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Supplementary Information

Novel *N*-Acylated Benzimidazolone Derivatives: Synthesis, 2D-QSAR and Targets Prediction

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NMR data for **11a01**-**11a15**

Ethyl 3-acetyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a01**): yield: 78%; m.p.: 126.7-128.4 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 8.5 Hz, CH_3), 1.56 (d, 6H, *J* 8.5 Hz, $2CH_3$), 2.74 (s, 3H, CH3), 4.38 (q, 2H, *J* 9.0 Hz, CH_2), 4.64-4.71 (m, 1H, CH), 7.76 (d, 1H, *J* 1.5 Hz, Ar–H), 7.83 (dd, 1H, *J* 2.0, 10.5 Hz, Ar–H), 8.22 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 25.8, 45.8, 61.3, 109.5, 115.2, 124.3, 126.6, 128.9, 129.8, 151.7, 166.2, 170.6; anal. calcd. for $C_{15}H_{18}N_2O_4$: C, 62.06; H, 6.25; N, 9.65; found: C, 62.22; H, 6.23; N, 9.62.

Ethyl 3-hexanoyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a02**): yield: 70%; m.p.: 63.9-65.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.93 (t, 3H, *J* 8.5 Hz, CH_3), 1.40-1.44 (m, 5H, CH_2, CH_3), 1.57-1.60 (m, 8H, CH_2, $2CH_3$), 1.74-1.82 (m, 2H, CH_2), 3.18 (t, 2H, *J* 9.0 Hz, CH_2), 4.40 (q, 2H, *J* 9.0 Hz, CH_2), 4.68-4.71 (m, 1H, CH), 7.78 (d, 1H, *J* 2.0 Hz, Ar–H), 7.88 (dd, 1H, *J* 1.5, 10.5 Hz, Ar–H), 8.28 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 14.4, 19.8, 22.5, 23.8, 31.3, 37.5, 45.7, 61.3, 109.5, 115.3, 124.3, 126.4, 128.9, 130.1, 151.6, 166.2, 174.0; anal. calcd. for $C_{19}H_{26}N_2O_4$: C, 65.87; H, 7.56; N, 8.09; found: C, 65.78; H, 7.51; N, 9.04.

Ethyl 3-heptanoyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a03**): yield: 68%; m.p.: 62.0-63.5 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.90 (t, 3H, *J* 8.5 Hz, CH_3), 1.32-1.36 (m, 4H, $2CH_2$), 1.40-1.44 (m, 5H, CH_2, CH_3), 1.58 (d, 6H, *J* 9.0 Hz, $2CH_3$), 1.74-1.80 (m, 2H, CH_2), 3.18 (t, 2H, *J* 9.0 Hz, CH_2), 4.40 (q, 2H, *J* 9.0 Hz, CH_2), 4.68-4.71 (m, 1H, CH), 7.78 (d, 1H, *J* 1.5 Hz, Ar–H), 7.88 (dd, 1H, *J* 2.0, 10.5 Hz, Ar–H), 8.28 (d, 1H, *J* 11.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.0, 14.4, 19.8, 22.5, 24.0, 28.8, 31.6, 37.5, 45.7, 61.3, 109.5, 115.3, 124.3, 126.4, 128.9, 130.1, 151.6, 166.2, 174.0; anal. calcd. for $C_{20}H_{28}N_2O_4$: C, 66.64; H, 7.83; N, 7.77; found: C, 66.52; H, 7.79; N, 7.71.

Ethyl 3-(cyclopropanecarbonyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a04**): yield: 82%; m.p.: 100.7-102.5 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.09-1.12 (m, 2H, CH_2), 1.28-1.30 (m, 3H, CH, CH_2), 1.41 (t, 3H, *J* 9.0 Hz, CH_3), 1.59 (d, 6H, *J* 9.0 Hz, $2CH_3$), 3.46-3.52 (m, 1H, CH), 4.37 (q, 2H, *J* 9.0 Hz, CH_2), 4.68-4.75 (m, 1H, CH), 7.77 (s, 1H, Ar–H), 7.83 (dd, 1H, *J* 1.5, 10.5 Hz, Ar–H), 8.22 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 11.5, 14.2, 14.4, 19.8, 45.8, 61.2, 109.5, 115.2, 124.3, 126.4, 128.6, 130.2, 152.1, 166.2, 174.9; anal. calcd. for $C_{17}H_{20}N_2O_4$: C, 64.54; H, 6.37; N, 8.86; found: C, 64.41; H, 6.37; N, 8.92.

Ethyl 3-(2-(4-chlorophenyl)acetyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a05**): yield: 62%; m.p.: 116.8-118.4 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.41 (t, 3H, *J* 9.0 Hz, CH_3), 1.60 (d, 6H, *J* 9.0 Hz, $2CH_3$), 4.39 (q, 2H, *J* 9.0 Hz, CH_2), 4.51 (s, 2H, CH_2), 4.68-4.72 (m, 1H, CH), 7.28-7.34 (m, 4H, Ar–H), 7.79 (s, 1H, Ar–H), 7.88 (dd, 1H, *J* 2.0, 11.0 Hz, Ar–H), 8.25 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.3, 19.7, 42.9, 45.9, 61.3, 109.6, 115.4, 124.4, 126.8, 128.7, 128.9, 129.9, 131.3, 131.9, 133.2, 151.5, 166.1, 171.3; anal. calcd. for $C_{21}H_{21}ClN_2O_4$: C, 62.92; H, 5.28; N, 6.99; found: C, 63.03; H, 5.31; N, 7.04.

Ethyl 3-(2-(4-chlorophenoxy)acetyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a06**): yield: 70%; m.p.: 125.6-127.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.42 (t, 3H, *J* 9.0 Hz, CH_3), 1.60 (d, 6H, *J* 9.0 Hz, $2CH_3$), 4.40 (q, 2H, *J* 9.0 Hz, CH_2), 4.69-4.72 (m, 1H, CH), 5.39 (s, 2H, CH_2), 6.93 (d, 2H, *J* 11.5 Hz, Ar–H), 7.24 (d, 2H, *J* 11.0 Hz, Ar–H), 7.81 (d, 1H, *J* 1.5 Hz, Ar–H), 7.89 (dd, 1H, *J* 2.0, 10.5 Hz, Ar–H), 8.26 (d, 1H, *J* 11.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.3, 19.7, 46.1, 61.4,

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68.6, 109.8, 115.1, 116.2, 124.6, 126.6, 127.1, 129.0, 129.4, 129.5, 151.4, 156.5, 165.9, 168.4; anal. calcd. for $C_{21}H_{21}ClN_2O_5$: C, 60.51; H, 5.08; N, 6.72; found: C, 60.54; H, 5.15; N, 6.67.

Ethyl 3-benzoyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a07**): yield: 66%; m.p.: 122.4-123.9 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.43 (t, 3H, *J* 9.0 Hz, CH_3), 1.57 (d, 6H, *J* 9.0 Hz, $2CH_3$), 4.42 (q, 2H, *J* 9.0 Hz, CH_2), 4.62-4.69 (m, 1H, CH), 7.50 (t, 2H, *J* 10.0 Hz, Ar–H), 7.58-7.62 (m, 1H, Ar–H), 7.78 (d, 1H, *J* 1.5 Hz, Ar–H), 7.83 (d, 1H, *J* 1.0 Hz, Ar–H), 7.90 (dd, 1H, *J* 1.5, 10.5 Hz, Ar–H), 7.97 (d, 1H, *J* 10.5 Hz, Ar–H), 8.10 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 45.9, 61.3, 109.9, 114.1, 124.2, 126.5, 128.1, 128.8, 129.5, 130.1, 133.0, 133.5, 151.3, 166.2, 168.9; anal. calcd. for $C_{20}H_{20}N_2O_4$: C, 68.17; H, 5.72; N, 7.95; found: C, 68.25; H, 5.59; N, 7.81.

Ethyl 3-(3-chlorobenzoyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a08**): yield: 66%; m.p.: 128.2-129.7 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.44 (t, 3H, *J* 9.0 Hz, CH_3), 1.58 (d, 6H, *J* 9.0 Hz, $2CH_3$), 4.41 (q, 2H, *J* 9.0 Hz, CH_2), 4.63-4.69 (m, 1H, CH), 7.42 (d, 1H, *J* 10.0 Hz, Ar–H), 7.55-7.58 (m, 1H, Ar–H), 7.62-7.65 (m, 1H, Ar–H), 7.72-7.76 (m, 1H, Ar–H), 7.83 (d, 1H, *J* 1.5 Hz, Ar–H), 7.91 (dd, 1H, *J* 2.0, 11.0 Hz, Ar–H), 7.99 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.7, 46.0, 61.3, 110.0, 114.3, 124.3, 126.8, 127.4, 129.3, 129.3, 129.4, 130.2, 132.7, 134.3, 135.3, 151.1, 166.1, 167.6; anal. calcd. for $C_{20}H_{19}ClN_2O_4$: C, 62.10; H, 4.95; N, 7.24; found: C, 62.14; H, 4.89; N, 7.42.

Ethyl 3-(4-chlorobenzoyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a09**): yield: 71%; m.p.: 73.4-75.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.44 (t, 3H, *J* 9.0 Hz, CH_3), 1.56 (d, 6H, *J* 9.0 Hz, $2CH_3$), 4.43 (q, 2H, *J* 9.0 Hz, CH_2), 4.62-4.66 (m, 1H, CH), 7.47 (d, 2H, *J* 11.0 Hz, Ar–H), 7.74 (d, 2H, *J* 10.5 Hz, Ar–H), 7.83 (d, 1H, *J* 1.5 Hz, Ar–H), 7.92 (dd, 1H, *J* 2.0, 10.5 Hz, Ar–H), 7.98 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.7, 46.0, 61.3, 110.0, 114.2, 124.3, 126.7, 128.5, 129.4, 130.3, 130.9, 131.8, 139.4, 151.2, 166.1, 167.8; anal. calcd. for $C_{20}H_{19}ClN_2O_4$: C, 62.10; H, 4.95; N, 7.24; found: C, 62.34; H, 4.85; N, 7.12.

Ethyl 3-acryloyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a10**): yield: 51%; m.p.: 121.5-123.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 9.0 Hz, CH_3), 1.57 (d, 6H, *J* 9.0 Hz, $2CH_3$), 4.38 (q, 2H, *J* 9.0 Hz, CH_2), 4.66-4.70 (m, 1H, CH), 6.00 (dd, 1H, *J* 2.0, 14.0 Hz, CH of acryloyl), 6.66 (dd, 1H, *J* 2.0, 21.0 Hz, CH of acryloyl), 7.74 (dd, 1H, *J* 13.0, 21.5 Hz, CH of acryloyl), 7.77 (d, 1H, *J* 1.5 Hz, Ar–H), 7.88 (dd, 1H, *J* 2.0, 10.5 Hz, Ar–H), 8.28 (d, 1H, *J* 11.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.7, 45.9, 61.3, 109.6, 115.4, 124.4, 126.7, 129.1, 129.2, 130.1, 132.3, 151.6, 165.3, 166.1; anal. calcd. for $C_{16}H_{18}N_2O_4$: C, 63.56; H, 6.00; N, 9.27; found: C, 63.47; H, 6.04; N, 9.32.

Ethyl 3-but-2-enoyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a11**): yield: 58%; m.p.: 148.7-150.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.42 (t, 3H, *J* 9.0 Hz, CH_3), 1.59 (d, 6H, *J* 9.0 Hz, $2CH_3$), 2.03 (dd, 3H, *J* 1.5, 9.0 Hz, CH_3), 4.40 (q, 2H, *J* 9.0 Hz, CH_2), 4.68-4.73 (m, 1H, CH), 7.30-7.36 (m, 1H, H-2 of 3-but-2-enoyl), 7.50 (dd, 1H, *J* 2.0, 17.5 Hz, H-3 of 3-but-2-enoyl), 7.78 (d, 1H, *J* 2.0 Hz, Ar–H), 7.88 (dd, 1H, *J* 1.5, 10.5 Hz, Ar–H), 8.28 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 18.7, 19.7, 45.8, 61.2, 109.5, 115.3, 124.3, 126.4, 129.1, 130.4, 147.7, 151.7, 165.4, 166.2; anal. calcd. for $C_{17}H_{20}N_2O_4$: C, 64.54; H, 6.37; N, 8.86; found: C, 64.55; H, 6.32; N, 8.79.

Ethyl 1-isopropyl-2-oxo-3-propionyl-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a12**): yield: 55%; m.p.: 104.5-106.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.28 (t, 3H, *J* 9.0 Hz, CH_3), 1.42 (t, 3H, *J* 9.0 Hz, CH_3), 1.59 (d, 6H, *J* 9.0 Hz, $2CH_3$), 3.19 (q, 2H, *J* 9.0 Hz, CH_2), 4.14 (q, 2H, *J* 9.0 Hz, CH_2), 4.68-4.71 (m, 1H, CH), 7.79 (d, 1H, *J* 1.5 Hz, Ar–H), 7.88 (dd, 1H, *J* 1.5, 10.5 Hz, Ar–H), 8.27 (d, 1H, *J* 11.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 8.2, 14.4, 19.8, 31.1, 45.7, 61.2, 109.5, 115.2, 124.3, 126.4, 128.9, 130.0, 151.6, 166.2, 174.6; anal. calcd. for $C_{16}H_{20}N_2O_4$: C, 63.14; H, 6.62; N, 9.20; found: C, 63.21; H, 6.47; N, 9.17.

Ethyl 3-butyryl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a13**): yield: 63%; m.p.: 76.0-77.3 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.06 (t, 3H, *J* 9.5 Hz, CH_3), 1.42 (t, 3H, *J* 9.0 Hz, CH_3), 1.59 (d, 6H, *J* 9.0 Hz, $2CH_3$), 1.78-1.84 (m, 2H, CH_2), 3.16 (t, 2H, *J* 9.0 Hz, CH_2), 4.39 (q, 2H, *J* 9.0 Hz, CH_2), 4.68-4.72 (m, 1H, CH), 7.79 (s, 1H, Ar–H), 7.88 (dd, 1H, *J* 1.5, 10.5 Hz, Ar–H), 8.28 (d, 1H, *J* 11.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.7, 14.4, 17.6, 19.8, 39.4, 45.7, 61.2, 109.5, 115.3, 124.3, 126.4, 128.9, 130.0, 151.6, 166.2, 173.8; anal. calcd. for $C_{17}H_{22}N_2O_4$: C, 64.13; H, 6.97; N, 8.80; found: C, 64.25; H, 6.94; N, 8.84.

Ethyl 1-isopropyl-3-(4-methylpentanoyl)-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a14**): yield: 54%; m.p.: 77.5-78.9 °C; ^{1}H NMR (500 MHz, $CDCl_3$)

δ 0.98 (d, 6H, *J* 8.0 Hz, $2CH_3$), 1.42 (t, 3H, *J* 9.0 Hz, CH_3), 1.58 (d, 6H, *J* 9.0 Hz, $2CH_3$), 1.68-1.73(m, 3H, CH, CH_2), 3.18 (t, 2H, *J* 9.0 Hz, CH_2), 4.41 (q, 2H, *J* 9.0 Hz, CH_2), 4.68-4.73 (m, 1H, CH), 7.78 (d, 1H, *J* 1.5 Hz, Ar–H), 7.88 (dd, 1H, *J* 2.0, 10.5 Hz, Ar–H), 8.28 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 22.4, 27.7, 32.9, 35.6, 45.7, 61.2, 109.5, 115.3, 124.3, 126.4, 128.9, 130.1, 151.6, 166.2, 174.2; anal. calcd. for $C_{19}H_{26}N_2O_4$: C, 65.87; H, 7.56; N, 8.09; found: C, 65.48; H, 7.55; N, 8.12.

Ethyl 1-isopropyl-2-oxo-3-(4-(trifluoromethyl-benzoyl)-2,3-dihydro-1*H*-benzo[*d*]imidazole-6-carboxylate (**11a15**): yield: 60%; m.p.: 126.0-127.8 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.44 (t, 3H, *J* 9.0 Hz, CH_3), 1.58 (d, 6H, *J* 9.0 Hz, $2CH_3$), 4.43 (q, 2H, *J* 9.0 Hz, CH_2), 4.60-4.67 (m, 1H, CH), 7.75 (d, 2H, *J* 10.0 Hz, Ar–H), 7.85-7.87 (m, 3H, Ar–H), 7.93 (dd, 1H, *J* 1.5, 10.5 Hz, Ar–H), 8.05 (d, 1H, *J* 10.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.7, 46.1, 61.4, 110.1, 114.5, 123.6 (q, $^1J_{CF}$ 340.0 Hz), 124.5, 125.1, 127.0, 129.4, 129.5, 130.1, 134.0 (q, $^2J_{CF}$ 41.3 Hz), 137.1, 151.1, 166.1, 167.8; anal. calcd. for $C_{21}H_{19}F_3N_2O_4$: C, 60.00; H, 4.56; N, 6.66; found: C, 60.24; H, 4.50; N, 6.61.

NMR spectra for 9b01-9b21

Ethyl 3-acetyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b01**): yield: 58%; m.p.: 151.6-152.9 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.57 (d, 6H, *J* 7.0 Hz, $2CH_3$), 2.77 (s, 3H, CH_3), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.68-4.74 (m, 1H, CH), 7.15 (d, 1H, *J* 8.5 Hz, Ar–H), 7.98 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.87 (d, 1H, *J* 1.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 25.8, 45.8, 61.0, 108.1, 117.0, 124.7, 126.1, 126.7, 132.5, 151.9, 166.3, 170.4; anal. calcd. for $C_{15}H_{18}N_2O_4$: C, 62.06; H, 6.25; N, 9.65; found: C, 62.20; H, 6.23; N, 9.72.

Ethyl 3-hexanoyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b02**): yield: 50%; m.p.: 63.1-65.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.93 (t, 3H, *J* 7.0 Hz, CH_3), 1.39-1.42 (m, 7H, $2CH_2$, CH_3), 1.57 (d, 6H, *J* 7.0 Hz, $2CH_3$), 1.78-1.81 (m, 2H, CH_2), 3.17 (t, 2H, *J* 7.0 Hz, CH_2), 4.38 (q, 2H, *J* 7.0 Hz, CH_2), 4.69-4.72 (m, 1H, CH), 7.15 (d, 1H, *J* 8.5 Hz, Ar–H), 7.98 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.90 (d, 1H, *J* 1.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 14.4, 19.8, 22.5, 23.8, 31.3, 37.4, 45.7, 61.0, 108.0, 117.0, 124.6, 126.3, 126.6, 132.5, 151.8, 166.4, 173.8; anal. calcd. for $C_{19}H_{26}N_2O_4$: C, 65.87; H, 7.56; N, 8.09; found: C, 65.49; H, 7.58; N, 7.06.

Ethyl 3-heptanoyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b03**): yield: 58%; m.p.: 60.0-61.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.90 (t, 3H, *J* 6.5 Hz, CH_3), 1.33-1.44 (m, 9H, $3CH_2$, CH_3), 1.57 (d, 6H, *J* 7.0 Hz, $2CH_3$), 1.77-1.80 (m, 2H, CH_2), 3.17 (t, 2H, *J* 7.5 Hz, CH_2), 4.38 (q, 2H, *J* 7.0 Hz, CH_2), 4.69-4.72 (m, 1H, CH), 7.15 (d, 1H, *J* 8.5 Hz, Ar–H), 7.98 (d, 1H, *J* 8.5 Hz, Ar–H), 8.90 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.0, 14.4, 19.8, 22.6, 24.1, 28.8, 31.6, 37.5, 45.7, 61.0, 108.0, 117.0, 124.6, 126.3, 126.6, 132.5, 151.8, 166.4, 173.8; anal. calcd. for $C_{20}H_{28}N_2O_4$: C, 66.64; H, 7.83; N, 7.77; found: C, 66.48; H, 7.86; N, 7.74.

Ethyl 3-(cyclopropanecarbonyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b04**): yield: 71%; m.p.: 130.2-131.6 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.11-1.13 (m, 2H, CH_2), 1.31-1.33 (m, 2H, CH_2), 1.39 (t, 3H, *J* 7.0 Hz, CH_3), 1.59 (d, 6H, *J* 7.0 Hz, $2CH_3$), 3.49-3.52 (m, 1H, CH),4.38 (q, 2H, *J* 7.0 Hz, CH_2), 4.70-4.73 (m, 1H, CH), 7.15 (d, 1H, *J* 8.5 Hz, Ar–H), 7.98 (d, 1H, *J* 8.5 Hz, Ar–H), 8.83 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 11.4, 14.1, 14.4, 19.8, 45.7, 61.0, 108.0, 117.0, 124.6, 126.3, 126.5, 126.6, 132.2, 152.4, 166.3, 174.7; anal. calcd. for $C_{17}H_{20}N_2O_4$: C, 64.54; H, 6.37; N, 8.86; found: C, 64.85; H, 6.25; N, 8.82.

Ethyl 3-(2-(4-chlorophenyl)acetyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b05**): yield: 68%; m.p.: 69.0-71.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.41 (t, 3H, *J* 7.0 Hz, CH_3), 1.61 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.54 (s, 2H, CH_2), 4.75-4.77 (m, 1H, CH), 7.19 (d, 1H, *J* 8.5 Hz, Ar–H), 7.30-7.38 (m, 4H, Ar–H), 8.02 (d, 1H, *J* 8.5 Hz, Ar–H), 8.90 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 42.9, 45.9, 61.1, 108.2, 117.1, 124.9, 126.1, 127.0, 128.8, 131.3, 131.9, 132.6, 133.3, 151.8, 166.2, 171.1; anal. calcd. for $C_{21}H_{21}ClN_2O_4$: C, 62.92; H, 5.28; N, 6.99; found: C, 62.83; H, 5.22; N, 6.94.

Ethyl 3-(2-(4-chlorophenoxy)acetyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b06**): yield: 75%; m.p.: 123.6-125.0 °C;^{1}H NMR (500 MHz, $CDCl_3$) δ 1.38 (t, 3H, *J* 7.0 Hz, CH_3), 1.59 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.38 (q, 2H, *J* 7.0 Hz, CH_2), 4.69-4.72 (m, 1H, CH), 5.40 (s, 2H, CH_2), 6.95 (d, 2H, *J* 9.0 Hz, Ar–H), 7.19 (d, 1H, *J* 8.5 Hz, Ar–H), 7.27 (d, 2H, *J* 8.5 Hz, Ar–H), 8.03 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.89 (d, 1H, *J* 1.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 46.1, 61.2, 68.6, 108.5, 116.2, 116.9, 125.2, 125.4, 126.7, 127.3, 129.5, 133.0, 151.6, 156.6, 166.0, 168.2; anal. calcd. for $C_{21}H_{21}ClN_2O_5$: C, 60.51; H, 5.08; N, 6.72; found: C, 60.34; H, 5.16; N, 6.59.

Ethyl 3-benzoyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b07**): yield: 75%; m.p.: 111.0-112.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.55 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.40 (q, 2H, *J* 7.0 Hz, CH_2), 4.64-4.67 (m, 1H, CH), 7.19 (d, 1H, *J* 8.0 Hz, Ar–H), 7.50 (t, 2H, *J* 8.0 Hz, Ar–H), 7.61 (t, 1H, *J* 7.5 Hz, Ar–H), 7.79 (d, 2H, *J* 7.5 Hz, Ar–H), 8.01 (d, 1H, *J* 7.5 Hz, Ar–H), 8.59 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 45.8, 61.1, 108.4, 115.8, 124.6, 126.6, 126.7, 128.1, 128.5, 129.4, 130.2, 133.0, 133.6, 151.5, 166.2, 168.8; anal. calcd. for $C_{20}H_{20}N_2O_4$: C, 68.17; H, 5.72; N, 7.95; found: C, 68.55; H, 5.66; N, 7.91.

Ethyl 3-(3-chlorobenzoyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b08**): yield: 78%; m.p.: 65.4-67.2 °C;^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.55 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.61-4.67 (m, 1H, CH), 7.19 (d, 1H, *J* 8.5 Hz, Ar–H), 7.43 (t, 1H, *J* 8.0 Hz, Ar–H), 7.56 (d, 1H, *J* 8.0 Hz, Ar–H), 7.64 (d, 1H, *J* 8.0 Hz, Ar–H), 7.74 (s, 1H, Ar–H), 8.01 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.62 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 46.0, 61.1, 108.5, 116.0, 123.7, 124.8, 126.4, 126.9, 127.4, 129.3, 132.7, 133.1, 134.3, 135.4, 151.3, 166.1, 167.5; anal. calcd. for $C_{20}H_{19}ClN_2O_4$: C, 62.10; H, 4.95; N, 7.24; found: C, 62.04; H, 4.97; N, 7.29.

Ethyl 3-(4-chlorobenzoyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b09**): yield: 80%; m.p.: 94.0-96.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.56 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.62-4.65 (m, 1H, CH), 7.19 (d, 1H, *J* 8.5 Hz, Ar–H), 7.46 (d, 2H, *J* 8.5 Hz, Ar–H), 7.73 (d, 2H, *J* 8.0 Hz, Ar–H), 8.01 (d, 1H, *J* 8.5 Hz, Ar–H), 8.59 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 46.0, 61.1, 108.5, 115.9, 124.8, 126.6, 126.8, 128.5, 129.0, 129.4, 130.9, 131.9, 133.1, 139.4, 151.4, 166.1, 167.7; anal. calcd. for $C_{20}H_{19}ClN_2O_4$: C, 62.10; H, 4.95; N, 7.24; found: C, 61.96; H, 4.86; N, 7.31.

Ethyl 3-acryloyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b10**): yield: 62%; m.p.: 137.3-139.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.41 (t, 3H, *J* 7.0 Hz, CH_3), 1.57 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.71-4.73 (m, 1H, CH), 6.02 (d, 1H, *J* 10.5 Hz, CH_2 of acryloyl), 6.71 (d, 1H, *J* 17.0 Hz, CH_2 of acryloyl), 7.16 (d, 1H, *J* 8.5 Hz, Ar–H), 7.74 (dd, 1H, *J* 17.0, 10.5 Hz, CH of acryloyl), 7.98 (d, 1H, *J* 8.5 Hz, Ar–H), 8.90 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 45.8, 61.1, 108.2, 117.1, 124.8, 126.3, 126.9, 129.1, 132.3, 132.8, 151.8, 165.2, 166.3; anal. calcd. for $C_{16}H_{18}N_2O_4$: C, 63.56; H, 6.00; N, 9.27; found: C, 63.77; H, 6.08; N, 9.22.

(*E*)-Ethyl 3-but-2-enoyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b11**): yield: 68%; m.p.: 141.5-143.5 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.57 (d, 6H, *J* 7.0 Hz, $2CH_3$), 2.03 (t, 3H, *J* 6.5 Hz, CH_3), 4.38 (q, 2H, *J* 7.0 Hz, CH_2), 4.67-4.71 (m, 1H, CH), 7.14 (d, 1H, *J* 8.5 Hz, Ar–H), 7.31-7.35 (m, 1H, H-2 of 3-but-2-enoyl), 7.50 (dd, 1H, *J* 1.5, 15.5 Hz, H-3 of 3-but-2-enoyl), 7.98 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.88 (d, 1H, *J* 1.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 18.7, 19.8, 45.8, 61.0, 108.0, 117.1, 123.6, 124.7, 126.5, 126.7, 132.7, 147.6, 151.9, 165.3, 166.4; anal. calcd. for $C_{17}H_{20}N_2O_4$: C, 64.54; H, 6.37; N, 8.86; found: C, 64.36; H, 6.42; N, 8.85.

Ethyl 3-(2-chloroacetyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b12**): yield: 48%; m.p.: 146.0-148.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.41 (t, 3H, *J* 7.0 Hz, CH_3), 1.57 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.67-4.69 (m, 1H, CH), 4.97(s, 2H, CH_2), 7.18 (d, 1H, *J* 8.0 Hz, Ar–H), 8.02 (dd, 1H, *J* 1.0, 8.0 Hz, Ar–H), 8.89 (d, 1H, *J* 1.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8 (2C), 45.2, 46.1, 61.2, 108.5, 117.0, 125.2, 125.6, 127.3, 132.8, 151.4, 166.0, 166.1; anal. calcd. for $C_{15}H_{17}ClN_2O_4$: C, 55.48; H, 5.28; N, 8.63; found: C, 55.79; H, 5.22; N, 8.61.

Ethyl 3-(2-bromopropanoyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b13**): yield: 49%; m.p.: 98.5-99.6 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.41 (t, 3H, *J* 7.0 Hz, CH_3), 1.58 (d, 6H, *J* 7.0 Hz, $2CH_3$), 1.96 (d, 3H, *J* 7.0 Hz, CH_3), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.71-4.76 (m, 2H, 2CH), 7.18 (d, 1H, *J* 8.0 Hz, Ar–H), 8.02 (d, 1H, *J* 8.5 Hz, Ar–H), 8.87 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 20.6, 40.4, 46.0, 61.2, 108.4, 117.2, 125.0, 126.1, 127.3, 132.7, 151.0, 166.1, 169.7; anal. calcd. for $C_{16}H_{19}BrN_2O_4$: C, 50.14; H, 5.00; N, 7.31; found: C, 49.85; H, 5.03; N, 7.26.

Ethyl 3-(2-ethylbutanoyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b14**): yield: 52%; m.p.: 64.0-65.4 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.97 (t, 6H, *J* 7.5 Hz, $2CH_3$), 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.57 (d, 6H, *J* 7.0 Hz, $2CH_3$), 1.63-1.68 (m, 2H, CH_2), 1.83-1.89 (m, 2H, CH_2), 3.95-3.98 (m, 1H, CH), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.71-4.74 (m, 1H, CH), 7.16 (d, 1H, *J* 8.0 Hz, Ar–H), 7.99 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.92 (d, 1H, *J* 1.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 11.6, 14.4, 19.8, 24.4, 45.7, 47.4, 61.0, 108.1, 117.2, 124.6, 126.5, 126.6,

132.5, 151.7, 166.4, 177.1; anal. calcd. for $C_{19}H_{26}N_2O_4$: C, 65.87; H, 7.56; N, 8.09; found: C, 66.08; H, 7.51; N, 8.14.

Ethyl 3-isobutyryl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b15**): yield: 64%; m.p.: 110.5-112.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.31 (d, 6H, *J* 7.0 Hz, $2CH_3$), 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.58 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.07-4.08 (m, 1H, CH), 4.38 (q, 2H, *J* 7.0 Hz, CH_2), 4.70-4.73 (m, 1H, CH), 7.15 (d, 1H, *J* 8.5 Hz, Ar–H), 7.98 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.89 (d, 1H, *J* 1.5 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 18.9, 19.8, 34.4, 45.7, 61.1, 108.0, 117.2, 124.6, 126.5, 126.6, 132.6, 151.5, 166.3, 178.1; anal. calcd. for $C_{17}H_{22}N_2O_4$: C, 64.13; H, 6.97; N, 8.80; found: C, 64.39; H, 6.91; N, 8.75.

Ethyl 3-(4-fluorobenzoyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b16**): yield: 65%; m.p.: 120.3-121.8 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.56 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.64-4.66 (m, 1H, CH), 7.15-7.20 (m, 3H, Ar–H), 7.84 (dd, 2H, *J* 5.0, 8.5 Hz, Ar–H), 8.01 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.57 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 46.0, 61.1, 108.5, 115.4 (d, $^2J_{CF}$ 22.5 Hz), 115.7 (d, $^2J_{CF}$ 22.5 Hz), 115.8, 124.7, 126.7, 129.6, 132.3 (d, $^3J_{CF}$ 8.8 Hz), 132.8 (d, $^3J_{CF}$ 8.8 Hz), 133.0, 151.5, 165.7 (d, $^1J_{CF}$ 253.8 Hz), 166.2, 167.6; anal. calcd. for $C_{20}H_{19}FN_2O_4$: C, 64.86; H, 5.17; N, 7.56; found: C, 64.68; H, 5.21; N, 7.52.

