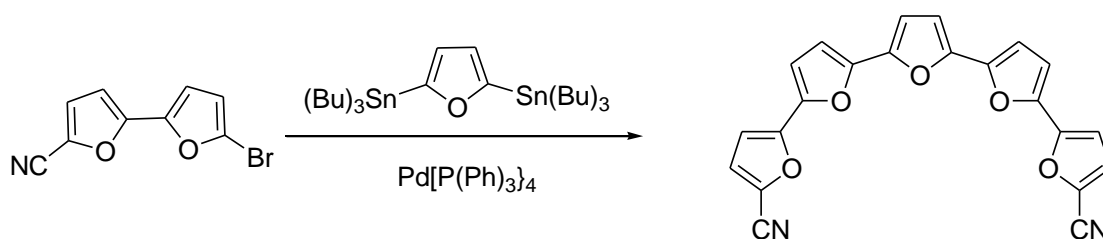


1 SUPPLEMENTAL MATERIAL

2 Chemistry experimental

3 Melting points were recorded using a Thomas-Hoover (Uni-Melt) capillary melting
4 point apparatus and are uncorrected. TLC analysis was carried out on silica gel 60 F₂₅₄
5 precoated aluminum sheets and detected under UV light. ¹H and ¹³C NMR spectra, were
6 recorded employing a Varian Unity Plus 300 spectrometer or Bruker 400 MHz, using the
7 indicated solvents, and chemical shifts (δ) are in ppm relative to TMS as internal standard.
8 Mass spectra were recorded on a VG analytical 70-SE spectrometer. Elemental analyses were
9 obtained from Atlantic Microlab Inc. (Norcross, GA). The compounds reported as salts
10 frequently analyzed correctly for fractional moles of water and/or other solvents; in each case
11 ¹H NMR spectra were consistent with the presence of water or organic solvent(s). All
12 chemicals and solvents were purchased from Aldrich Chemical Co., VWR, Frontier Scientific
13 or Combi-Blocks, Inc. The bis-nitriles required for synthesis of DB1464, DB1465 and
14 DB1645 have been previously reported (1) and were used as described below. The synthesis
15 of the bis-nitriles needed to prepare DB1680 and 1692 are outlined below. Brief synthetic
16 Schemes are provided with each compound set.

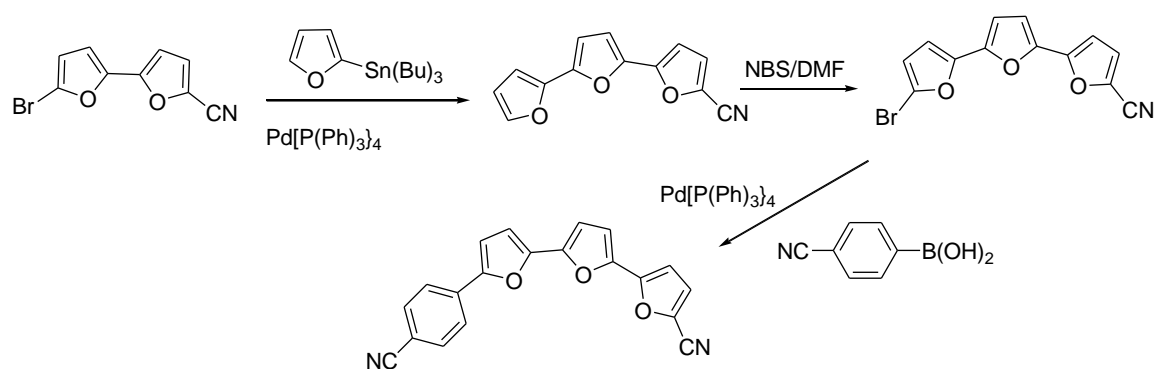
17 5,5''''-Dicyano-2,2':5',2'':5'',2''':5''',2''''-quinguefuran.



