitrile (5 mL) in an ice bath. The reaction mixture was stirred at room temperature overnight. With the disappearance of the starting material, the organic solvent was removed under reduced pressure to yield a crude oil product. Dry ether (20 mL) was added into the crude material and the mixture was stirred at room temperature for 4 h. The precipitate was filtered and washed with dry ether. The filtrate was dissolved in water, the solution was cooled to 0 ^oC in an ice bath and 10% NaOH was added until pH reach to approximately 10. The free base was participated, and then extracted into dichloromethane (2 × 200 mL). The organic layer was washed with distilled water, dried over K_2CO_3, filtrated and removed under reduced pressure. The resulting solid was crystallized with dichloromethane/hexane mixture and filtrated. The free base solid was characterized with NMR.

(ii) Hydrochloride salt formation: The free base was suspended in dry ethanol (10 mL) and cooled to 0 ^oC in an ice bath. Freshly prepared hydrochloric ethanol (2 mL) was added into the suspension and the mixture was stirred at room temperature overnight. The resulting solution was concentrated under vacuo. The crude solid was crystallized with dry ethanol and dry ether.

2,5-Bis[2-isobutoxyl-4-(2-pyridylimino)aminophenyl]-furan hydrochloride (4a, DB1890). Orange-red solid, yield 60%, mp 201-203 ^oC. ^1H NMR (DMSO-d_6+D_2O): δ 8.90 (d, *J* = 4.8 Hz, 2H), 8.51 (d, *J* = 7.5 Hz, 2H), 8.22 (dd, *J* = 7.5, 7.5 Hz, 2H),8.14 (d, *J* = 8.0 Hz, 2H) 7.85 (m, 2H), 7.32 (s, 2H), 7.19 (m, 4H), 3.99 (d, *J* = 6 Hz, 4H), 2.24 (m, 2H), 1.10 (d, *J* = 7 Hz, 12H); ^{13}C NMR (MeOD): δ 160.3, 156.1, 150.0, 148.4, 144.1, 138.2, 133.4, 128.4, 126.7, 122.9, 120.1, 117.2, 113.1, 109.3, 75.2, 28.1, 18.4; ESI-MS: *m/z* calcd. for $C_{36}H_{38}N_6O_3$ (base): 602.3; Found: 603.4 $(M+H)^+$. Anal. Calcd. for $C_{36}H_{38}N_6O_3$-2HCl -2.85H_2O: C, 59.47; H, 6.33; N, 11.56; Found: C, 59.45; H, 6.36; N, 11.19.

2,5-Bis-[2-isopentyloxy-4-(2-pyridylimino)aminophenyl]furan hydrochloride (4b, DB1950). Orange solid, yield 68%, mp>280 ^oC (dec); ^{1}HNMR (DMSO-d_6+D_2O) δ 8.92 (d, *J* = 4 Hz, 2H), 8.55 (br s, 2H), 8.22 (m, 2H), 8.13 (m, 2H), 7.85 (m, 2H), 7.36 (s, 2H), 7.18 (m, 4H), 4.22 (br t, 4H), 2.51 (m, 2H), 1.86 (m, 4H), 1.01 (d, *J* = 6.5 Hz, 12H); ^{13}CNMR (DMSO-

d_6) δ 159.8, 155.6, 150.3, 148.6, 144.9, 138.8, 134.7, 129.0, 126.8, 124.6, 118.9, 118.4, 113.4, 110.8, 67.5, 31.1, 25.4, 22.9; ESI-MS: *m/z* calcd. for $C_{38}H_{42}N_6O_3$ (base): 630.78, Found: 631.5 $(M+H)^+$; Anal. Calcd. for $C_{38}H_{42}N_6O_3$-2HCl-2.3H_2O: C, 61.25; H, 6.57; N, 11.27. Found: C, 60.87; H, 6.48; N, 11.00.

2,5-Bis[2-cyclopentoxyl-4-(2-pyridylimino)aminophenyl]-furan hydrochloride (4c, DB1852). Red-orange solid,Yield 36%. mp: 208-210 ^oC. ^1H NMR (DMSO-d_6+D_2O): δ 8.90 (br s, 2H), 8.56 (br s, 2H), 8.21 (m, 2H), 8.11 (m, 2H),7.85 (s, 2H), 7.29 (s, 2H), 7.13 (m, 4H), 5.05 (br s, 2H), 2.01-1.68 (br m, 16H). ^{13}C NMR (DMSO-d_6): δ 159.9, 154.6, 150.3, 148.5, 144.9, 138.8, 134.6, 129.0, 127.0, 124.4, 119.4, 118.1, 113.3, 111.5, 80.4, 32.7, 24.1; ESI-MS: *m/z* calcd. for $C_{38}H_{38}N_6O_3$ (base): 626.3; Found: 627.2 $(M+H)^+$. Anal. Calc. for $C_{38}H_{38}N_6O_3$-3.5HCl-0.6$C_4H_{10}O$: C, 60.74; H, 5.99; N, 10.52; Found: C, 60.75; H, 6.02; N, 10.47.

