

Supporting Information

for

A novel and facile synthesis of 3-(2-benzofuroyl)- and 3,6-bis(2-benzofuroyl)carbazole derivatives

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Characterization data of the title compounds and NMR and HRMS spectra

Characterization data for products 3a–l

3-(2-Benzofuroyl)-*N*-ethyl-9*H*-carbazole (3a). Yellow solid. IR (KBr) ν/cm^{-1} : 3068, 2972, 2938, 1638, 1591, 1436, 1231, 1062, 809, 747; ^1H NMR (300 MHz, CDCl_3): δ 1.51 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.46 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.36 (d, $J = 8.0$ Hz, 1H, ArH), 7.38 (d, $J = 8.0$ Hz, 1H, ArH), 7.48–7.55 (m, 4H, ArH), 7.61 (s, 1H, furan-H), 7.70 (d, $J = 8.2$ Hz, 1H, ArH), 7.78 (d, $J = 7.8$ Hz, 1H, ArH), 8.19 (d, $J = 7.8$ Hz, 1H, ArH), 8.29 (dd, $J = 8.7, 1.50$ Hz, 1H, ArH), 8.93 (d, $J = 1.3$ Hz, 1H, ArH); HRMS–ESI: (m/z) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{NNaO}_2$: 362.1151; found: 362.1150.

3-[2-(5-Methylbenzofuroyl)]-*N*-ethyl-9*H*-carbazole (3b). Yellow solid. IR (KBr) ν/cm^{-1} : 3065, 2963, 2915, 1640, 1591, 1432, 1022, 816, 775; ^1H NMR (600 MHz, CDCl_3): δ 1.49 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 2.54 (s, 3H, CH_3), 4.42 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.17 (d, $J = 7.8$ Hz, 1H, ArH), 7.32 (t, $J = 7.8$ Hz, 1H, ArH), 7.47–7.50 (m, 4H, ArH), 7.53 (d, $J = 7.2$ Hz, 1H, ArH), 7.54 (s, 1H, furan-H), 7.62 (d, $J = 7.8$ Hz, 1H, ArH), 8.26 (dd, $J = 8.4, 1.8$ Hz, 1H, ArH), 8.90 (d, $J = 1.2$ Hz, 1H, ArH); ^{13}C NMR (150 MHz, CDCl_3): δ 13.84, 22.09, 37.89, 108.21, 109.03, 112.49, 115.75, 120.04, 120.84, 122.56, 122.79, 123.29, 124.78, 125.56, 126.53, 127.76, 128.42, 138.75, 140.68, 142.74, 152.75, 156.41, 183.89; Anal. calcd for $\text{C}_{24}\text{H}_{19}\text{NO}_2$: C, 81.56; H, 5.42; N, 3.96; found: C, 81.42; H, 5.70; N, 3.75.

3-[2-(6-Methylbenzofuroyl)]-*N*-ethyl-9*H*-carbazole (3c). Yellow solid. IR (KBr) ν/cm^{-1} : 3071, 2962, 2911, 1641, 1590, 1432, 1022, 816, 776; ^1H NMR (600 MHz,

CDCl₃): δ 1.49 (t, J = 7.2 Hz, 3H, CH₃CH₂), 2.48 (s, 3H, CH₃), 4.43 (q, J = 7.2 Hz, 2H, CH₃CH₂), 7.30-7.33 (m, 2H, ArH), 7.47 (d, J = 7.8 Hz, 1H, ArH), 7.49 (d, J = 8.4 Hz, 1H, ArH), 7.51 (s, 1H, furan-H), 7.53 (d, J = 7.8 Hz, 2H, ArH), 7.56 (d, J = 8.4 Hz, 1H, ArH), 8.18 (d, J = 7.8 Hz, 1H, ArH), 8.27 (dd, J = 8.4, 1.8 Hz, 1H, ArH), 8.90 (s, 1H, ArH); ¹³C NMR (150 MHz, CDCl₃): δ 13.83, 21.34, 37.89, 108.21, 109.03, 112.04, 115.34, 120.05, 120.83, 122.58, 122.80, 123.52, 123.35, 126.54, 127.32, 127.80, 128.33, 129.41, 133.40, 140.68, 142.76, 153.26, 154.39, 183.91; Anal. calcd for C₂₄H₁₉NO₂: C, 81.56; H, 5.42; N, 3.96; found: C, 81.38; H, 5.43; N, 3.82.

3-[2-(7-Methylbenzofuroyl)]-N-ethyl-9H-carbazole (3d). Yellow solid. IR (KBr) ν/cm^{-1} : 3069, 2966, 2916, 1641, 1590, 1432, 1021, 815, 779; ¹H NMR (600 MHz, CDCl₃): δ 1.48 (t, J = 7.2 Hz, 3H, CH₃CH₂), 2.53 (s, 3H, CH₃), 4.42 (q, J = 7.2 Hz, 2H, CH₃CH₂), 7.16 (d, J = 7.8 Hz, 1H, ArH), 7.31 (d, J = 7.8 Hz, 1H, ArH), 7.45-7.53 (m, 5H, ArH and furan-H), 7.61 (d, J = 7.8 Hz, 1H, ArH), 8.17 (d, J = 7.8 Hz, 1H, ArH), 8.25 (d, J = 8.4 Hz, 1H, ArH), 8.89 (s, 1H, ArH); ¹³C NMR (150 MHz, CDCl₃): δ 13.81, 22.07, 37.85, 108.18, 109.00, 112.45, 115.73, 120.01, 120.81, 122.54, 122.76, 123.26, 124.76, 125.54, 126.51, 127.73, 128.38, 138.72, 140.65, 142.70, 152.73, 156.39, 183.84; Anal. calcd for C₂₄H₁₉NO₂: C, 81.56; H, 5.42; N, 3.96; found: C, 81.76; H, 5.24; N, 3.75.

3-[2-(5-Methoxybenzofuroyl)]-N-ethyl-9H-carbazole (3e). Yellow solid. IR (KBr) ν/cm^{-1} : 3071, 2962, 2911, 1641, 1590, 1432, 1036, 816, 776; ¹H NMR (600 MHz, CDCl₃): δ 1.50 (t, J = 7.2 Hz, 3H, CH₃CH₂), 3.89 (s, 3H, OCH₃), 4.44 (q, J = 7.2 Hz, 2H, CH₃CH₂), 7.12 (dd, J = 9.0, 2.4 Hz, 1H, ArH), 7.15 (d, J = 2.4 Hz, 1H, ArH), 7.32 (t, J =

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7.2 Hz, 1H, ArH), 7.48 (d, $J = 8.4$, 1H, ArH), 7.50 (d, $J = 9.0$ Hz, 1H, ArH), 7.57 (d, $J = 9.0$ Hz, 1H, ArH), 7.51-7.55 (m, 2H, ArH and furan-H), 8.19 (d, $J = 7.8$ Hz, 1H, ArH), 8.27 (dd, $J = 8.4$, 1.2 Hz, 1H, ArH), 8.91 (s, 1H, ArH); ^{13}C NMR (150 MHz, CDCl_3): δ 13.84, 37.90, 55.89, 103.93, 108.23, 109.04, 113.17, 115.50, 117.85, 120.07, 120.84, 122.80, 123.26, 123.39, 126.56, 127.70, 127.83, 128.26, 140.68, 142.79, 151.08, 153.89, 156.59, 183.73; Anal. calcd for $\text{C}_{24}\text{H}_{19}\text{NO}_3$: C, 78.03; H, 5.18; N, 3.79; found: C, 77.82; H, 5.36; N, 3.57.

3-[2-(5-Chlorobenzofuroyl)]-N-ethyl-9H-carbazole (3f). Yellow solid. IR (KBr) v/cm^{-1} : 3091, 2983, 2940, 1641, 1591, 1435, 1232, 1062, 1022, 816, 773; ^1H NMR (300 MHz, CDCl_3): δ 1.50 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.47 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.26 (d, $J = 7.8$ Hz, 1H, ArH), 7.44-7.58 (m, 5H, ArH), 7.63 (s, 1H, furan-H), 7.79 (d, $J = 2.0$ Hz, 1H, ArH), 8.24 (d, $J = 7.8$ Hz, 1H, ArH), 8.29 (dd, $J = 8.7$, 1.6 Hz, 1H, ArH), 8.90 (d, $J = 1.4$ Hz, 1H, ArH); Anal. calcd for $\text{C}_{23}\text{H}_{16}\text{ClNO}_2$: C, 73.90; H, 4.31; N, 3.75; found: C, 74.07; H, 4.24; N, 3.73.

3-[2-(5-Bromobenzofuroyl)]-N-ethyl-9H-carbazole (3g). Yellow solid. IR (KBr) v/cm^{-1} : 3063, 2982, 2937, 1642, 1591, 1434, 1232, 1022, 970, 814, 772, 622; ^1H NMR (300 MHz, CDCl_3): δ 1.49 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.48 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.41-7.52 (m, 4H, ArH), 7.58-7.64 (m, 3H, ArH), 7.88 (s, 1H, furan-H), 8.17 (d, $J = 7.8$ Hz, 1H, ArH), 8.25 (dd, $J = 8.6$, 1.5 Hz, 1H, ArH), 8.89 (d, $J = 1.4$ Hz, 1H, ArH); Anal. calcd for $\text{C}_{23}\text{H}_{16}\text{BrNO}_2$: C, 66.04; H, 3.86; N, 3.35; found: C, 66.26; H, 3.72; N, 3.25.

3-[2-(5,7-Dibromobenzofuroyl)]-N-ethyl-9H-carbazole (3h). Yellow solid. IR (KBr) ν/cm^{-1} : 3069, 2966, 2916, 1641, 1590, 1432, 1021, 815, 779, 662; ^1H NMR (600 MHz, CDCl_3): δ 1.37 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.55 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.32 (t, $J = 7.2$ Hz, 1H, ArH), 7.56 (t, $J = 7.8$ Hz, 1H, ArH), 7.73 (d, $J = 8.4$ Hz, 1H, ArH), 7.83 (d, $J = 8.4$ Hz, 1H, ArH), 7.88 (s, 1H, furan-H), 8.04 (d, $J = 1.8$ Hz, 1H, ArH), 8.12 (d, $J = 1.8$ Hz, 1H, ArH), 8.19 (dd, $J = 8.4, 1.2$ Hz, 1H, ArH), 8.32 (d, $J = 7.8$ Hz, 1H, ArH), 8.99 (s, 1H, ArH); ^{13}C NMR (150 MHz, DMSO): δ 13.82, 37.44, 105.35, 109.44, 109.96, 115.59, 116.42, 120.16, 121.04, 122.15, 122.53, 123.40, 125.64, 126.86, 127.19, 127.46, 129.95, 132.35, 140.46, 142.65, 151.38, 153.64, 182.16; Anal. calcd for $\text{C}_{23}\text{H}_{15}\text{Br}_2\text{NO}_2$: C, 55.56; H, 3.04; N, 2.82; found: C, 55.28; H, 3.09; N, 2.58.

3-[2-(5-*tert*-Butyl-7-fluorobenzofuroyl)]-N-ethyl-9H-carbazole (3i). Yellow solid. IR (KBr) ν/cm^{-1} : 3065, 2972, 2881, 1641, 1592, 1435, 1231, 1192, 1024, 815, 778; ^1H NMR (300 MHz, CDCl_3): δ 1.40 (s, 9H, *t*-butyl), 1.50 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.44 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.29-7.35 (m, 2H, ArH), 7.46-7.54 (m, 4H, ArH), 7.60 (d, $J = 2.7$ Hz, 1H, ArH), 8.18 (d, $J = 7.7$ Hz, 1H, ArH), 8.32 (dd, $J = 8.6, 1.4$ Hz, 1H, ArH), 8.97 (s, 1H, ArH); HRMS-ESI: (m/z) [$\text{M} + \text{Na}$] $^+$ calcd for $\text{C}_{27}\text{H}_{24}\text{FNNaO}_2$: 436.1683; found: 436.1688.

3-[2-(5-*tert*-Butyl-7-chlorobenzofuroyl)]-N-ethyl-9H-carbazole (3j). Yellow solid. IR (KBr) ν/cm^{-1} : 3058, 2964, 2870, 1640, 1589, 1430, 1229, 1084, 1022, 815, 777; ^1H NMR (300 MHz, CDCl_3): δ 1.42 (s, 9H, *t*-butyl), 1.50 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.45 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.32-7.41 (m, 1H, ArH), 7.47-7.58 (m, 5H, ArH), 7.64 (s,

1H, furan-H), 8.20 (d, $J = 7.7$ Hz, 1H, ArH), 8.38 (d, $J = 8.6$ Hz, 1H, ArH), 9.08 (s, 1H, ArH); Anal. calcd for $C_{27}H_{24}ClNO_2$: C, 75.43; H, 5.63; N, 3.26 found: C, 75.21; H, 5.52; N, 3.34.

3-[2-(7-Bromo-5-*tert*-butylbenzofuroyl)]-*N*-ethyl-9*H*-carbazole (3k). Yellow solid. IR (KBr) ν/cm^{-1} : 3070, 2963, 2869, 1640, 1587, 1431, 1228, 1022, 815, 780, 658; 1H NMR (300 MHz, $CDCl_3$): δ 1.24 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 1.40 (s, 9H, *t*-butyl), 3.73 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.29-7.34 (m, 2H, ArH), 7.45-7.55 (m, 3H, ArH), 7.66 (s, 1H, furan-H), 7.71 (s, 1H, ArH), 8.19 (d, $J = 7.6$ Hz, 1H, ArH), 8.37 (d, $J = 8.6$ Hz, 1H, ArH), 9.12 (s, 1H, ArH); Anal. calcd for $C_{27}H_{24}BrNO_2$: C, 68.36; H, 5.10; N, 2.95; found: C, 68.22; H, 5.34; N, 2.87.

3-(2-Naphtho[2,1-*b*]furoyl)-*N*-ethyl-9*H*-carbazole (3l). Brown solid. IR (KBr) ν/cm^{-1} : 3071, 2972, 2931, 1642, 1590, 1436, 1232, 1065, 808, 765; 1H NMR (300 MHz, $CDCl_3$): δ 1.52 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.48 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.32-7.37 (m, 1H, ArH), 7.49 (d, $J = 8.0$ Hz, 1H, ArH), 7.53-7.60 (m, 3H, ArH), 7.64-7.69 (m, 1H, ArH), 7.81 (d, $J = 8.8$ Hz, 1H, ArH), 7.94 (d, $J = 9.0$ Hz, 1H, ArH), 8.01 (d, $J = 8.0$ Hz, 1H, ArH), 8.10 (d, $J = 0.5$ Hz, 1H, ArH), 8.22 (d, $J = 7.8$ Hz, 2H, ArH), 8.34 (dd, $J = 8.6, 1.7$ Hz, 1H, ArH), 8.98 (d, $J = 1.4$ Hz, 1H, ArH); HRMS–ESI: (m/z) $[M + Na]^+$ calcd for $C_{27}H_{19}NNaO_2$: 412.1308. Found: 412.1309.

Characterization data for products 5a–l

3,6-Bis(benzofuroyl)-*N*-ethyl-9*H*-carbazole (5a). Yellow solid. IR (KBr) ν/cm^{-1} : 3071, 2972, 2938, 1643, 1591, 1436, 1062, 809, 747; ^1H NMR (600 MHz, CDCl_3): δ 1.55 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.50 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.36 (t, $J = 7.8$ Hz, 2H, ArH), 7.52 (t, $J = 7.8$ Hz, 2H, ArH), 7.59 (d, $J = 9.0$ Hz, 2H, ArH), 7.62 (s, 2H, furan-H), 7.69 (d, $J = 8.4$ Hz, 2H, ArH), 7.77 (d, $J = 7.8$ Hz, 2H, ArH), 8.33 (dd, $J = 8.4, 1.2$ Hz, 2H, ArH), 8.97 (d, $J = 1.2$ Hz, 2H, ArH); Anal. calcd for $\text{C}_{32}\text{H}_{21}\text{NO}_4$: C, 79.49; H, 4.38; N, 2.90; found: C, 79.40; H, 4.53; N, 2.77.

