Product characterisation

(5-(Benzylamino-methyl)-furan-2-yl)methanol (1)

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 2.12 (2H, br s, OH, NH); 3.75 (2H, s, furylCH_2NH); 3.78 (2H, s, NHCH_2phenyl); 4.54 (2H, s, CH_2OH); 6.12 (1H, d, J=2.8, $H_{furyl}4$); 6.19 (1H, d, J=3.0, $H_{furyl}3$); 7.20-7.43 (5H, m, phenyl); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 45.48 (furylCH_2NH); 52.90 (NHCH_2phenyl); 57.45 (CH_2OH); 108.05 ($C_{furyl}4$); 108.34 ($C_{furyl}3$); 127.19 ($C_{phenyl}4$); 128.38 ($C_{phenyl}2$, $C_{phenyl}6$); 128.56 ($C_{phenyl}3$, $C_{phenyl}5$); 139.73 (CH_2phenyl); 153.71 ($C_{furyl}5$, $C_{furyl}2$); IR (cm^{-1}) ν_{max}: 697; 737; 792; 920; 1012; 1073; 1182; 1359; 1453; 1495; 1560; 1603; 2849; 2920; 3028; 3061; 3301; MS (ES+) m/z: 218.2 ($M+H^+$); yellow viscous liquid.

(5-Allylaminomethyl-furan-2-yl)methanol (2)

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 3.27 (2H, dt, J=6.1, J=1.3, NHCH_2CH); 3.77 (2H, s, CH_2NH); 4.57 (2H, s, CH_2OH); 5.09 (1H, d, J=10.5, CHH_{cis}CHCH$_2$); 5.13 (1H, d, J=17.6, CHH_{trans}CHCH2); 5.82 (1H, ddt, J_{cis}=17.1, J_{trans}=10.5, J_{CH2}=6.1, NHCH$_2$CHCH$_2$); 6.13 (1H, d, J=3.3, $H_{furyl}4$); 6.21 (1H, d, J=3.3, $H_{furyl}3$); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 45.17 (NHCH_2CH); 51.22 (CH_2NH); 57.02 (CH_2OH); 108.06 ($C_{furyl}4$); 108.14 ($C_{furyl}3$); 116.93 (CH_2CH); 135.94 (CH_2CH); 153.00($C_{furyl}5$); 154.17 ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 790; 921; 1012; 1075; 1143; 1186; 1355; 1447; 1560; 1643; 2919; 2840; 3078; 3286; MS (ES+) m/z: 168.2 ($M+H^+$); yellow viscous liquid.

(5-(2-Phenylethyl)-aminomethyl-furan-2-yl)methanol (3) (CAS 66356-43-2)

Elemental analysis data are reported elsewhere.[a] Additional characterisation is given.

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 2.77-2.95 (4H, m, CH_2CH_2NH); 3.77 (2H, s, furylCH_2NH); 4.56 (2H, s, CH_2OH); 6.09 (1H, d, J=2.8, $H_{furyl}4$); 6.19 (1H, d, J=2.8, $H_{furyl}3$); 7.34-7.18 (5H, m, phenyl); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 36.22 (NHCH$_2$$CH_2$); 46.27 (NH$CH_2CH_2$); 50.39 (furyl$CH_2$NH); 57.62 ($CH_2$OH); 107.92 ($C_{furyl}4$); 108.46 ($C_{furyl}3$); 126.32 ($C_{phenyl}4$); 128.60 ($C_{phenyl}2$, $C_{phenyl}6$); 128.80 ($C_{phenyl}3$, $C_{phenyl}5$); 139.91 ($C_{phenyl}1$); 153.48 ($C_{furyl}5$); 153.80 ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 698; 747; 791; 921; 1012; 1086; 1188; 1358; 1453; 1495; 1560; 1603; 2849; 2922; 3026; 3293; MS (ES+) m/z: 232.3 ($M+H^+$); yellow viscous liquid.

