

Supporting Information

Nucleophilic reactivities of tributylstannyl substituted
furans and thiophenes

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General: ^1H (300 MHz) and ^{13}C (75.5 MHz) NMR spectra of solutions in CDCl_3 ($\delta_{\text{H}} = 7.24$, $\delta_{\text{C}} = 77.0$) were calibrated to the solvent signal.

2-(Ferrocenylphenylmethyl)-5-(tributylstannyl)furan

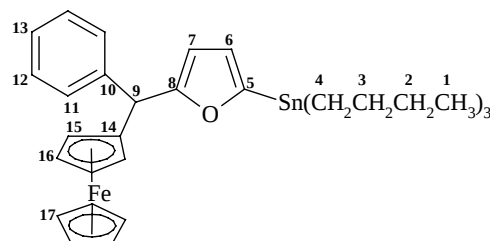
Separation and purification by column chromatography on basic alumina (activity III, pentane/ether = 30/1 (v/v)), red oil;

^1H NMR (CDCl_3 , 300 MHz): $\delta = 0.87$ (t, $J = 7.3$ Hz, 9 H, 1-H), 1.05-1.09 (m, 6 H, 4-H), 1.27-1.36 (m, 6 H, 2-H), 1.52-1.58 (m, 6 H, 3-H), 4.00-4.24 (m, 4 H, 15-H, 16-H), 4.01 (s, 5 H, 17-H), 5.12 (s, 1 H, 9-H), 6.04 (d, $J = 3.0$ Hz, 1 H, 7-H), 6.48 (d, $J = 3.0$ Hz, 1 H, 6-H), 7.15-7.24 (m, 5 H, 11-H, 12-H, 13-H);

^{13}C NMR (CDCl_3 , 75.5 MHz): $\delta = 10.2$ (t, C-4), 13.7 (q, C-1), 27.2 (t, C-2), 29.0 (t, C-3), 45.7 (d, C-9), 67.3, 67.5, 68.4, 68.5 (4 d, C-15, C-16), 68.8 (d, C-17), 90.4 (s, C-14), 106.2 (d, C-7), 122.1 (d, C-6), 126.2 (d, C-13), 128.0, 128.1 (2 d, C-11, C-12), 143.4 (s, C-10), 158.7 (s, C-8), 161.8 (s, C-5);

MS (EI, 70 eV), m/z (%): 637, 636, 635, 634, 633, 632, 631, 630, 629, 628 (M^+ , 4.5, 12, 4.6, 15, 28, 100, 43, 75, 31, 36), 576, 575, 574, 573, 572, 571 ($\text{M}^+ - \text{C}_4\text{H}_9$, 2.3, 6.9, 3.5, 5.4, 2.6, 3.0), 519 ($\text{M}^+ - \text{C}_8\text{H}_{17}$, > 1), 466, 464, 463, 462, 461, 460, 459, 458 (6.0, 6.4, 8.9, 42, 17, 33, 13, 17), 343, 342, 341 ($\text{M}^+ - \text{C}_{12}\text{H}_{17}\text{Fe}$, 4.2, 16, 4.0), 275 (27), 231 (11);

$\text{C}_{33}\text{H}_{44}\text{FeOSn}$ calcd. 632.1763 found 632.1784 (HRMS).



2-(Ferrocenylphenylmethyl)-5-(tributylstannyl)thiophene

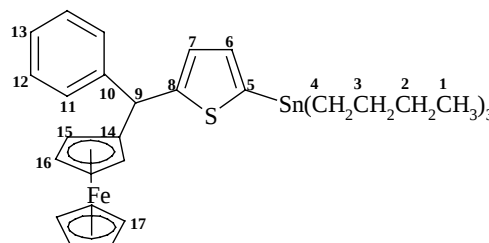
Separation and purification by column chromatography on basic alumina (activity III, pentane), orange oil;

^1H NMR (CDCl_3 , 300 MHz): δ = 0.88 (t, 3J = 7.2 Hz, 9 H, 1-H), 1.03-1.09 (m, 6 H, 4-H), 1.26-1.38 (m, 6 H, 2-H), 1.50-1.60 (m, 6 H, 3-H), 4.02 (br s, 5 H, 17-H), 4.02-4.15 (m, 4 H, 15-H, 16-H), 5.36 (br s, 1 H, 9-H), 6.82 (d, 3J = 3.0 Hz, 1 H, 7-H), 6.95 (d, 3J = 3.0 Hz, 1 H, 6-H), 7.25 (m, 5 H, 11-H, 12-H, 13-H);