3,6-Bis[2-(5-methylbenzofuroyl)]-*N*-ethyl-9*H*-carbazole (5b). Yellow solid. IR (KBr) ν/cm^{-1} : 3071, 2962, 2911, 1641, 1590, 1432, 1022, 816, 776; ^1H NMR (600 MHz, CDCl_3): δ 1.57 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 2.53 (s, 6H, CH_3), 4.50 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.18 (d, $J = 8.4$ Hz, 2H, ArH), 7.48 (s, 2H, ArH), 7.57 (d, $J = 8.4$ Hz, 2H, ArH), 7.58 (s, 2H, furan-H), 7.63 (d, $J = 7.8$ Hz, 2H, ArH), 8.32 (dd, $J = 9.0, 1.8$ Hz, 2H, ArH), 8.97 (s, 2H, ArH); ^{13}C NMR (150 MHz, CDCl_3): δ 13.91, 22.10, 38.29, 108.91, 112.51, 116.14, 122.68, 123.04, 123.49, 124.72, 125.68, 128.50, 129.56, 139.02, 143.43, 152.51, 156.50, 183.70; HRMS–ESI: (m/z) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{34}\text{H}_{25}\text{NNaO}_4$: 534.1676; found: 534.1678.

3,6-Bis[2-(6-methylbenzofuroyl)]-*N*-ethyl-9*H*-carbazole (5c). Yellow solid. IR (KBr) ν/cm^{-1} : 3069, 2966, 2916, 1641, 1590, 1432, 1021, 815, 779; ^1H NMR (600 MHz, CDCl_3): δ 1.54 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 2.48 (s, 6H, CH_3), 4.51 (q, $J = 7.2$ Hz, 2H,

CH_3CH_2), 7.31 (d, $J = 9.0$ Hz, 2H, ArH), 7.53-7.58 (m, 8H, ArH and furan-H), 8.32 (d, $J = 9.0$ Hz, 2H, ArH), 8.97 (s, 2H, ArH); ^{13}C NMR (150 MHz, CDCl_3): δ 13.91, 21.34, 38.29, 108.94, 112.06, 115.75, 122.70, 123.05, 123.55, 127.25, 128.55, 129.50, 129.65, 133.53, 143.47, 152.99, 154.48, 183.74; HRMS–ESI: (m/z) [$\text{M} + \text{Na}$] $^+$ calcd for $\text{C}_{34}\text{H}_{25}\text{NNaO}_4$: 534.1676; found: 534.1672.

3,6-Bis[2-(7-methylbenzofuroyl)]-*N*-ethyl-9*H*-carbazole (5d). Yellow solid. IR (KBr) v/cm^{-1} : 3065, 2963, 2915, 1640, 1591, 1432, 1022, 816, 775; ^1H NMR (600 MHz, CDCl_3): δ 1.55 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 2.48 (s, 6H, CH_3), 4.50 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.32 (d, $J = 9.0$ Hz, 2H, ArH), 7.54-7.59 (m, 8H, ArH and furan-H), 8.33 (d, $J = 9.0$ Hz, 2H, ArH), 8.97 (d, $J = 1.2$ Hz, 2H, ArH); HRMS–ESI: (m/z) [$\text{M} + \text{Na}$] $^+$ calcd for $\text{C}_{34}\text{H}_{25}\text{NNaO}_4$: 534.1676; found: 534.1700.

3,6-Bis[2-(5-methoxybenzofuroyl)]-*N*-ethyl-9*H*-carbazole (5e). Yellow solid. IR (KBr) v/cm^{-1} : 3071, 2962, 2911, 1641, 1590, 1432, 1036, 816, 776; ^1H NMR (600 MHz, CDCl_3): δ 1.49 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 3.88 (s, 6H, OCH_3), 4.46 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.13 (dd, $J = 9.0, 2.4$ Hz, 2H, ArH), 7.15 (d, $J = 2.4$ Hz, 2H, ArH), 7.56-7.58 (m, 6H, ArH and furan-H), 8.38 (dd, $J = 8.4, 1.2$ Hz, 2H, ArH), 8.89 (s, 2H, ArH); ^{13}C NMR (150 MHz, CDCl_3): δ 13.91, 38.29, 55.87, 103.93, 108.94, 113.20, 115.93, 118.19, 123.04, 123.56, 127.63, 128.57, 129.41, 143.48, 151.12, 153.56, 156.65, 183.54; HRMS–ESI: (m/z) [$\text{M} + \text{Na}$] $^+$ calcd for $\text{C}_{34}\text{H}_{25}\text{NNaO}_6$: 566.1574; found: 566.1570.

3,6-Bis[2-(5-chlorobenzofuroyl)]-N-ethyl-9H-carbazole (5f). Yellow solid. IR (KBr) ν/cm^{-1} : 3072, 2983, 2940, 1641, 1591, 1436, 1062, 1022, 816, 783; ^1H NMR (600 MHz, CDCl_3): δ 1.56 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.52 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.21 (d, $J = 8.4$ Hz, 2H, ArH), 7.46 (s, 2H, ArH), 7.57 (s, 2H, furan-H), 7.62 (d, $J = 8.4$ Hz, 2H, ArH), 7.66 (d, $J = 7.8$ Hz, 2H, ArH), 8.35 (dd, $J = 9.0, 1.8$ Hz, 2H, ArH), 8.96 (s, 2H, ArH); HRMS–ESI: (m/z) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{32}\text{H}_{19}^{35}\text{Cl}_2\text{NNaO}_4$: 574.0583; found: 574.0589.

3,6-Bis[2-(5-bromobenzofuroyl)]-N-ethyl-9H-carbazole (5g). Yellow solid. IR (KBr) ν/cm^{-1} : 3063, 2982, 2937, 1642, 1591, 1434, 1022, 814, 772, 622; ^1H NMR (600 MHz, CDCl_3): δ 1.56 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.51 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.56-7.61 (m, 8H, ArH and furan-H), 7.90 (d, $J = 1.8$ Hz, 2H, benzofuran-H), 8.33 (dd, $J = 8.4, 1.2$ Hz, 2H, ArH), 8.96 (s, 2H, ArH); Anal. calcd for $\text{C}_{32}\text{H}_{19}\text{Br}_2\text{NO}_4$: C, 59.93; H, 2.99; N, 2.18; found: C, 60.22; H, 2.79; N, 2.07.

3,6-Bis[2-(5,7-dibromobenzofuroyl)]-N-ethyl-9H-carbazole (5h). Yellow solid. IR (KBr) ν/cm^{-1} : 3069, 2966, 2916, 1641, 1590, 1432, 1021, 815, 779, 662; ^1H NMR (600 MHz, CDCl_3): δ 1.55 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.48 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.27 (d, $J = 7.2$ Hz, 2H, ArH), 7.51 (s, 2H, furan-H), 7.57 (d, $J = 8.4$ Hz, 2H, ArH), 7.63 (d, $J = 7.2$ Hz, 2H, ArH), 8.37 (q, $J = 1.2$ Hz, 2H, ArH), 9.14 (s, 2H, ArH); HRMS–ESI: (m/z) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{32}\text{H}_{17}^{79}\text{Br}_4\text{NNaO}_4$: 817.7784; found: 817.7792. Anal. calcd for $\text{C}_{32}\text{H}_{17}\text{Br}_4\text{NO}_4$: C, 48.10; H, 2.14; N, 1.75; found: C, 48.34; H, 1.86; N, 1.76.

3,6-Bis[2-(5-*tert*-butyl-7-fluorobenzofuroyl)]-*N*-ethyl-9*H*-carbazole (5i). Yellow solid. IR (KBr) ν/cm^{-1} : 3065, 2972, 2881, 1641, 1592, 1435, 1192, 1024, 815, 778; ^1H NMR (600 MHz, CDCl_3): δ 1.40 (s, 18H, *t*-butyl), 1.56 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.51 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.27-7.31 (m, 2H, ArH), 7.51 (s, 2H, furan-H), 7.58 (d, $J = 8.4$ Hz, 2H, ArH), 7.62 (d, $J = 2.4$ Hz, 2H, ArH), 8.36 (dd, $J = 8.4, 1.2$ Hz, 2H, ArH), 9.00 (s, 2H, ArH); ^{13}C NMR (150 MHz, CDCl_3): δ 13.91, 31.56, 35.04, 38.31, 109.10, 112.12, 112.23, 114.48, 115.71, 123.02, 123.73, 128.62, 129.07, 130.02, 141.22, 141.30, 143.58, 146.86, 148.52, 148.75, 153.99, 182.98; HRMS–ESI: (m/z) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{40}\text{H}_{35}\text{F}_2\text{NNaO}_4$: 654.2426; found: 654.2424.

3,6-Bis[2-(5-*tert*-butyl-7-chlorobenzofuroyl)]-*N*-ethyl-9*H*-carbazole (5j). Yellow solid. IR (KBr) ν/cm^{-1} : 3058, 2964, 2870, 1640, 1589, 1430, 1062, 1022, 815, 777; ^1H NMR (600 MHz, CDCl_3): δ 1.32 (s, 18H, *t*-butyl), 1.46 (t, $J = 7.2$ Hz, 3H, CH_3CH_2), 4.40 (q, $J = 7.2$ Hz, 2H, CH_3CH_2), 7.46 (d, $J = 1.8$ Hz, 2H, benzofuran-H), 7.49 (d, $J = 8.4$ Hz, 2H, carbazole-H), 7.55 (s, 2H, furan-H), 7.57 (d, $J = 1.8$ Hz, 2H, benzofuran-H), 8.29 (dd, $J = 8.4, 1.2$ Hz, 2H, carbazole-H), 8.96 (d, $J = 0.6$ Hz, 2H, carbazole-H); ^{13}C NMR (150 MHz, CDCl_3): δ 13.93, 31.58, 35.01, 38.27, 109.14, 115.83, 116.94, 117.76, 122.96, 123.79, 126.15, 128.64, 128.61, 128.96, 143.52, 148.52, 149.88, 153.79, 182.71; HRMS–ESI: (m/z) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{40}\text{H}_{35}^{35}\text{Cl}_2\text{NNaO}_4$: 686.1835; found: 686.1835.

3,6-Bis[2-(5-*tert*-butyl-7-bromobenzofuroyl)]-*N*-ethyl-9*H*-carbazole (5k). Yellow solid. IR (KBr) ν/cm^{-1} : 3070, 2963, 2869, 1640, 1587, 1431, 1022, 815, 780, 658; ^1H

S10

NMR (600 MHz, CDCl₃): δ 1.41 (s, 18H, *t*-butyl), 1.56 (t, J = 7.2 Hz, 3H, CH₃CH₂), 4.52 (q, J = 7.2 Hz, 2H, CH₃CH₂), 7.60 (d, J = 9.0 Hz, 2H, carbazole-H), 7.68 (s, 2H, furan-H), 7.71 (s, 2H, benzofuran-H), 7.73 (s, 2H, benzofuran-H), 8.42 (dd, J = 8.4, 1.2 Hz, 2H, carbazole-H), 9.13 (d, J = 1.2 Hz, 2H, carbazole-H); ¹³C NMR (150 MHz, CDCl₃): δ 13.97, 31.62, 35.01, 38.31, 104.34, 109.18, 115.91, 118.45, 123.06, 123.95, 127.89, 128.68, 129.00, 129.07, 143.58, 148.88, 151.31, 153.83, 182.64; HRMS–ESI: (m/z) [M + Na]⁺ calcd for C₄₀H₃₅⁷⁹Br₂NNaO₄: 774.0825; found: 774.0814.

3,6-Bis(2-naphtho[2,1-*b*]furoyl)-*N*-ethyl-9*H*-carbazole (5I). Brown solid. IR (KBr) ν/cm^{-1} : 3071, 2972, 2931, 1642, 1590, 1436, 1232, 1065, 808, 765; ¹H NMR (600 MHz, CDCl₃): δ 1.57 (t, J = 7.2 Hz, 3H, CH₃CH₂), 4.50 (q, J = 7.2 Hz, 2H, CH₃CH₂), 7.55 (t, J = 7.8 Hz, 2H, ArH), 7.59 (d, J = 8.4 Hz, 2H, ArH), 7.63 (t, J = 7.8 Hz, 2H, ArH), 7.77 (d, J = 9.0 Hz, 2H, ArH), 7.89 (d, J = 9.0 Hz, 2H, ArH), 7.97 (d, J = 8.4 Hz, 2H, ArH), 8.10 (s, 2H, furan-H), 8.21 (d, J = 7.8 Hz, 2H, ArH), 8.38 (dd, J = 8.4, 1.2 Hz, 2H, ArH), 9.04 (s, 2H, ArH); ¹³C NMR (150 MHz, CDCl₃): δ 13.91, 38.25, 108.97, 112.86, 114.87, 122.98, 123.05, 123.47, 123.53, 125.46, 127.33, 128.18, 128.54, 129.04, 129.52, 129.68, 130.54, 143.40, 152.59, 154.34, 183.08 ppm; Anal. calcd for C₄₀H₂₅NO₄: C, 82.32; H, 4.32; N, 2.40; found: C, 82.68; H, 4.25; N, 2.57.

[illegible]

Figure S2: HRMS spectrum of **3a**.

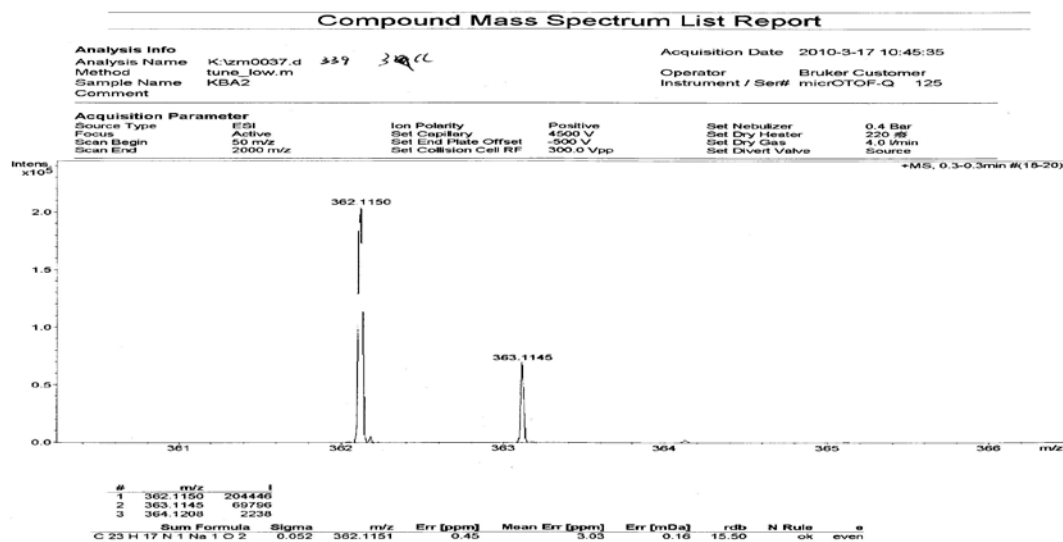


Figure S2: HRMS spectrum of **3a**.