Ethyl 3-(2-methylbenzoyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b17**): yield: 82%; m.p.: 80.0-81.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.41 (t, 3H, *J* 7.0 Hz, CH_3), 1.52 (d, 6H, *J* 7.0 Hz, $2CH_3$), 2.40 (s, 3H, CH_3), 4.41 (q, 2H, *J* 7.0 Hz, CH_2), 4.61-4.63 (m, 1H, CH), 7.18 (d, 1H, *J* 8.5 Hz, Ar–H), 7.28-7.31 (m, 2H, Ar–H), 7.38-7.45 (m, 2H, Ar–H), 8.02 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.82 (d, 1H, *J* 1.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.4, 19.8, 45.8, 61.1, 108.4, 116.4, 124.7, 126.2, 126.9, 127.3, 130.6, 130.8, 131.9, 132.8, 133.0, 135.7, 151.0, 166.2, 169.3; anal. calcd. for $C_{21}H_{22}N_2O_4$: C, 68.84; H, 6.05; N, 7.65; found: C, 68.76; H, 5.97; N, 7.60.

Ethyl 3-(4-methylbenzoyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b18**): yield: 75%; m.p.: 90.2-91.8 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.39 (t, 3H, *J* 7.0 Hz, CH_3), 1.55 (d, 6H, *J* 7.0 Hz, $2CH_3$), 2.44 (s, 3H, CH_3), 4.38 (q, 2H, *J* 7.0 Hz, CH_2), 4.63-4.66 (m, 1H, CH), 7.19 (d, 1H, *J* 8.5 Hz, Ar–H), 7.29 (d, 2H, *J* 6.5 Hz, Ar–H), 7.71 (d, 2H, *J* 8.0 Hz, Ar–H), 7.99 (d, 1H, *J* 8.0 Hz, Ar–H), 8.55 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 21.8, 45.9, 61.1, 108.4, 115.7, 124.5, 126.4, 126.9, 128.9, 129.2, 129.8, 133.0, 144.0, 151.6, 166.3, 168.7; anal. calcd. for $C_{21}H_{22}N_2O_4$: C, 68.84; H, 6.05; N, 7.65; found: C, 68.79; H, 6.09; N, 7.66.

Ethyl 1-isopropyl-3-methacryloyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b19**): yield: 56%; 135.0-136.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.57 (d, 6H, *J* 7.0 Hz, $2CH_3$), 2.15 (s, 3H, CH_3), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.65-4.68 (m, 1H, CH), 5.59, 5.60 (s, 2H, CH_2 of methacryloyl), 7.17 (d, 1H, *J* 8.5 Hz, Ar–H), 7.98 (d, 1H, *J* 8.5 Hz, Ar–H), 8.58 (s, 1H, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 18.8, 19.8, 45.8, 61.1, 108.3, 115.8, 122.1, 124.5, 126.4, 126.6, 133.0, 140.4, 151.1, 166.2, 170.1; anal. calcd. for $C_{17}H_{20}N_2O_4$: C, 64.54; H, 6.37; N, 8.86; found: C, 64.63; H, 6.36; N, 8.89.

Ethyl 3-(2*E*,4*E*)-hexa-2,4-dienoyl-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b20**): yield: 42%; m.p.: 74.0-75.6 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (t, 3H, *J* 7.0 Hz, CH_3), 1.57 (d, 6H, *J* 7.0 Hz, $2CH_3$), 1.91 (d, 3H, *J* 6.5 Hz, CH_3), 4.39 (q, 2H, *J* 7.0 Hz, CH_2), 4.68-4.71 (m, 1H, CH), 6.27-6.42 (m, 2H, H-2, H-5 of sorbic acid), 7.15 (d, 1H, *J* 8.0 Hz, Ar–H), 7.46 (d, 1H, *J* 15.0 Hz, H-4 of sorbic acid), 7.58-7.64 (m, 1H, H-3 of sorbic acid), 7.98 (dd, 1H, *J* 1.5, 8.5 Hz, Ar–H), 8.91 (d, 1H, *J* 1.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 18.8, 19.8, 45.8, 61.0, 108.0, 117.0, 119.6, 124.6, 126.1, 126.6, 130.6, 132.6, 141.5, 147.6, 151.9, 165.8, 166.4; anal. calcd. for $C_{19}H_{22}N_2O_4$: C, 66.65; H, 6.48; N, 8.18; found: C, 66.27; H, 6.61; N, 8.03.

(*E*)-Ethyl 3-(3-(furan-2-yl)acryloyl)-1-isopropyl-2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (**9b21**): yield: 55%; m.p.: 178.5-180.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.41 (t, 3H, *J* 7.0 Hz, CH_3), 1.59 (d, 6H, *J* 7.0 Hz, $2CH_3$), 4.40 (q, 2H, *J* 7.0 Hz, CH_2), 4.70-4.73 (m, 1H, CH), 6.51 (dd, 1H, *J* 1.5, 3.0 Hz, H-4 of furan), 6.75 (d, 1H, *J* 3.5 Hz, H-3 of furan), 7.16 (d, 1H, *J* 8.5 Hz, Ar–H), 7.54 (s, 1H, H-5 of furan), 7.76 (d, 1H, *J* 15.0 Hz, H-2 of acryloyl), 7.99 (dd, 1H, *J* 1.5, 8.0 Hz, Ar–H), 8.03 (d, 1H, *J* 15.5 Hz, H-3 of acryloyl), 8.94 (d, 1H, *J* 1.0 Hz, Ar–H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 19.8, 45.9, 61.0, 108.1, 112.6, 116.2, 116.3, 117.2, 124.7, 126.6, 126.7, 132.7, 132.8, 145.4, 151.6, 151.9, 165.4, 166.4; anal. calcd. for $C_{20}H_{20}N_2O_5$: C, 65.21; H, 5.47; N, 7.60; found: C, 65.05; H, 5.49; N, 7.64.

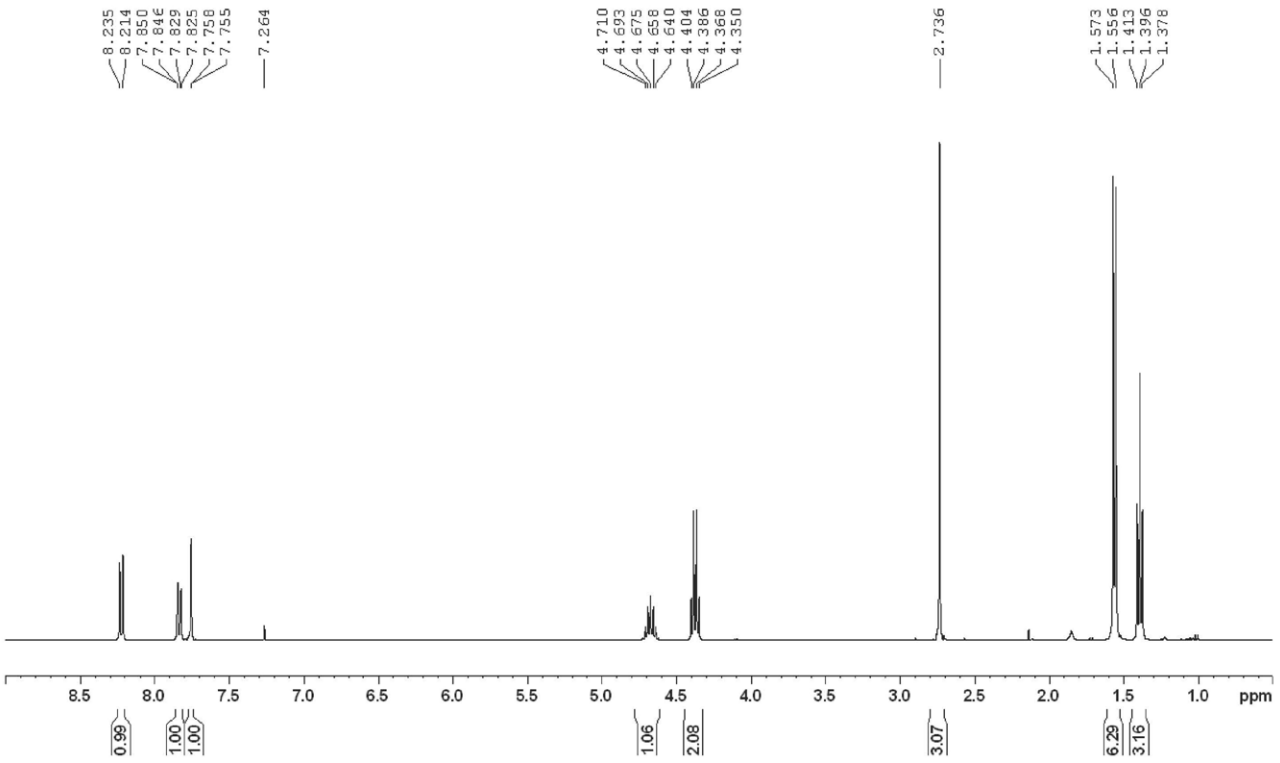

Figure S1. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a01**.

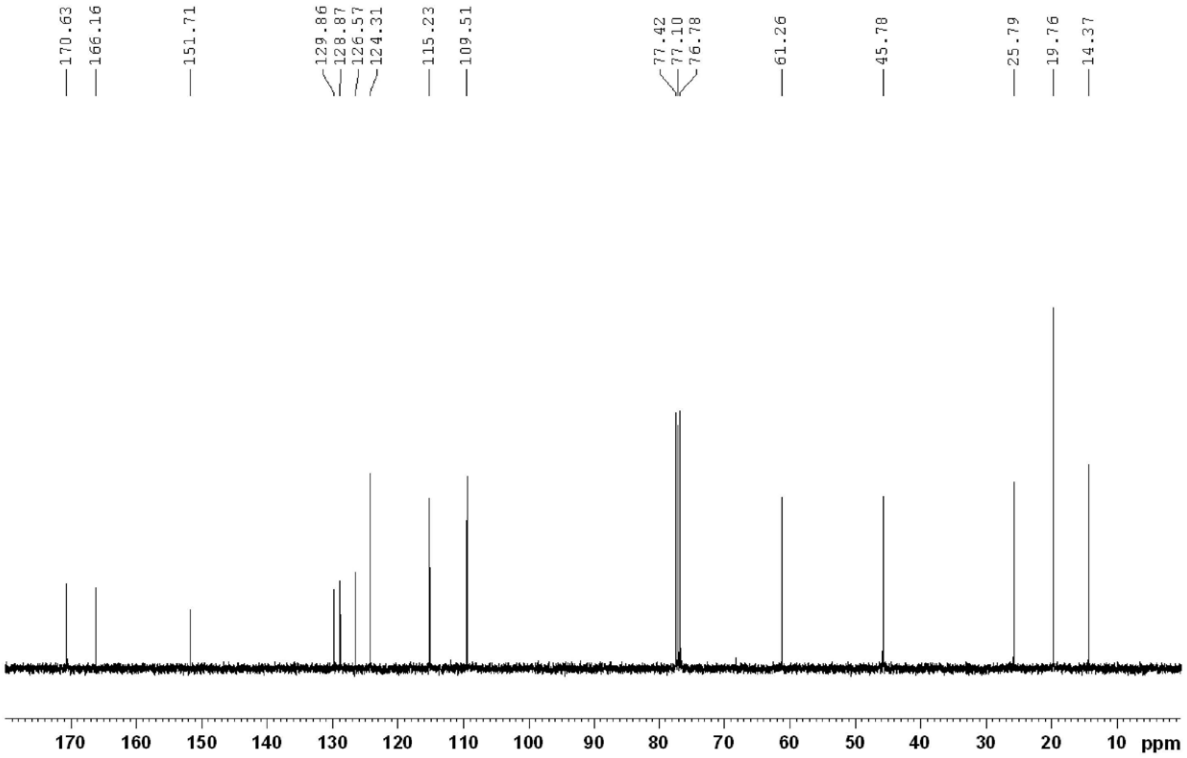

Figure S2. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a01**.

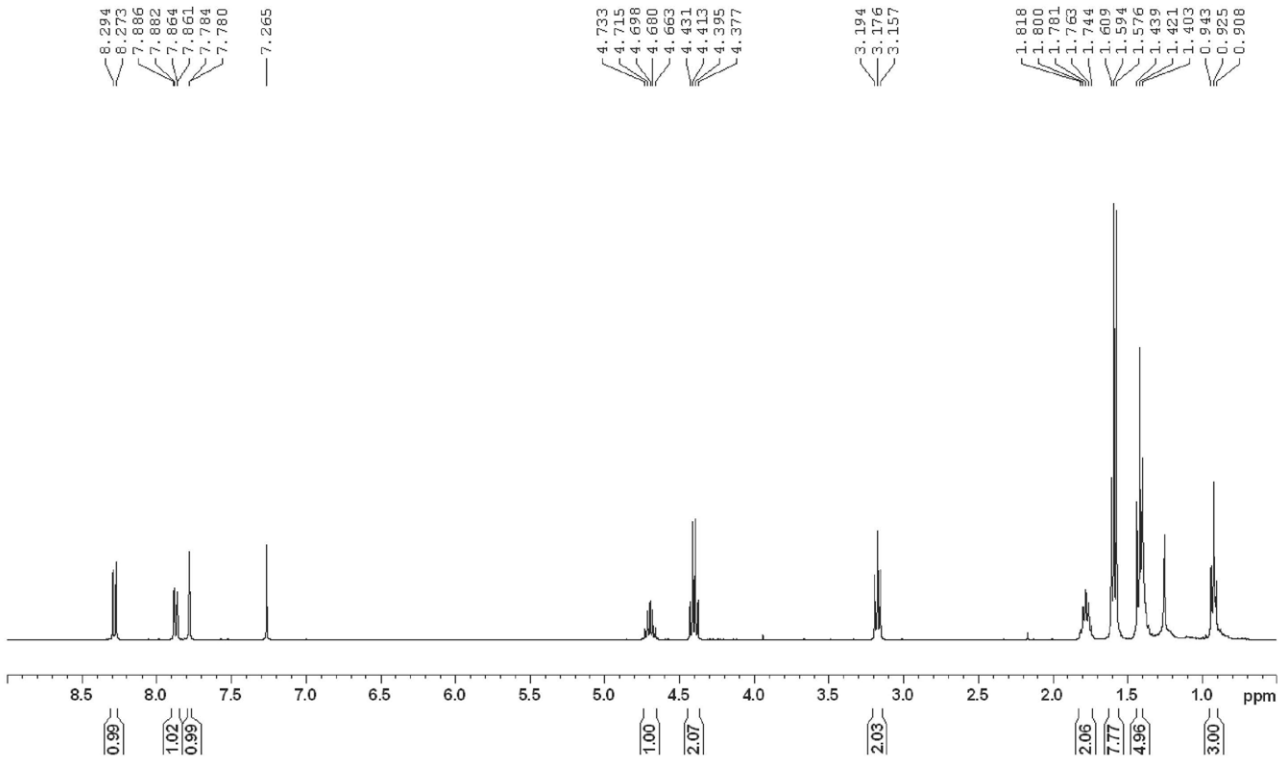

Figure S3. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a02**.

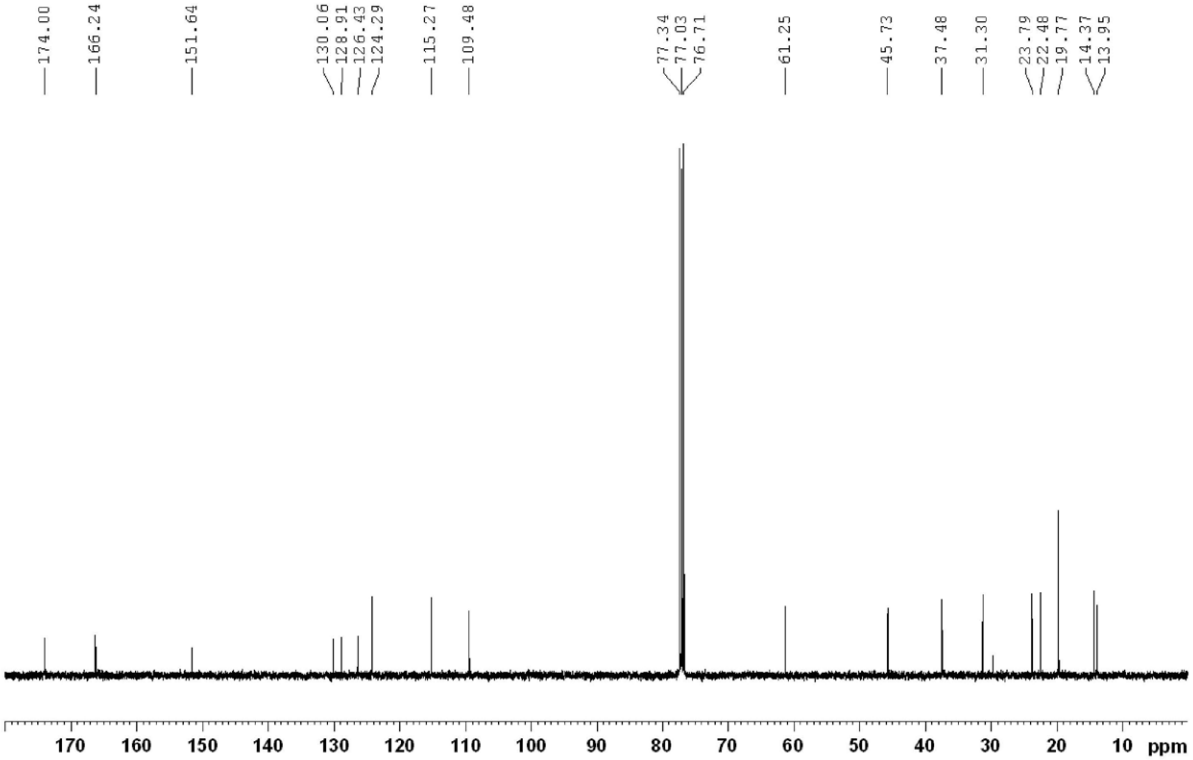

Figure S4. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a02**.

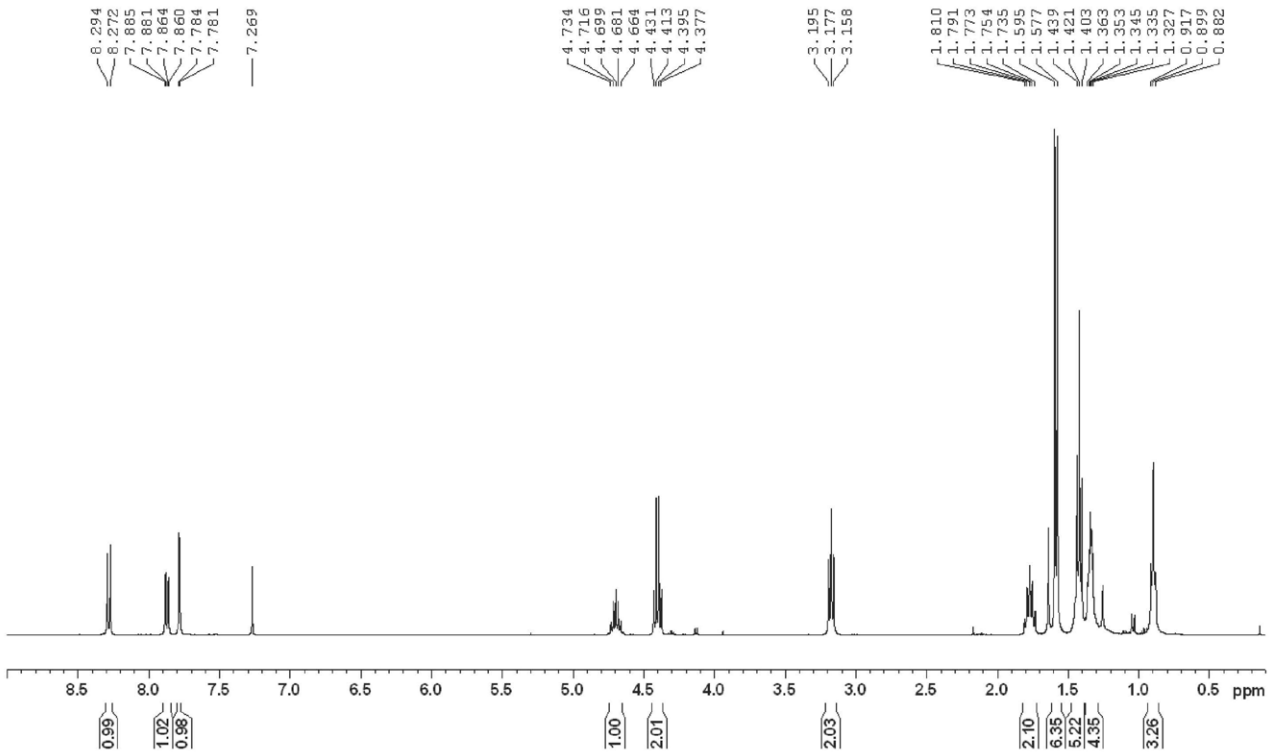

Figure S5. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a03**.

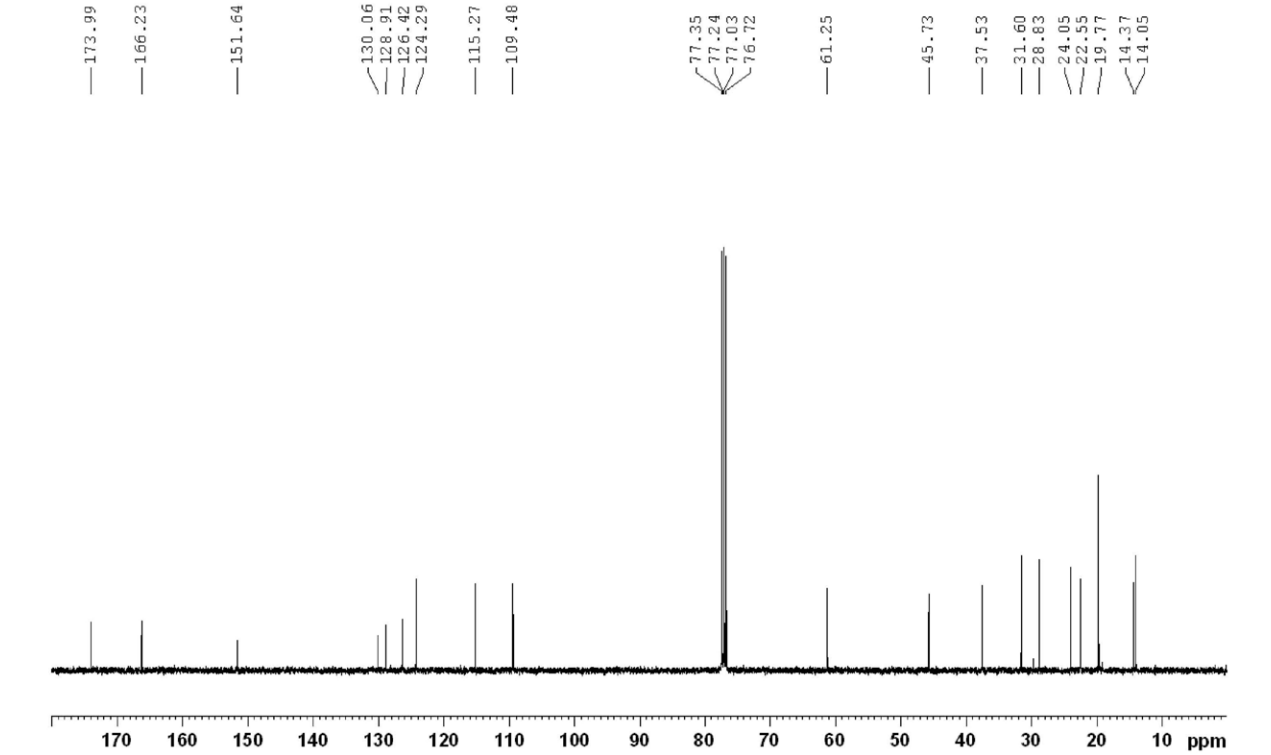

Figure S6. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a03**.

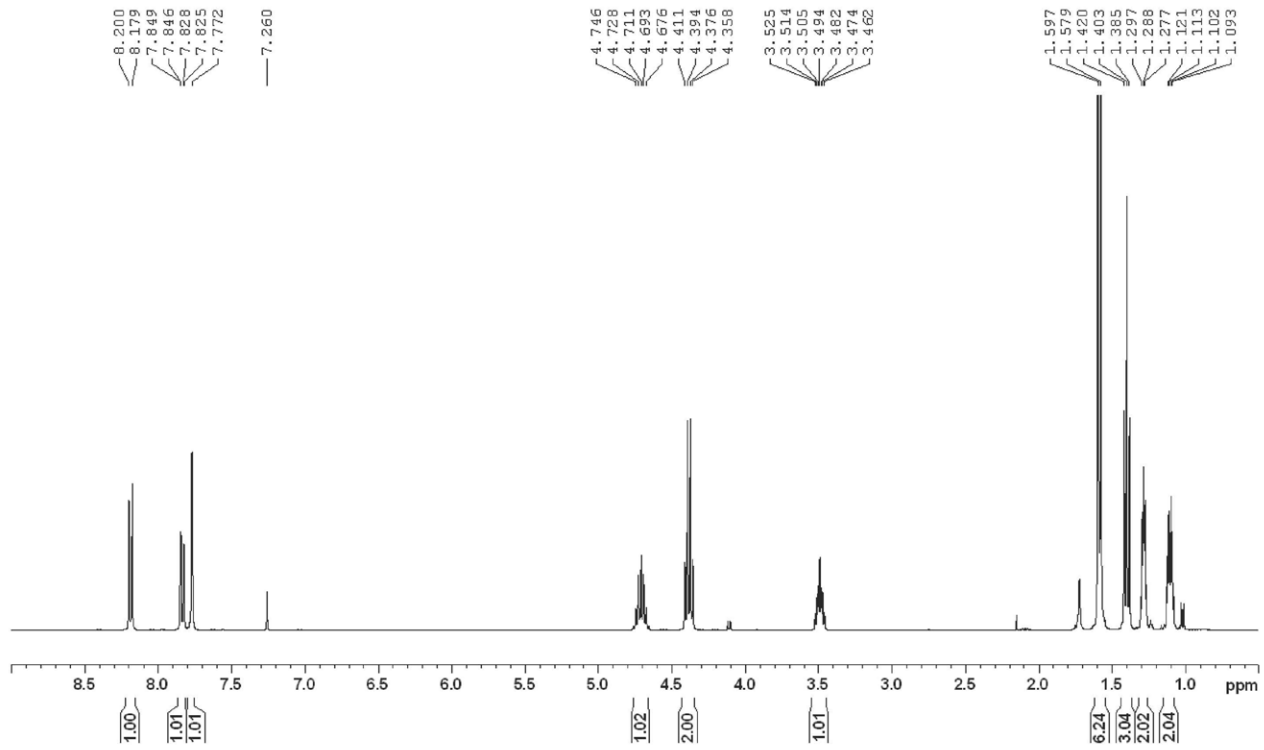

Figure S7. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a04**.

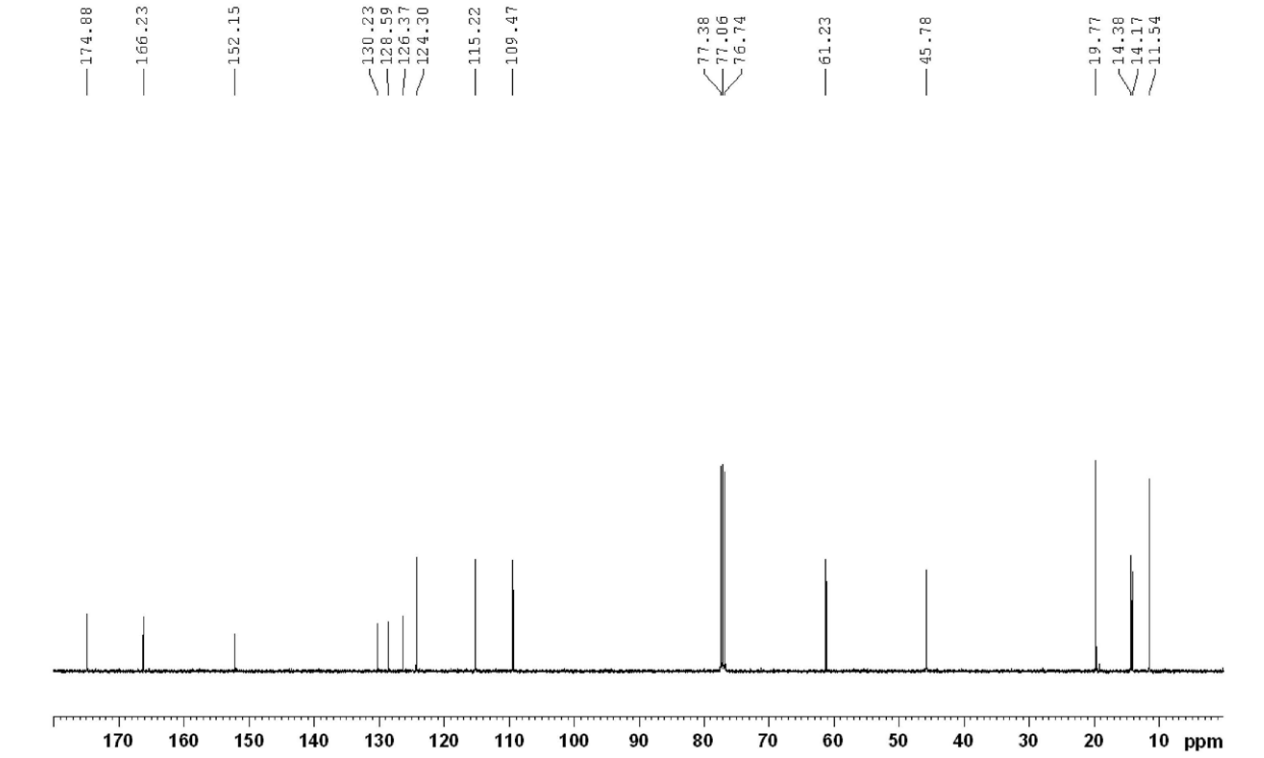

Figure S8. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a04**.

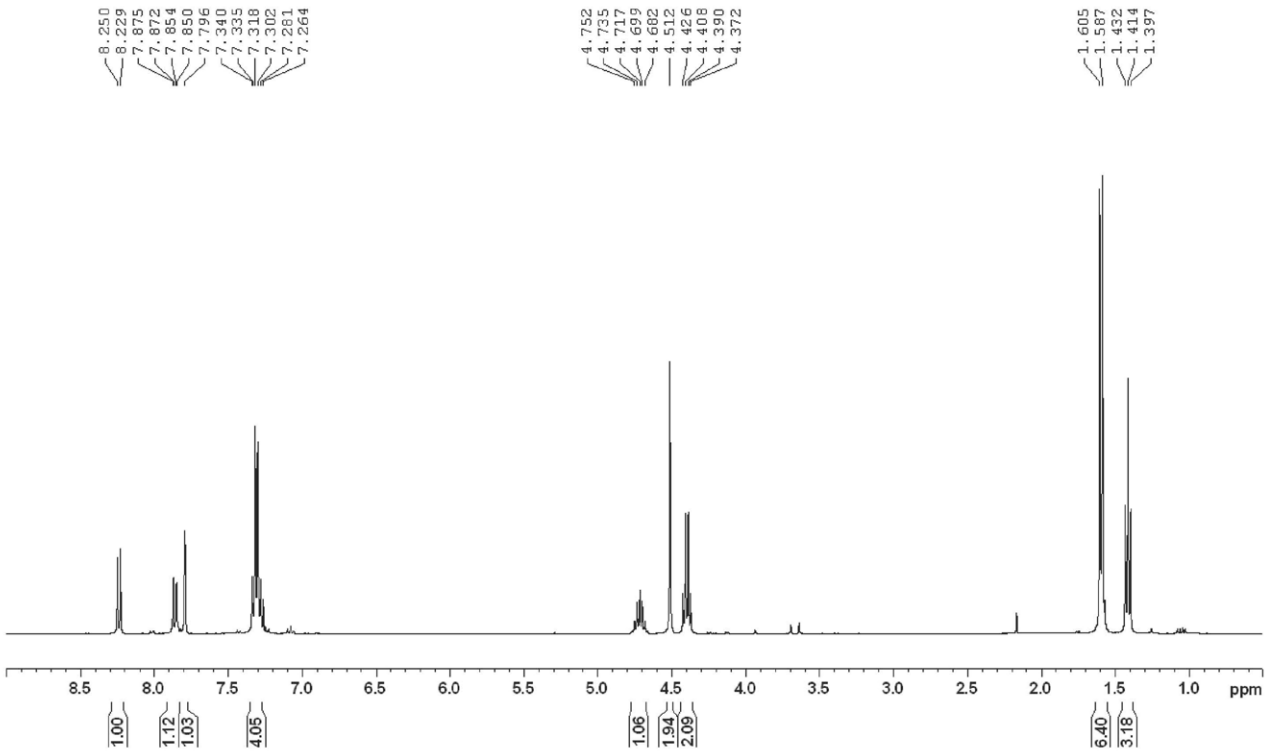

Figure S9. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a05**.