(5-Dodecylaminomethyl-furan-2-yl)methanol (4)

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 0.88 (3H, t, J=6.6 CH_3); 1.25 (18H, s, CH_2); 1.48 (2H, t, J=6.3, NHCH$_2$CH_2); 2.58 (2H, t, J=7.4, NHCH_2CH$_2$); 3.74 (2H, s, CH_2NH); 4.51 (2H, s, CH_2OH); 6.11 (1H, d, J=2.8, $H_{furyl}4$); 6.17 (1H, d, J=3.3, $H_{furyl}3$); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 14.22 (C12); 22.78 (C11); 27.41 (C3); 29.45 (C4, C9); 29.70 (C5-C8); 30.03 (C2); 32.01 (C10); 46.44 (C1); 49.39 (furylCH_2NH); 57.59 (CH_2OH); 107.71 ($C_{furyl}4$); 108.43 ($C_{furyl}3$); 153.45 ($C_{furyl}5$); 154.17 C ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 718; 791; 883; 897; 938; 1008; 1016; 1115; 1198; 1351; 1470; 1572; 1604; 2788; 2849; 2915; 2954; 1744; 3156; 3263; MS (ES+) m/z: 296.3 ($M+H^+$); mp=35°C; white fatty solid.

(5-Propylaminomethyl-furan-2-yl)methanol (5)

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 0.92 (3H, t, J=7.4, CH_3); 1.52 (2H, sext, J=7.4, CH_2CH_3); 2.59 (2H, t, J=7.2, NHCH_2CH$_2$); 3.77 (2H, s, furylCH_2NH); 4.58 (2H, s, CH_2OH); 6.13 (1H, d, J=3.3, $H_{furyl}4$); 6.21 (1H, d, J=3.3, $H_{furyl}3$); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 11.82 (CH_3); 23.03 (CH_2CH_3); 46.29 (NHCH_2CH$_2$); 51.11 (furylNHCH_2); 57.70 (CH_2OH); 107.81 ($C_{furyl}4$); 108.50 ($C_{furyl}3$); 153.51 ($C_{furyl}5$); 153.94 ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 791; 1013; 1072; 1096; 1189; 1358; 1458; 1560; 1637; 2873; 2931; 2958; 3279; MS (ES+) m/z: 170.2 ($M+H^+$); yellow viscous liquid.

(5-(Isopropylamino-methyl)-furan-2-yl)methanol (6) (CAS 66356-44-3)

Elemental analysis is reported elsewhere.[30,31] Additional characterisation is given.

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 1.09 (6H, d, J=6.1, CH(CH_3)$_2$); 1.97 (2H, br s, NH, OH); 2.84 (1H, sept, J=6.2 $CH(CH_3)_2$); 3.77 (2H, s, CH_2NH); 4.57 (2H, s, CH_2OH); 6.12 (1H, d, J=3.3, $H_{furyl}4$); 6.20 (1H, d, J=3.3, $H_{furyl}3$); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 22.74 (CH_3); 44.01 (NHCH); 47.91 (CH_2NH); 57.59 (CH_2OH); 107.63 ($C_{furyl}4$); 108.50 ($C_{furyl}3$); 153.50 ($C_{furyl}5$); 154.14 ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 788; 1013; 1064; 1129; 1173; 1339; 1383; 1443; 1467; 1560; 1654; 2864; 2922; 2965; 3270; MS (ES+) m/z: 170.5 ($M+H^+$); yellow viscous liquid.

(5-((2-Methoxy-phenylamino)-methyl)-furan-2-yl)methanol (7)

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 3.84 (3H, s, OCH_3); 4.32 (2H, s, CH_2NH); 4.58 (2H, s, CH_2OH); 6.19 (1H, d, *J*=3.3, $H_{furyl}4$); 6.22 (1H, d, J=3.3, $H_{furyl}3$); 6.65-6.90 (4H, m, phenyl); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 41.39 (CH_2NH); 55.54 (OCH_3); 57.48 (CH_2OH); 107.83 ($C_{furyl}4$); 108.60 ($C_{phenyl}6$); 109.76 ($C_{furyl}3$); 110.57 ($C_{phenyl}3$); 117.42 ($C_{phenyl}4$); 121.33 ($C_{phenyl}5$); 137.67 ($C_{phenyl}1$); 147.21 ($C_{phenyl}2$); 153.04 ($C_{furyl}5$); 153.65 ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 735; 791; 1012; 1178; 1221; 1246; 1339; 1456; 1508; 1601; 2836; 2867; 3066; 3400; MS (ES+) m/z: 234.3 ($M+H^+$); yellow viscous liquid.