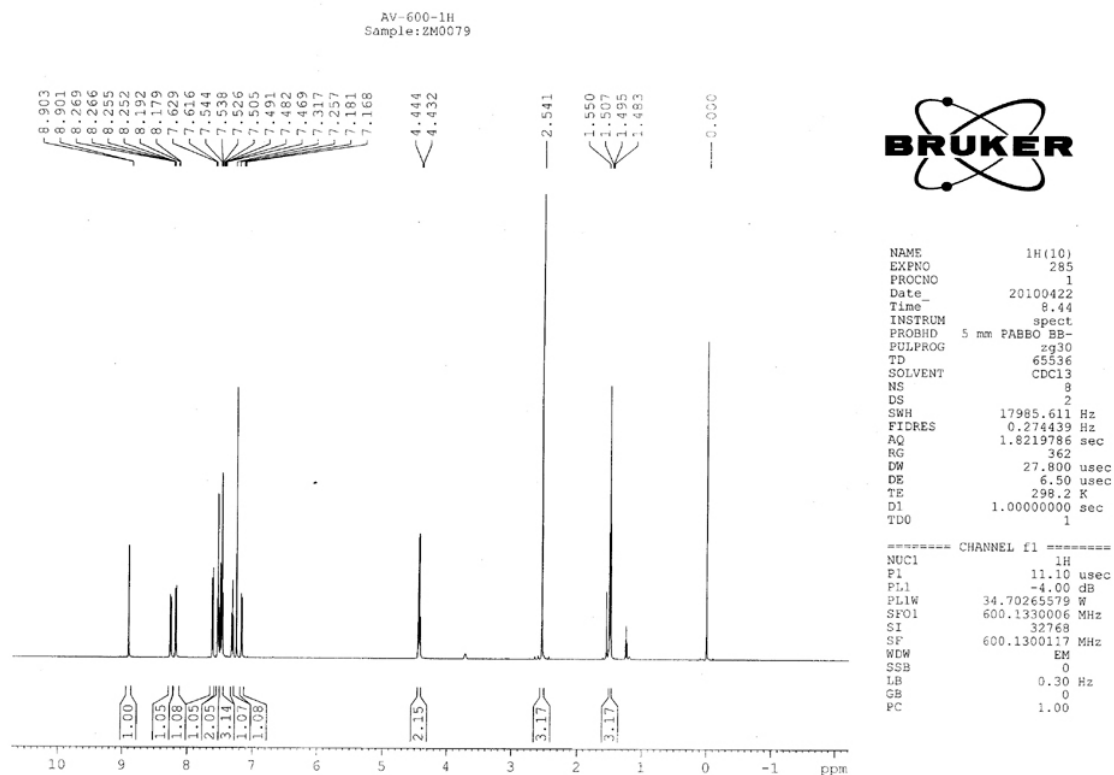


Figure S3: ^1H NMR spectrum of **3b**.

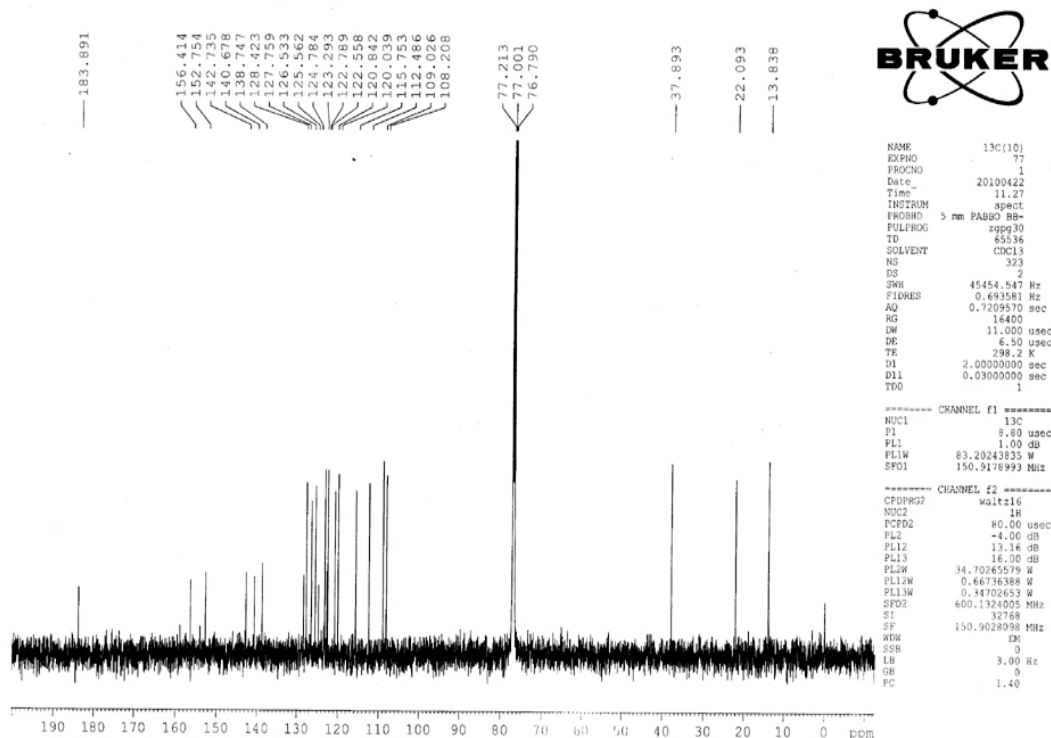


Figure S4: ^{13}C NMR spectrum of **3b**.

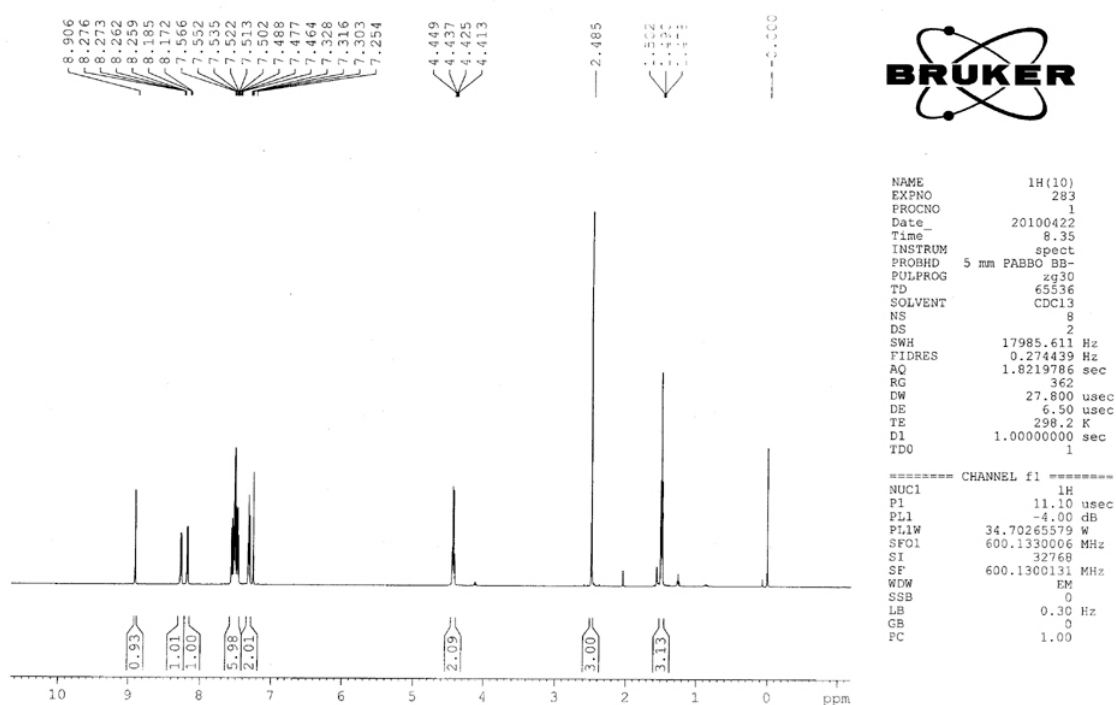


Figure S5: ^1H NMR spectrum of **3c**.

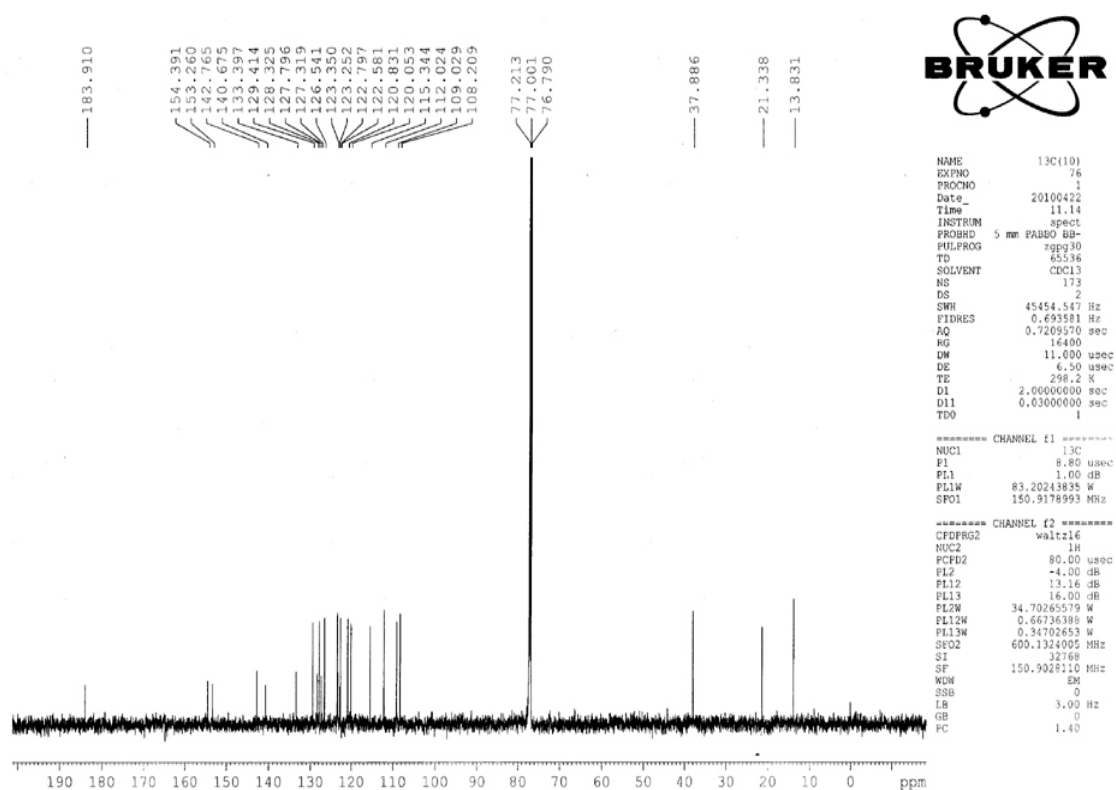


Figure S6: ^{13}C NMR spectrum of **3c**.

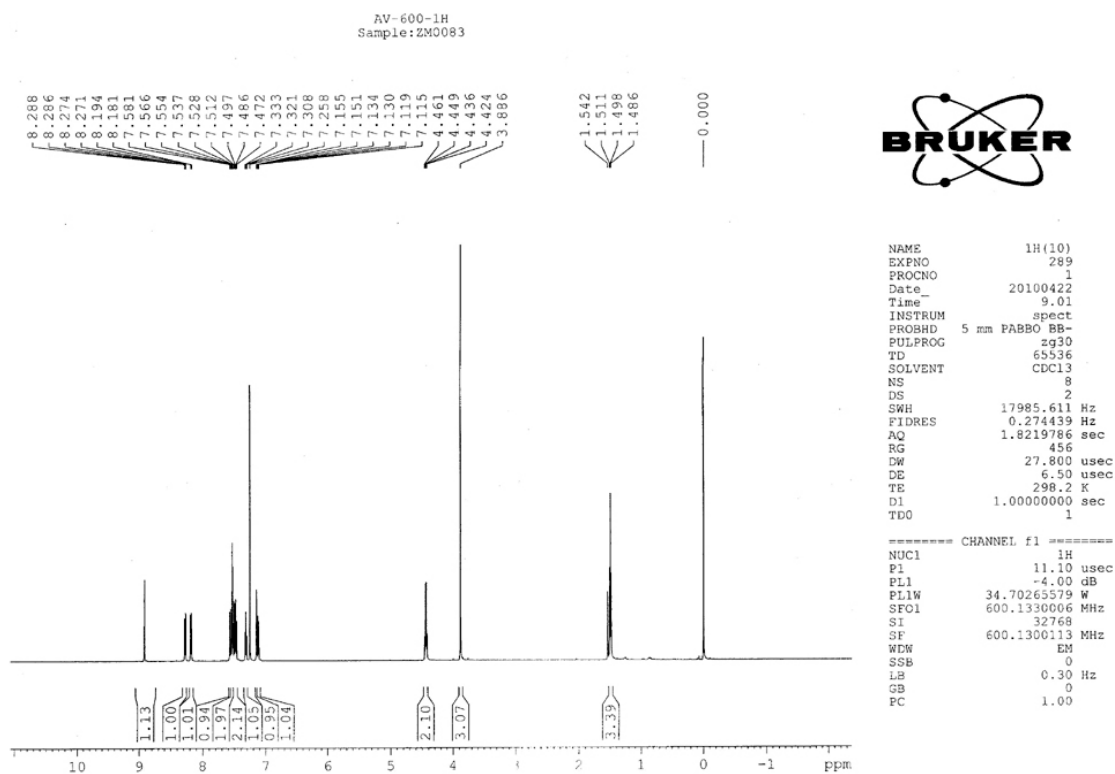


Figure S9: ^1H NMR spectrum of **3e**.

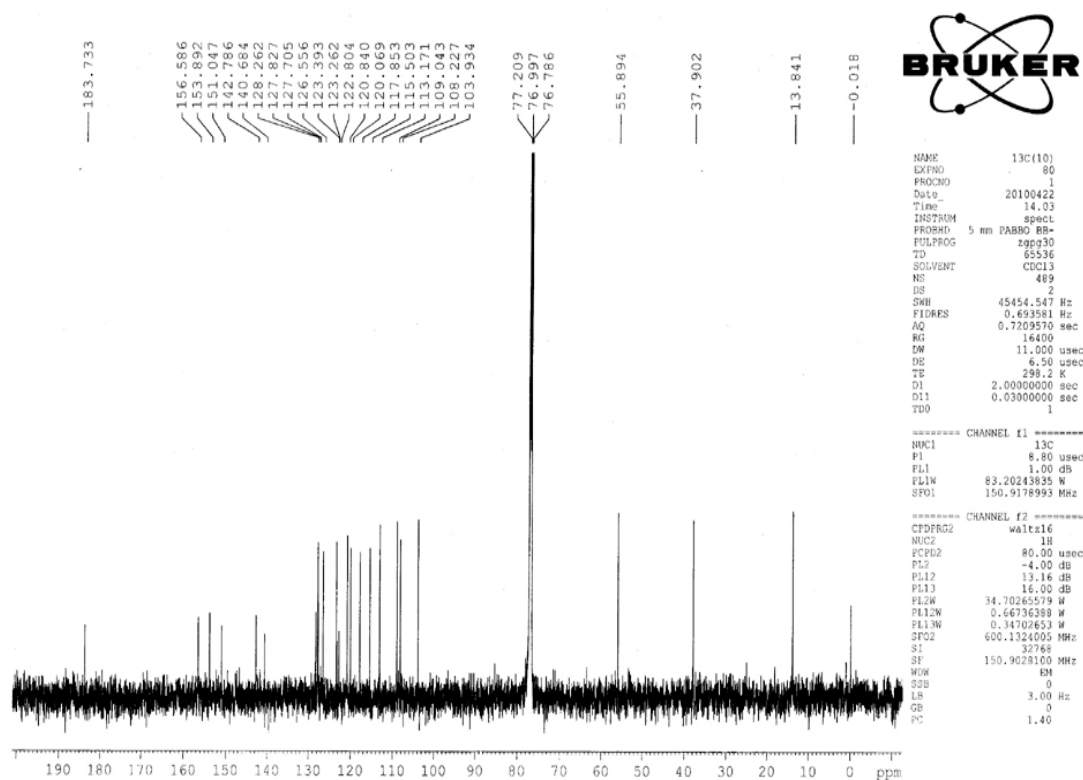


Figure S10: ^{13}C NMR spectrum of **3e**.