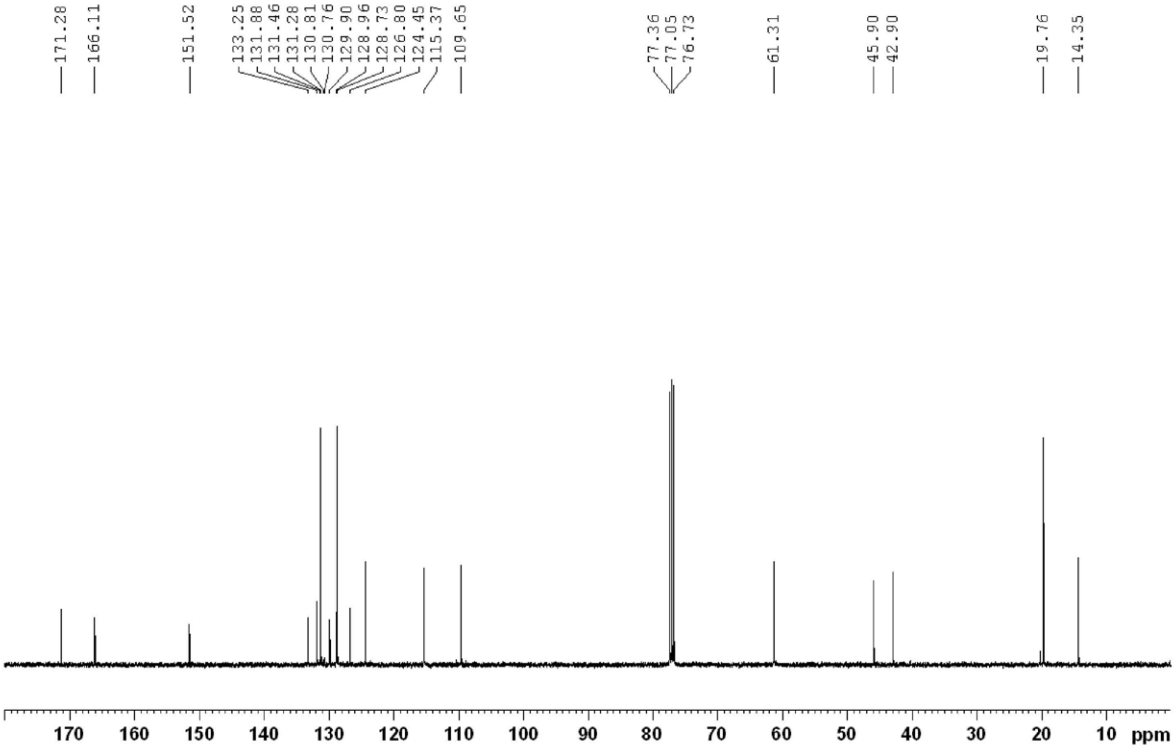

Figure S10. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a05**.

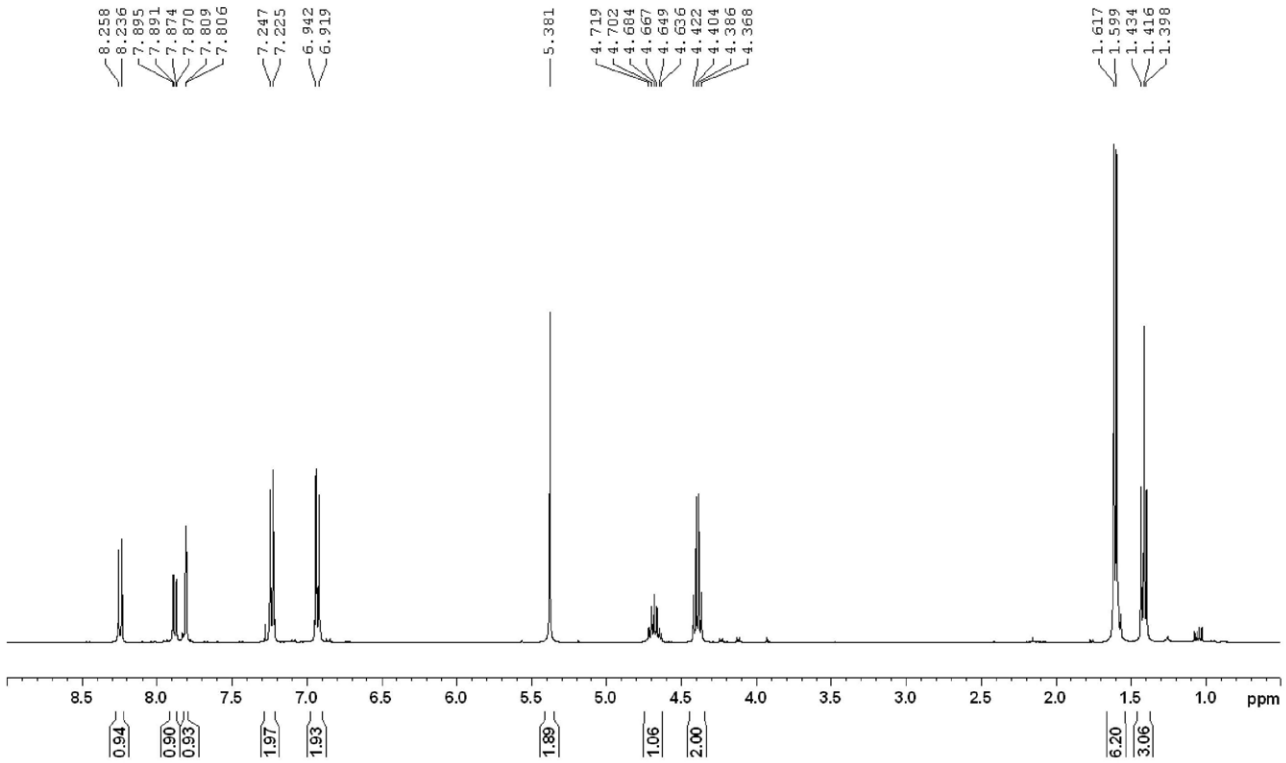

Figure S11. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a06**.

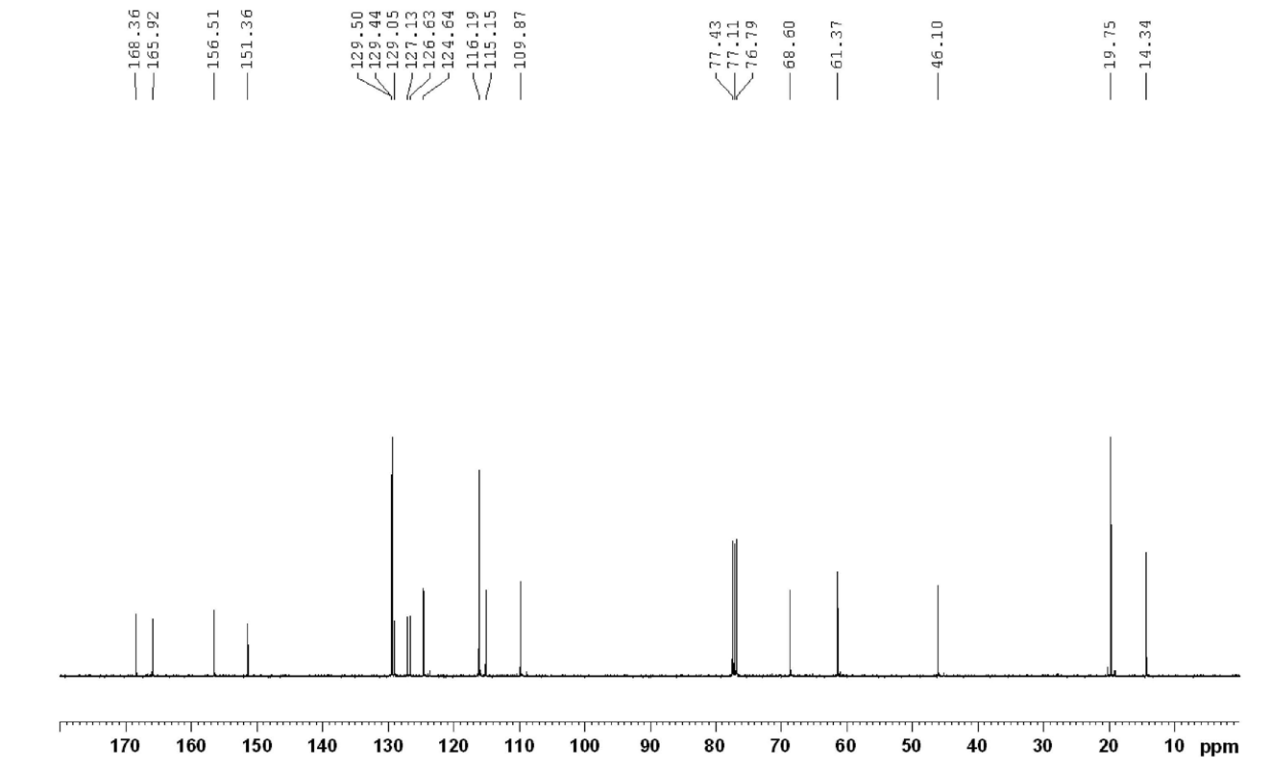

Figure S12. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a06**.

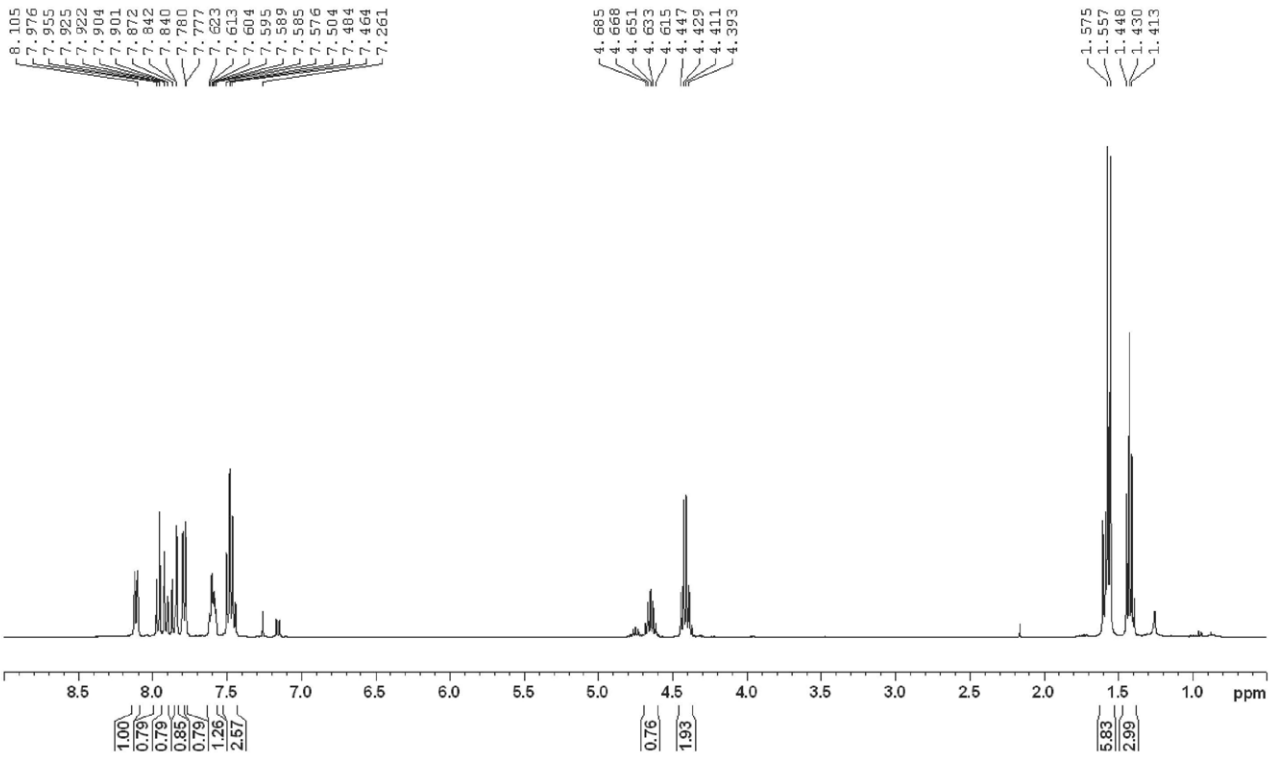

Figure S13. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a07**.

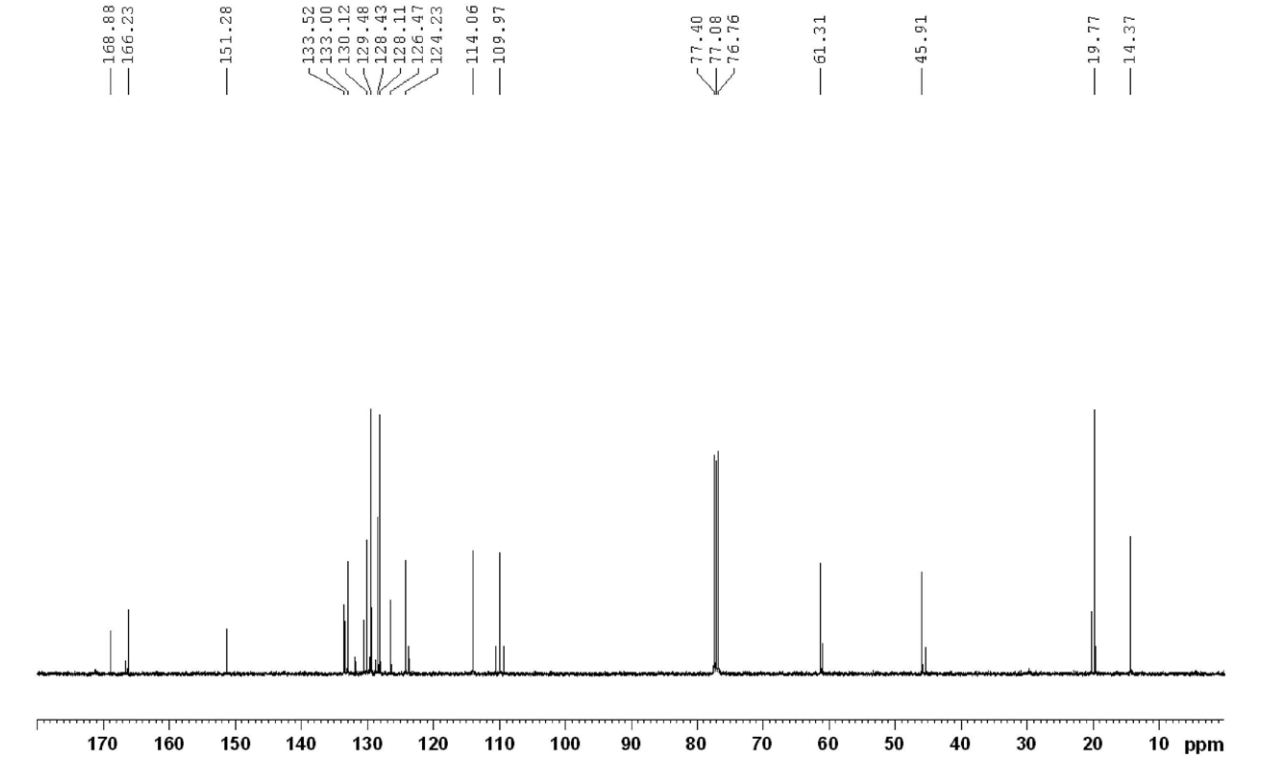

Figure S14. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a07**.

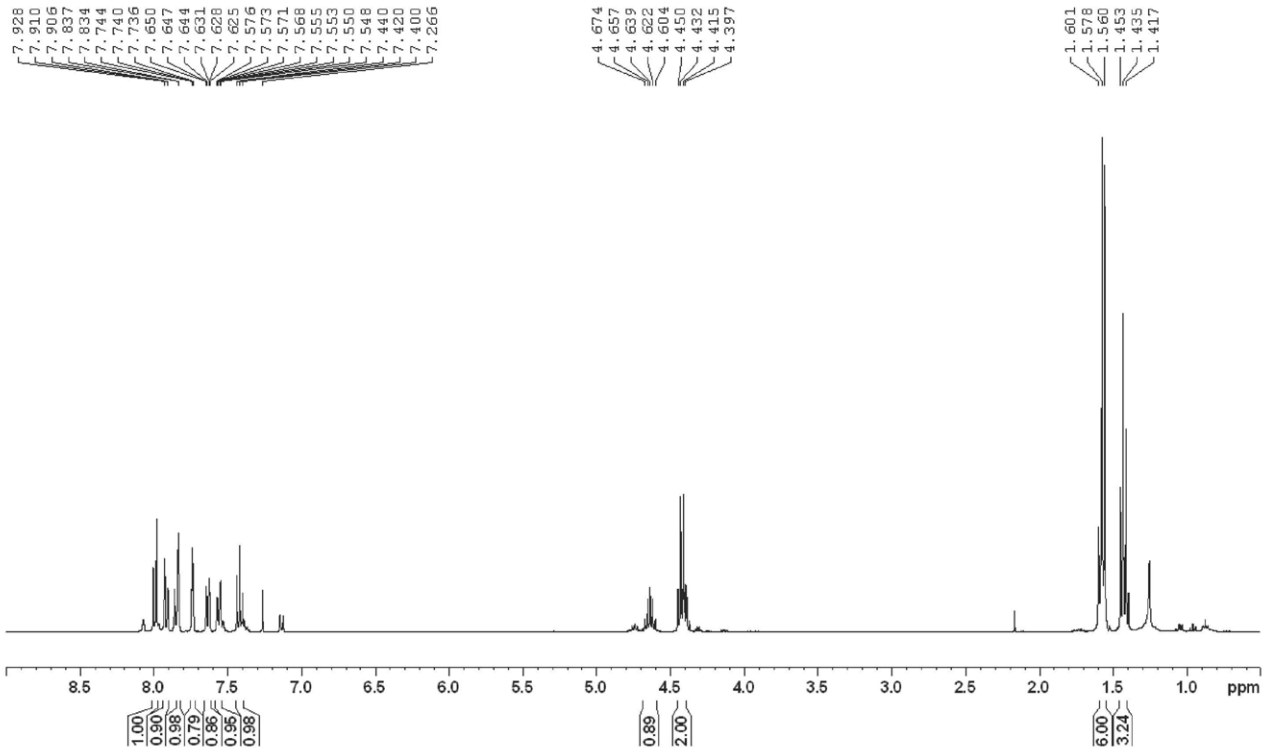

Figure S15. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a08**.

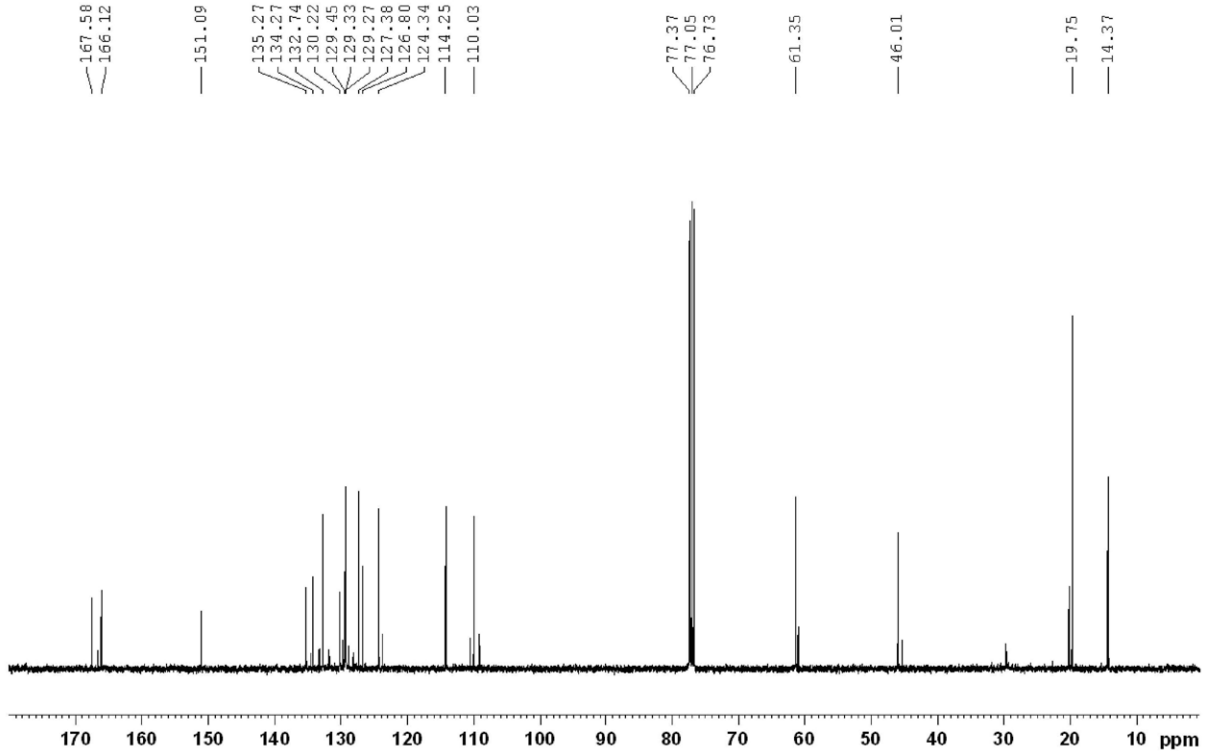

Figure S16. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a08**.

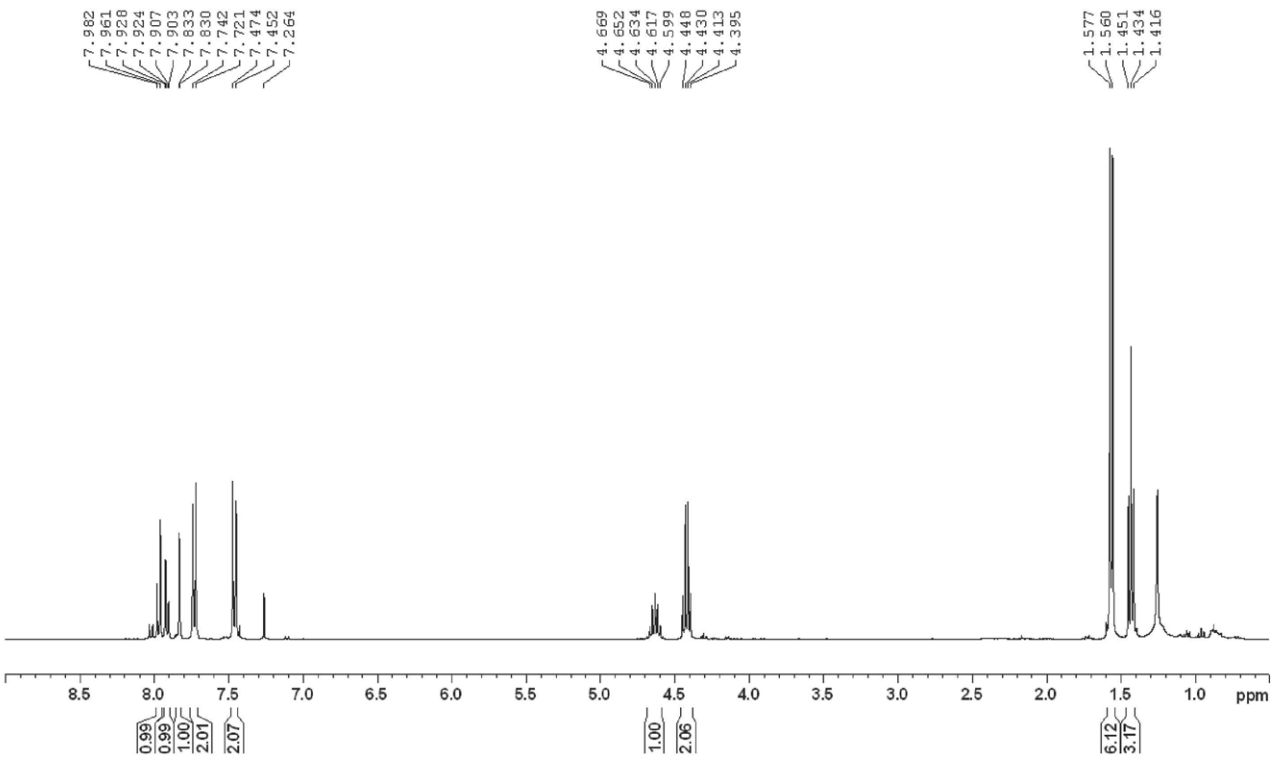

Figure S17. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a09**.

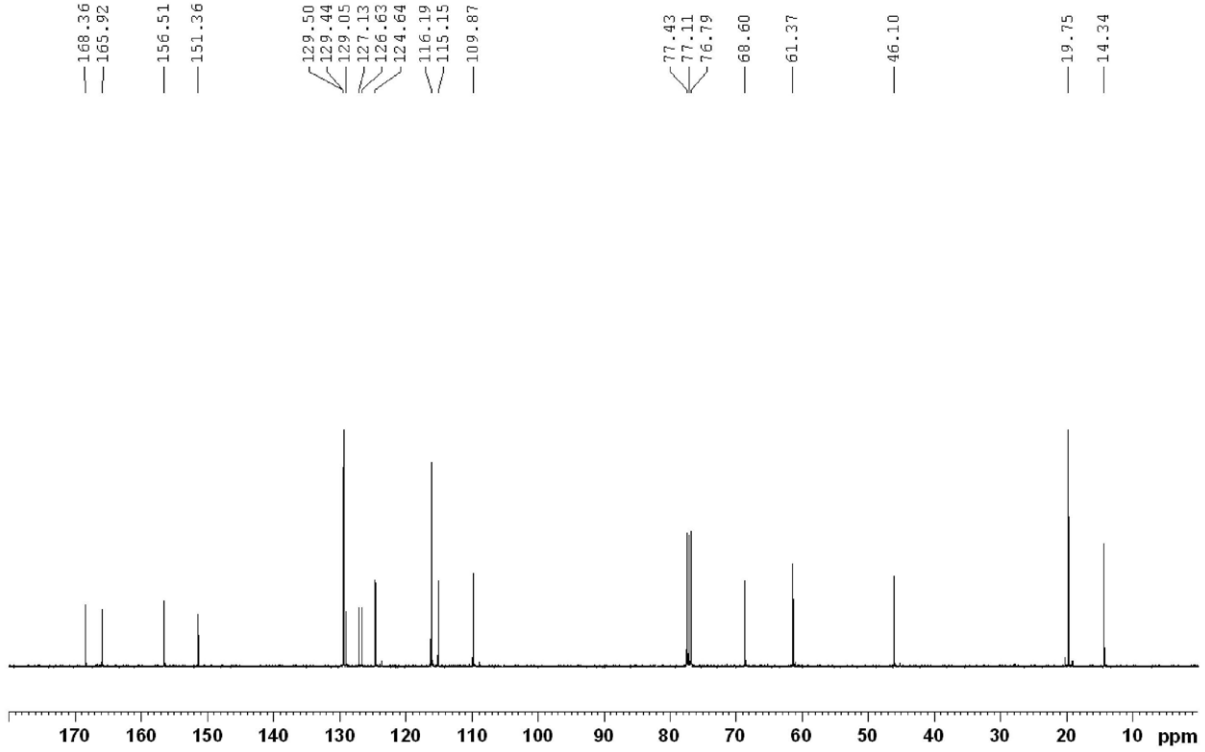

Figure S18. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a09**.

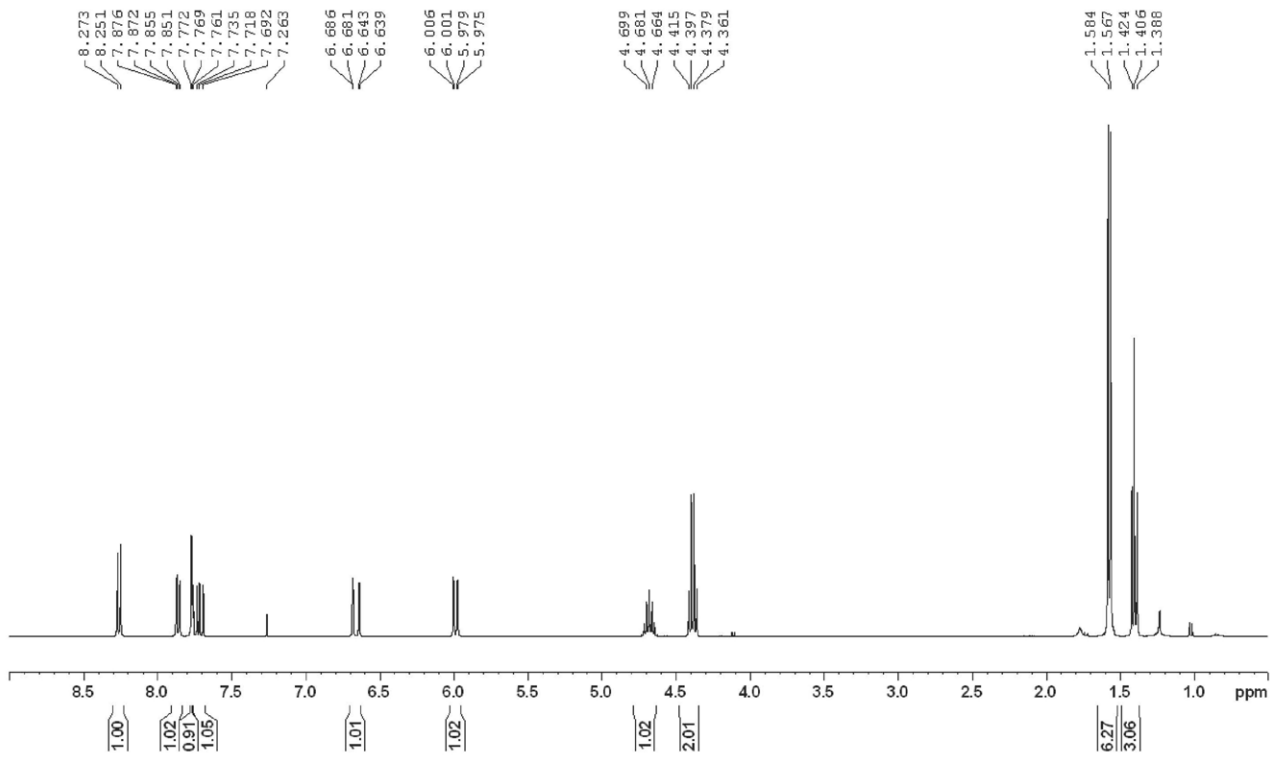

Figure S19. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a10**.