19 A mixture of 5'-bromo-2,2'-bifuran-5-carbonitrile (1) (1.19 g, 5 mmol), 2,5-bis(tri-*n*-
20 butylstannyl)furan (1.6 g, 2.5 mmol) and tetrakis(triphenylphosphine)palladium(0) (125 mg)
21 in dry 1,4-dioxane (40 ml) was heated under nitrogen at reflux (100-110 °C) for 24 h. The

22 precipitate which formed was collected, washed with hexanes and recrystallized from DMF to
23 afford the product in 76% yield, mp 237-239 °C. ¹H NMR (DMSO-*d*₆); δ 7.08-7.23 (m, 8H),
24 7.78 (s, 2H). ¹³C NMR (DMSO-*d*₆); δ 149.3, 145.8, 144.6, 143.3, 125.7, 124.0, 112.0, 109.7,
25 109.0, 107.7, 107.5. Anal. Calcd. for C₂₂H₁₀N₂O₅: C, 69.11; H, 2.64. Found: C, 68.83; H,
26 2.87.

27 **5-Cyano-5''-(4-cyanophenyl)-2,2':5',2''-terfuran.**



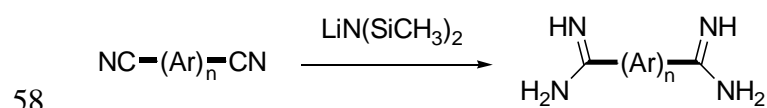
29 A similar procedure described for 5,5''''-dicyano-2,2':5',2''':5'',2''''-quinguefuran
30 was used by employing 5'-bromo-2,2'-bifuran-5-carbonitrile (1) (1 equiv) and 2-(tri-*n*-
31 butylstannyl)furan (1 equiv) to furnish 5-cyano-2,2':5',2''-terfuran in 83% yield, mp 123.5-
32 124 °C (EtOH). ¹H NMR (DMSO-*d*₆); δ 6.66-6.67 (m, 1H), 6.89-6.91 (m, 2H), 7.05 (d, J =
33 3.6 Hz, 1H), 7.17 (d, J = 3.6 Hz, 1H), 7.75 (d, J = 3.6 Hz, 1H), 7.81-7.82 (m, 1H). ¹³C NMR
34 (DMSO-*d*₆); δ 149.4, 146.6, 144.5, 143.8, 142.8, 125.6, 123.9, 112.1, 111.9, 111.7, 107.8,
35 107.4, 107.1. MS (EI) *m/e* (rel.int.); 225 (M⁺, 30), 196 (6), 169 (15), 140 (55), 51 (100). The
36 product was used directly in the next step.

37 To a solution of cyano-2,2':5',2''-terfuran (2.25 g, 10 mmol) in DMF (25 ml) was added
38 portionwise *N*-bromosuccinimide (1.78 g, 10 mmol) with stirring. The reaction mixture was
39 stirred overnight at room temperature, then poured onto cold-water. The precipitate which
40 formed was collected, washed with water and dried to give 5-bromo-5''-cyano-2,2':5',2''-

41 terfuran in 92% yield, mp 154-155 °C. ¹H NMR (DMSO-*d*₆); δ 6.79 (d, J = 3.6 Hz, 1H), 6.93-
42 6.96 (m, 2H), 7.07 (d, J = 3.6 Hz, 1H), 7.17 (d, J = 3.6 Hz, 1H), 7.75 (d, J = 3.6 Hz, 1H). ¹³C
43 NMR (DMSO-*d*₆); δ 149.2, 146.5, 145.3, 143.1, 125.6, 124.0, 122.5, 114.2, 111.9, 111.7,
44 109.9, 108.5, 107.5. MS (EI) m/e (rel.int.); 303, 305 (M⁺, 8, 11), 224 (15), 196 (100). The
45 product was used directly in the next step.

46 To a stirred solution of 5-bromo-5''-cyano-2,2':5',2''-terfuran (1.51 g, 5 mmol), and
47 tetrakis(triphenylphosphine) palladium (288 mg) in toluene (20 ml) under a nitrogen
48 atmosphere was added 10 ml of a 1 M aqueous solution of NaHCO₃ followed by 4-
49 cyanophenylboronic acid (875 mg, 6 mmol) in 5 ml of methanol. The vigorously stirred
50 mixture was warmed to 80 °C for 24 h, then cooled, and the precipitate was filtered and
51 recrystallized from DMF to afford the bis-nitrile in 67% yield, mp 241-243 °C. ¹H NMR
52 (DMSO-*d*₆); δ 7.08-7.14 (m, 3H), 7.24 (d, J = 4.4 Hz, 1H), 7.44 (d, J = 4.4 Hz, 1H), 7.78 (d, J
53 = 4.4 Hz, 1H), 7.93 (d, J = 8.8 Hz, 2H), 7.98 (d, J = 8.8 Hz, 2H). ¹³C NMR (DMSO-*d*₆); δ
54 151.5, 149.3, 146.0, 145.5, 143.5, 133.4, 133.04, 133.00, 128.1, 125.7, 124.1, 112.0, 111.7,
55 111.3, 110.0, 109.7, 109.3, 107.6. MS (EI) m/e (rel.int.); 326 (M⁺, 25), 270 (5), 214 (12), 140
56 (75), 75 (100). Anal. Calcd. for C₂₀H₁₀N₂O₃: C, 73.62; H, 3.09. Found: C, 73.25; H, 3.18.