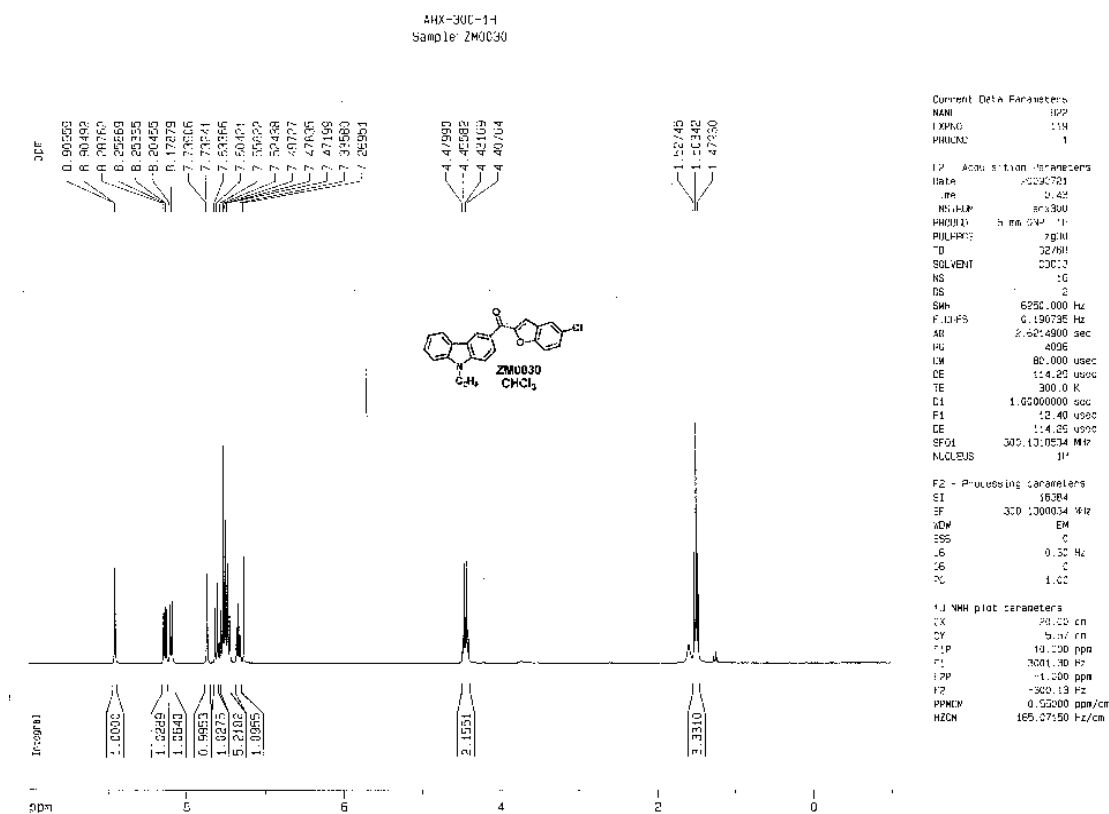


Figure S11: ¹H NMR spectrum of 3f.

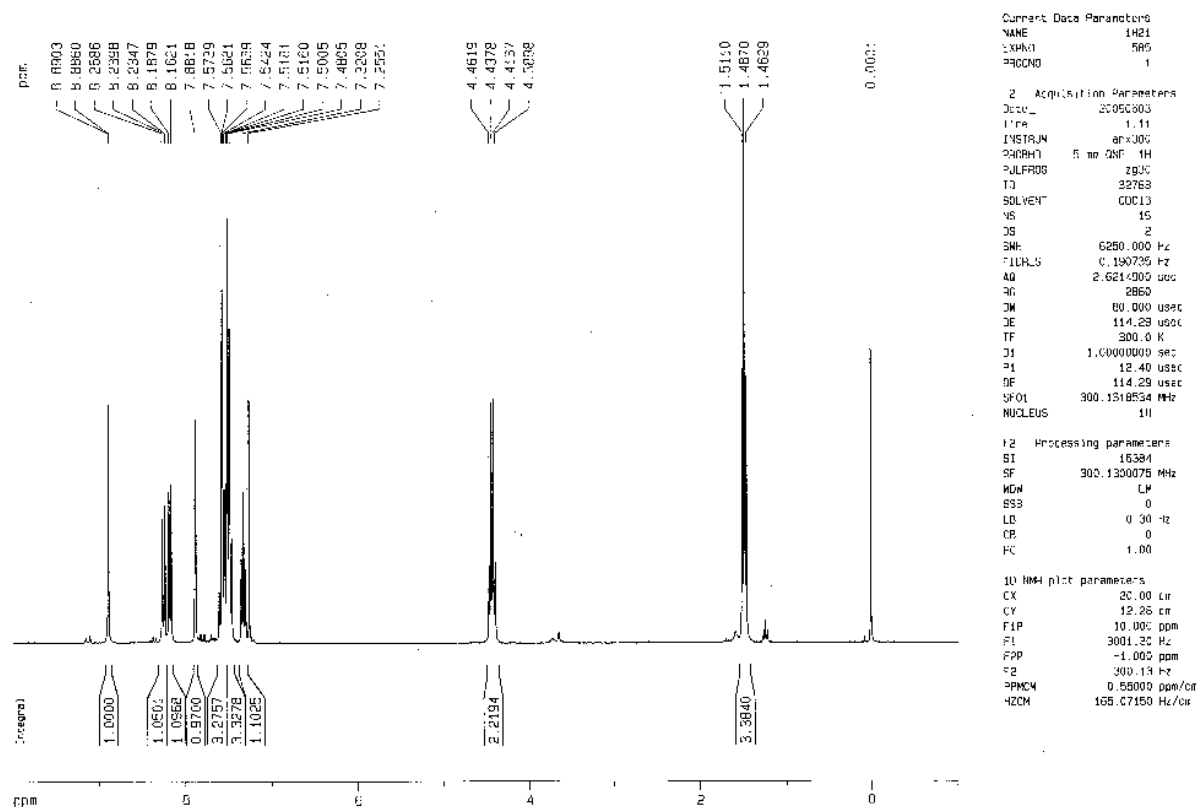


Figure S12: ¹H NMR spectrum of 3g.

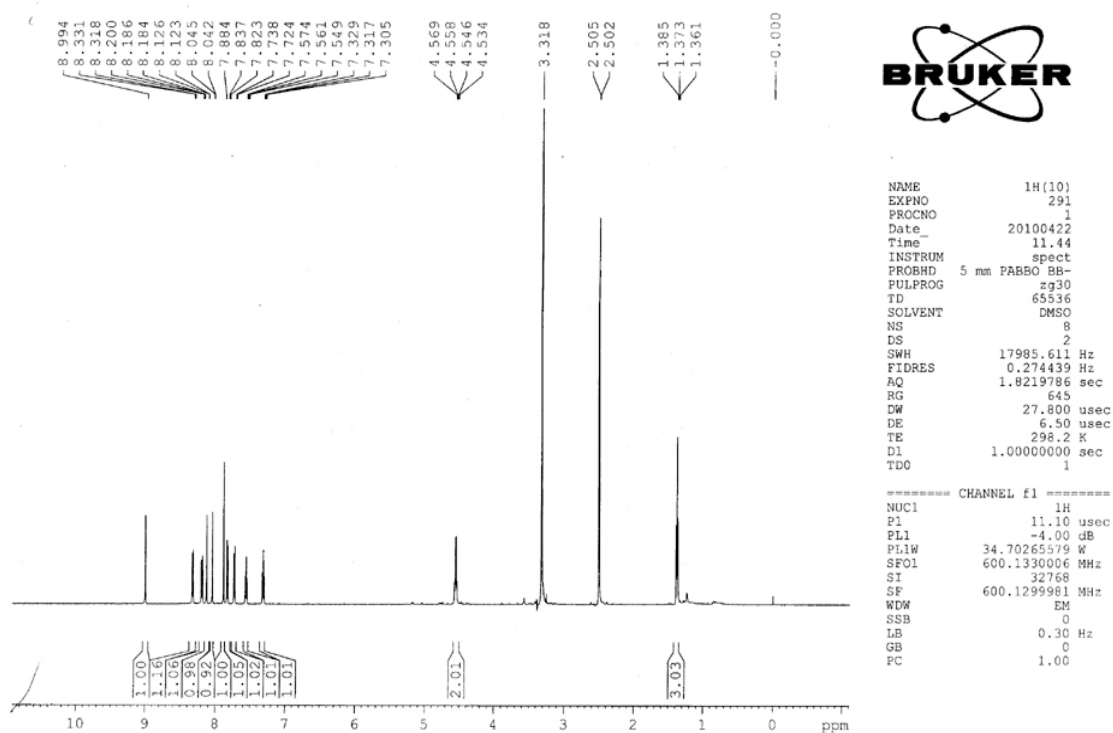


Figure S13: ^1H NMR spectrum of 3h.

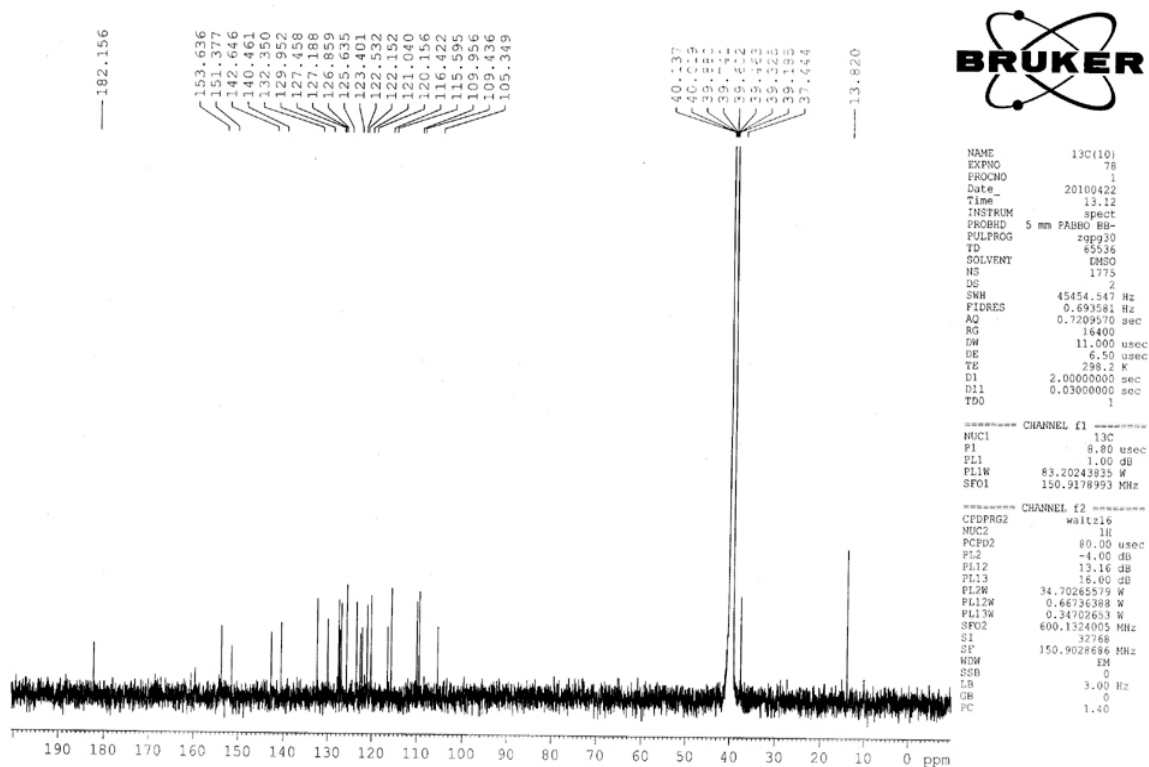


Figure S14: ^{13}C NMR spectrum of 3h.

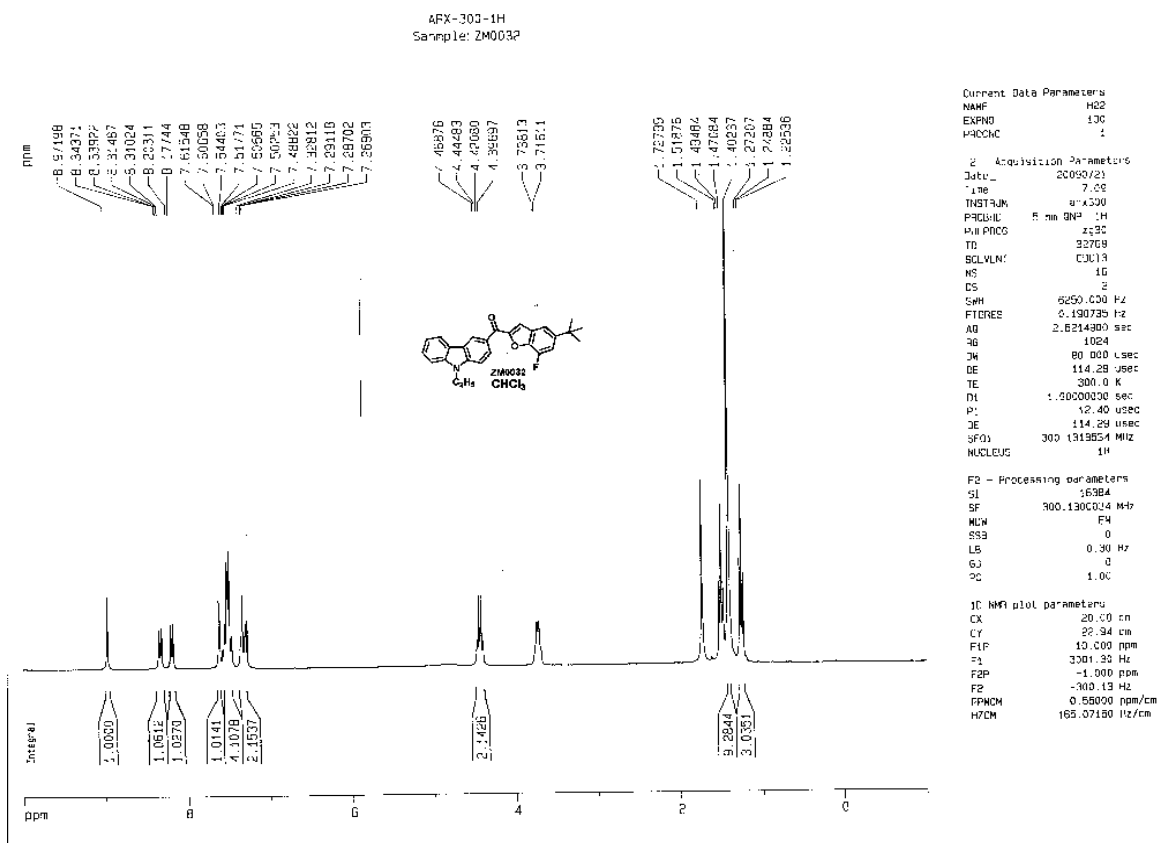


Figure S15: ¹H NMR spectrum of 3i.