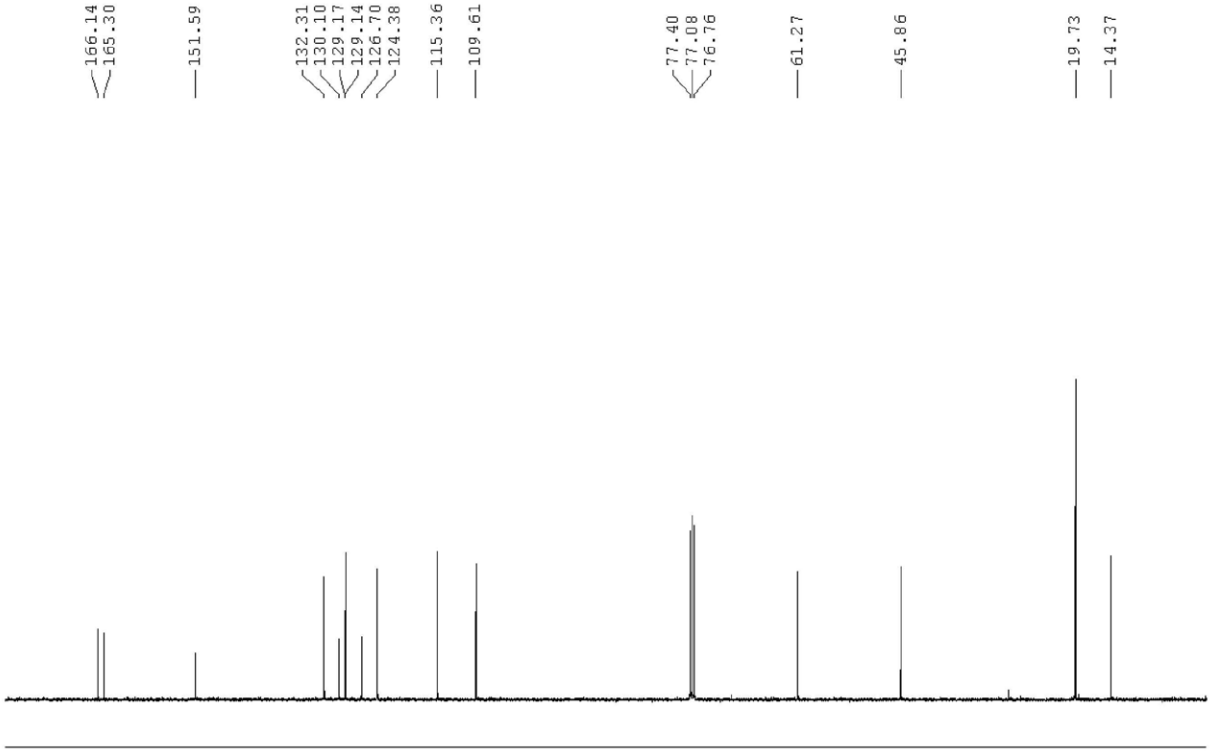

Figure S20. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a10**.

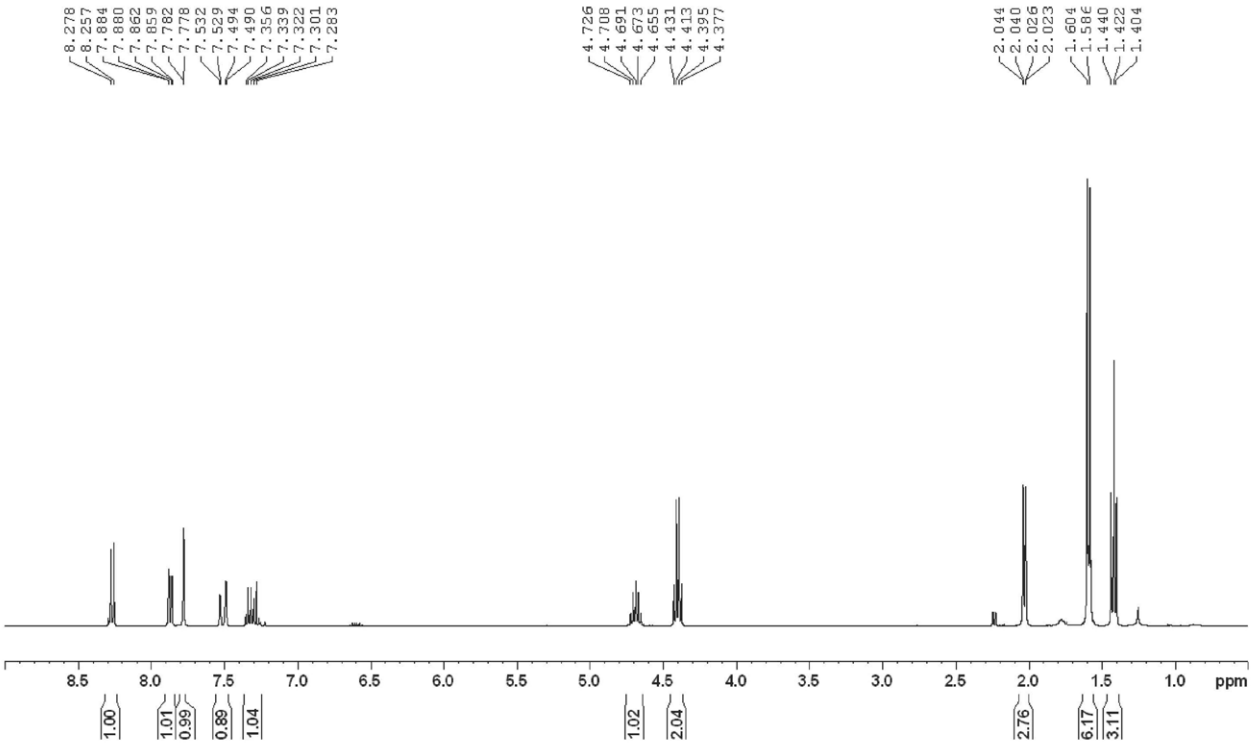

Figure S21. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a11**.

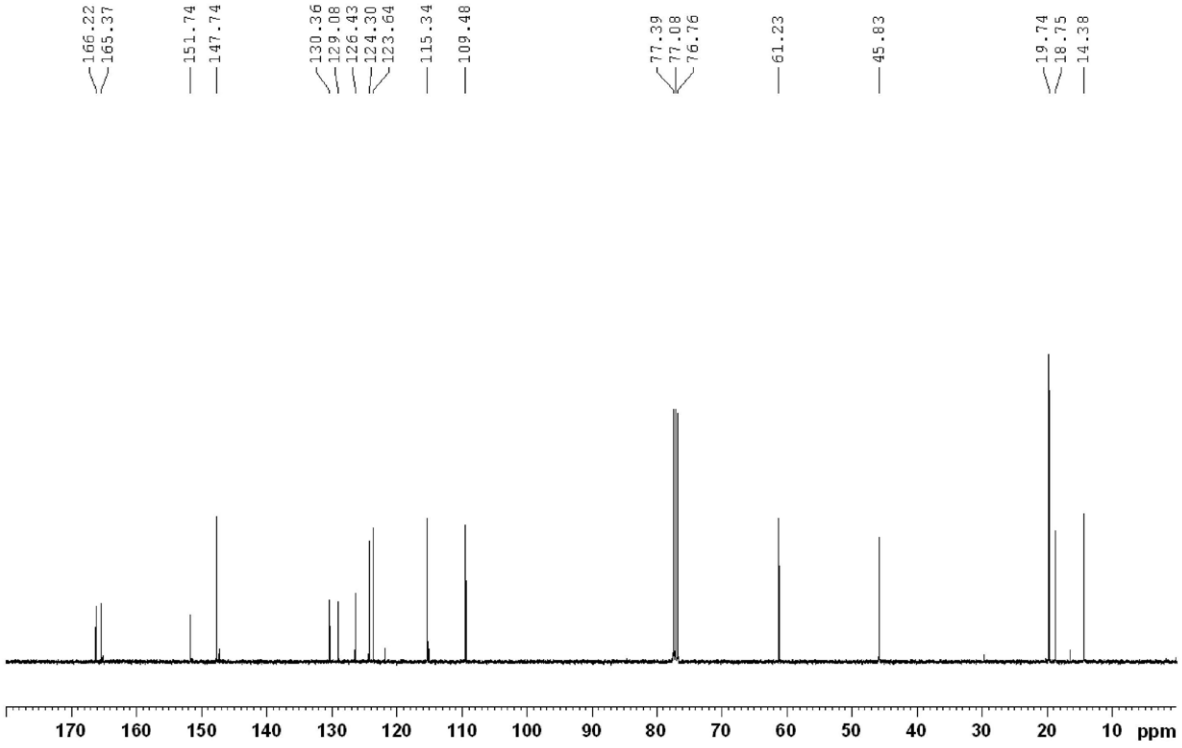

Figure S22. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a11**.

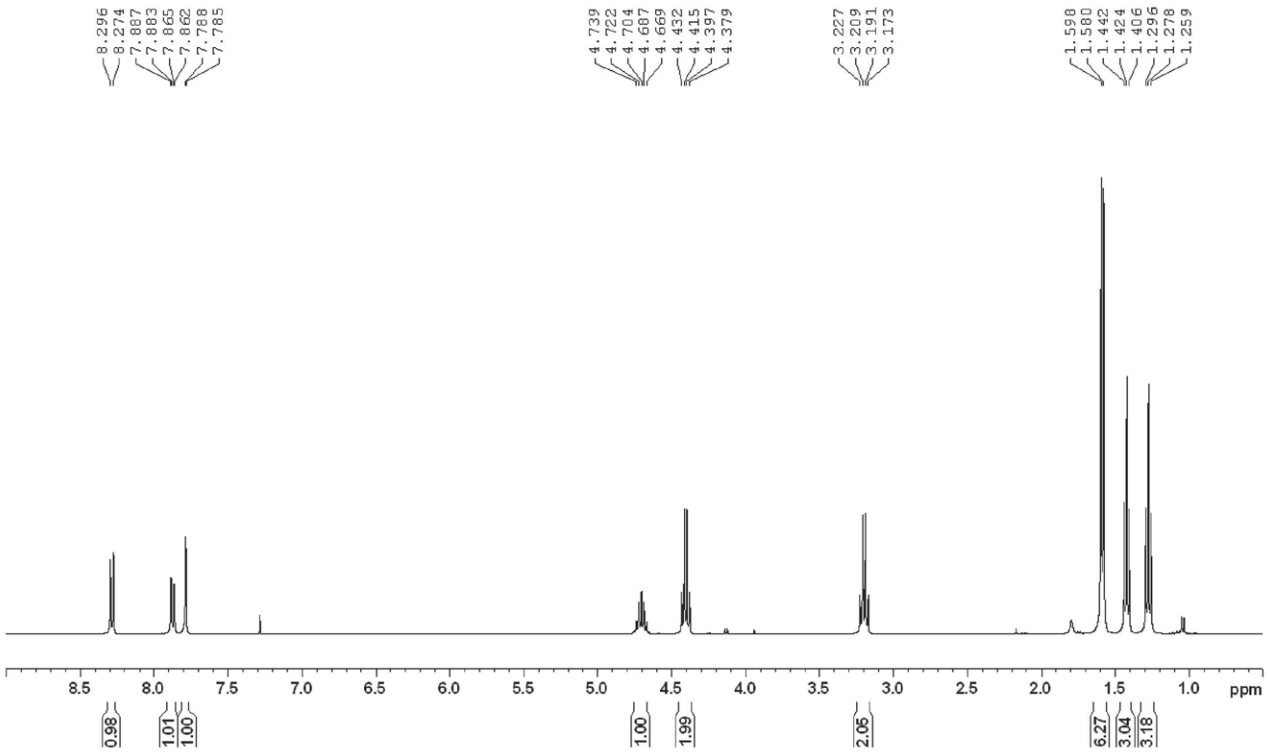

Figure S23. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a12**.

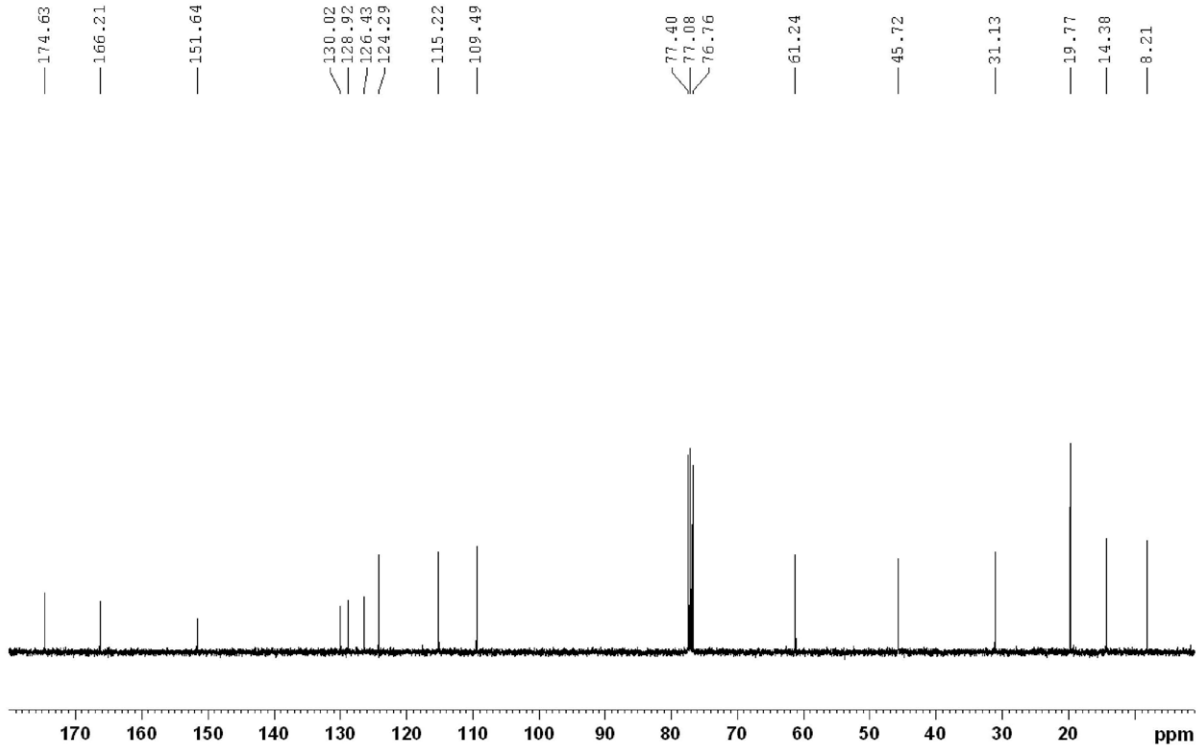

Figure S24. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a12**.

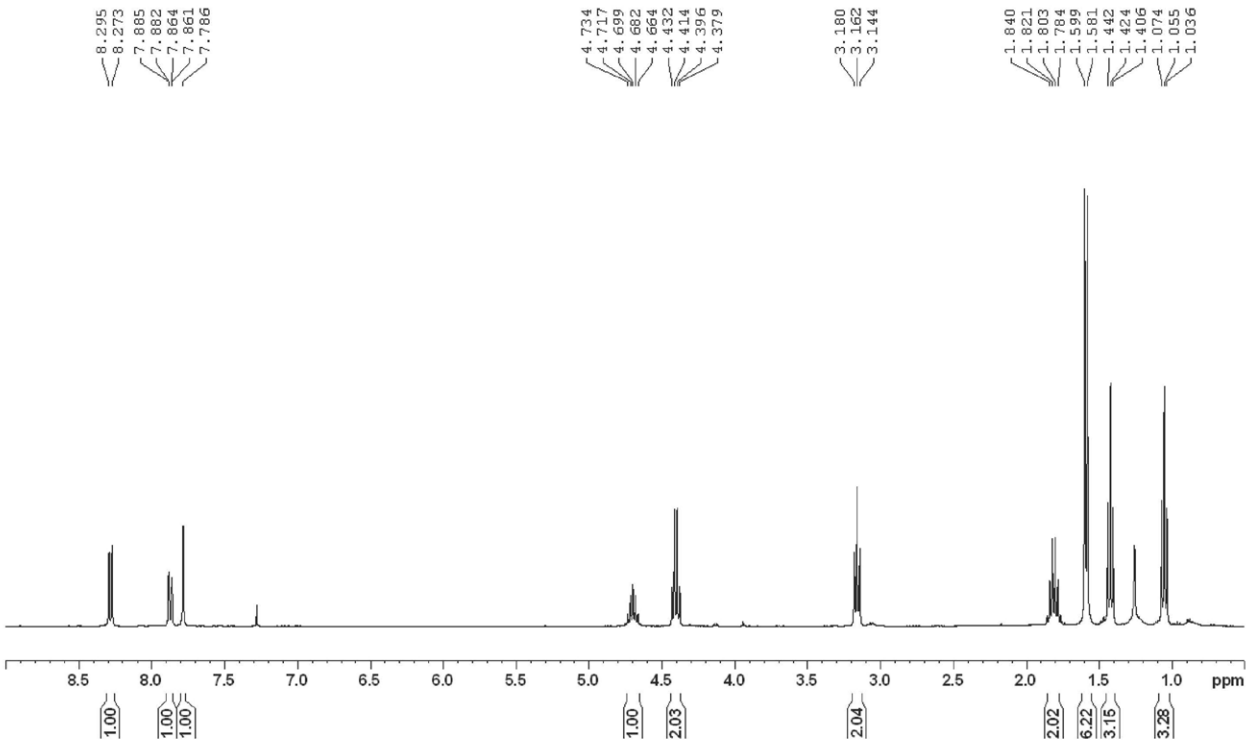

Figure S25. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a13**.

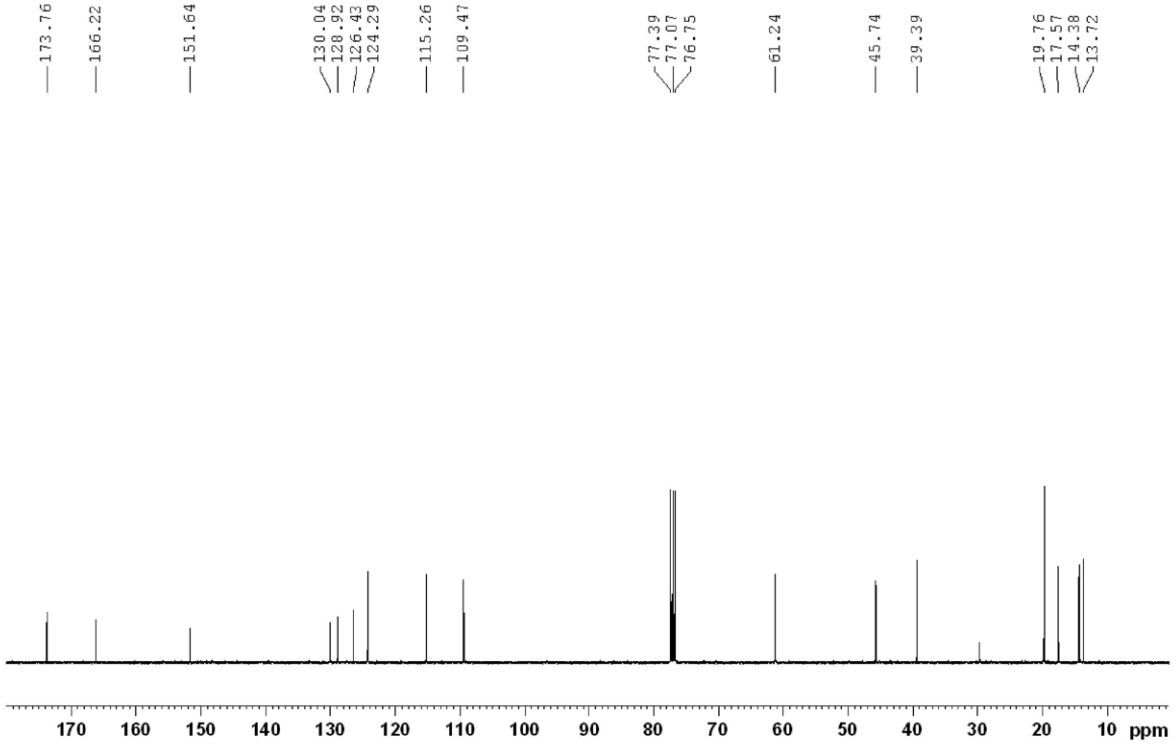

Figure S26. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a13**.

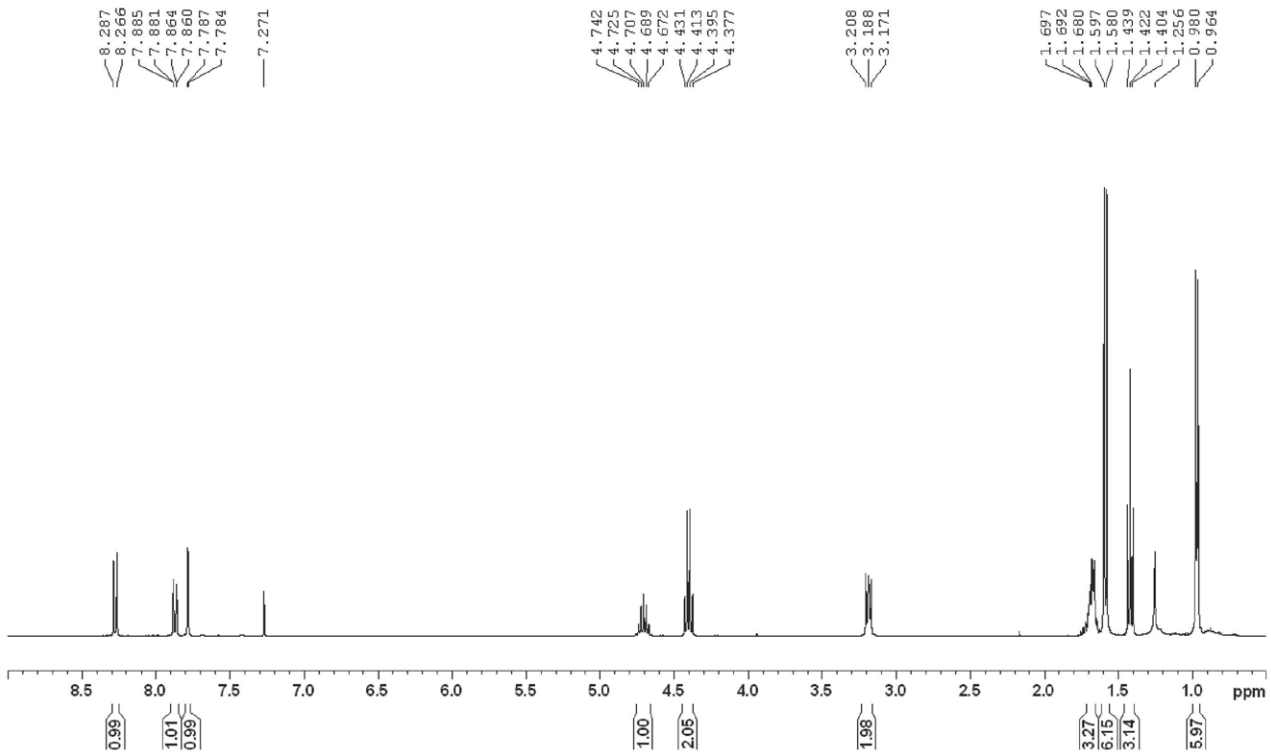

Figure S27. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a14**.

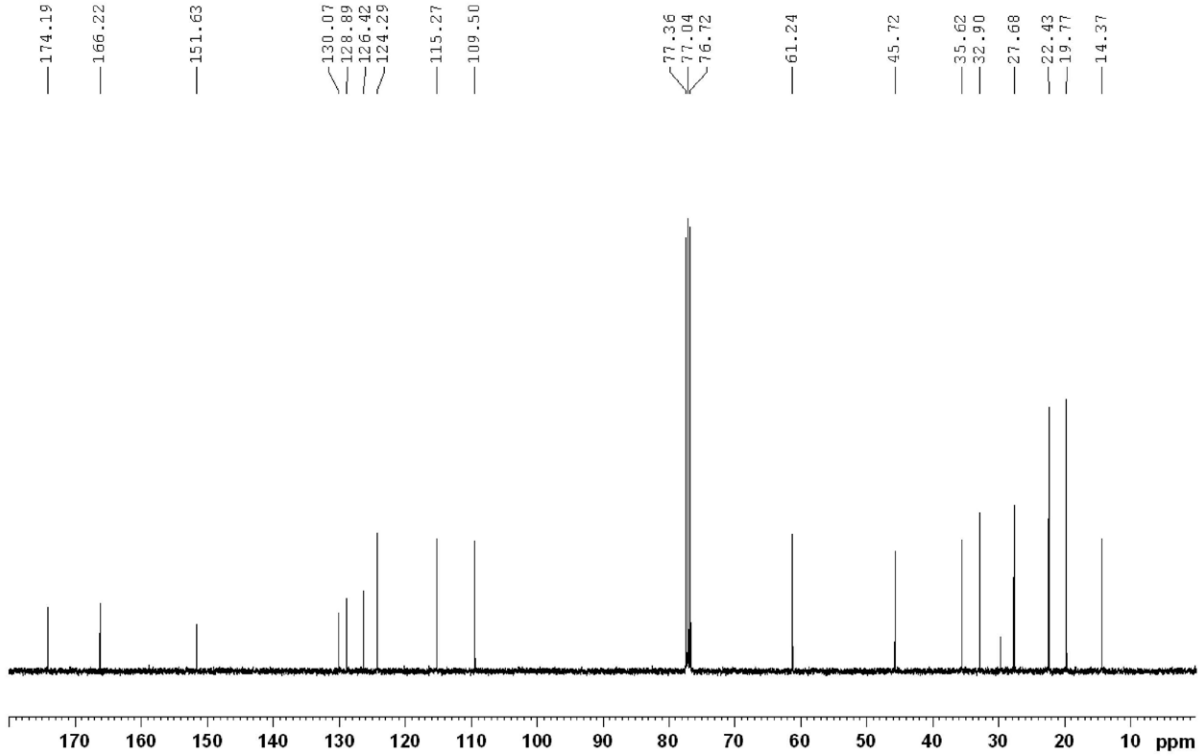

Figure S28. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a14**.

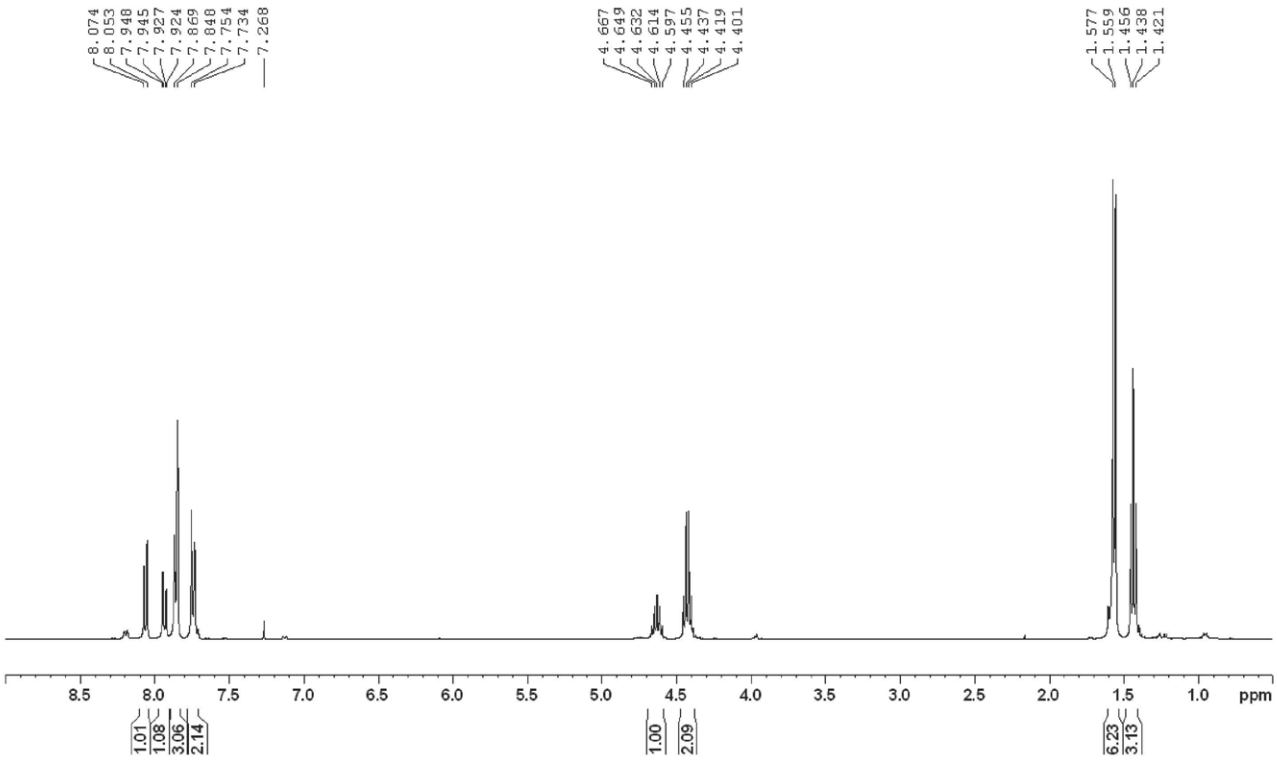

Figure S29. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **11a15**.

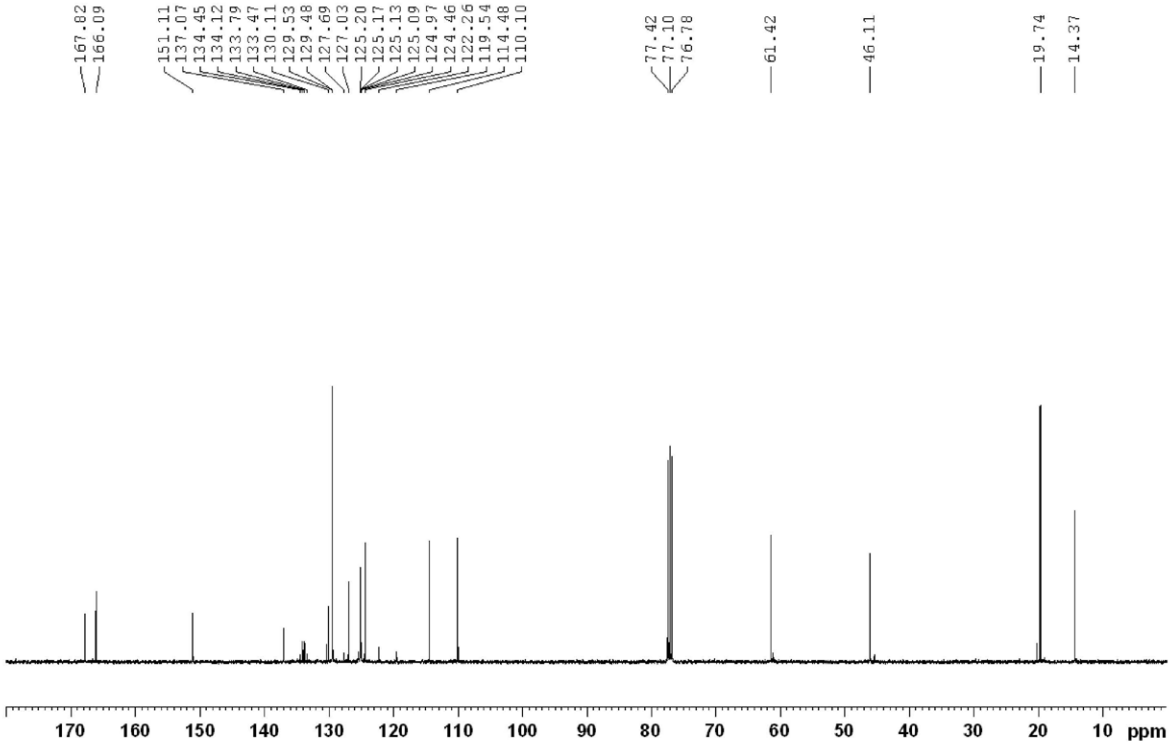

Figure S30. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **11a15**.