57 **Bis-amidino oligochalcophenes.**



59 **5,5'-Bis(5-amidino-2-furanyl)-2,2'-bifuran hydrochloride (DB1464).**

60 The bis-nitrile 5,5'-bis(5-cyano-2-furanyl)-2,2'-bifuran (1) (316 mg, 1 mmol), suspended in
61 freshly distilled THF (5 ml), was treated with lithium trimethylsilylamide (1M solution in
62 THF, 6 ml, 6 mmol) and the reaction was allowed to stir for 48 hr. The reaction mixture was

63 then cooled to 0 °C to which was added HCl saturated ethanol (60 ml) whereupon a
64 precipitate started forming. The mixture was left to run overnight whereafter it was diluted
65 with ether and the resultant solid was collected by filtration. The diamidine was purified by
66 neutralization with 1N NaOH followed by filtration of the resultant solid and washing with
67 water (3×). Finally, the free base was stirred with ethanolic HCl overnight, diluted with ether,
68 and the solid formed was filtered and dried to give the diamidine salt DB1464 in 62% yield,
69 mp >300 °C. ¹H NMR (D₂O/DMSO-*d*₆): δ 7.02 (d, J = 3.6 Hz, 2H), 7.05 (d, J = 3.9 Hz, 2H),
70 7.19 (d, J = 3.6 Hz, 2H), 7.74 (d, J = 3.9 Hz, 2H). ¹³C NMR (D₂O/DMSO-*d*₆); δ 153.8, 149.9,
71 146.3, 144.3, 140.1, 121.7, 112.9, 110.2, 109.4. MS (ESI) m/e (rel. int.): 351 (M⁺+1, 78), 176
72 (100). HRMS calcd. for C₁₈H₁₅N₄O₄: 351.1093. Observed: 351.1091. Anal. Calcd. For
73 C₁₈H₁₄N₄O₄·2.0HCl·2.4H₂O: C, 46.34; H, 4.49; N, 12.01. Found: C, 46.09; H, 4.26; N, 11.68.

74 **5,5'-Bis(5-amidino-2-furanyl)-2,2'-bithiophene hydrochloride (DB1465).**

75 The diamidine DB1465 was prepared from 5,5'-bis(5-cyano-2-furanyl)-2,2'-bithiophene
76 following the procedure used for DB1464 in a 60% yield, mp >300 °C. ¹H NMR
77 (D₂O/DMSO-*d*₆): δ 7.11 (d, J = 3.9 Hz, 2H), 7.49 (d, J = 3.9 Hz, 2H), 7.72 (d, J = 3.9 Hz,
78 2H), 7.79 (d, J = 3.9 Hz, 2H). ¹³C NMR (D₂O/DMSO-*d*₆); δ 153.7, 153.5, 139.8, 138.0, 130.3,
79 128.7, 126.6, 122.1, 109.6. MS (ESI) m/e (rel. int.): 383 (M⁺+1, 80), 192 (100). HRMS calcd
80 for C₁₈H₁₅N₄O₂S₂: 383.0636. Observed: 383.0643. Anal. Calcd. For C₁₈H₁₄N₄O₂S₂·2.0HCl·
81 1.7H₂O·0.25EtOH: C, 44.66; H, 4.23; N, 11.26. Found: C, 44.75; H, 3.99; N, 10.95.