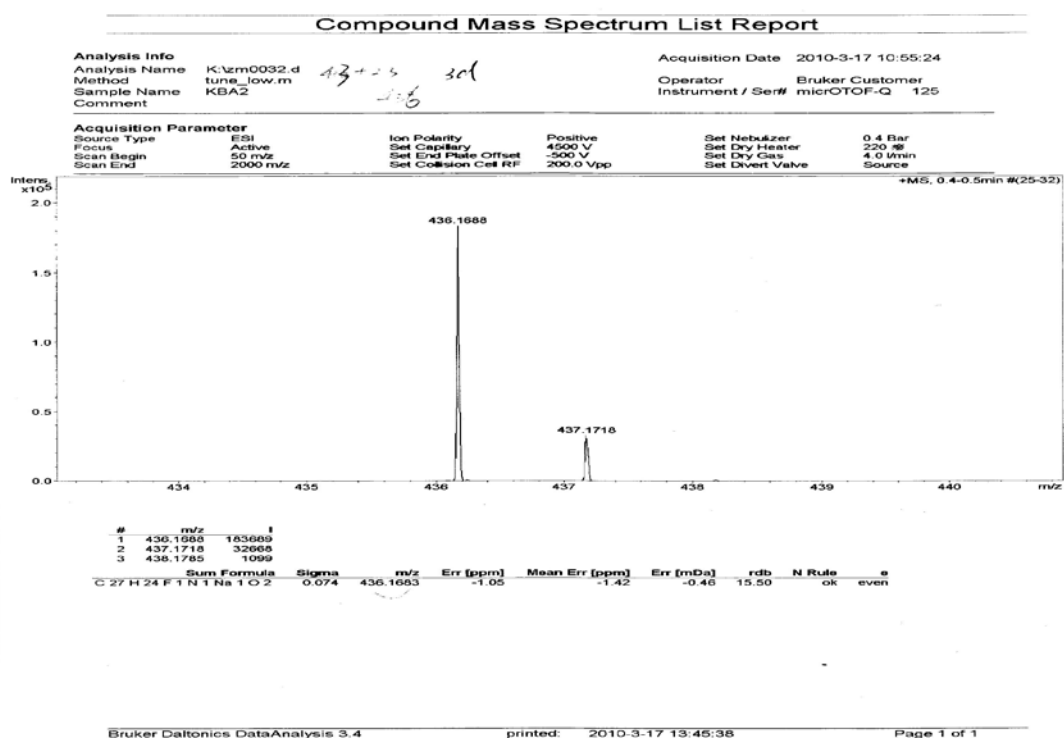


Figure S16: HRMS spectrum of 3i.

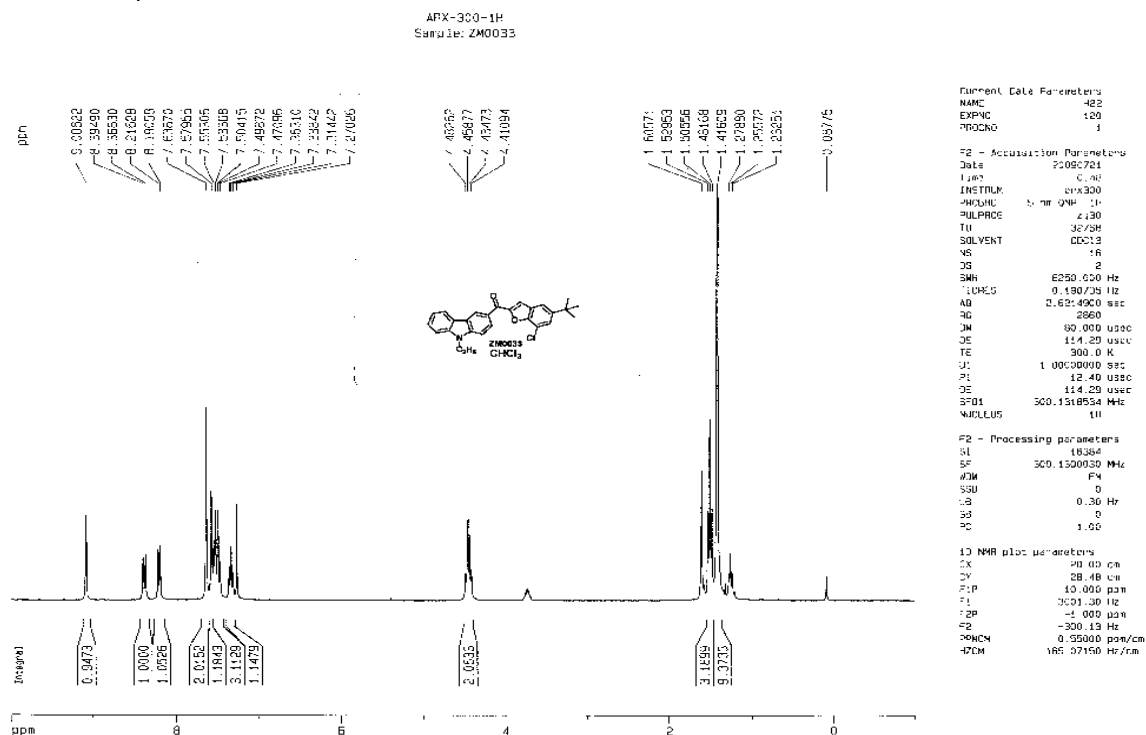


Figure S17: ^1H NMR spectrum of 3j.

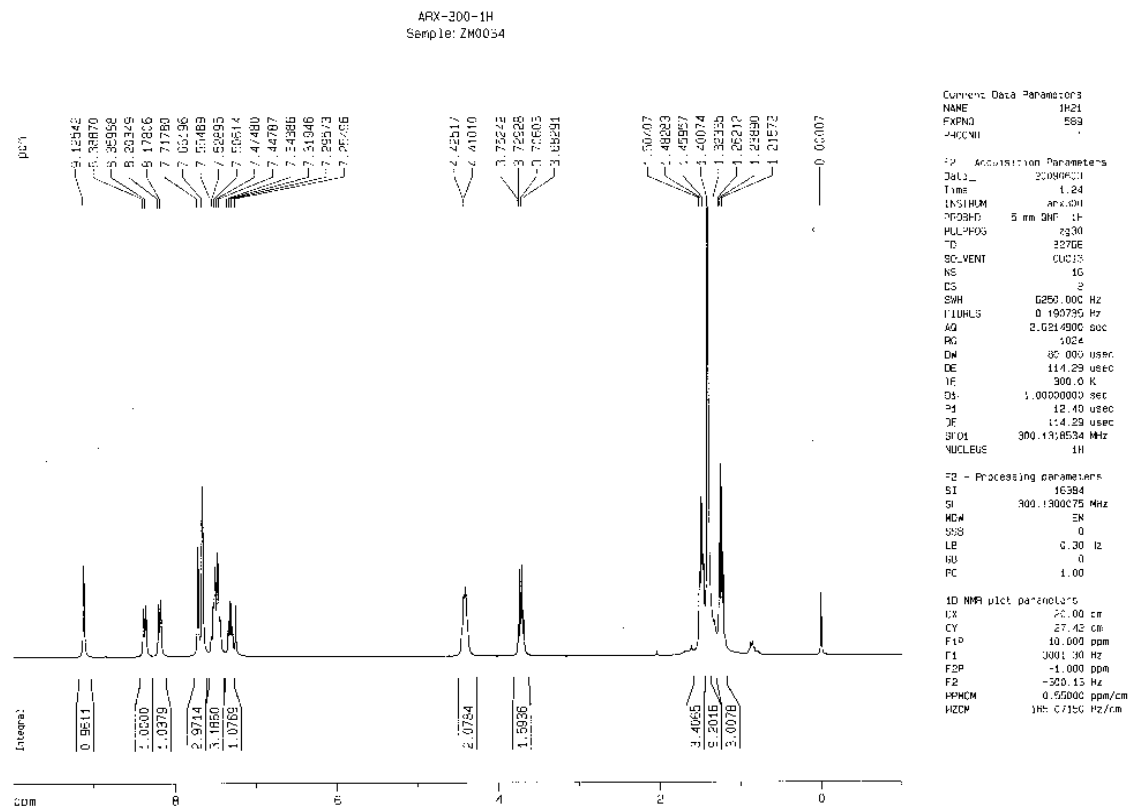


Figure S18: ^1H NMR spectrum of 3k.

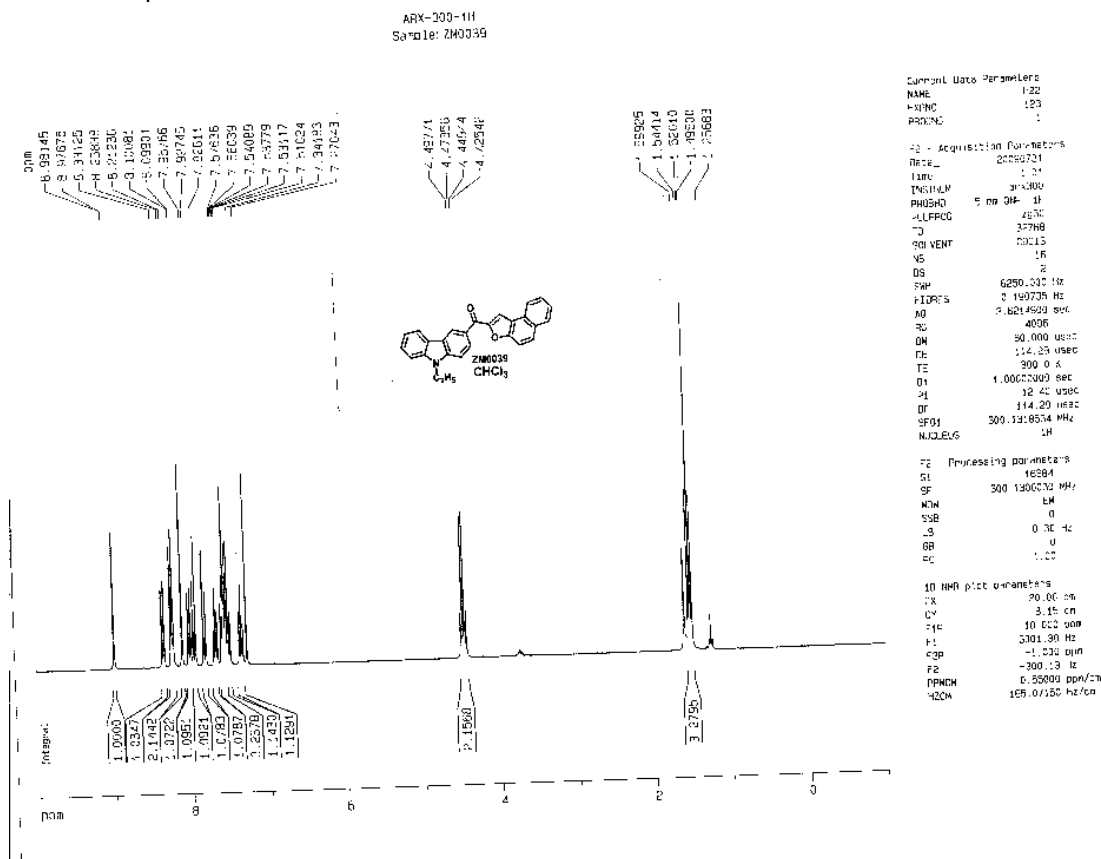


Figure S19: ^1H NMR spectrum of 31.

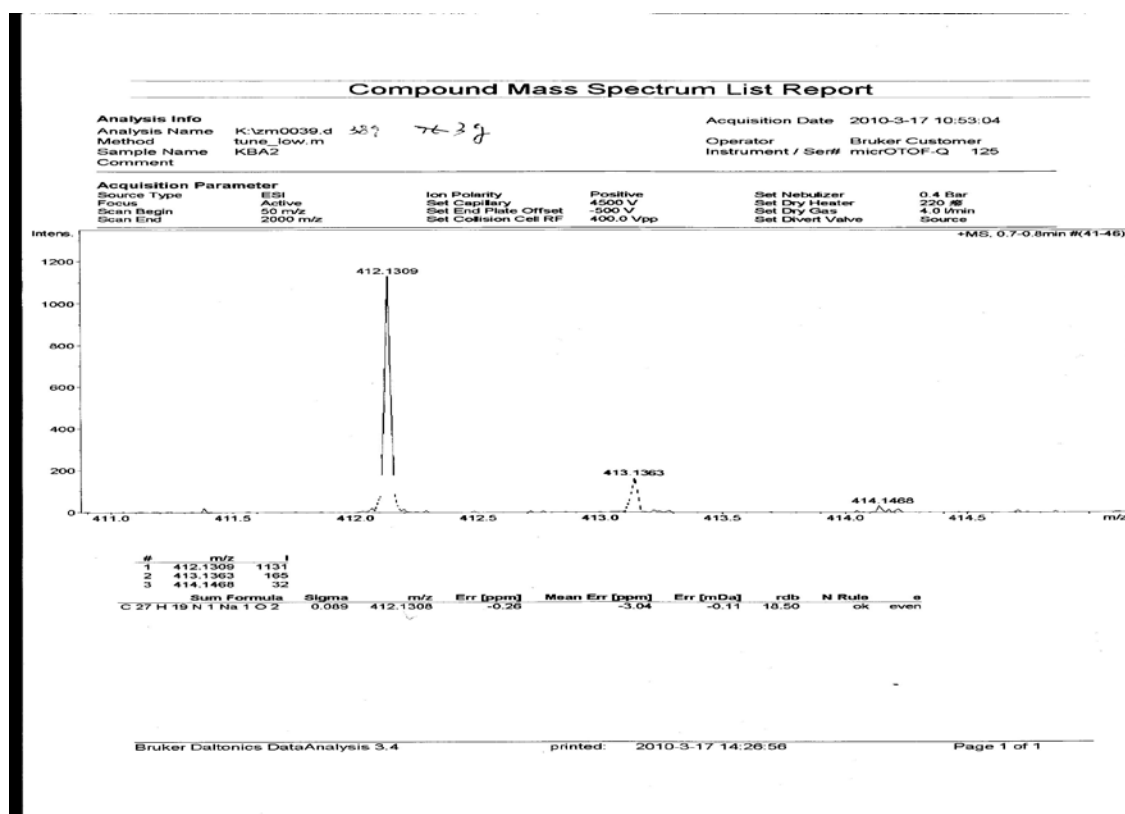


Figure S20: HRMS spectrum of 31.

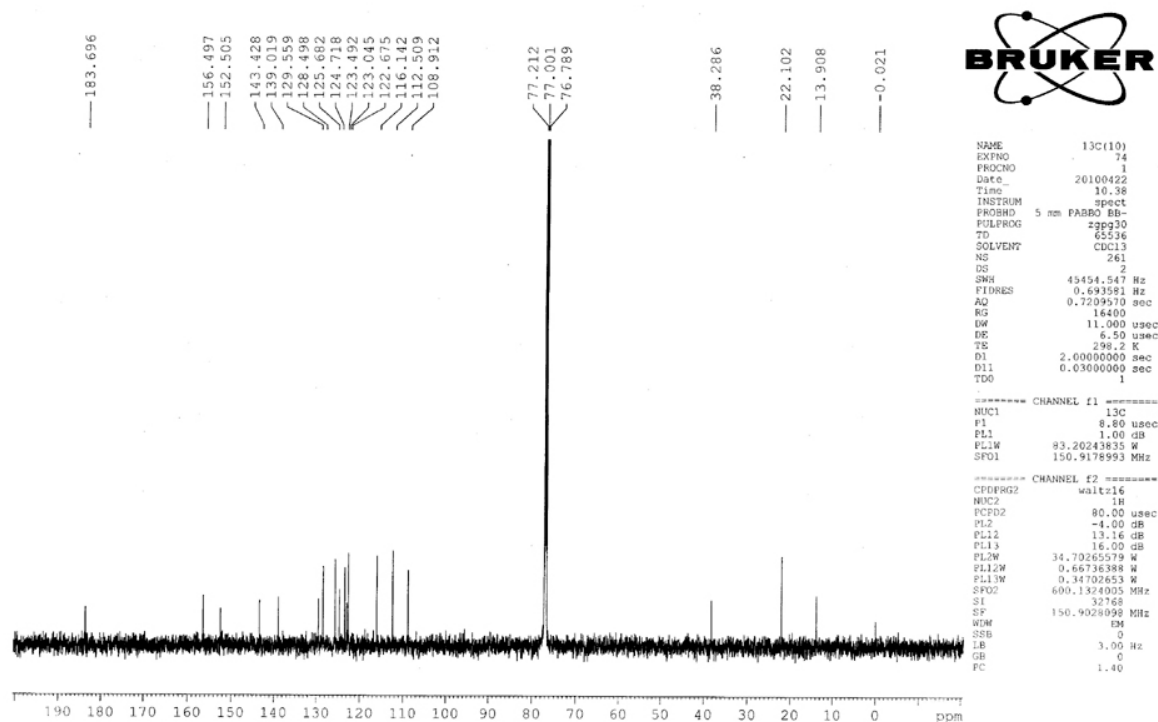


Figure S23: ^{13}C NMR spectrum of 5b.