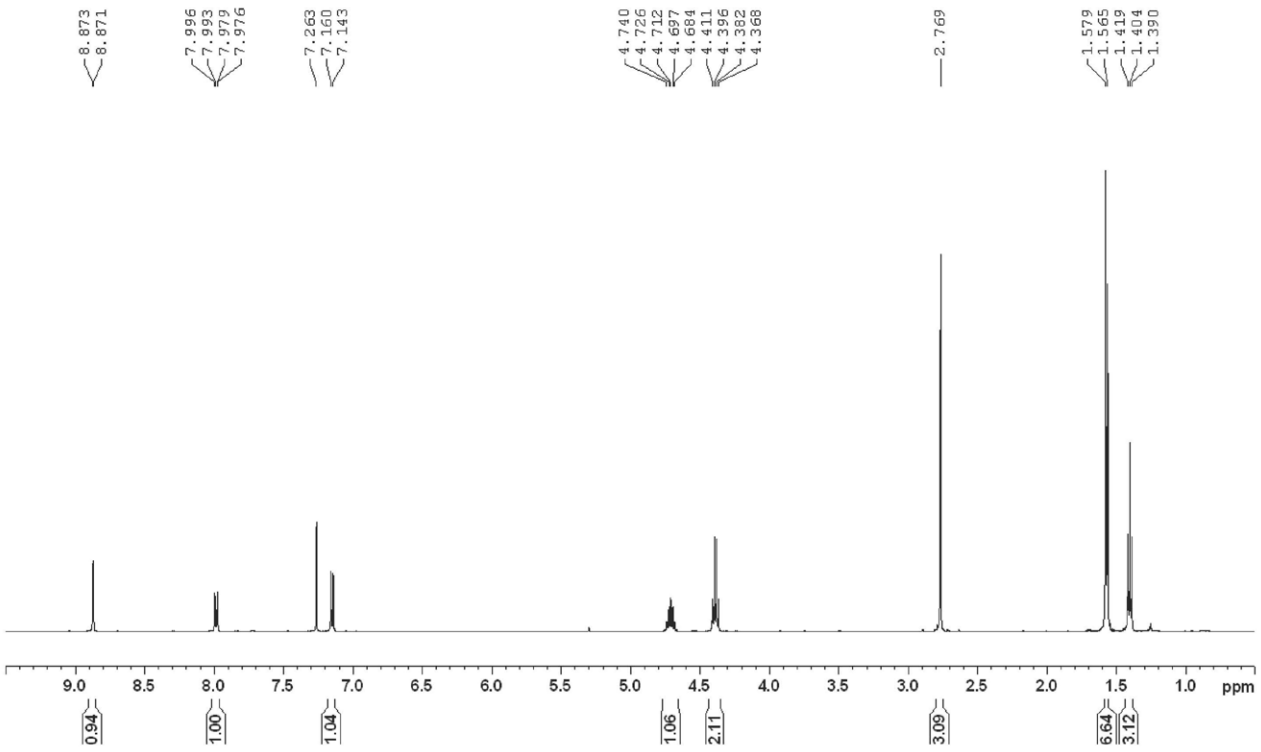

Figure S31. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b01**.

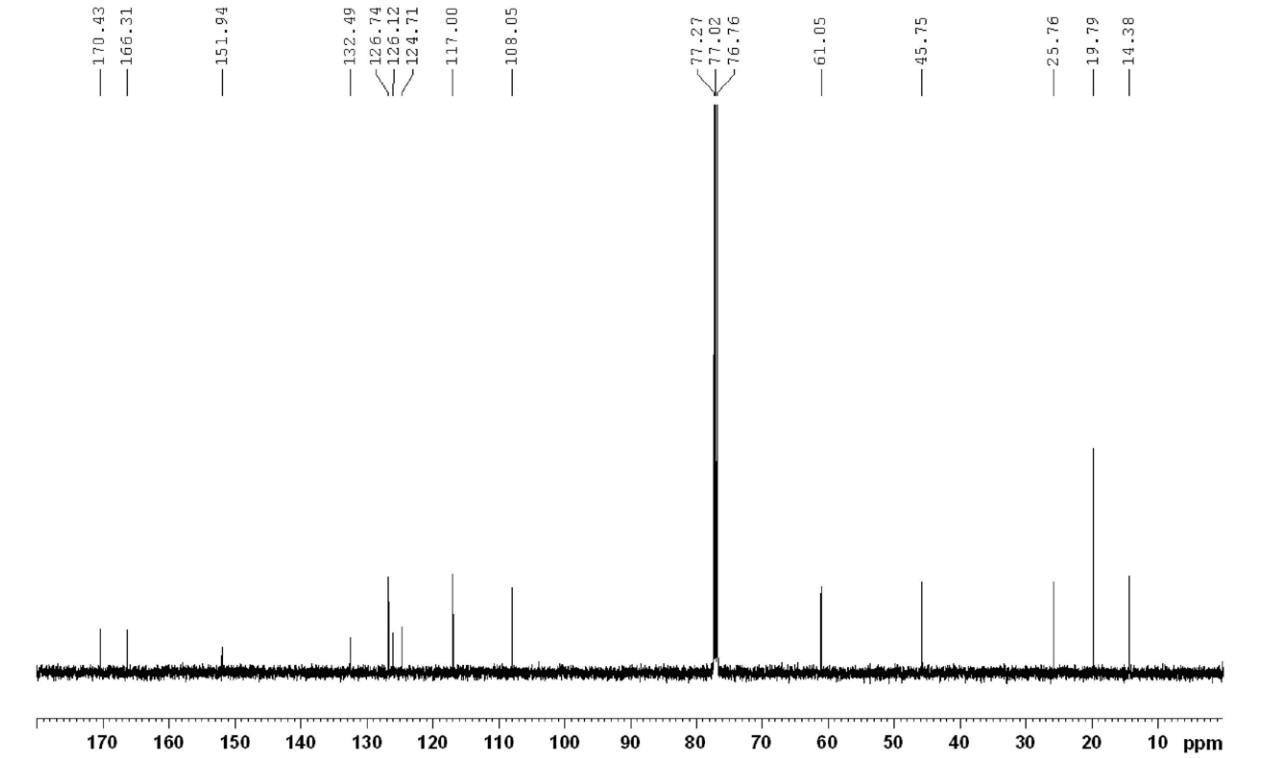

Figure S32. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b01**.

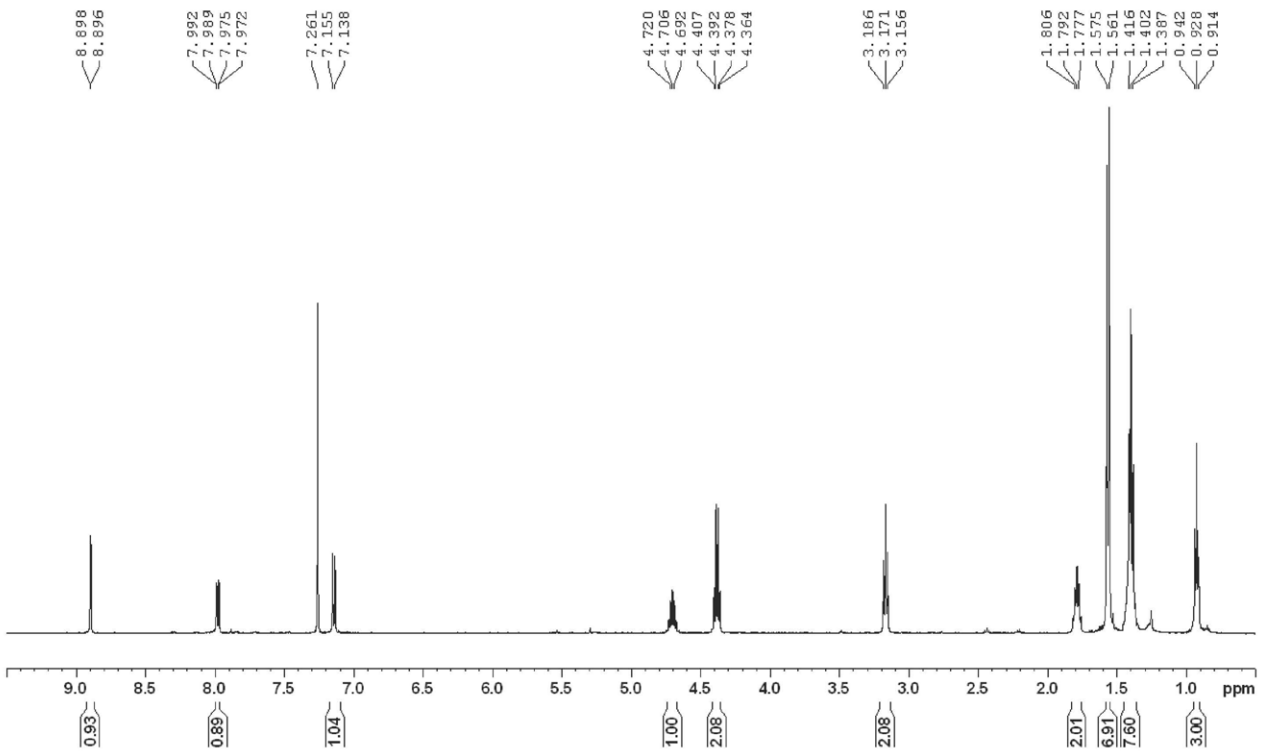

Figure S33. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b02**.

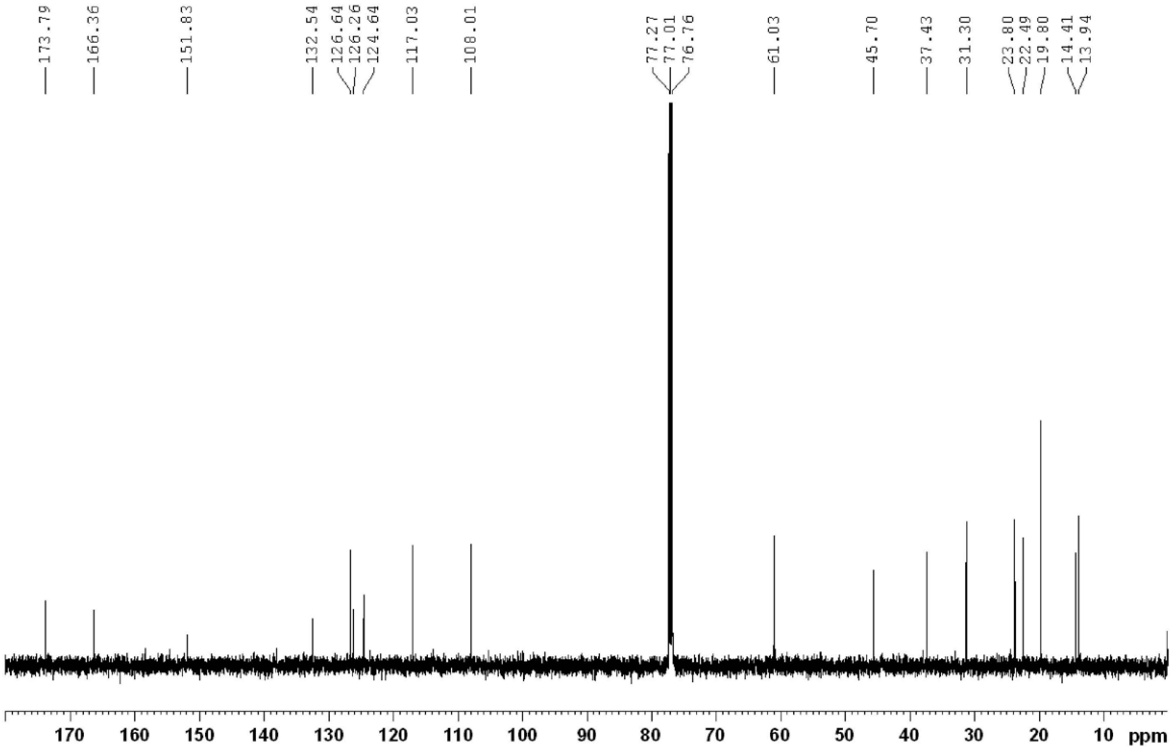

Figure S34. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b02**.

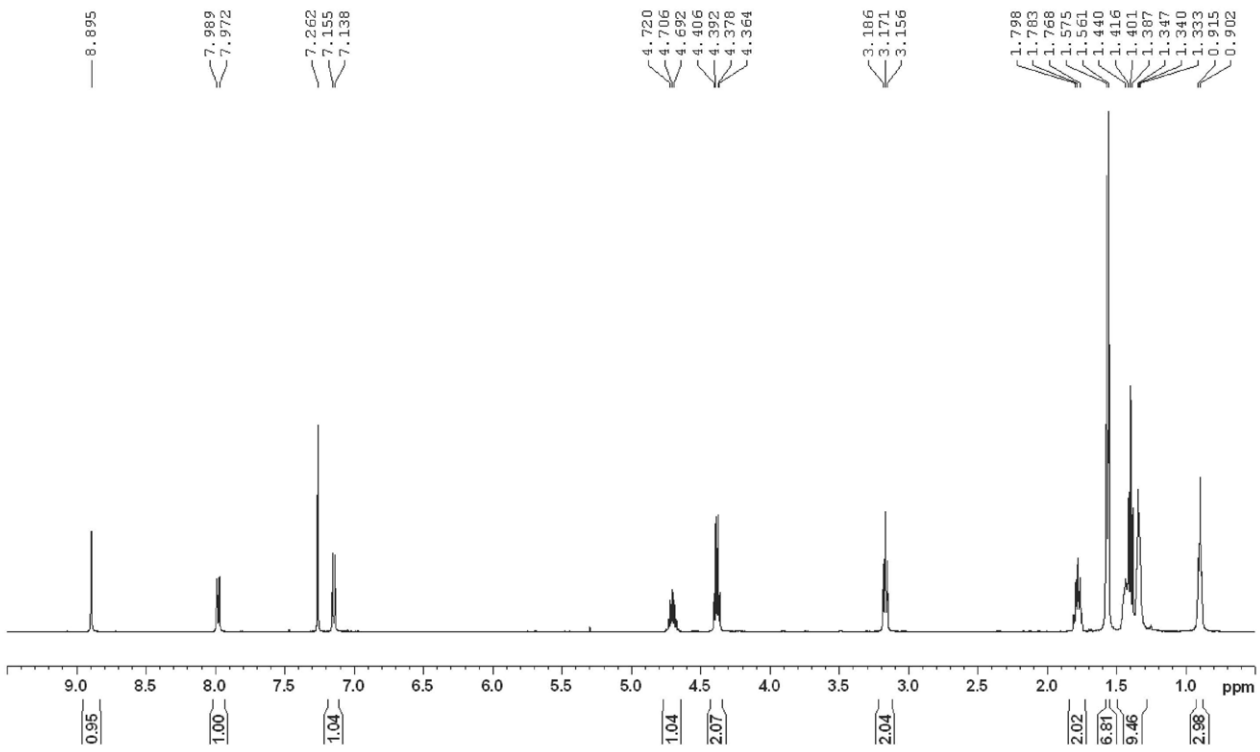

Figure S35. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b03**.

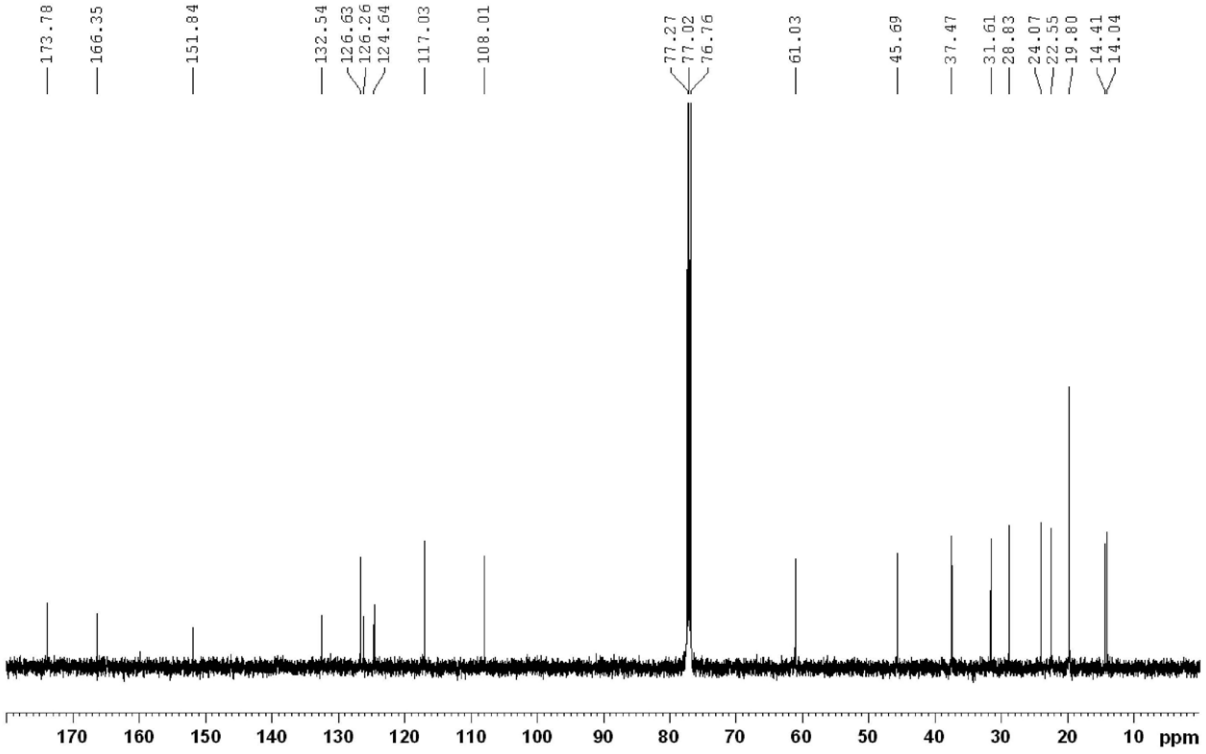

Figure S36. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b03**.

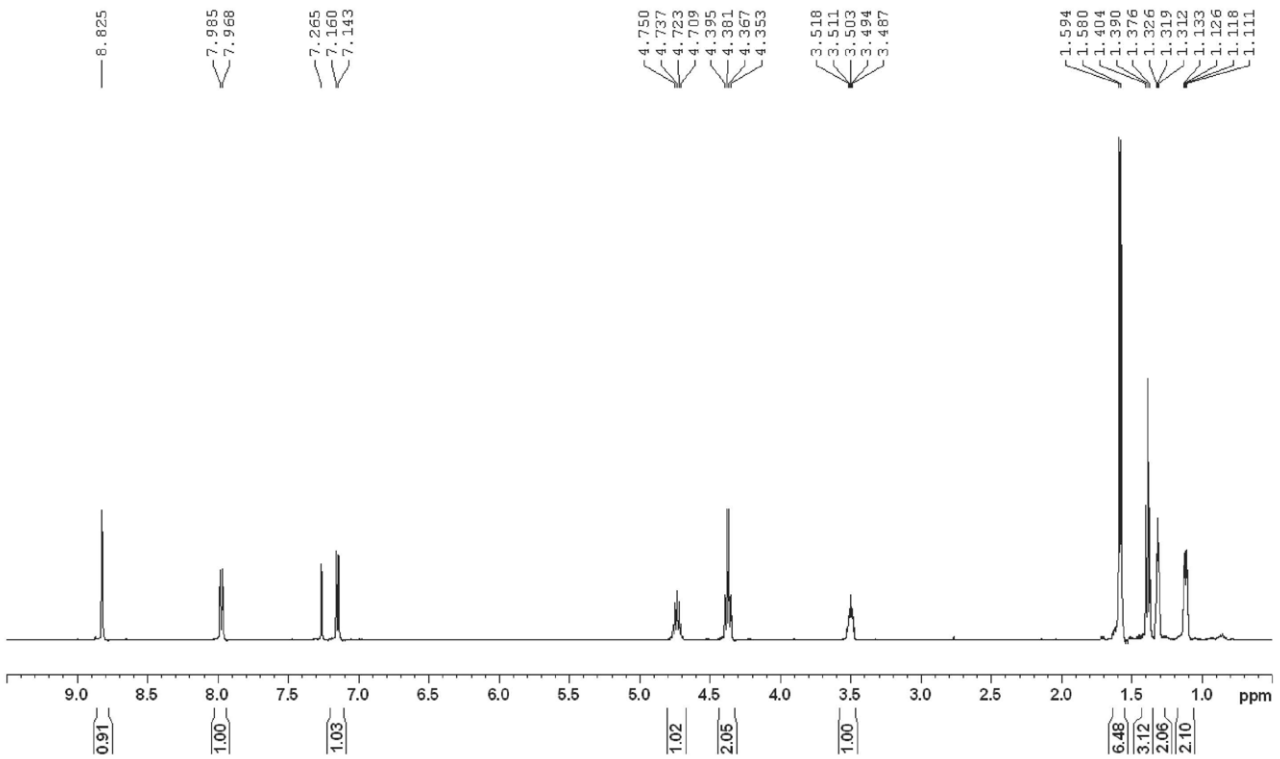

Figure S37. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b04**.

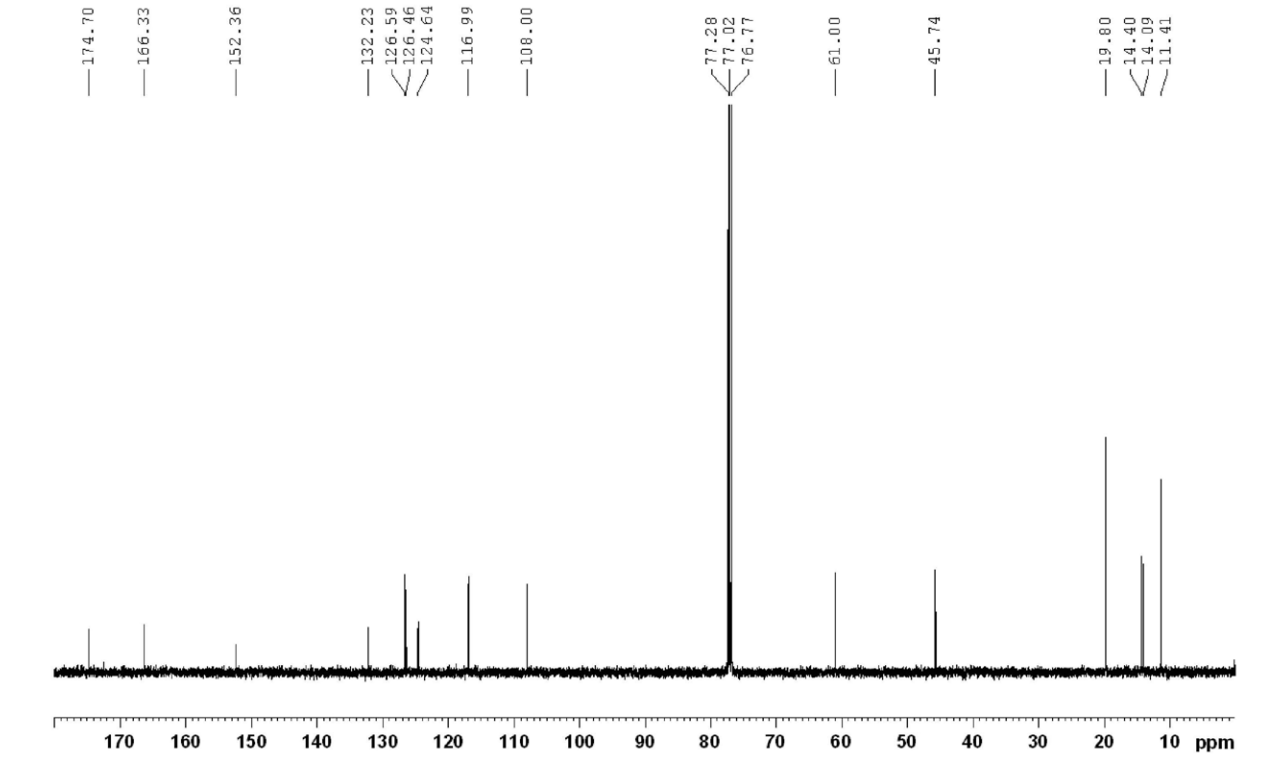

Figure S38. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b04**.

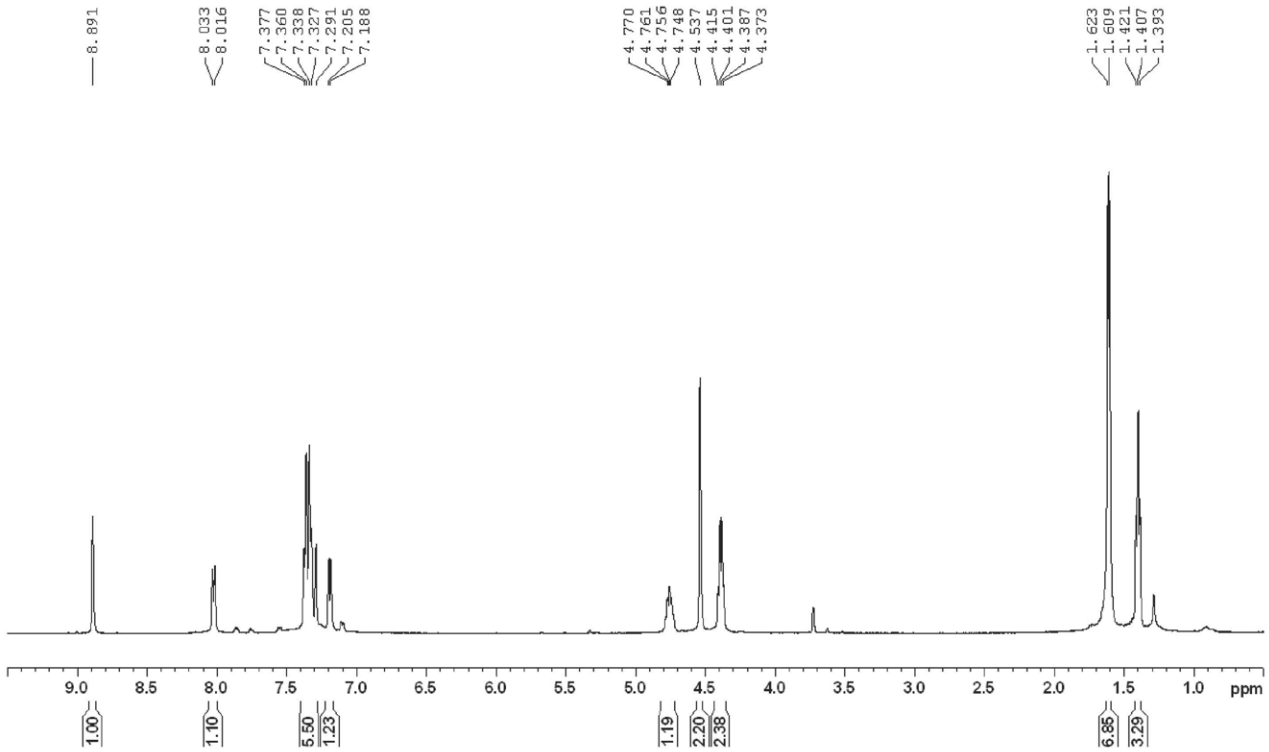

Figure S39. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b05**.

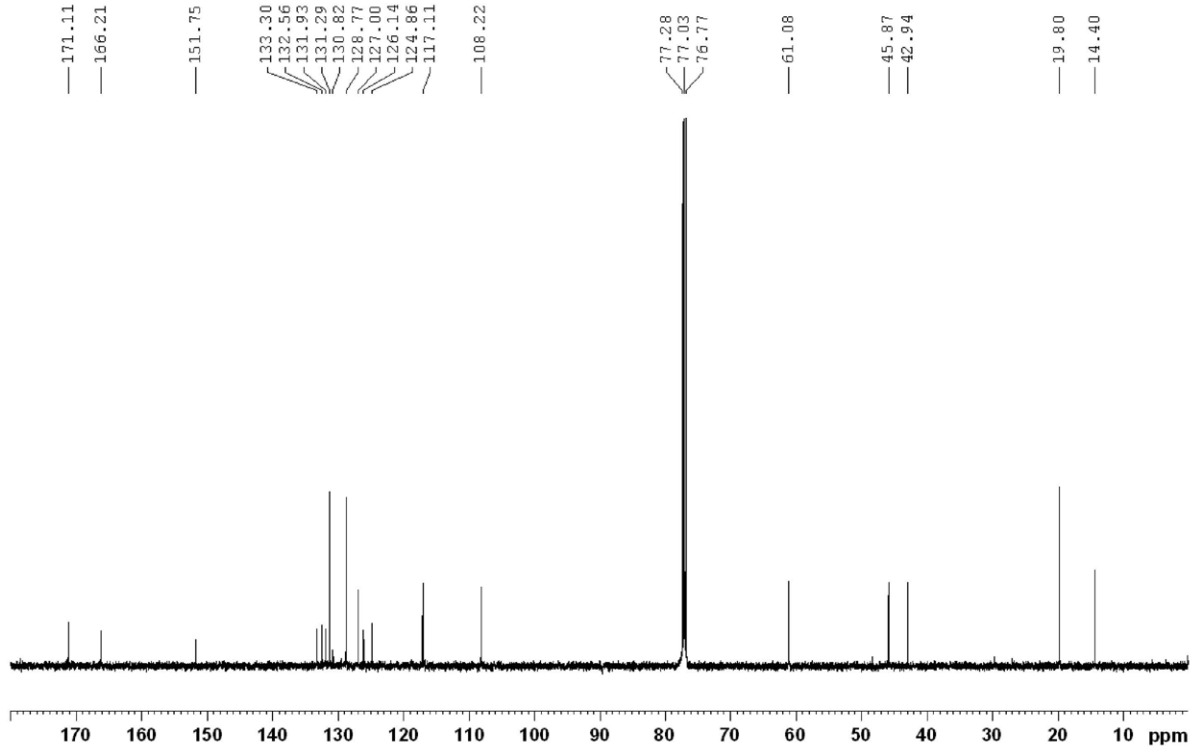

Figure S40. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b05**.

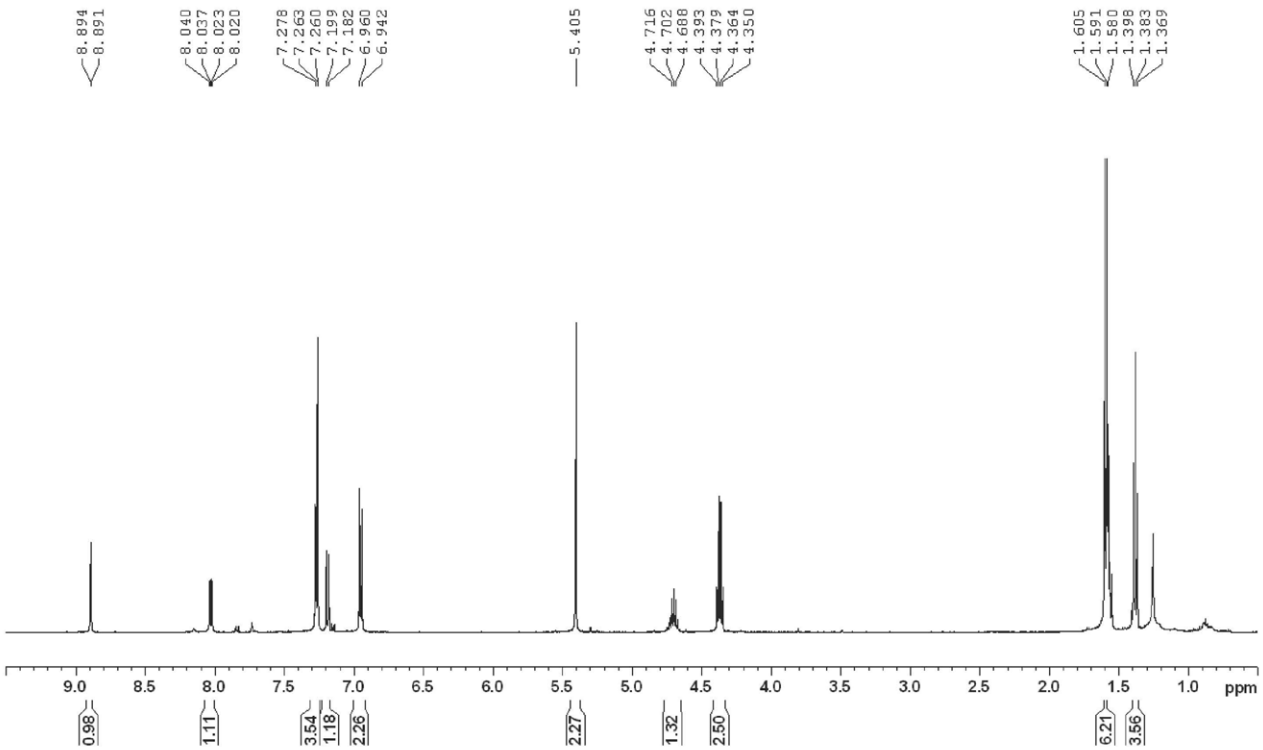

Figure S41. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b06**.