82 **5, 5'-Bis(5-amidino-2-thienyl)-2, 2'-bifuran hydrochloride (DB1645).**

83 The diamidine DB1645 was prepared from 5, 5'-bis(5-cyano-2-thienyl)-2, 2'-bifuran
84 following the procedure used for DB1464 in a 67% yield of dark reddish solid; mp >300 °C
85 dec.; ¹H NMR (DMSO-*d*₆): 7.05 (d, J = 3.5 Hz), 7.27 (d, J = 3.5 Hz), 7.68 (d, J = 4.0 Hz), 8.03
86 (d, J = 4.0 Hz), 9.15 (vbr, 4H), 9.38 (vbr, 4H); ¹³C NMR (DMSO-*d*₆): 147.1, 145.2, 140.2,

87 138.9, 123.9, 114.4, 111.7, 110.0, 106.2; MS: m/e 383 ($M^+ + 1$); Anal. Calcd. For
88 $C_{18}H_{14}N_4O_2S_2 \cdot 2HCl \cdot 1.5H_2O$ (482.4): C, 44.81; H, 3.96; N, 11.61; Found: C, 44.75; H, 3.98;
89 N, 11.31.

90 **5,5''''-Diamidino-2,2':5',2'':5'',2''':5''',2''''-quinguefuran hydrochloride (DB1680).**

91 The diamidine was prepared from 5,5''''-Dicyano-2,2':5',2'':5'',2''':5''',2''''-quinguefuran
92 following the procedure used for DB1464 in a 65 % yield. mp 297-300 °C. 1H NMR
93 ($D_2O/DMSO-d_6$); δ 7.03-7.05 (m, 4H), 7.12 (d, $J = 4.0$ Hz, 2H), 7.31 (d, $J = 4.0$ Hz, 2H), 7.94
94 (d, $J = 4.0$ Hz, 2H). ^{13}C NMR ($D_2O/DMSO-d_6$); δ 153.6, 150.0, 146.6, 145.3, 144.1, 140.2,
95 121.7, 113.0, 110.4, 109.7, 109.3. MS (ESI) m/e (rel.int.); 417 ($M^+ + 1$, 65), 400 (4), 351 (10),
96 275 (4), 242 (40), 209 (100). HRMS calcd. for $C_{22}H_{17}N_4O_5$: 417.1199. Observed: 417.1184.
97 Anal. Calcd. for $C_{22}H_{16}N_4O_5 \cdot 2.0HCl \cdot 1.75H_2O$: C, 50.73; H, 4.16; N, 10.75. Found: C, 50.65;
98 H, 4.02; N, 10.56.

99 **5-Amidino-5''-(4-amidinophenyl)-2,2':5',2''-terfuran hydrochloride (DB1692).**

100 The diamidine was prepared from 5-cyano-5''-(4-cyanophenyl)-2,2':5',2''-terfuran following
101 the procedure used for DB1464 in a 73 % yield mp >300 °C. 1H NMR ($D_2O/DMSO-d_6$); δ
102 7.09 (d, $J = 3.6$ Hz, 1H), 7.14 (d, $J = 3.6$ Hz, 1H), 7.19 (d, $J = 3.6$ Hz, 1H), 7.33 (d, $J = 3.6$ Hz,
103 1H), 7.47 (d, $J = 3.6$ Hz, 1H), 7.96-8.05 (m, 5H). ^{13}C NMR ($D_2O/DMSO-d_6$); δ 164.8, 153.2,
104 151.7, 149.0, 146.1, 145.5, 143.8, 140.1, 134.1, 129.0, 126.4, 123.6, 121.0, 112.3, 111.4,
105 109.9, 109.3, 108.6. MS (ESI) m/e (rel.int.); 361 ($M^+ + 1$, 100), 275 (12), 242 (94). HRMS
106 calcd. for $C_{20}H_{17}N_4O_3$: 361.1301. Observed: 361.1298. Anal. Calcd. for $C_{20}H_{16}N_4O_3 \cdot 2.0HCl \cdot$
107 $2.25H_2O \cdot 0.25C_2H_5OH$: C, 50.73; H, 4.98; N, 11.54. Found: C, 50.76; H, 4.54; N, 11.10.

108 **REFERENCE**

- 109 1. **Ismail MA.** 2006. An efficient synthesis of 5'-(4-cyanophenyl)-2,2'-bifuran-5-
110 carbonitrile and analogues. J. Chem. Res. S:733-737.