(5-Butylaminomethyl-furan-2-yl)methanol (8)

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 0.91 (3H, t, J=7.2 CH_3); 1.34 (2H, sext, J=7.3, CH_2CH_3); 1.49 (2H, sext, J=7.4, $CH_2CH_2CH_3$); 2.63 (2H, t, J=7.2, NHCH$_2$CH$_2$); 3.78 (2H, s, furylCH$_2$NH); 4.58 (2H, s, CH$_2$OH); 6.14 (1H, d, J=2.8, $H_{furyl}4$); 6.21 (1H, d, J=2.8, $H_{furyl}3$); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 13.98 (CH_3); 20.42 ($CH_2CH_2CH_3$); 31.55 ($CH_2CH_2CH_3$); 45.87 (NHCH_2CH$_2$); 48.55 (furylNHCH_2); 56.89 (CH_2OH); 107.94 ($C_{furyl}4$); 108.20 ($C_{furyl}3$); 152.63($C_{furyl}5$); 154.37 ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 789; 1012; 1071; 1097; 1188; 1258; 1357; 1458; 1560; 1662; 2860; 2928; 2928; 2956; 3280; MS (ES+) m/z: 184.5 ($M+H^+$); dark yellow viscous liquid.

(5-((2,4-Dimethoxy-phenylamino)-methyl)-furan-2-yl)methanol (9)

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 3.75 (3H, s, OCH_3(p)); 3.82 (3H, s, OCH_3(o)); 4.28 (2H, s, CH_2NH); 4.58 (2H, s, CH_2OH); 6.17 (1H, d, J=2.8, $H_{furyl}4$); 6.22 (1H, d, J=3.3, $H_{furyl}3$); 6.39 (1H, dd, J=2.8, J=2.8, $H_{phenyl}3$); 6.46 (1H, d, J=2.8, $H_{phenyl}5$); 6.59 (1H, d, J=8.8, $H_{phenyl}6$); $Si(CH_3)_4$, $CDCl_3$, $Si(CH_3)_4$) δ: 42.16 (CH_2NH); 55.57 (OCH_3(o)); 55.83 (OCH_3(p)); 57.65 (CH_2OH); 99.27 ($C_{phenyl}3$); 103.76 ($C_{phenyl}5$); 107.73 ($C_{furyl}4$); 108.69 ($C_{furyl}3$); 110.99 ($C_{phenyl}6$); 131.90 ($C_{phenyl}1$); 148.34 ($C_{phenyl}2$); 152.51 ($C_{phenyl}4$); 153.39

($C_{furyl}5$); 153.42 ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 790; 1012; 1030; 1136; 1154; 1204; 1287; 1359; 1455; 1513; 2834; 2936; 3396; MS (ES+) m/z: 264.2 ($M+H^+$); dark yellow viscous liquid.

(5-(Quinolin-6-yl-aminomethyl)-furan-2-yl)methanol (10)

^{1}H-NMR (ppm, $(CD_3)_2CO$, $Si(CH_3)_4$) δ: 4.42 (2H, s, CH_2NH); 4.70 (2H,s, CH_2OH); 6.19 (1H, d, J=3.3, $H_{furyl}4$); 6.28 (1H, d, J=3.3, $H_{furyl}3$); 7.22-7.31 (2H, m, $H_{quin}5$, $H_{quin}7$); 7.33 (1H, d, J=2.7, $H_{quin}3$); 7.77 (1H, d, $H_{quin}4$); 7.97 (1H, d, J=8.3, $H_{quin}8$); 8.53 (1H, dd, J=6.2, J=6.2, $H_{quin}2$); ^{13}C-NMR (ppm, $(CD_3)_2CO$, $Si(CH_3)_4$) δ: 40.68 (CH_2NH); 56.50 (CH_2OH); 102.75 ($C_{quin}5$); 107.60 ($C_{furyl}4$); 107.76 ($C_{furyl}3$); 121.28 C ($C_{quin}3$); 121.50 ($C_{quin}7$); 130.08 ($C_{quin}4a$); 130.26 ($C_{quin}8$); 133.33 CH ($C_{quin}4$); 143.45 ($C_{quin}8a$); 145.74 ($C_{quin}6$); 146.51 ($C_{quin}2$); 152.27 ($C_{furyl}5$); 155.07 ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 796; 832; 942; 1011; 1031; 1124; 1186; 1252; 1318; 1378; 1546; 1624; 2734; 2826; 2895; 3073; 3310; MS (ES+) m/z: 255.2 ($M+H^+$); El.anal. (%) Calc. for $C_{15}H_{14}N_2O_2$: C 70.85; H 5.55; N 11.02; O 12.58; found: C 69.75; H 5.44; N 10.60; mp=148°C; dark orange powder.