^{13}C NMR (CDCl_3 , 75.5 MHz): δ = 10.8 (t, C-4), 13.7 (q, C-1), 27.2 (t, C-2), 29.0 (t, C-3), 45.2 (d, C-9), 67.3, 67.6, 68.2, 68.9 (4 d, C-15, C-16), 68.9 (d, C-17), 92.2 (s, C-14), 126.4 (d, C-13), 126.6 (d, C-7), 128.1, 128.3 (2 d, C-11, C-12), 134.6 (d, C-6), 134.7 (s, C-8), 145.1 (s, C-10), 154.1 (s, C-5);

MS (EI, 70 eV), m/z (%): 653, 652, 651, 650, 649, 648, 647, 646, 645, 644 (M^+ , 6, 16, 7, 23, 35, 100, 50, 77, 36, 41), 591, 589 (M^+ - C_4H_9 , 9, 7), 482, 480, 479, 478, 477, 476, 475, 474 (M^+ - $\text{C}_{12}\text{H}_{26}$, 13, 16, 20, 82, 37, 65, 27, 36), 360, 359, 358, 357, 356, 355 (M^+ - $\text{C}_{12}\text{H}_{26}\text{Sn}$, 7, 24, 93, 22, 10, 5), 281 (M^+ - $\text{C}_{18}\text{H}_{32}\text{Sn}$, 12), 240, 239, 238, 237, 236, 235, 234 (7, 27, 15, 31, 14, 19, 7, 6, 5, 6), 204, 203, 202 (9.5, 21, 28), 184, (17), 182 (14), 121 (M^+ - $\text{C}_{33}\text{H}_{44}\text{SFe}$, 20);

$\text{C}_{33}\text{H}_{44}\text{FeSSn}$ calcd. 648.1535 found 648.1556 (HRMS).



2-[Bis(4-methoxyphenyl)methyl]-5-(tributylstannyl)thiophene

Separation and purification by column chromatography on basic alumina (activity III, pentane), colorless oil;

^1H -NMR (CDCl_3 , 300 MHz): δ = 0.88 (t, 3J = 7.3 Hz, 9-H, 1-H), 1.03-1.07 (m, 6 H, 4-H), 1.26-1.36 (m, 6 H, 2-H), 1.50-1.57 (m, 6 H, 3-H), 3.78 (s, 6 H, 14-H), 5.61 (br s, 1 H, 9-H), 6.75 (dd, 3J = 3.2 Hz, 4J = 0.9 Hz, 1 H, 7-H), 6.81-6.84 (AA'BB'-system, J_{AB} = 8.8 Hz, 4 H, 12-H), 6.97 (d, 3J = 3.2 Hz, 1 H, 6-H), 7.11-7.13 (AA'BB'-system, J_{AB} = 8.8 Hz, 4 H, 11-H);

^{13}C -NMR (CDCl_3 , 75.5 MHz): δ = 10.7 (t, C-4), 13.7 (q, C-1), 27.2 (t, C-2), 28.9 (t, C-3), 50.7 (d, C-9), 55.2 (q, C-14), 113.6, (d, C-12), 127.4 (d, C-7), 129.7 (d, C-11), 134.9 (d, C-6), 135.6 (s, C-8), 136.8 (s, C-10), 154.3 (s, C-5), 158.2 (s, C-13);

MS (EI, 70 eV), m/z (%): 604, 603, 602, 601, 600, 599, 598, 597, 596, 595 (M^+ , 0.2, 0.1, 0.2, 0.4, 1.1, 0.9, 0.6, 0.5, 0.1), 573, 571, 570, 569, 568, 567, 566, 565 (M^+ - OCH_3 , 0.2, 0.3, 0.4, 1.2, 0.5, 0.9, 0.4, 0.4), 548, 547, 546, 545, 544, 543, 542, 541, 540, 539 (M^+ - C_4H_8 , 4, 15, 5, 19, 27, 100, 42, 72, 30, 36), 491, 489, 488, 487, 486, 485, 484, 483 (M^+ - C_8H_{17} , 2.1, 2.5, 3.1, 12, 5.2, 9.2, 3.9, 4.9), 435, 433, 432, 431, 430, 429, 428, 427, 426, 425 (M^+ - $\text{C}_{12}\text{H}_{26}$, 2.0, 3.4, 2.8, 13, 6.2, 15, 6.0, 9.6, 2.2, 2.9), 310 (M^+ - $\text{C}_{12}\text{H}_{26}\text{Sn}$, 18), 227 (M^+ - $\text{C}_{16}\text{H}_{29}\text{SSn}$, 18);

$\text{C}_{31}\text{H}_{44}\text{O}_2\text{SSn}$ calcd. 600.2084 found 600.2080 (HRMS).