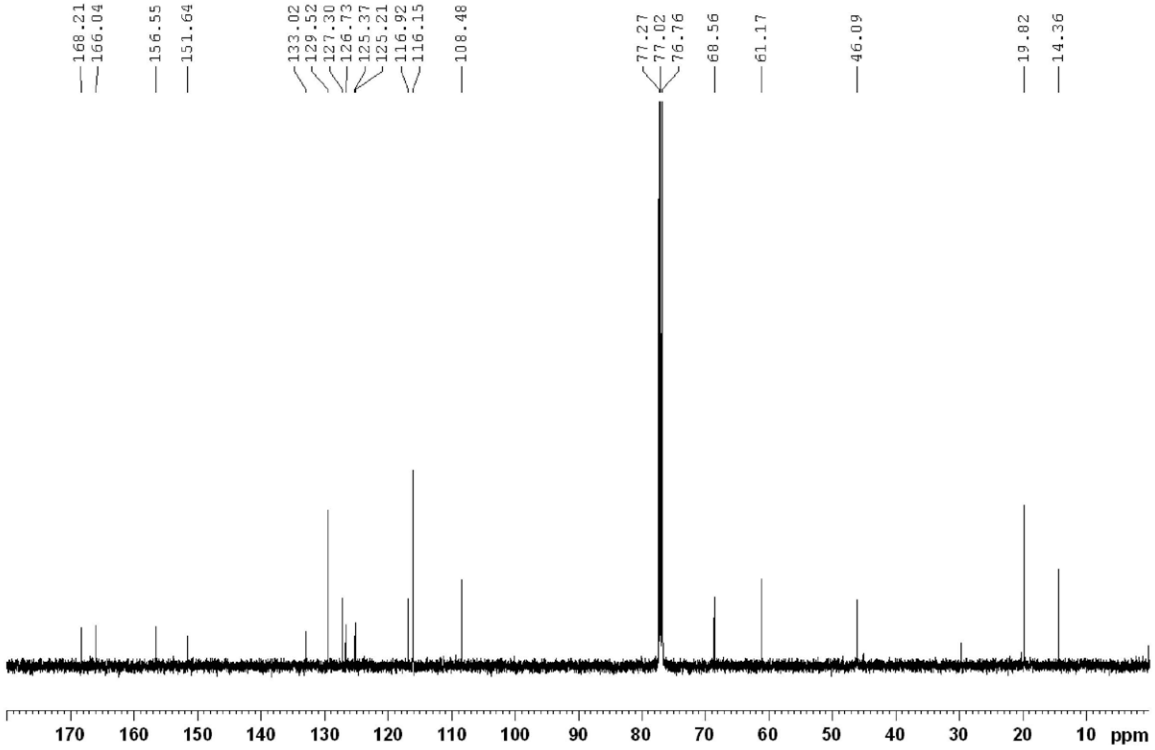

Figure S42. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b06**.

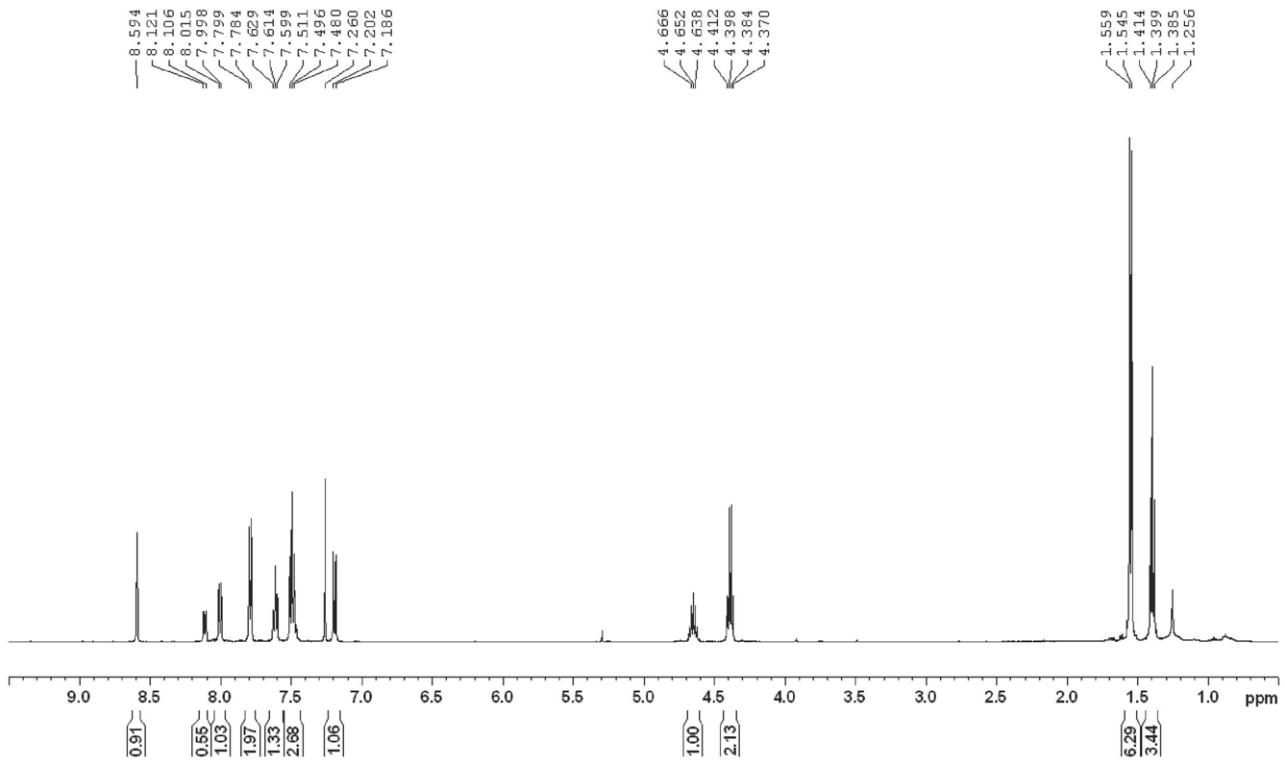

Figure S43. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b07**.

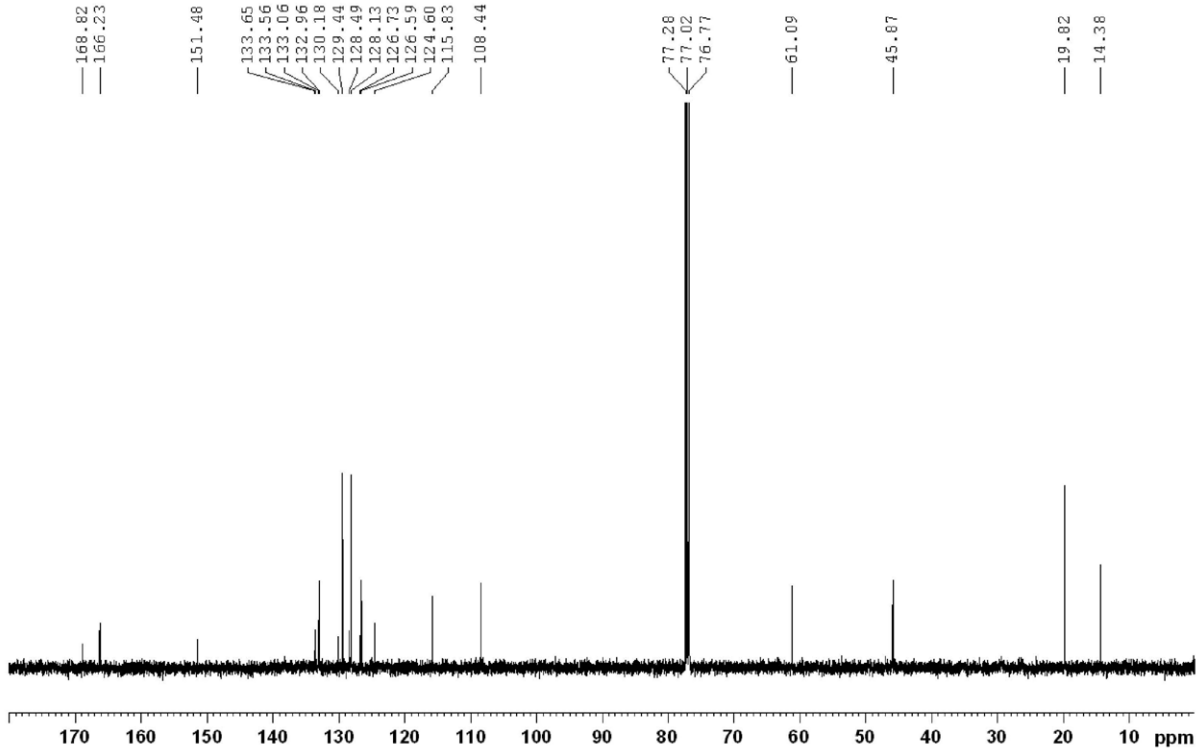

Figure S44. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b07**.

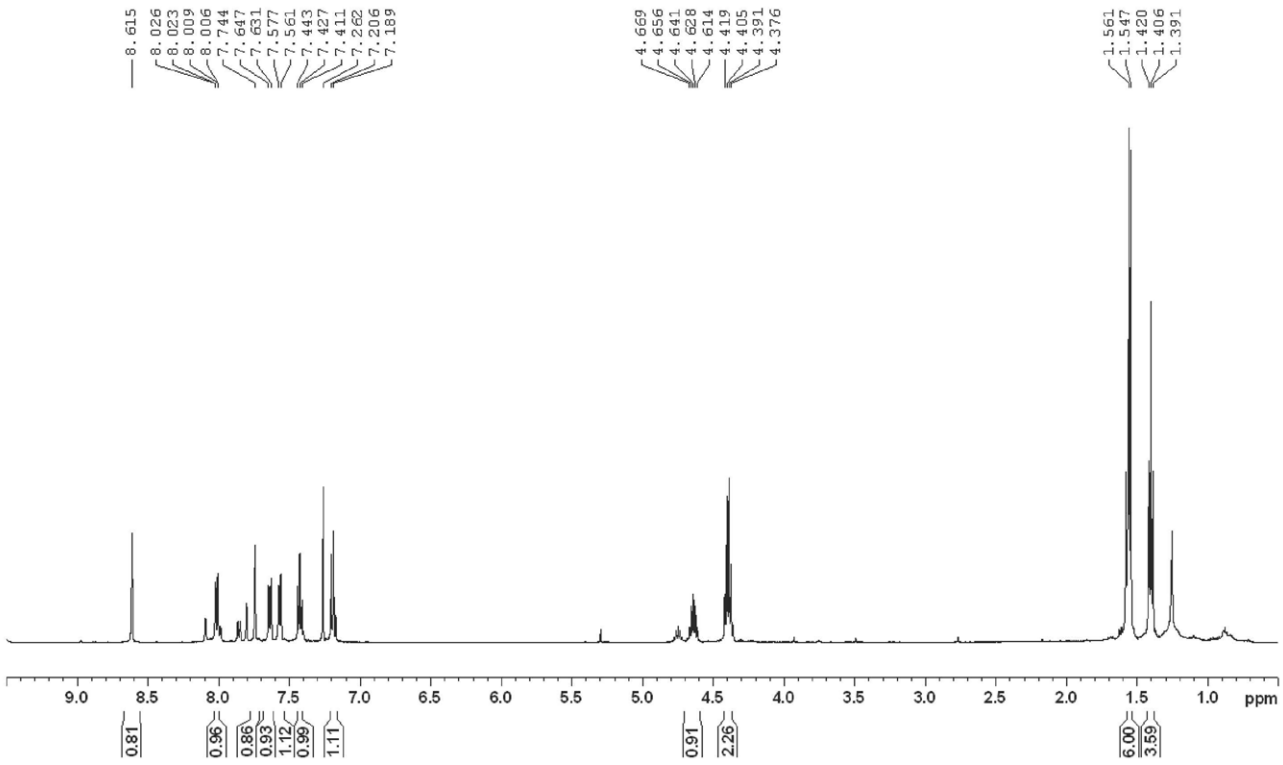

Figure S45. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b08**.

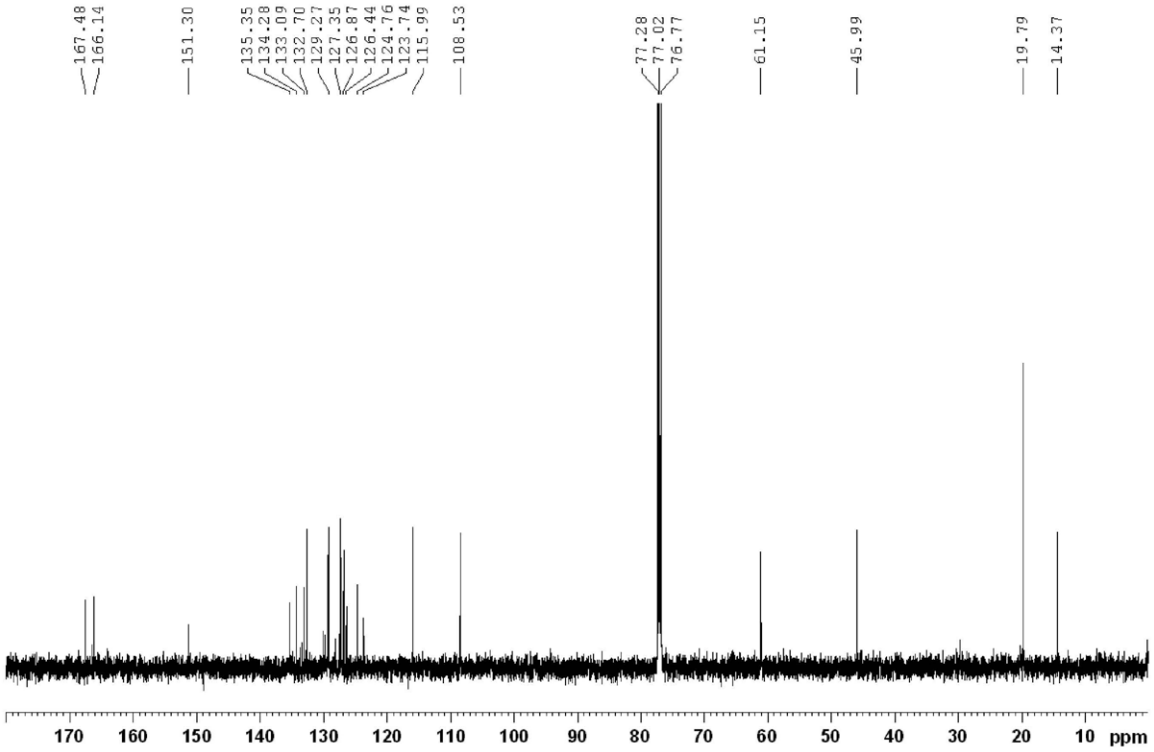

Figure S46. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b08**.

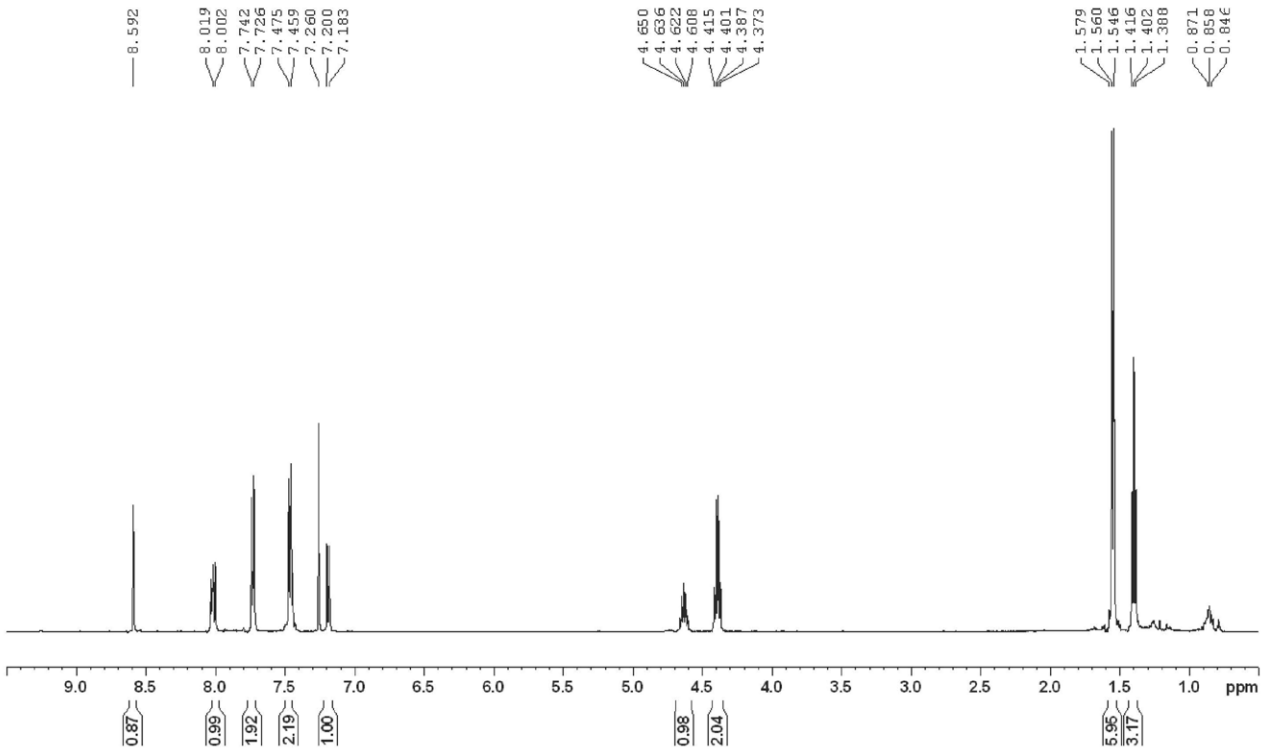

Figure S47. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b09**.

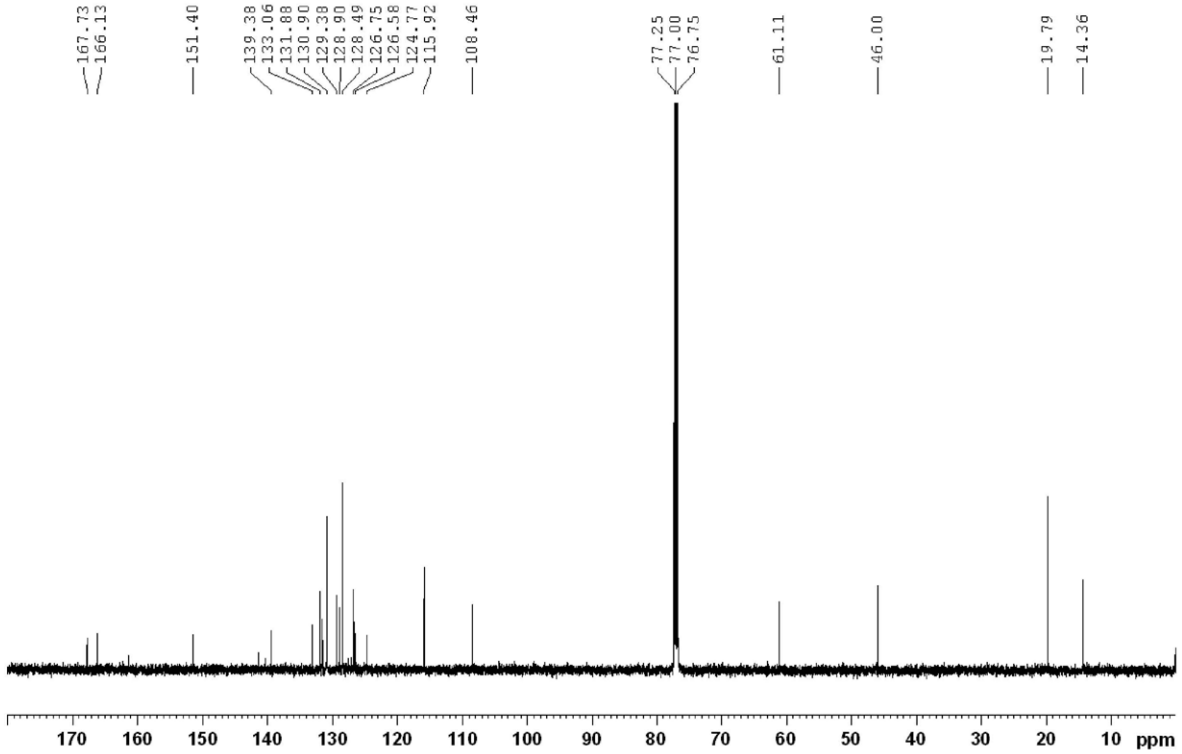

Figure S48. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b09**.

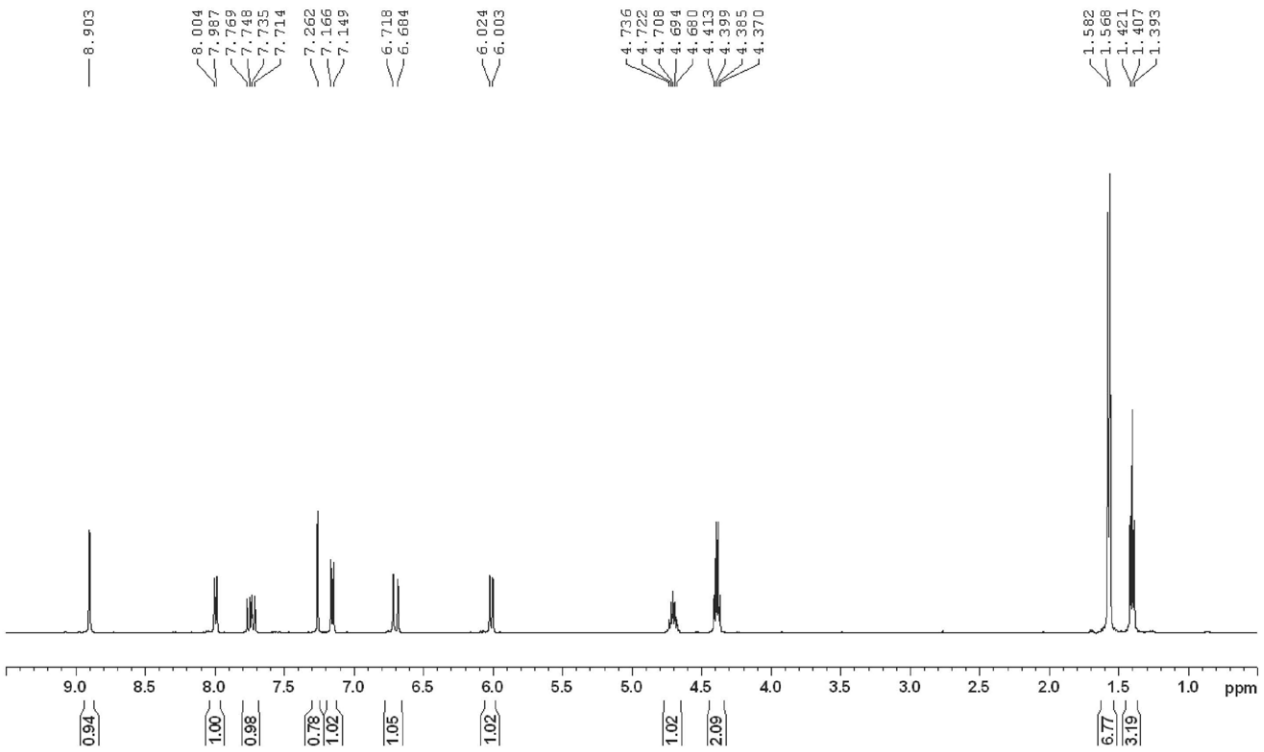

Figure S49. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b10**.

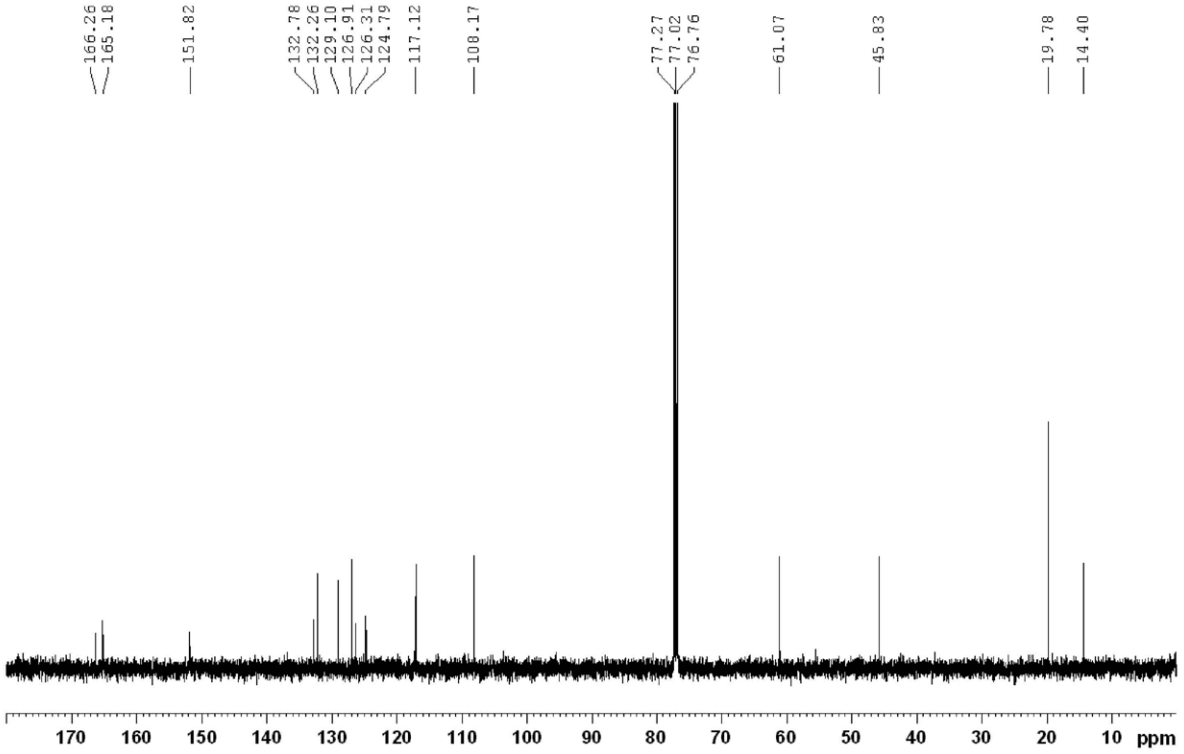

Figure S50. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b10**.

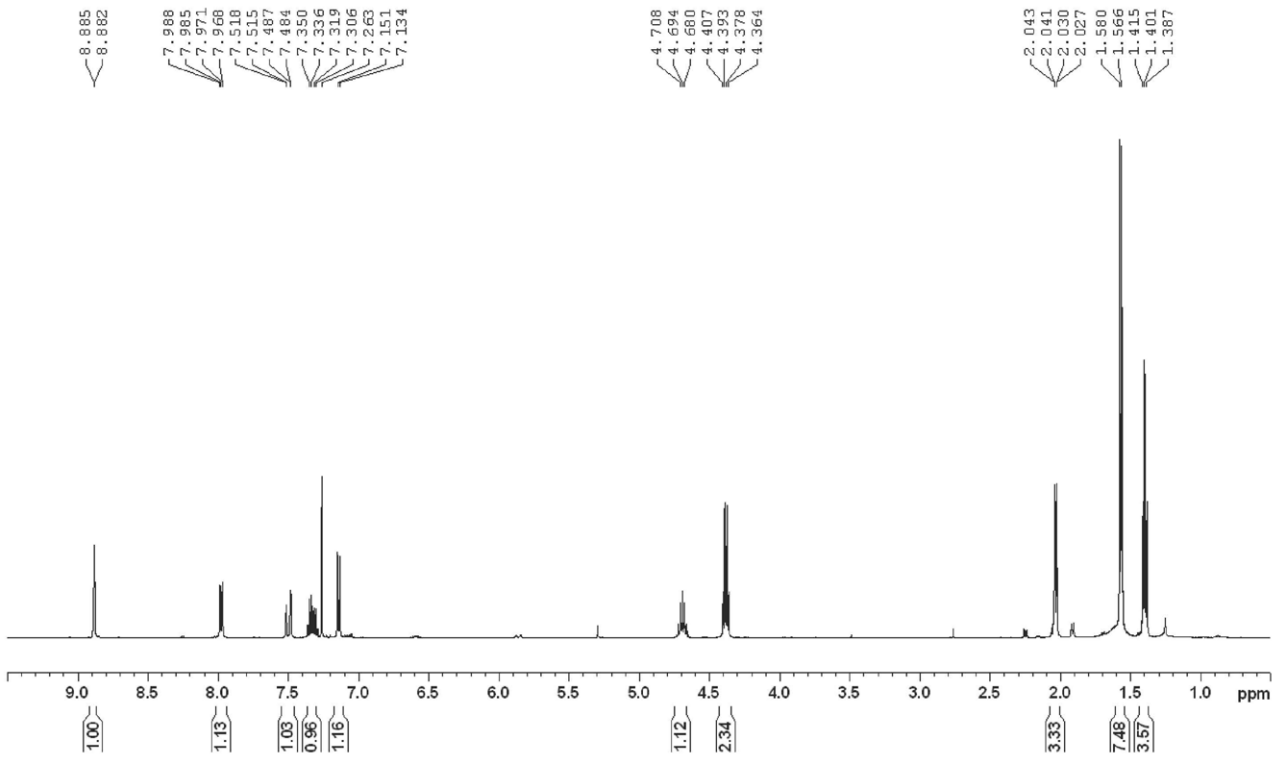

Figure S51. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b11**.

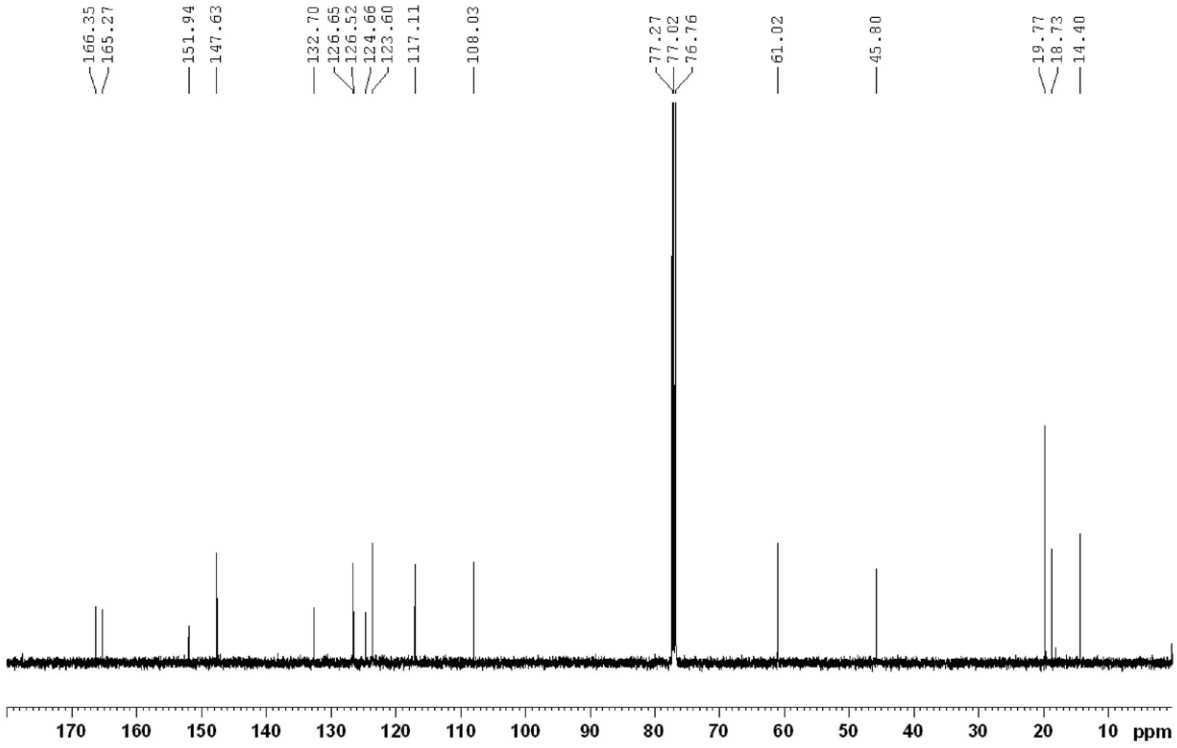

Figure S52. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b11**.