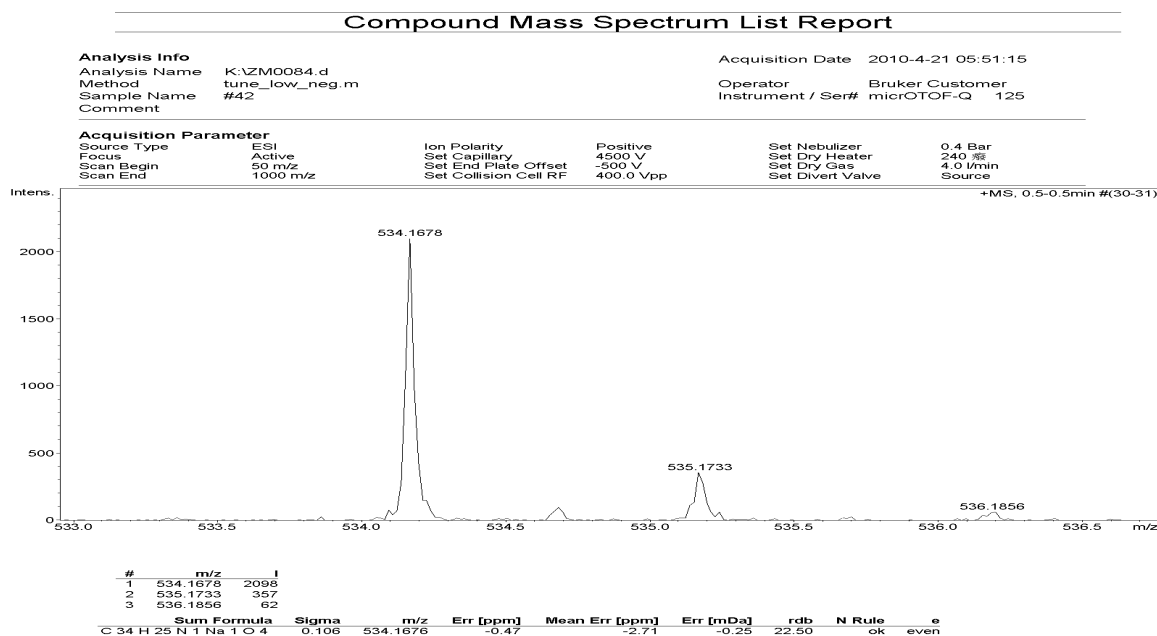


Figure S24: HRMS spectrum of 5b.

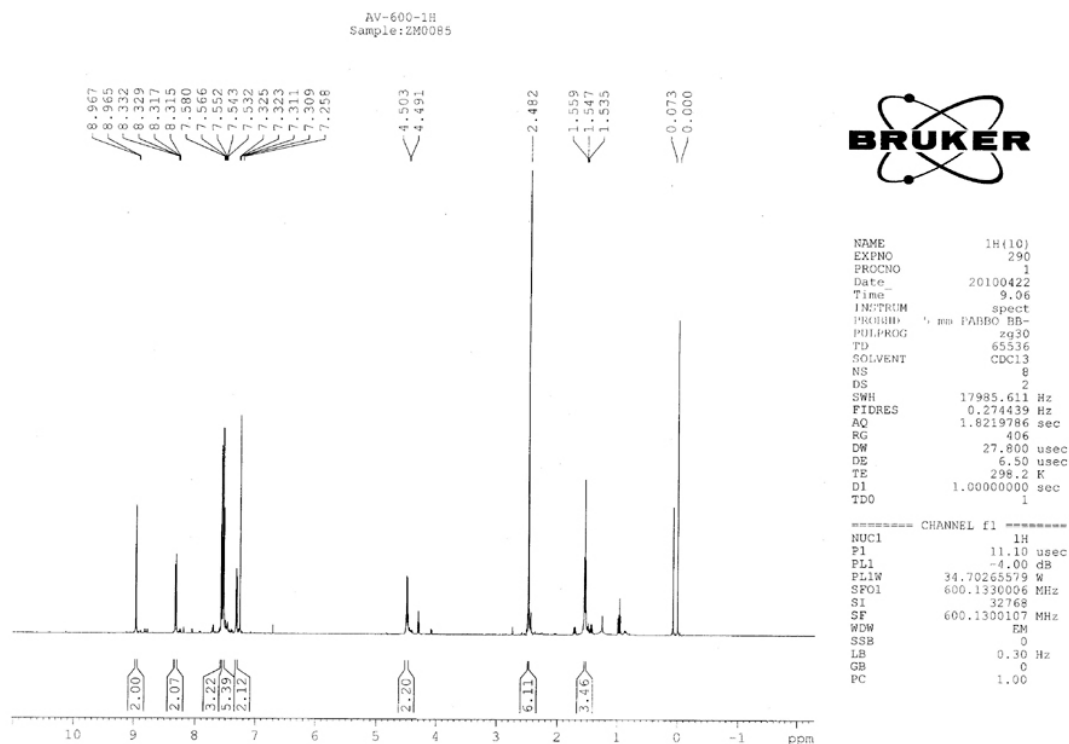


Figure S25: ^1H NMR spectrum of 5c.

AV-600-13C
Sample: ZM0085

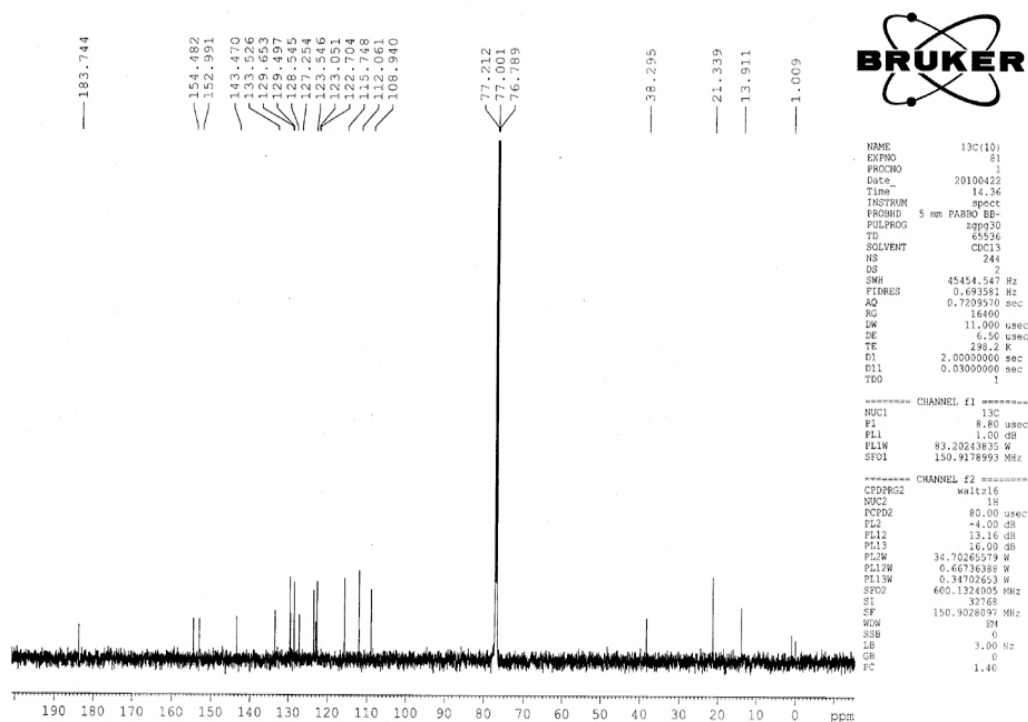


Figure S26: ^{13}C NMR spectrum of 5c.

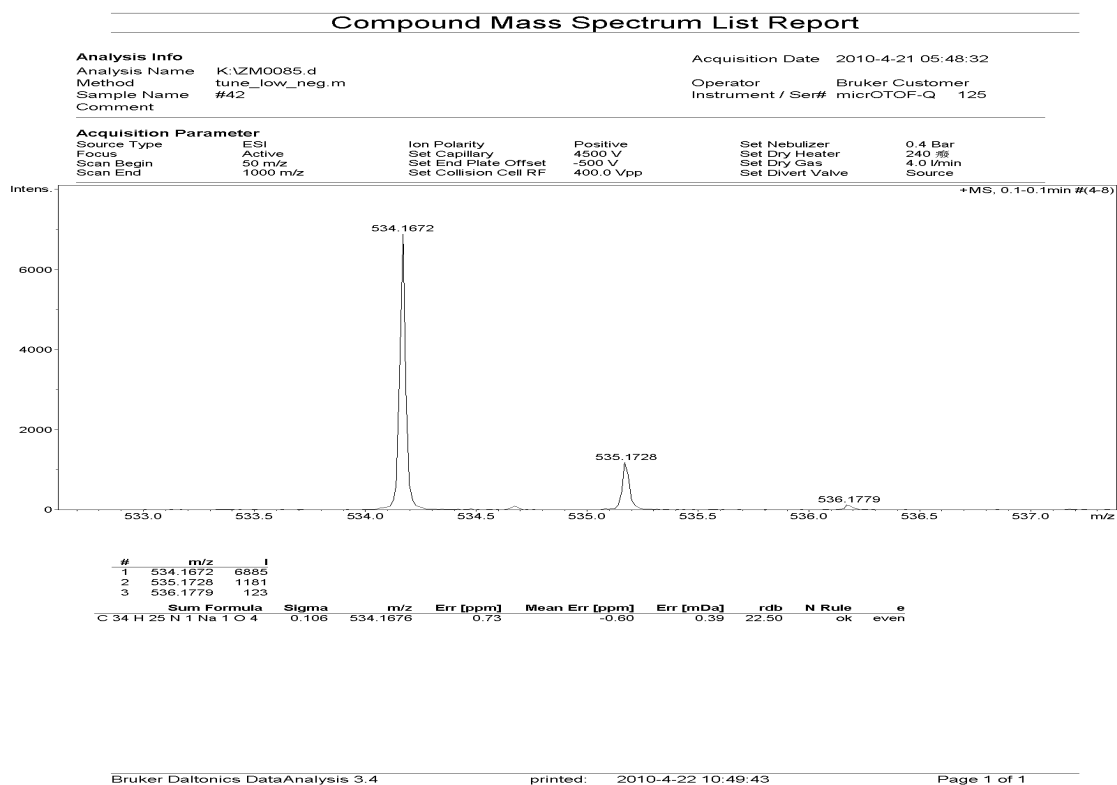


Figure S27: HRMS spectrum of 5c.

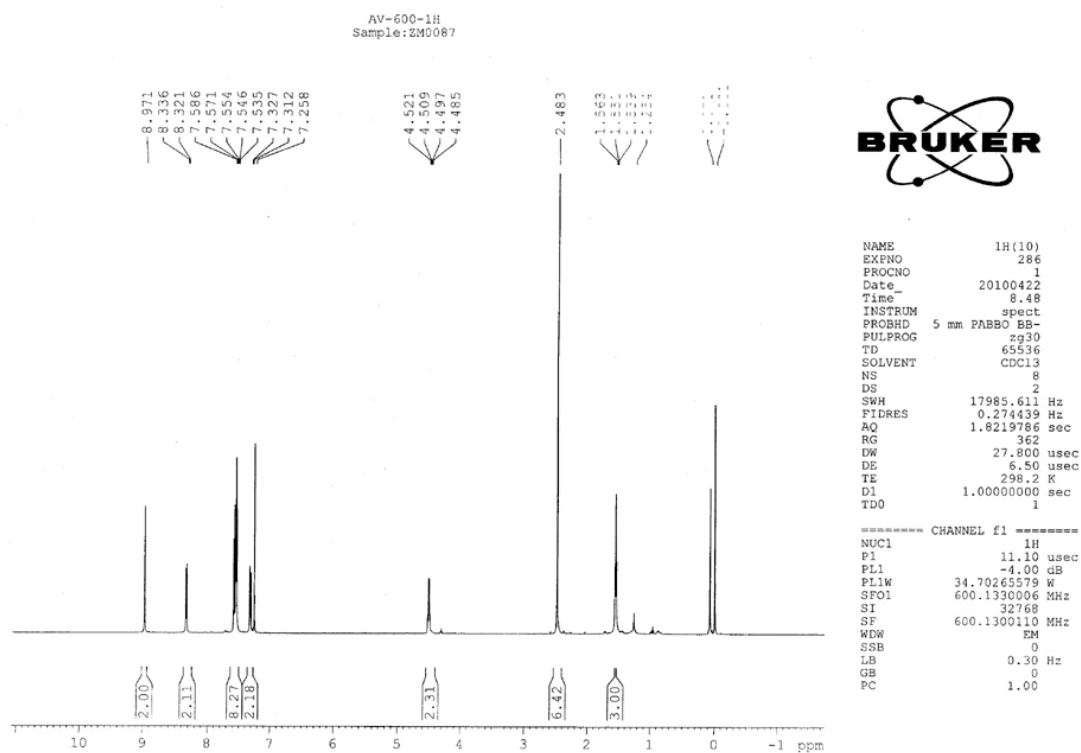


Figure S28: ¹H NMR spectrum of 5d.

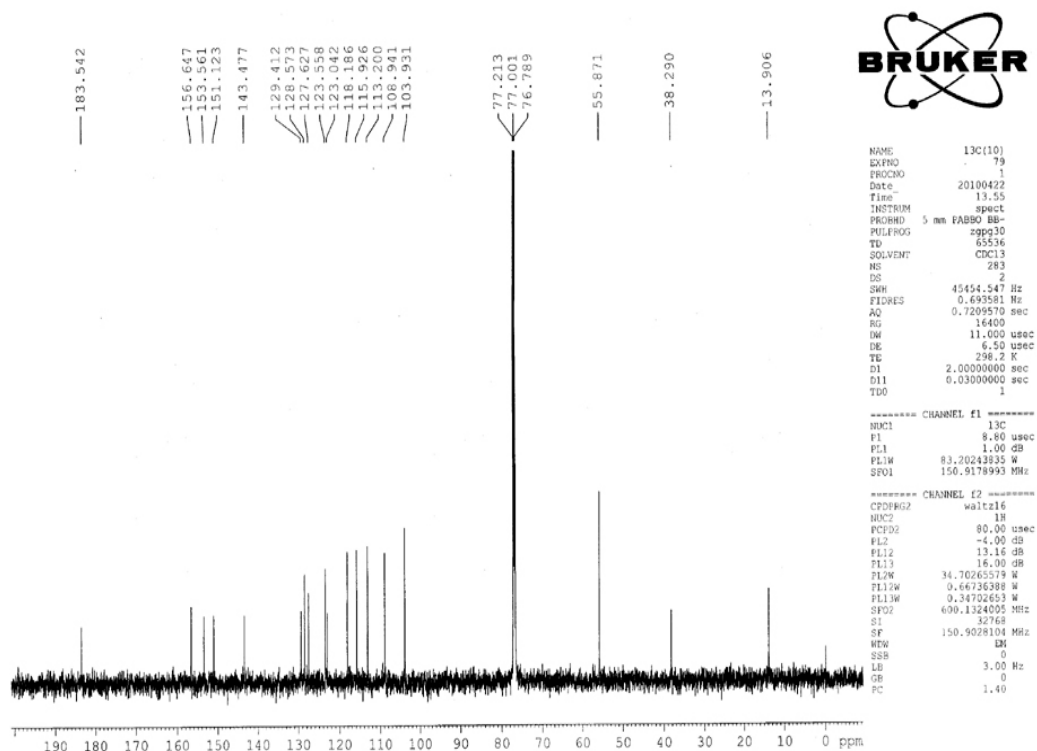


Figure S31: ^{13}C NMR spectrum of 5e.