(5-((2,6-Dimethyl-phenylamino)-methyl)- furan-2-yl)methanol (11) (CAS 241128-35-8)

^{1}H- and ^{13}C-NMR data and elemental analysis are reported elsewhere.[b] Additional characterisation is given.

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 2.26 (6H, s, $(CH_3)_2$); 3.40 (1H, br s, NH); 4.11 (2H, s, CH_2NH); 4.57 (2H, d, J=5.8, CH_2OH); 6.05 (1H, d, J=3.6, $H_{furyl}4$); 6.19 (1H, d, J=3.6, $H_{furyl}3$); 6.84 (1H, t, J=7.4, $H_{phenyl}4$); 6.99 (2H, d, J=7.7, $H_{phenyl}3$, $H_{phenyl}5$); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 18.36 $(CH_3)_2$; 45.24 (CH_2NH); 57.68 (CH_2OH); 107.70 ($C_{furyl}4$); 108.76 ($C_{furyl}3$); 122.55 ($C_{phenyl}4$); 128.83 ($C_{phenyl}2$, $C_{phenyl}6$); 130.14 ($C_{phenyl}3$, $C_{phenyl}5$); 145.15 ($C_{phenyl}1$); 153.39 ($C_{furyl}5$); 154.11 ($C_{furyl}2$); IR (cm^{-1}) ν_{max}: 777; 798; 849; 1014; 1028; 1172; 1357; 1448; 1471; 1557; 1592; 2849; 2894; 2930; 2955; 3224; 3352; MS (ES+) m/z: 232.2 ($M+H^+$); *mp*=96°C; light yellow crystals.

(5-((3-Methoxy-phenylamino)-methyl)-furan-2-yl)methanol (12)

^{1}H-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 3.65 (3H, s, OCH_3); 4.16 (2H, s, CH_2NH); 4.42 (2H, s, CH_2OH); 6.8 (2H, dd, J=3.3, J=3.3, $H_{furyl}3$, $H_{furyl}4$); 6.13 (1H, t, J=2.2, $H_{phenyl}3$); 6.20 (2H, td, J_t=8.5, J_d=2.0, $H_{phenyl}3$, $H_{phenyl}5$); 6.98 (1H, t, J=8.0, $H_{phenyl}5$); ^{13}C-NMR (ppm, $CDCl_3$, $Si(CH_3)_4$) δ: 41.56 (OCH_3); 55.19 (CH_2NH); 57.42 (CH_2OH); 99.47 ($C_{phenyl}2$); 103.30 ($C_{phenyl}4$); 106.44 ($C_{phenyl}6$); 107.79 ($C_{furyl}4$); 108.66 ($C_{furyl}3$); 130.08 ($C_{phenyl}5$); 149.12 C ($C_{phenyl}1$); 152.77 ($C_{furyl}5$); 153.62 ($C_{furyl}2$); 160.84 C ($C_{phenyl}3$); IR (cm^{-1}) ν_{max}: 687; 727; 908; 1010; 1161; 1209; 1341; 1496; 1509; 1600; 1613; 2836; 2933; 3387; MS (ES+) m/z: 234.2 ($M+H^+$); yellow viscous liquid.

[a] B. J. Price, J. W. Clitherow and J. Bradshaw, *CH Pat.,* 647517, 1985

[b] M. A. Flores, M. R. Manzoni, R. Baumann, W. M. Davis and R. R. Schrock, *Organometallics,* 1999, **18**, 3220-3227.