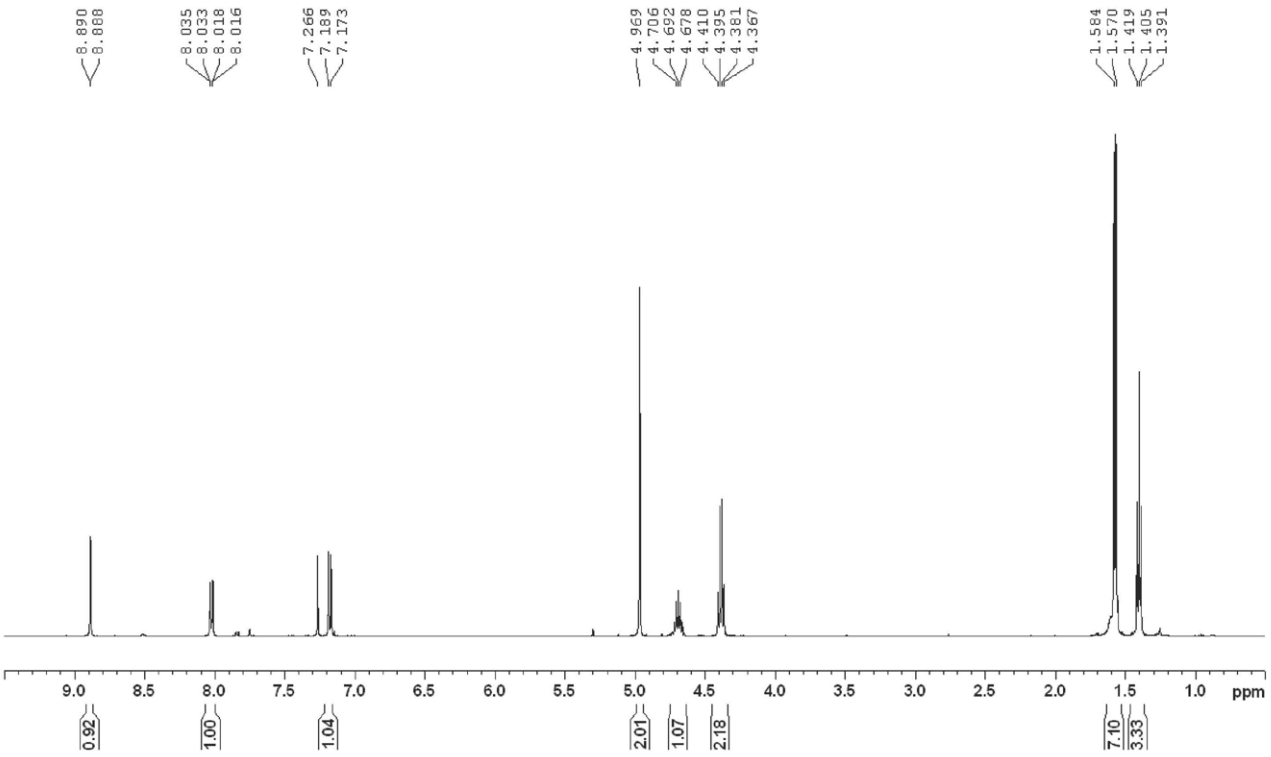

Figure S53. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b12**.

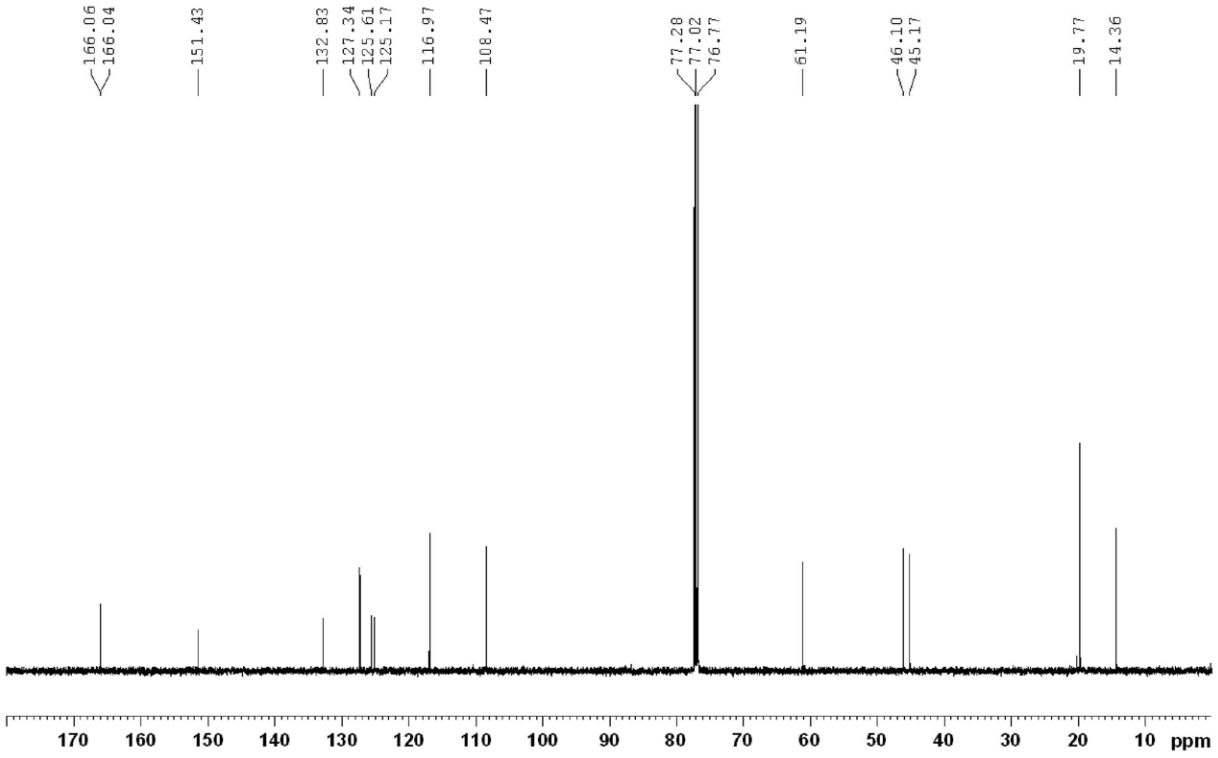

Figure S54. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b12**.

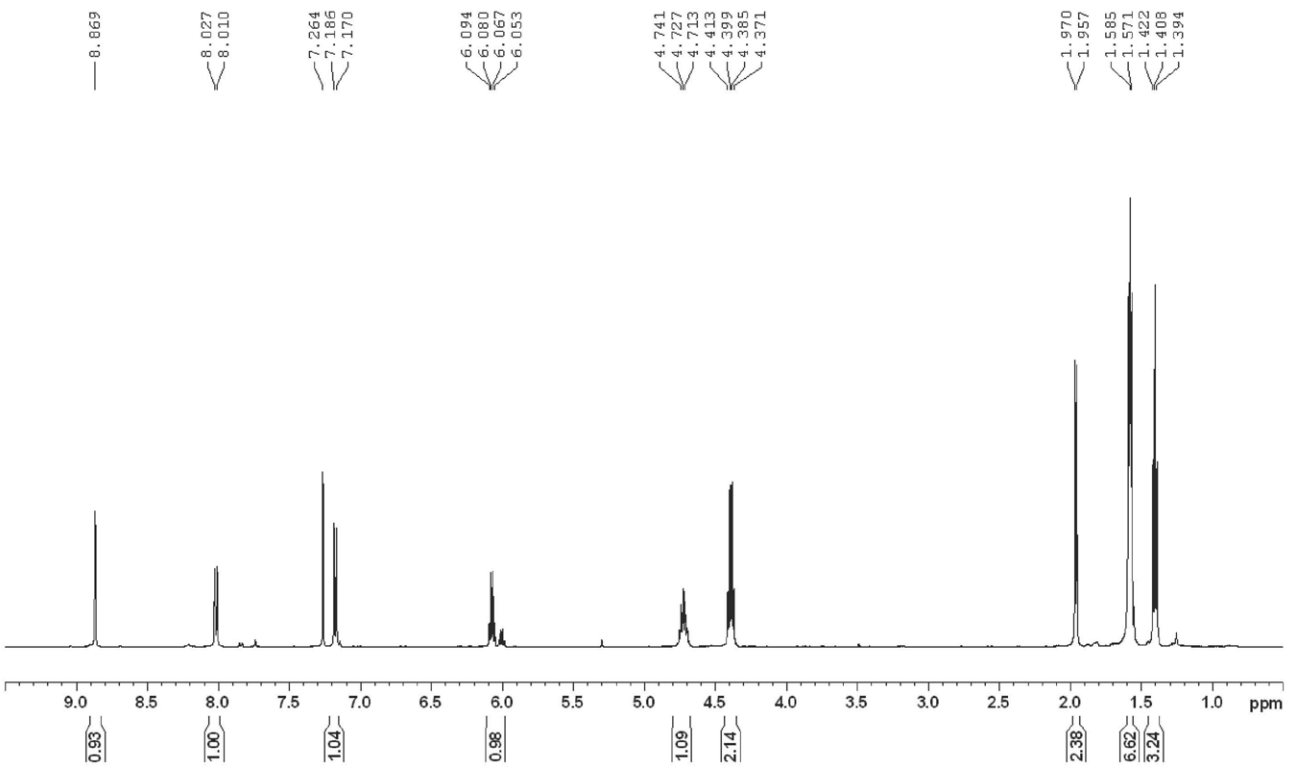

Figure S55. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b13**.

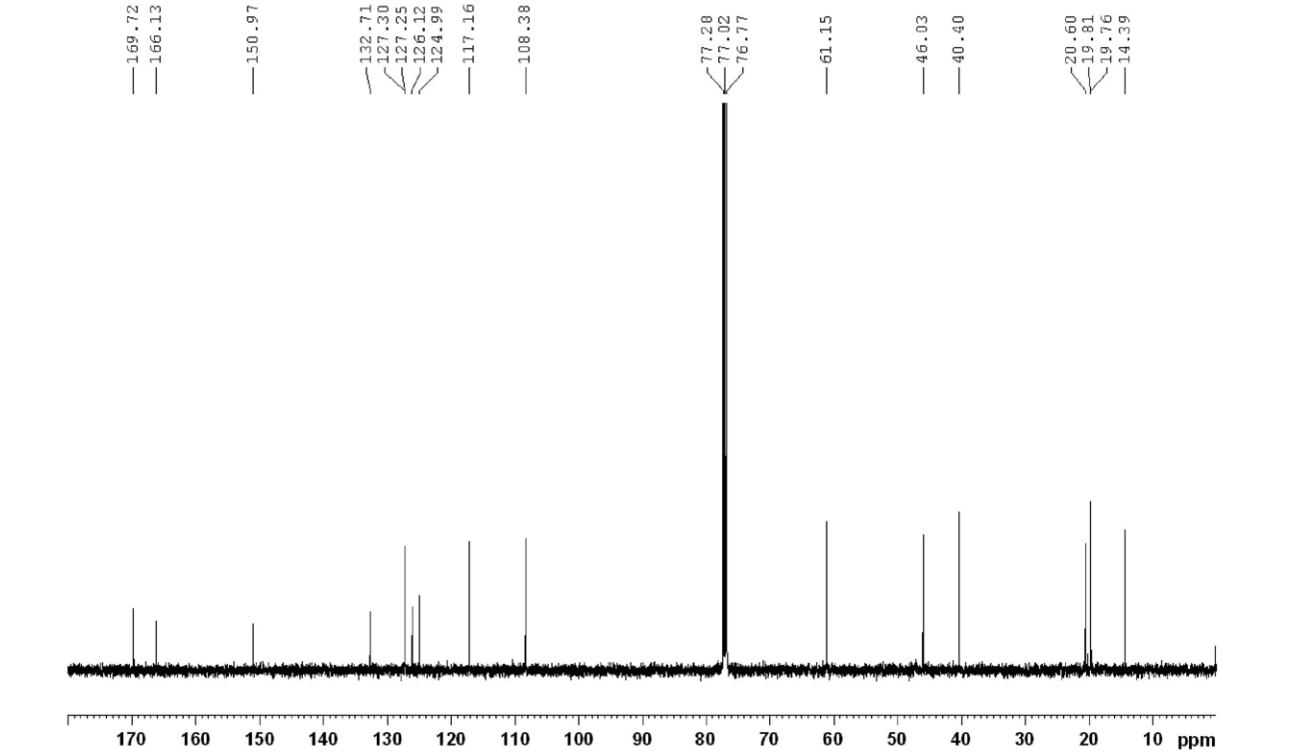

Figure S56. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b13**.

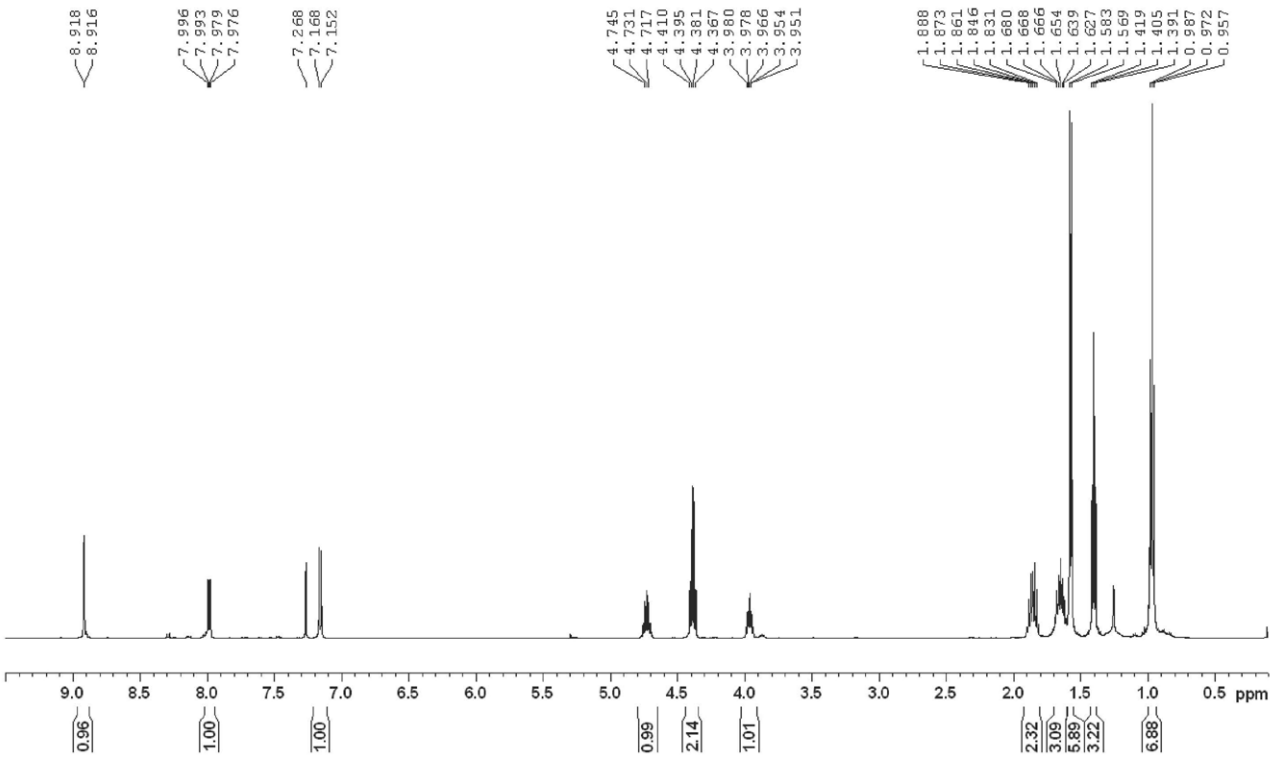

Figure S57. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b14**.

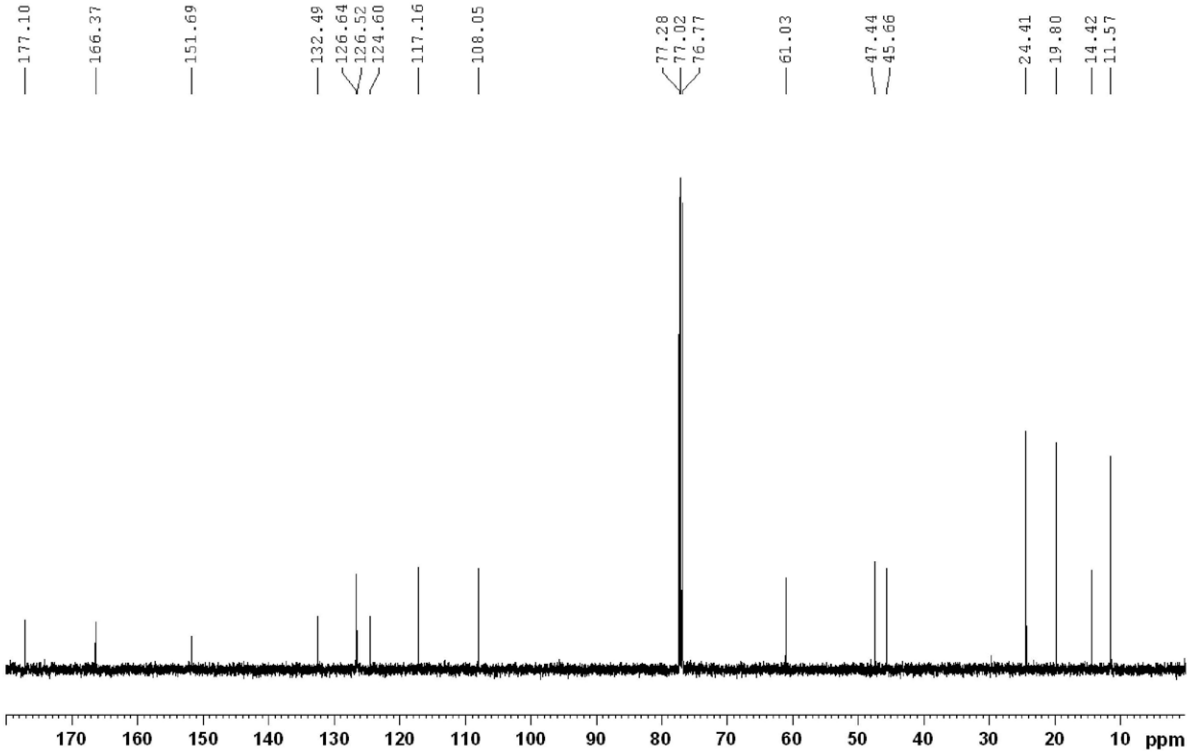

Figure S58. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b14**.

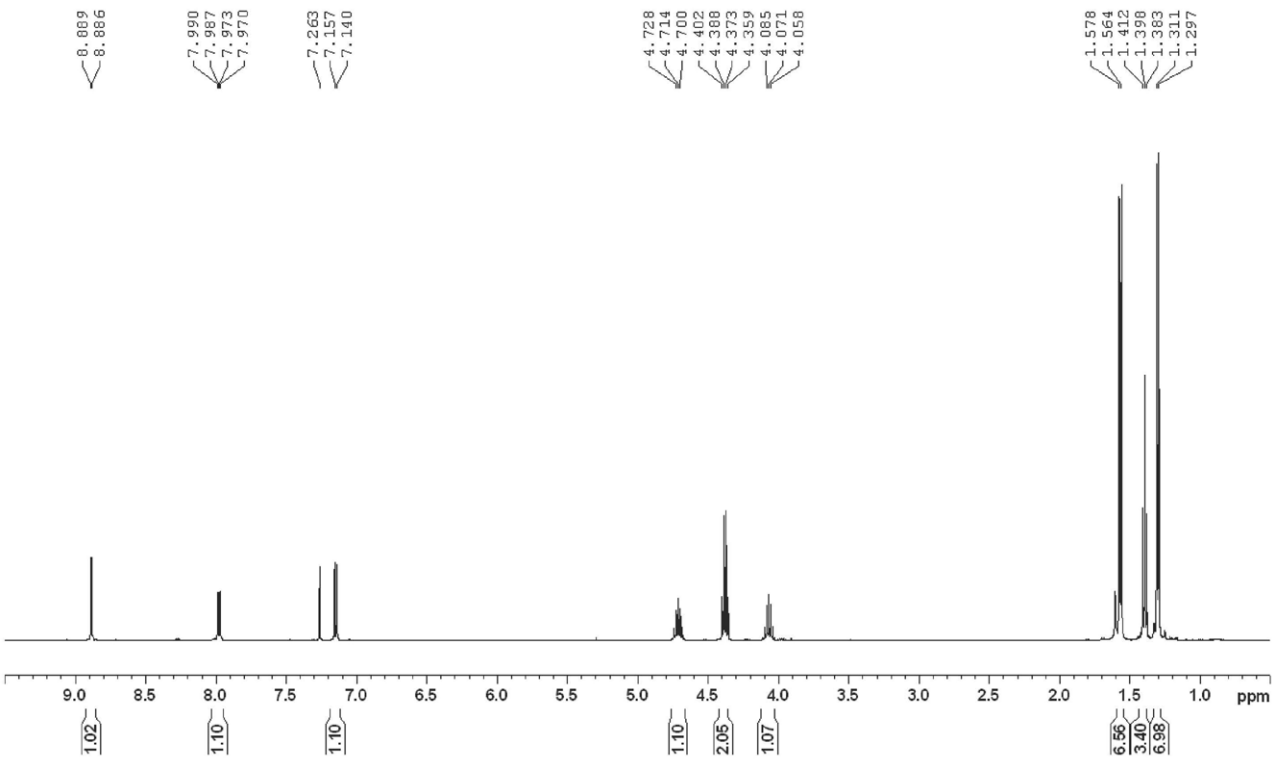

Figure S59. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b15**.

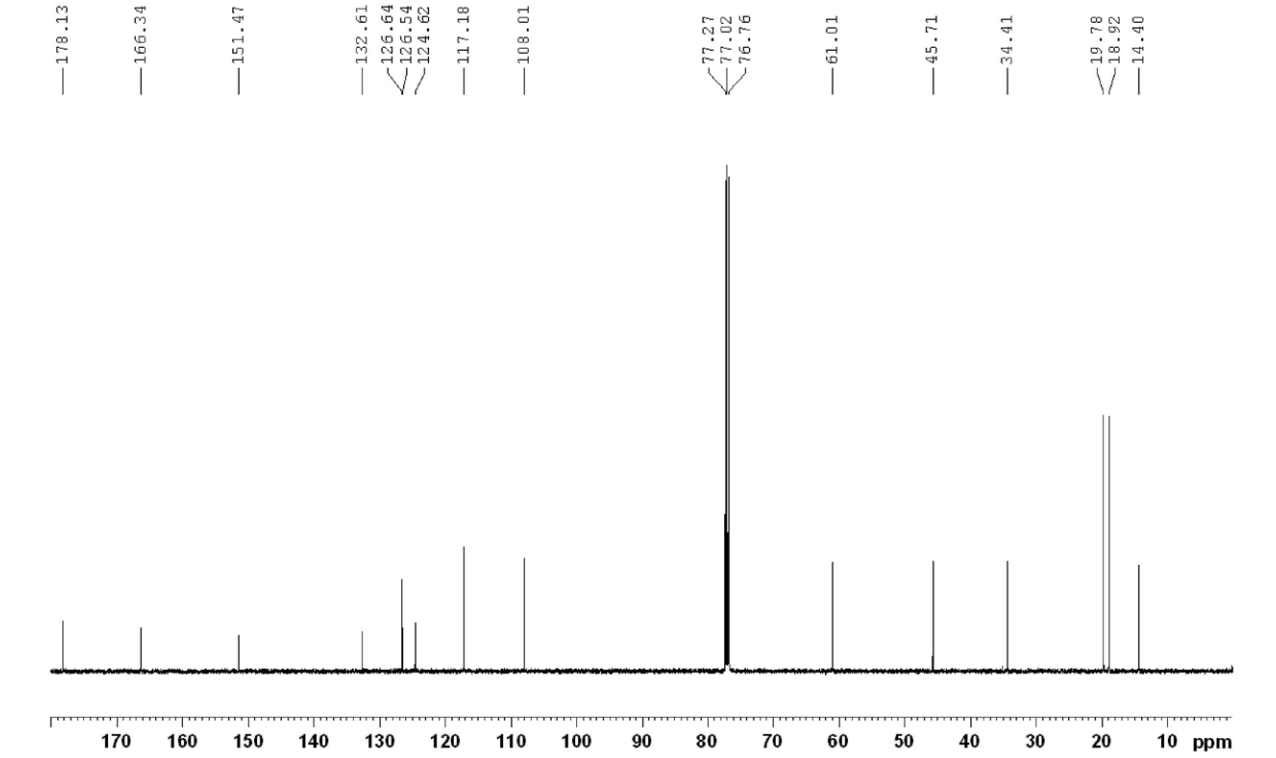

Figure S60. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b15**.

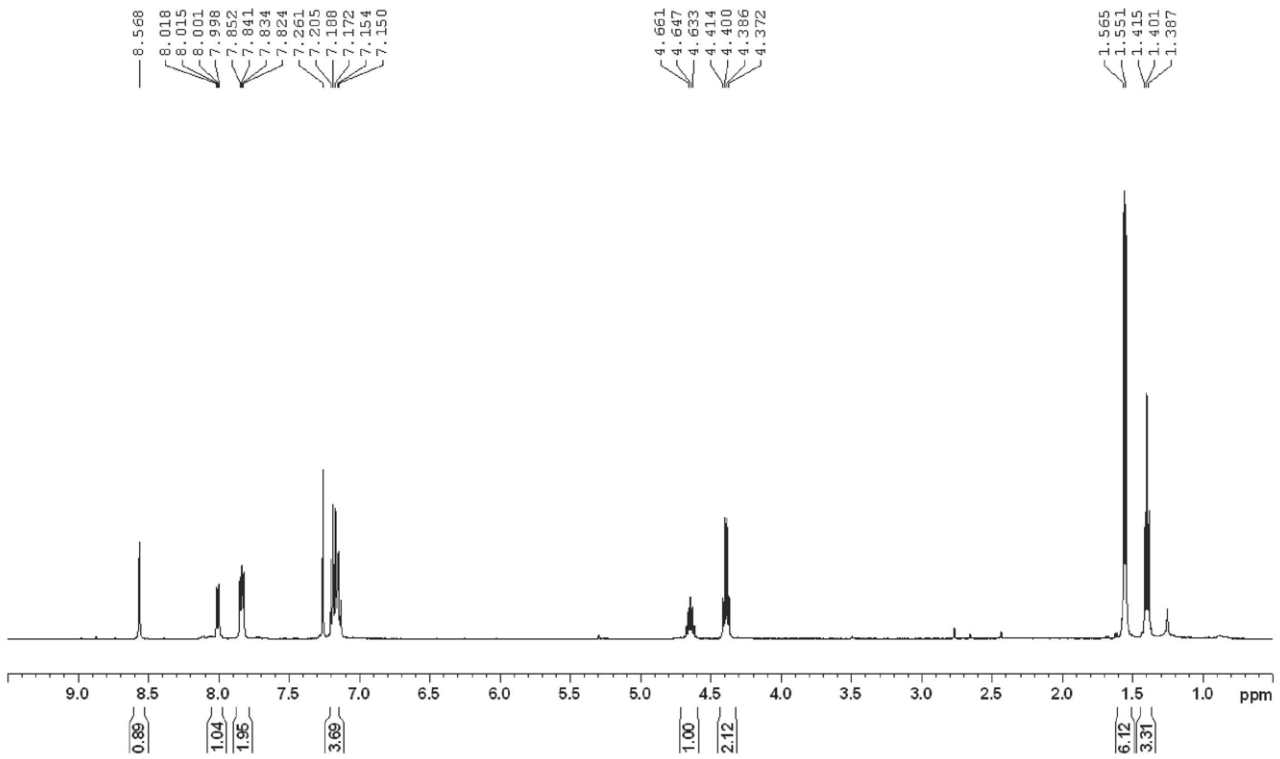

Figure S61. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b16**.

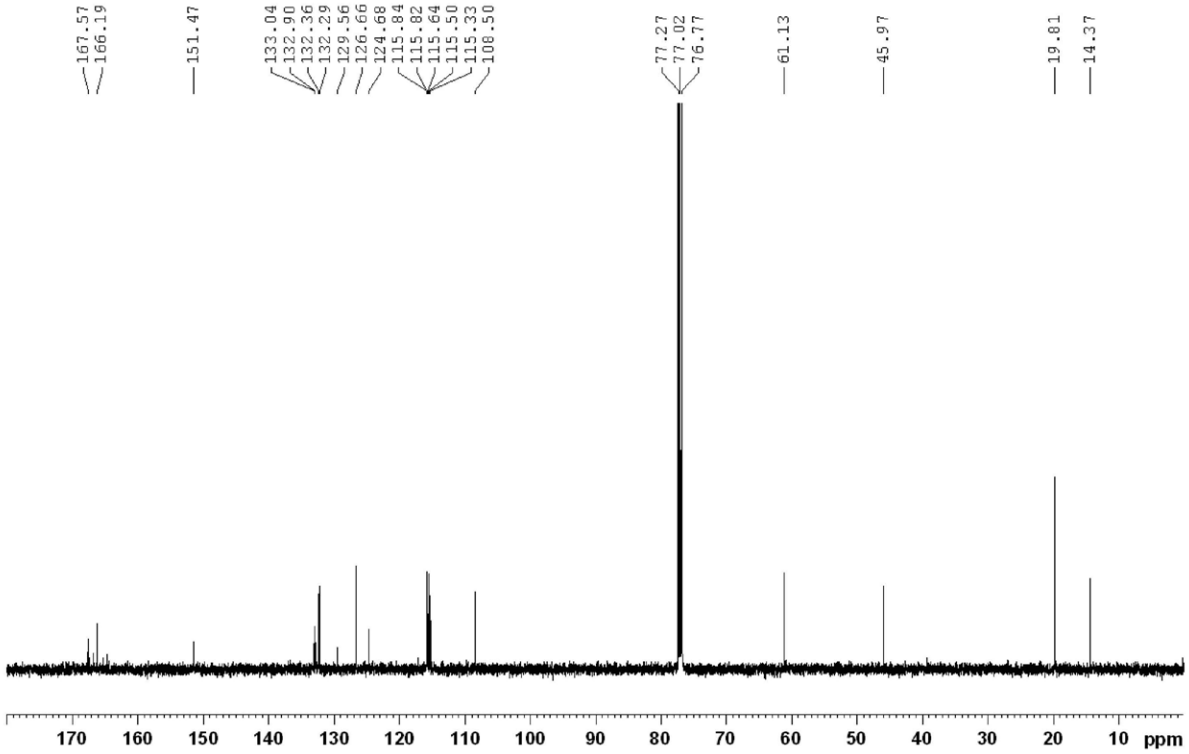

Figure S62. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b16**.