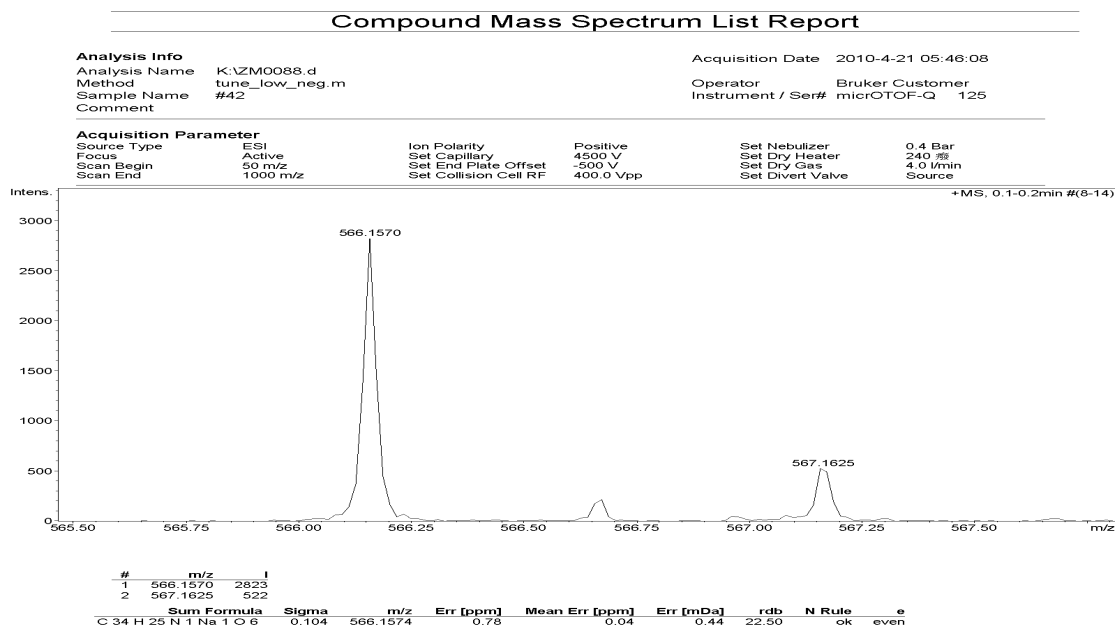


Figure S32: HRMS spectrum of 5e.

8.953
8.935
8.933
8.921
8.919
7.908
7.905
7.612
7.609
7.602
7.598
7.595
7.588
7.577
7.562
7.270

4.576
4.518
4.506
4.432

— 3.716

1.572
1.560
1.549

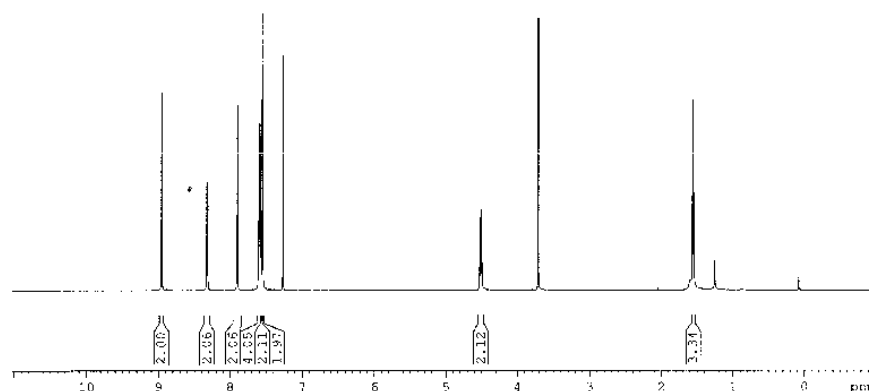


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EQUINO        663
PRECED        1
DATE          2009.07.31
TIME          20.79
INSTNUM       000001
PRECED        0  MUL PASS=0 BE-
CULTRNG       24300
TC            63584
SCIENTIST     CM13
NO            0
DS            2
SWH           17985.611 KHz
FREQS         0.274439 Hz
AQ            1.327978e sec
RG            10%
DC            27.400 40000
DC            6.50 40000
TF            231.3 K
BI            1.0 20000000 sec.
TFO           1

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P1	-4.00 00
P1+K	34.70265578 W
SPC1	600.1324005 MHz
SI	12.54
ST	600.1300000 MHz
WCM	FX
SRP	0
LR	0.30 Hz
GD	0
PC	1.00



AV-600-1H
Sample: ZM0043

Year	Population (millions)
1960	3.5
1965	3.825
1970	4.15
1975	4.475
1980	4.8
1985	5.125
1990	8.974

4.522
4.510
4.498
4.486

1.565
1.553
1.541

34

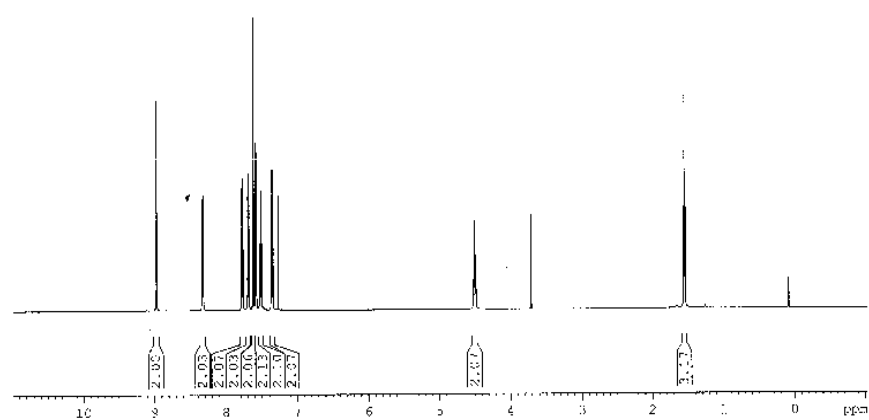


NAME	1411291
EXPNO	666
PROCNO	1
Date_	20031230
TIME	19:22
INSTNAM	SPARK
F2PROC	0 mm SPARK-M
FILENAM	sp30
TD	65336
SOLVENT	CDCl3
NS	4
DS	2
SWH	17665.811 Hz
FIDRES	0.274139 Hz
AS	1.8219486 mm
RG	256
DW	27.330 sec
TE	4.30 K
TD	230.9 K
DC	1.0009230 sec
TD0	1

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----- CHANNEL 01 -----
NUC1      1R
ZL        11.10  GSC
BT1        -4.00  G3
PI1W      34.7026553  G
SF01      600.1374000  K47
J1         17.68
JF        600.1374000  K42
WTFW      2R
SSB        0
LB         0 30  K7
GB         0
PC         1.00

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S29

AV-600-111
Sample: ZM0345

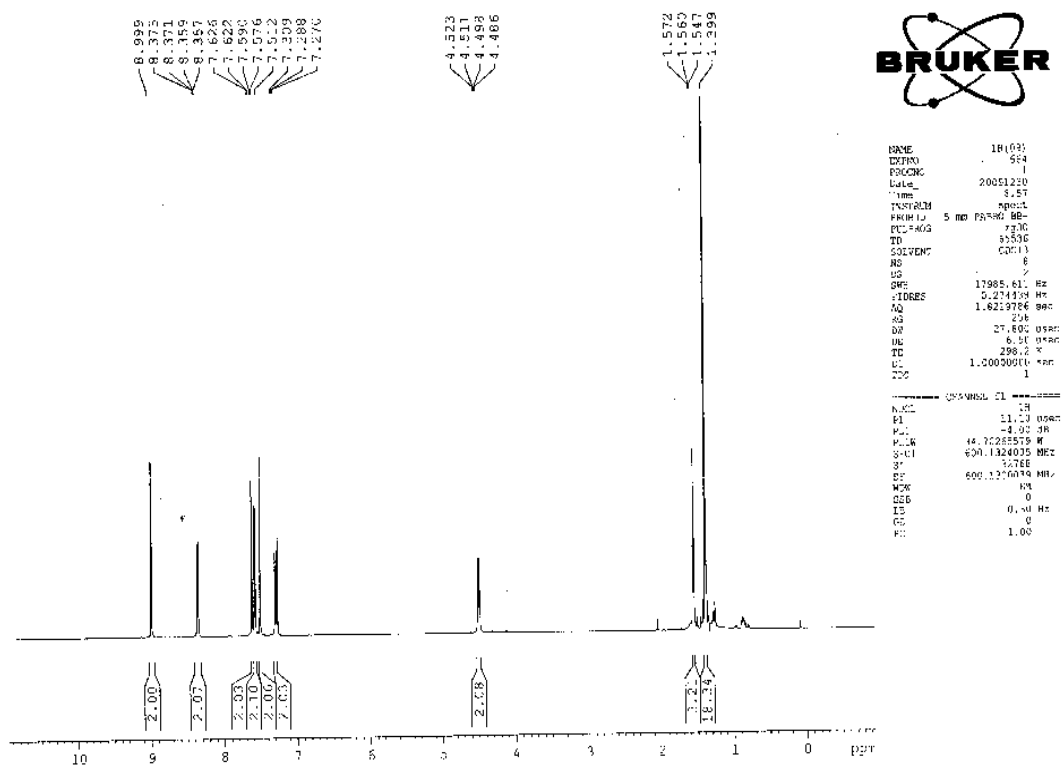


Figure S37: ^1H NMR spectrum of 5i.

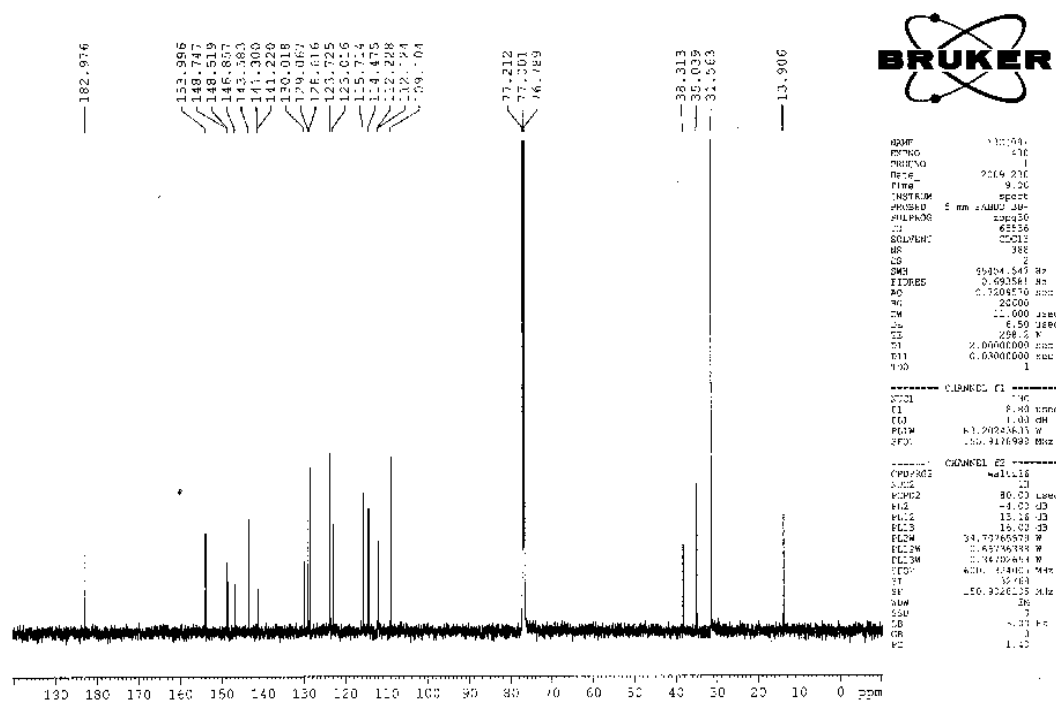


Figure S38: ^{13}C NMR spectrum of 5i.

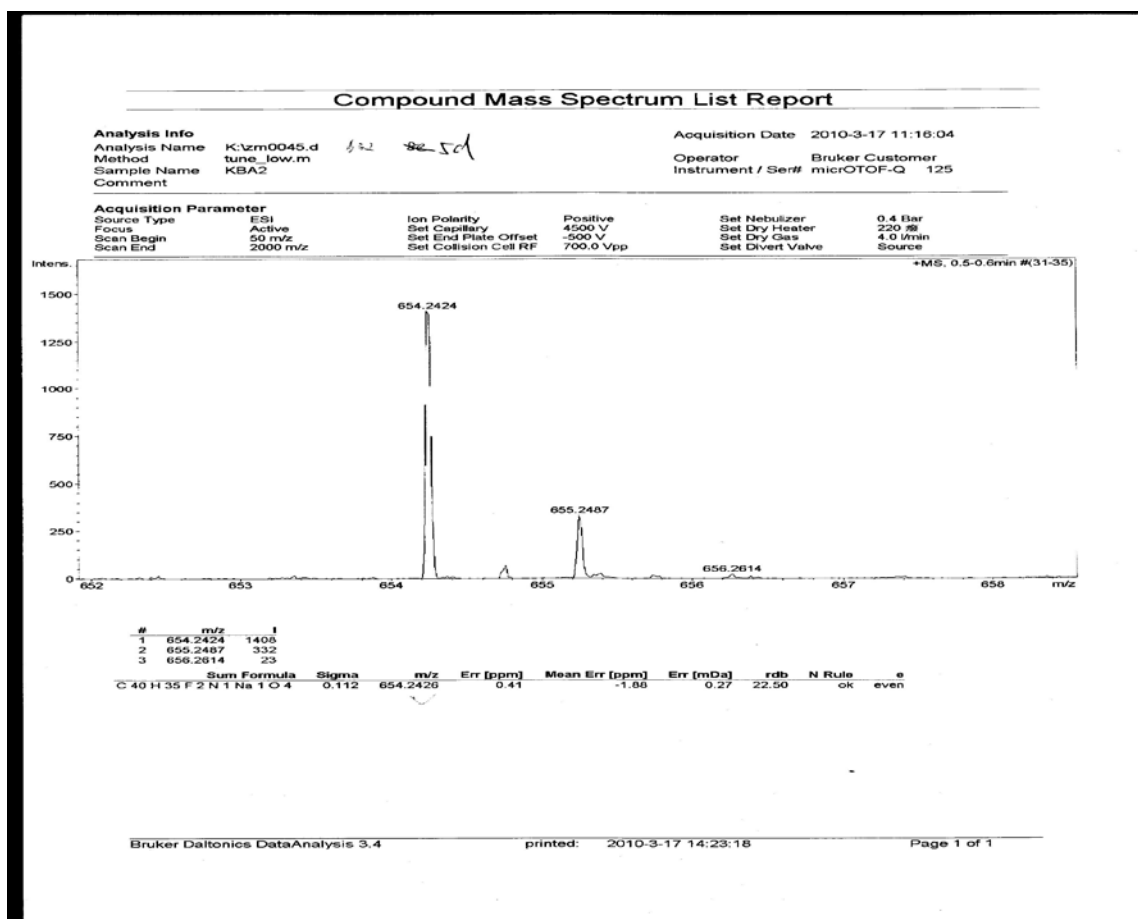


Figure S39: HRMS spectrum of 5i.