N,N'-[4,4'-(furan-2,5-diyl)bis(3-(piperidin-4-yloxy)-4,1-phenylene)] dipicolinimidamide tetrahydrochloride salt (4d, DB1880). Orange solid, yield 85%. mp 252 ^oC (dec).^1H NMR (DMSO-d_6+D_2O): δ 8.91 (d, *J* = 4 Hz, 2H), 8.56 (d, *J* = 7.5 Hz, 2H), 8.24 (dd, *J* = 8.5, 8.5 Hz, 2H), 8.14 (d, *J* = 8.5 Hz, 2H), 7.86 (m, 2H), 7.44 (s, 2H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.16 (s, 2H), 4.90 (br s, 2H), 3.28 (br s, 4H), 3.12 (br s, 4H), 2.29 (br s, 4H), 2.10 (br s, 4H). ^{13}C NMR (DMSO-d_6): δ 159.4, 153.2, 149.8, 148.1, 144.4, 138.4, 134.4, 128.7, 127.0, 124.2, 119.2, 118.6, 113.1, 111.7, 70.4, 40.7, 27.1. LRMS ESI: *m/z* Calcd. for $C_{38}H_{40}N_8O_3$ (base): 656.3, Found: 329.3 $(M+2H)^{+2}$. Anal. Calcd. for $C_{34}H_{40}N_8O_3$-4HCl-2.5H_2O: C, 53.84; H, 5.83; N, 13.22. Found C, 53.71; H, 5.99; N, 13.05.

N,N'-[4,4'-(furan-2,5-diyl)bis(3-(1-isopropylpiperidin-4-yloxy)-4,1-phenylene)] dipicolinimidamide tetrahydrochloride salt (4e, DB1876). Orange solid, yield 97%, mp 247 ^oC (dec). ^1H NMR (4 DMSO-d_6+D_2O): δ 8.90 (d, *J* = 4Hz, 2H), 8.86 (d, *J* = 7.5 Hz, 2H), 8.23 (dd *J* = 7.5, 7.5 Hz, 2H), 8.14 (m, 2H), 7.86 (br s, 2H), 7.44 (br s, 2H), 7.22 (br s, 2H), 7.14 (br s, 2H), 4.95 (m, 2H), 3.46 (m, 6H), 3.10 (m, 4H), 2.26-2.46 (m, 8H),1.30 (d, *J* = 6 Hz, 12H). ^{13}C NMR (DMSO-d_6): δ 159.2, 153.3, 149.7, 148.2, 144.4, 138.3, 134.8, 128.5, 126.8, 124.2, 119.2, 118.6, 113.0, 112.1, 71.7, 56.5, 45.9, 28.1, 16.2. LRMS ESI: *m/z* Calcd. for $C_{44}H_{52}N_8O_3$ (base): 740.4, Found: 741.5 $(M+H)^+$. Anal. Calcd. for $C_{44}H_{52}N_8O_3$-4HCl-2H_2O: C, 57.27; H, 6.55; N, 12.13. Found: C, 57.00; H, 6.65; N, 11.90.

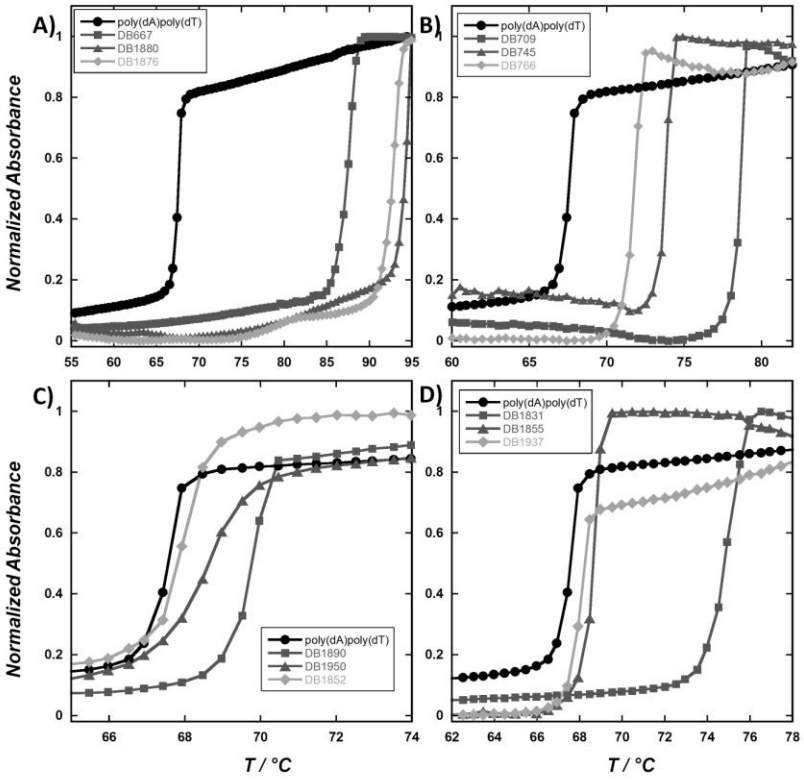

Figure S1. Melting profiles at 260nm for AIAs A) DB667, DB1880 and DB1876; B) DB709, DB745 and DB766; C) DB1890, DB1950 and DB1852; D) DB1831, DB1855 and DB1937 with poly(dA)·poly(dT).