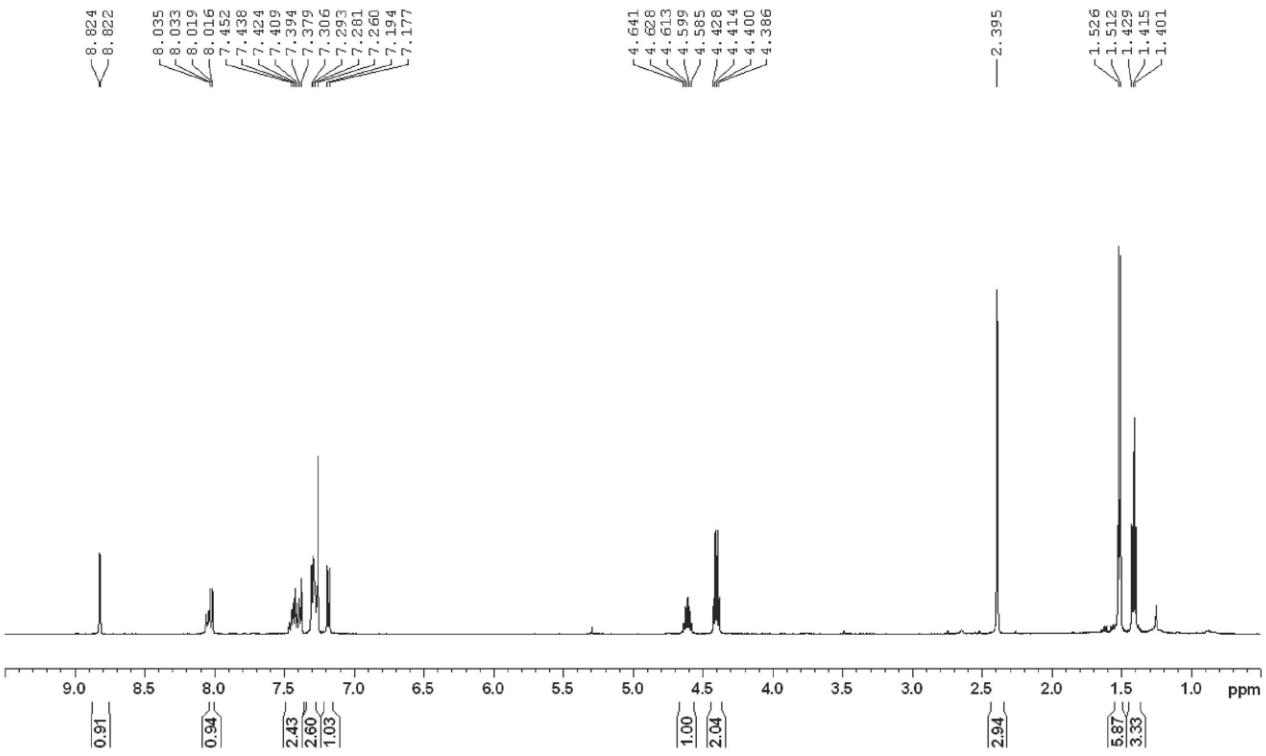

Figure S63. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b17**.

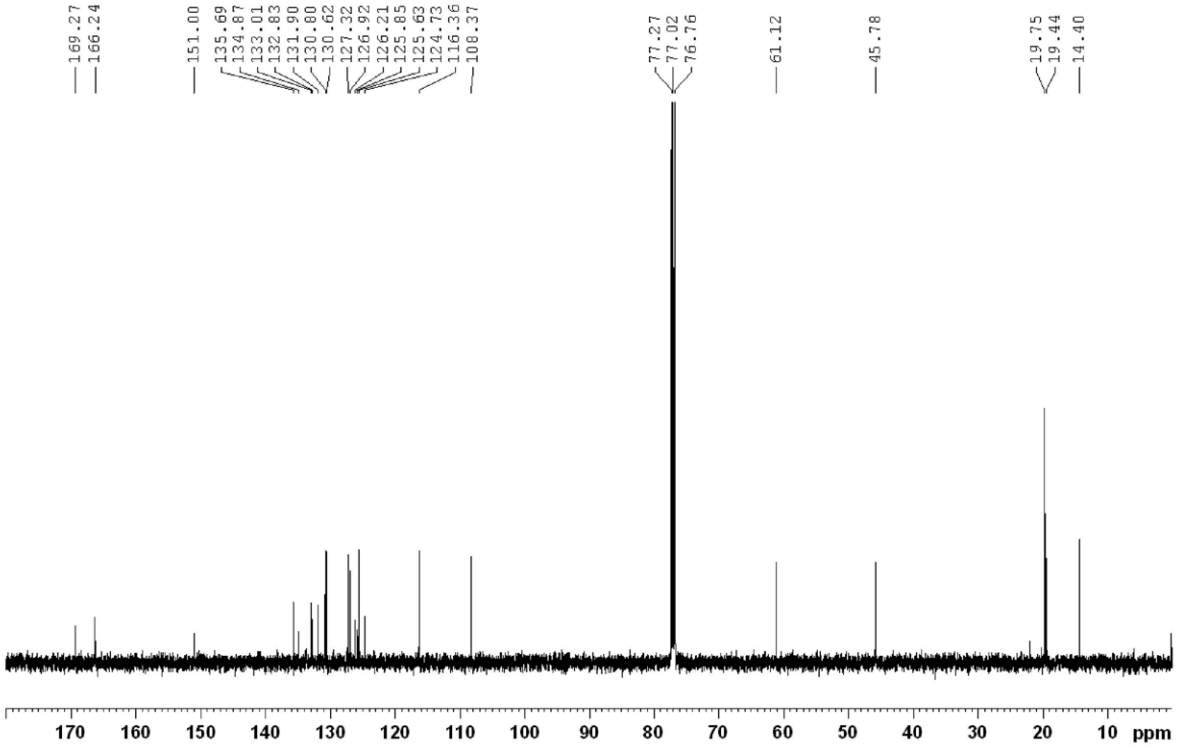

Figure S64. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b17**.

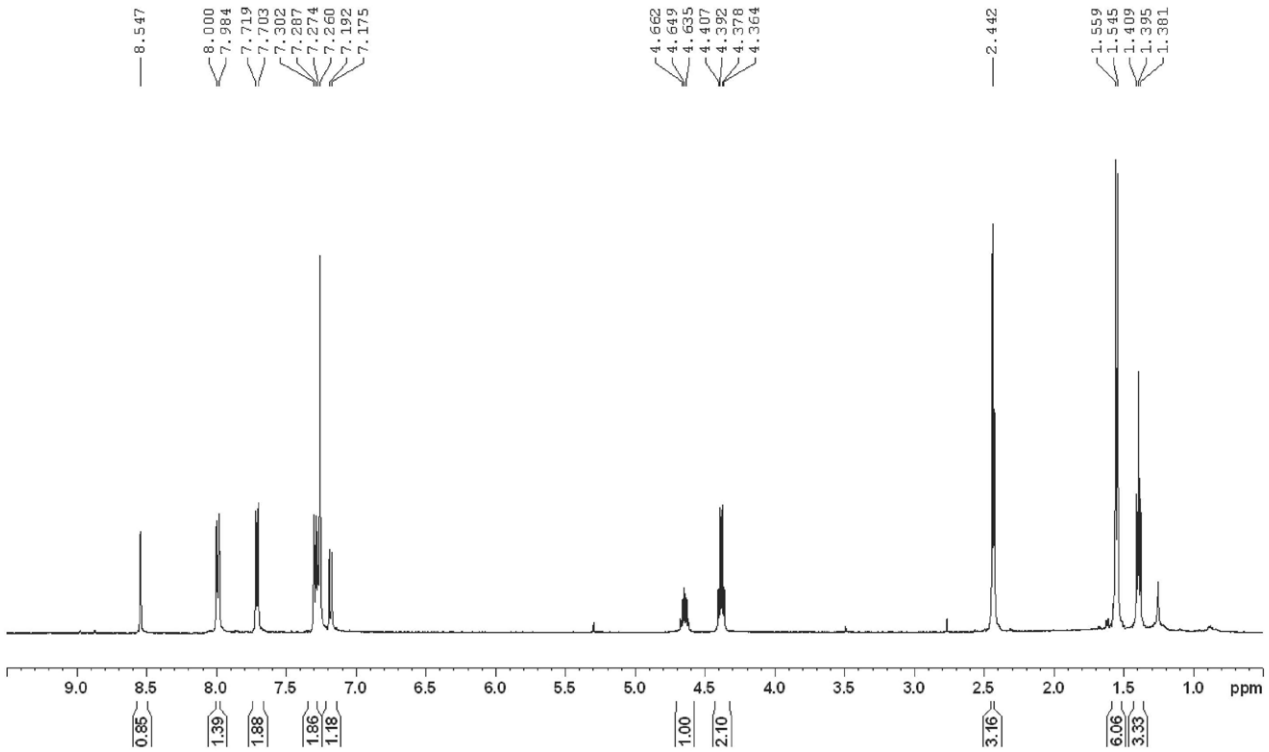

Figure S65. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b18**.

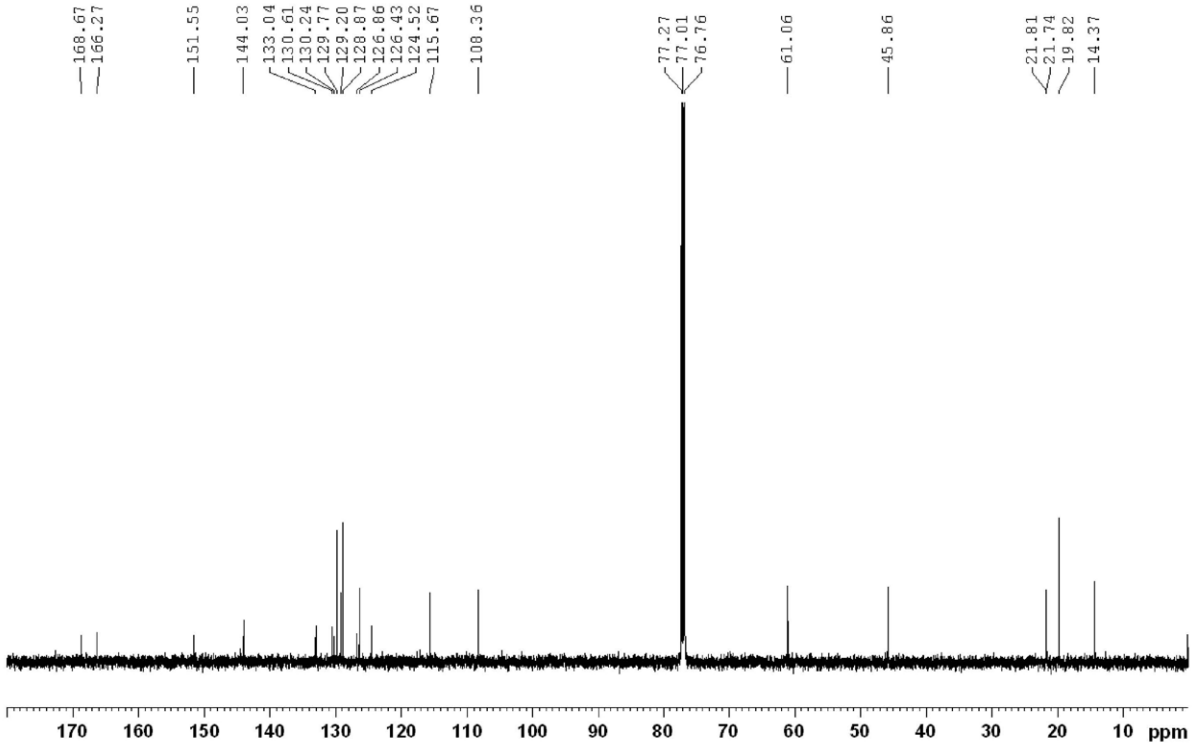

Figure S66. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b18**.

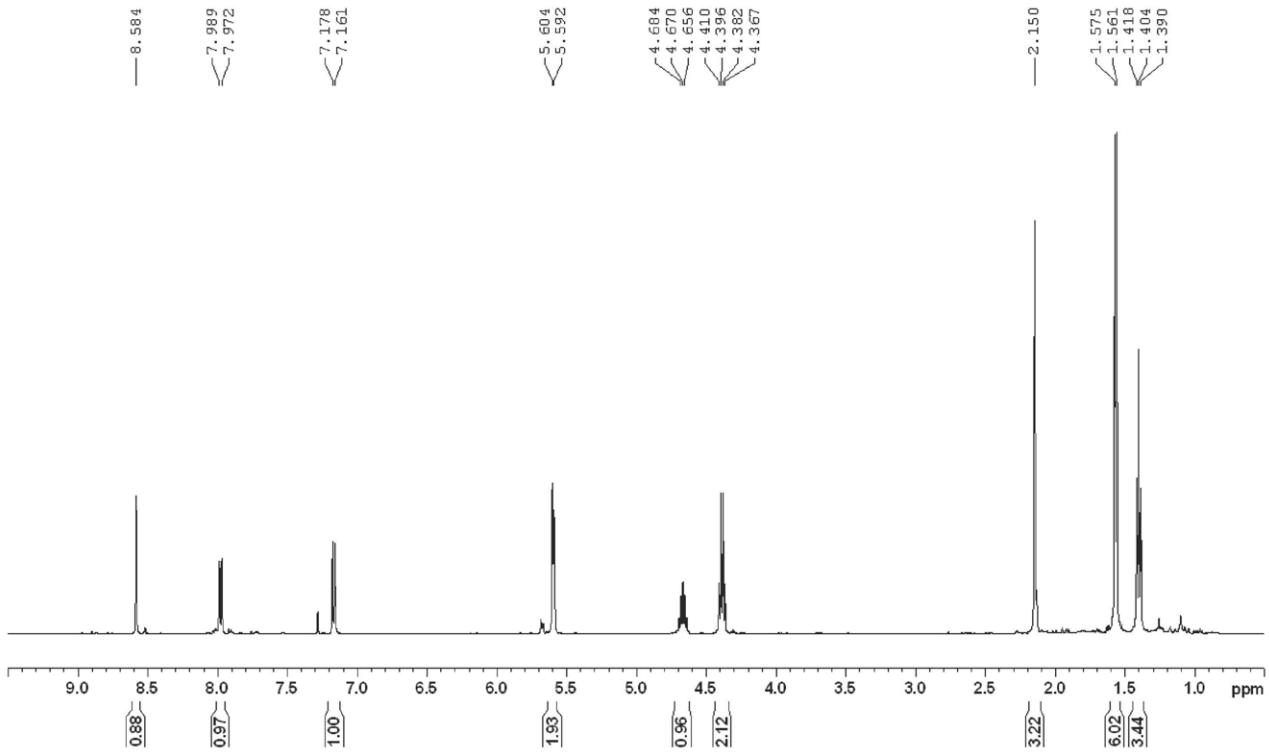

Figure S67. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b19**.

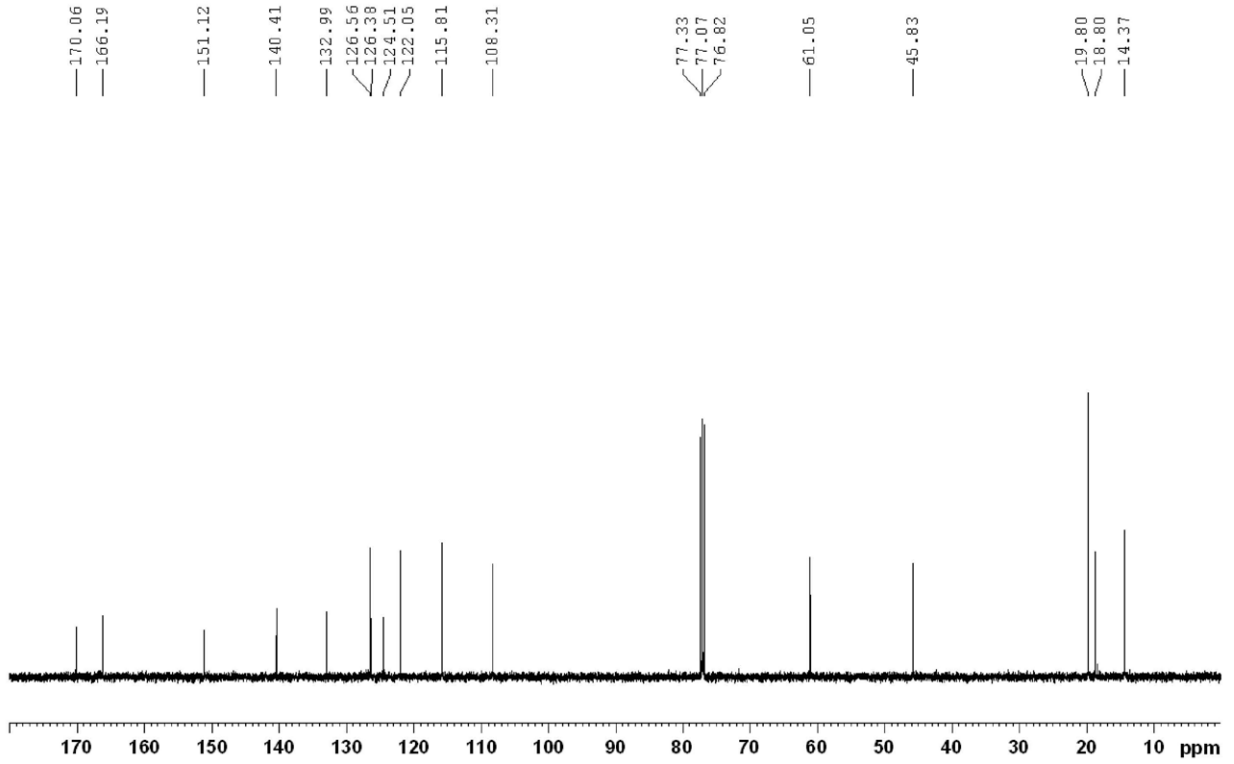

Figure S68. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b19**.

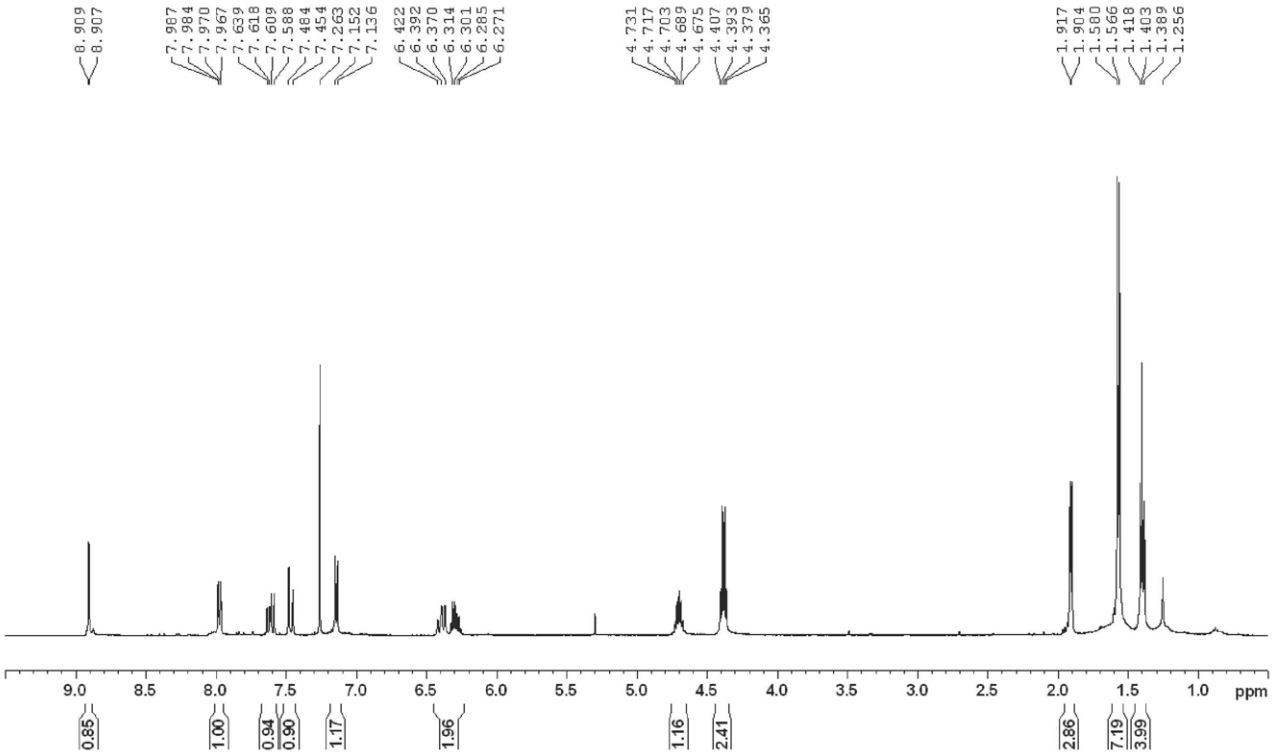

Figure S69. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b20**.

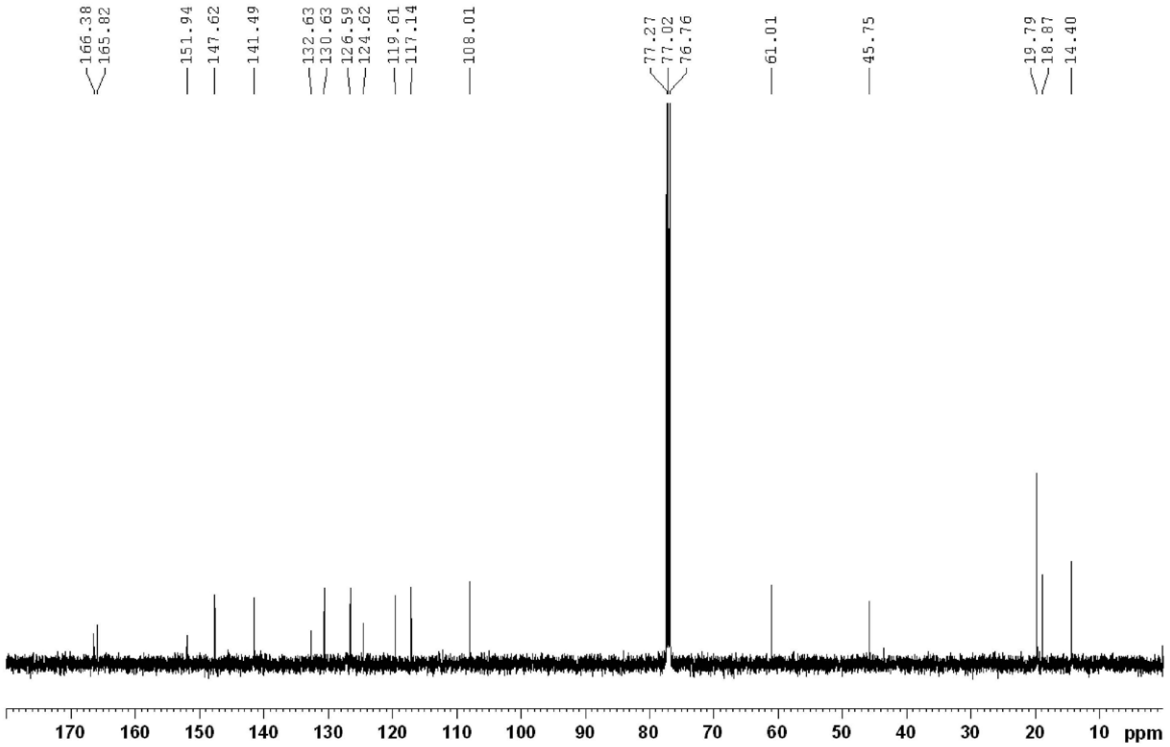

Figure S70. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b20**.

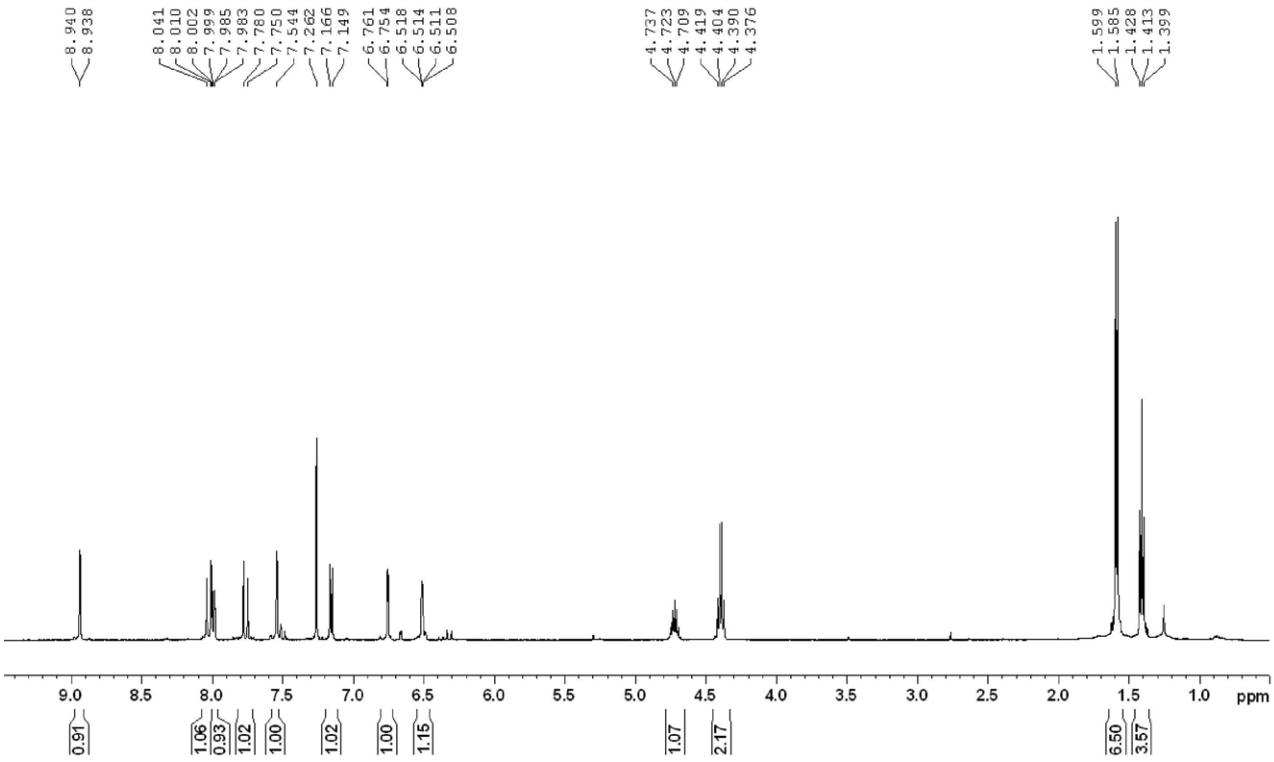

Figure S71. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **9b21**.

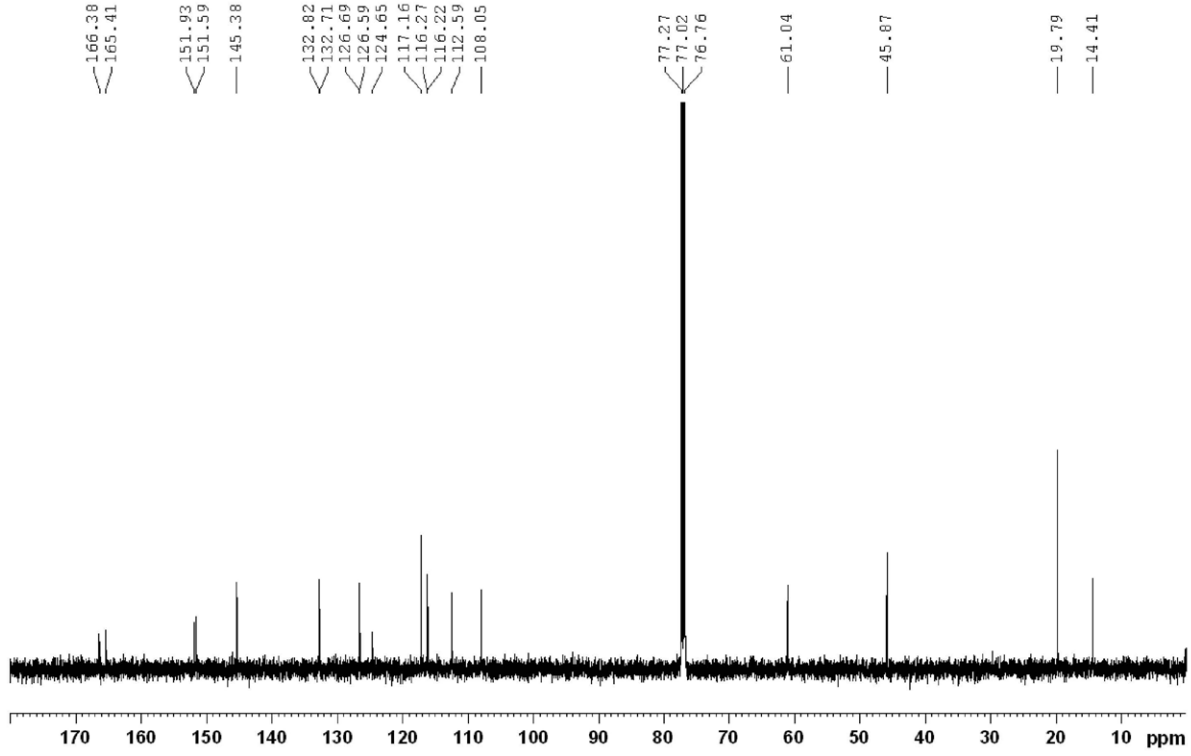

Figure S72. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **9b21**.

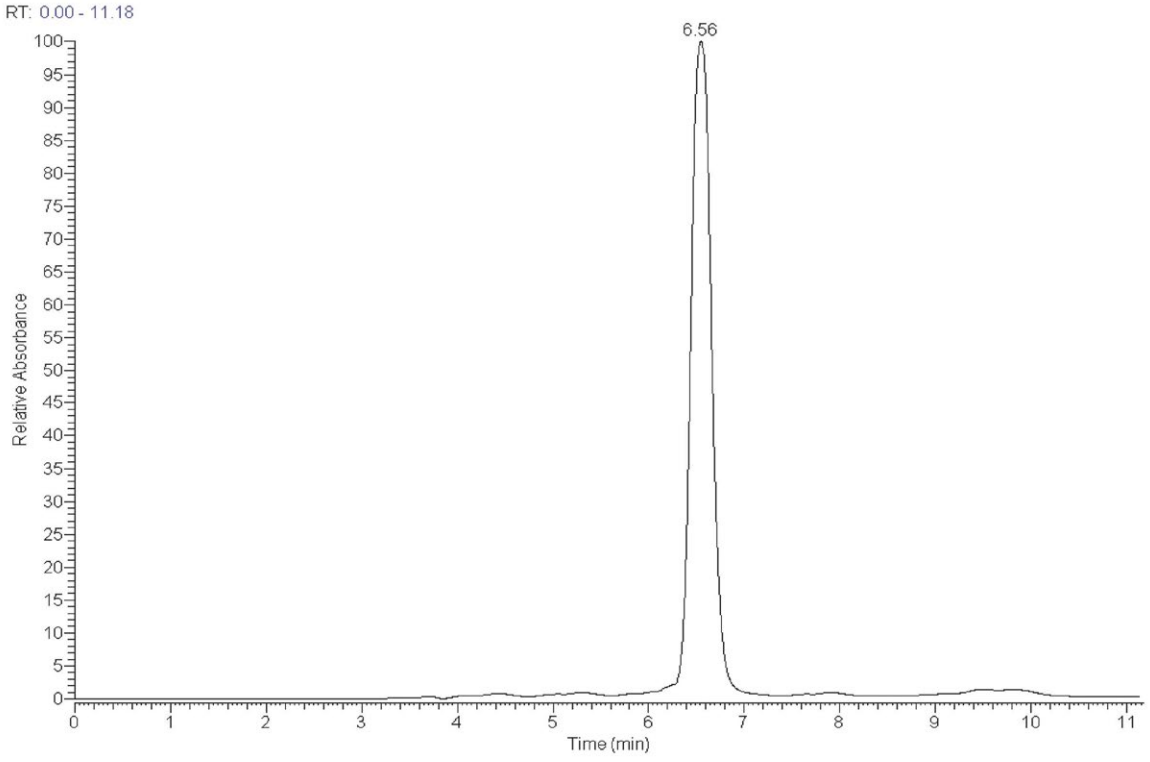

Figure S73. HPLC spectrum of **11a06**.