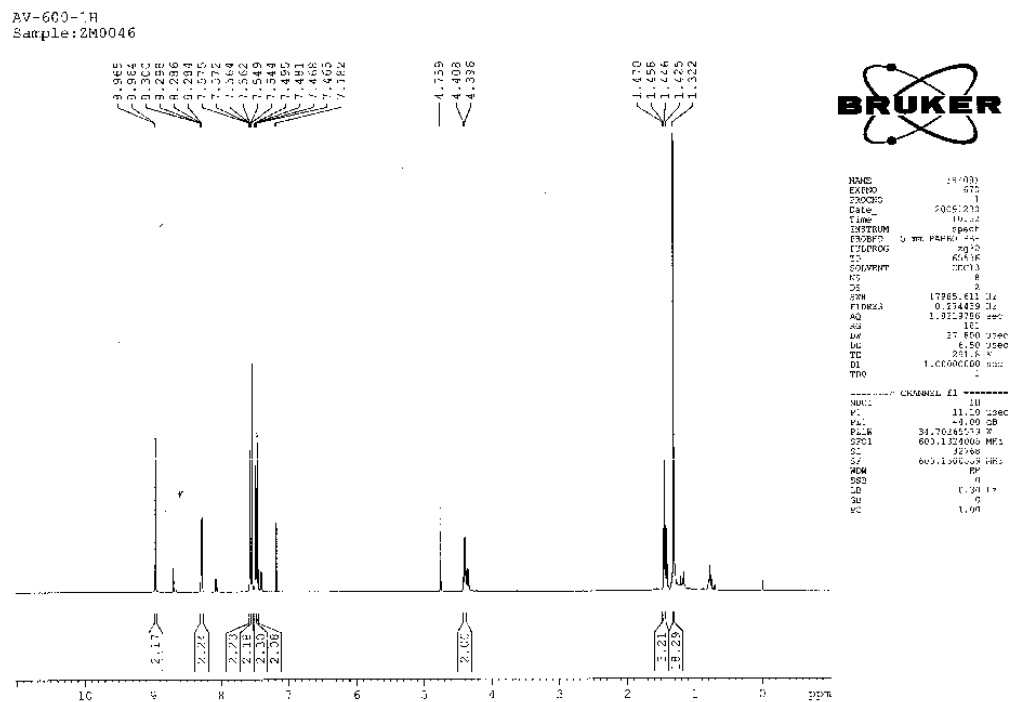
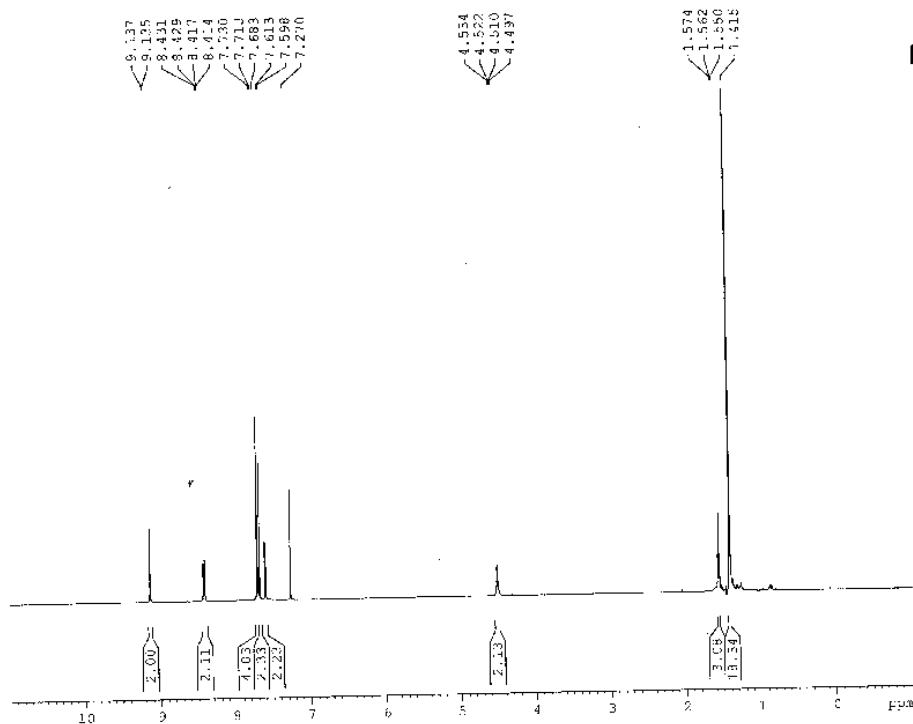


Figure S40: ¹H NMR spectrum of 5j.

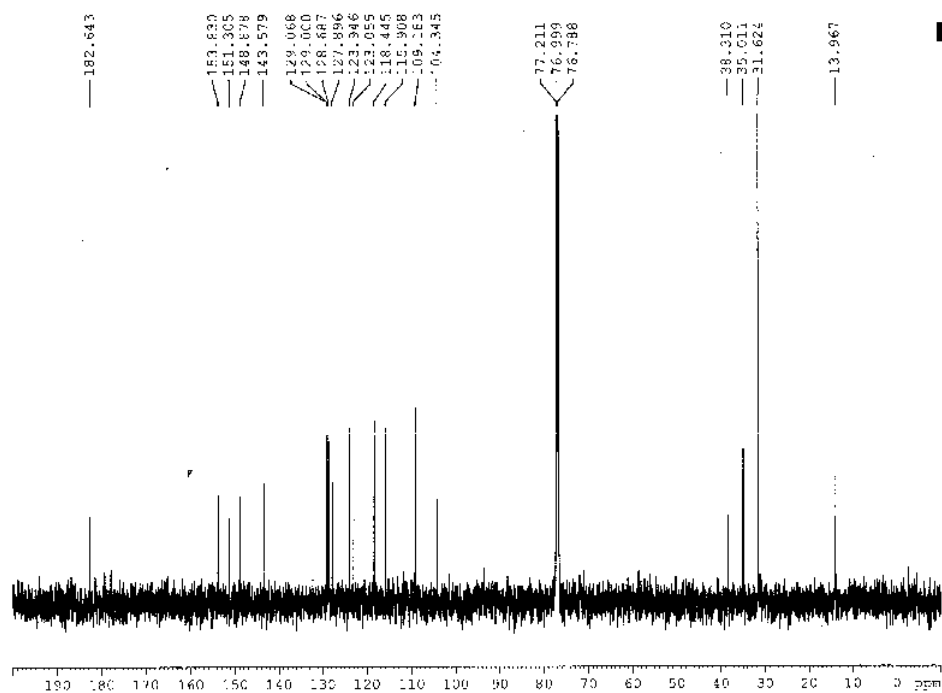
AV-600-1H
Sample: ZM0041



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EXPNO: 671
PROCNO: 1
Date_: 20091230
Time: 17.05
INSTRUM: spect
PROBHD: 5 mm PABBO BBO-
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO-d6
NS: 4
DS: 2
SWH: 17463.311 Hz
FIDRES: 0.2744339 Hz
AQ: 1.8215766 sec
RG: 327
DQ: 192
RFX: 27.890 MHz
DE: 6.50 MHz
TE: 281.8 K
D1: 1.0000000 sec
TD0: 1

----- CHANNEL f1 -----
NUC1: 1H
P1: 11.10 usec
PL1: -4.50 dB
PL12: 34.7026513 MHz
SFO1: 500.132000 MHz
WDW: EM
SSB: 0
GB: 0.30 Hz
PC: 1.10

Figure S43: ^1H NMR spectrum of 5k.



NAME: 13C001
EXPNO: 429
PROCNO: 1
Date_: 20091230
Time: 17.13
INSTRUM: spect
PROBHD: 5 mm PABBO BBO-
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO-d6
NS: 2
DS: 2
SWH: 25454.547 MHz
FIDRES: 0.6935081 Hz
AQ: 0.7203516 sec
RG: 3080
DQ: 11.005 MHz
DE: 6.50 MHz
TE: 281.7 K
D1: 2.0000000 sec
D11: 0.7000000 sec
TD0: 1

----- CHANNEL f1 -----
NUC1: 13C
P1: 8.30 usec
PL1: 1.20 dB
PL12: 63.2324535 MHz
SFO1: 125.7611893 MHz

----- CHANNEL f2 -----
CPDPRG2: waltz16
NUC2: 1H
P2P2G: 36.50 MHz
PL2: -4.50 dB
PL12: 12.16 dB
PL13: 16.30 dB
PL22: 34.7124535 MHz
P12P2: 0.6935081 MHz
P12P3: 0.3470265 MHz
SFO2: 500.132000 MHz
WDW: EM
SSB: 0
GB: 0.30 Hz
PC: 1.10

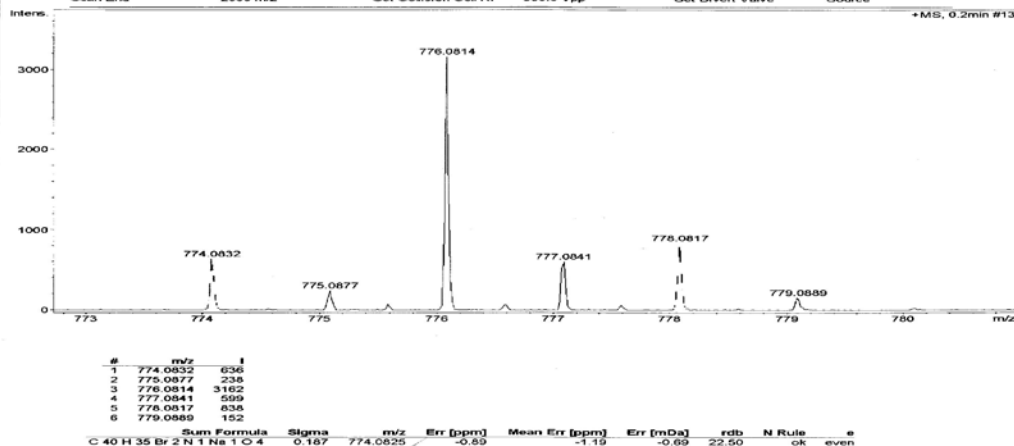
Figure S44: ^{13}C NMR spectrum of 5k.

Analysis Info		Acquisition Date 2010-3-17 11:09:36	
Analysis Name	K:\zm0047.d	Operator	Bruker Customer
Method	tune_low.m	Instrument / Serial	micrOTOF-Q 125
Sample Name	KBA2		
Comment	7.51 2.5f		

Analysis Info		Acquisition Date 2010-3-17 11:09:36	
Analysis Name	K:\zm0047.d	Operator	Bruker Customer
Method	tune_low.m	Instrument / Serial	micrOTOF-Q 125
Sample Name	KBA2		
Comment	7.51 2.5f		

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	220 度
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

776.0814



α	m/ν	l
1	774.0832	636
2	775.0877	238
3	776.0814	3162
4	777.0841	599
5	778.0817	839
6	779.0869	152

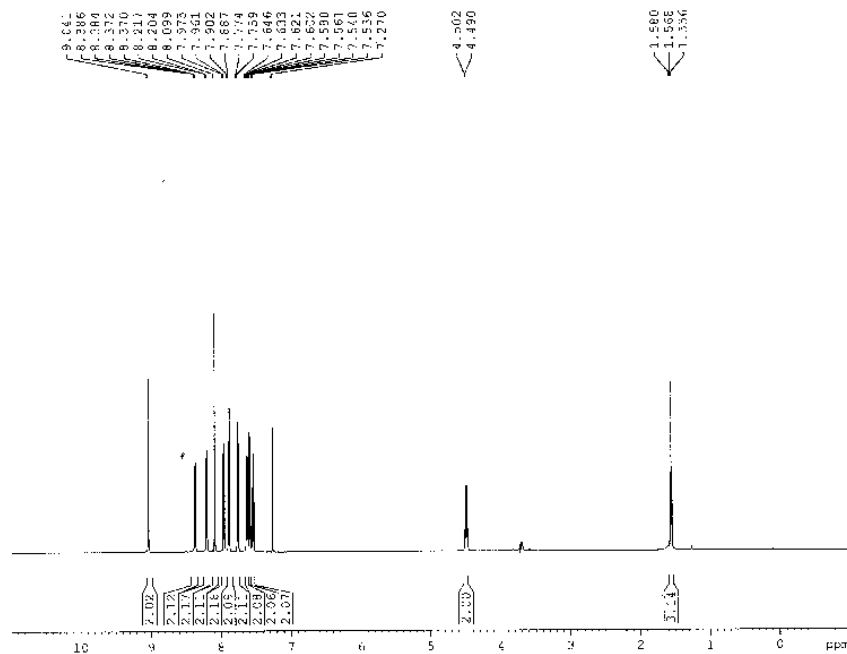
Bruker Daltonics DataAnalysis 3.4

printed: 2010-3-17 14:06:07

Page 1 of 1

Figure S45: HRMS spectrum of **5k**.

AV-600-1H
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PRM	5.22
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T2P005	20 qd
TE	65.56
20081231	20.13
NG	8
AGE	8
SEX	1.965, 1.11 Lz
PIORIS	2.57435 Lz
NO	1.8223786 PAR
NS	0
QK	29.27 CAC
QK	8.55 CAC
TC	298.7 K
D1	1.6000136 sec
TDO	3

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===== CHANNEL 1 =====
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PL           11.10 0540
PL           -4.00 dB
PLM          14.03265519 M
STRT         600.1324605 MHz
SI           32768
SC          600.1324605 MHz
SDM          1M
SSS          0
L4           0.30 Hz
L5           0
LC           1.00

```

Figure S46: ^1H NMR spectrum of **5l**.

AV-600-13C
Sample: 7M0053

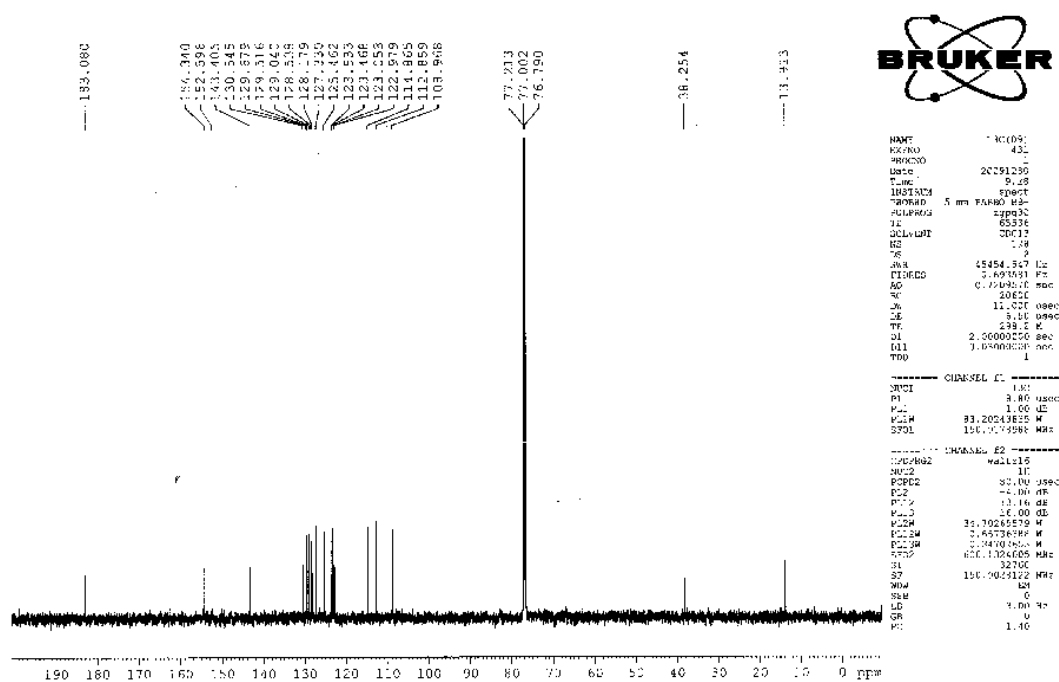


Figure S47: ^{13}C NMR spectrum of 5l.