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Supporting Information for

Supramolecular catalysis by β-cyclodextrin for the synthesis of kojic acid derivatives in water

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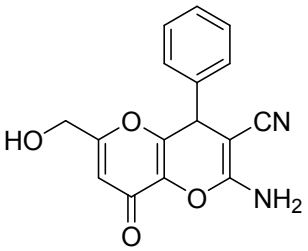
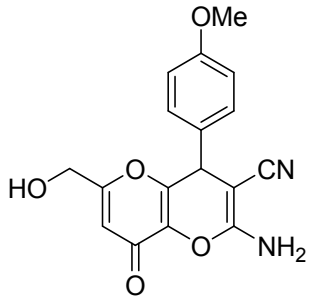
Spectral data for products:

2-amino-6-(hydroxymethyl)-8-oxo-4-phenyl-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2a):



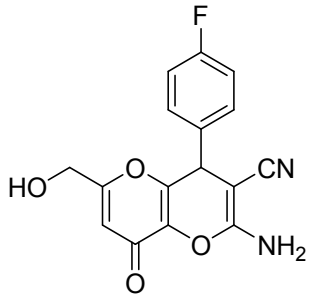
White solid, m.p.226-224 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.3-7.23 (m, 5H), 6.61 (bs, 2H, NH_2), 6.36 (s, 1H), 5.40 (bs, 1H, OH), 4.61 (s, 1H), 4.30-4.01 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 197.4, 168.3, 166.7, 158.0, 147.2, 138.9, 134.9, 127.2, 126.2, 126.1, 117.6, 109.7, 57.7, 54.1, 39.2 ppm; IR (KBr): υ 3361, 3280, 3066, 2223, 1668, 987 cm^{-1}; MS (ESI): *m/z* ([M+H]$^{+}$): 297; HRMS (ESI): *m/z* calcd for $C_{16}H_{13}N_2O_4$: 297.0876; found: 297.0875.

2-amino-6-(hydroxymethyl)-4-(4-methoxyphenyl)-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2b):



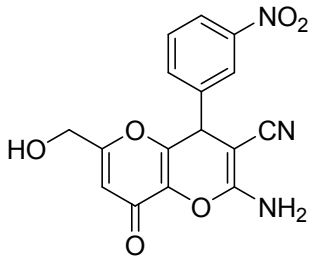
White solid, m.p.218-216 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.17 (d, *J* = 8.2 Hz, 2H), 6.8 (d, *J* = 8.5 Hz, 2H), 6.56 (bs, 2H, NH_2), 6.35 (s, 1H), 5.41 (bs, 1H, OH), 4.56 (s, 1H), 4.24 (dd, *J* = 3.2 Hz, *J* = 15.8 Hz, 1H), 4.16 (dd, *J* = 3.2 Hz, *J* = 15.7 Hz, 1H), 3.79 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 196.4, 169.2, 158.5, 158.1, 148.0, 11.1, 127.7, 118.2, 113.1, 110.3, 58.5, 58.5, 54.0, 38.5 ppm; IR (KBr): υ 3360, 3275, 3132, 2232, 1601, 883 cm^{-1}; MS (ESI): *m/z* ($[M+H]^+$): 327.

2-amino-4-(4-fluorophenyl)-6-(hydroxymethyl)-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2c):



White solid, m.p.242-240 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.31-7.28 (m, 2H), 7.06 (t, *J* = 8.3 Hz, 2H), 6.75 (bs, 2H, NH_2), 6.35 (s, 1H), 5.46 (bs, 1H, OH), 4.64 (s, 1H), 4.23 (d, *J* = 16 Hz, 1H), 4.14 (d, *J* = 15.9 Hz, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$): δ 197.8, 168.8, 167.1, 158.4, 147.6, 139.3, 15.3, 127.6, 126.7, 126.5, 118.0, 110.1, 59.0, 54.4, 39.6 ppm; IR (KBr): υ 3331, 3253, 3203, 2286, 1654, 978 cm^{-1}; MS (ESI): *m/z* ($[M+H]^+$): 315.

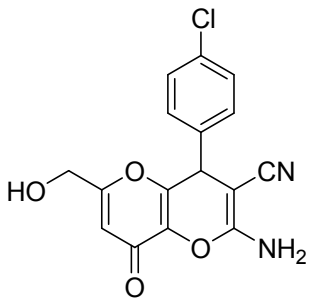
2-amino-6-(hydroxymethyl)-4-(3-nitrophenyl)-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2d):



White solid, m.p.230-228 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.67 (s, 1H), 7.38-7.26 (m, 4H), 6.61 (bs, 2H, NH_2), 6.36 (s, 1H), 5.39 (bs, 1H, OH), 4.61 (s, 1H), 4.31-4.01 (m, 2H) ppm; ^{13}C NMR (75 MHz,

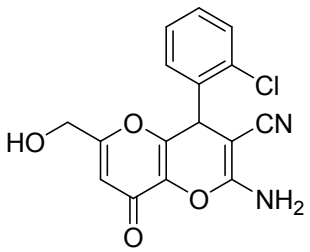
$CDCl_3$): δ 196.7, 169.7, 167.7, 158.8, 158.5, 148.5, 131.5, 128.1, 118.5, 113.5, 110.7, 58.9, 54.4, 39.5 ppm; IR (KBr): υ 3356, 3204, 2236, 1951, 1650, 905 cm^{-1}; MS (ESI): *m/z* ($[M+H]^+$): 342.

2-amino-4-(4-chlorophenyl)-6-(hydroxymethyl)-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2e):



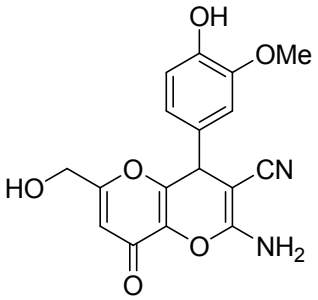
White solid, m.p.202-200 °C; ^1H NMR (300 MHz, $CDCl_3$): δ 7.32 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 6.73 (bs, 2H, NH_2), 6.35 (s, 1H), 5.49 (t, *J* = 5.6 Hz, 1H, OH), 4.64 (s, 1H), 4.23 (dd, *J* = 5.6 Hz, *J* = 15.7 Hz, 1H), 4.15 (dd, *J* = 5.7 Hz, *J* = 15.9 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 195.2, 169.4, 168.1, 159.1, 148.3, 139.6, 136.3, 132.4, 129.6, 119.0, 111.3, 58.9, 55.2, 39.5 ppm; IR (KBr): υ 3355, 3287, 3154, 2219, 1678, 875 cm^{-1}; MS (ESI): *m/z* ($[M+Na]^+$): 353; HRMS (ESI): *m/z* calcd for $C_{16}H_{11}ClN_2O_4Na$: 353.0305; found: 353.0307.

2-amino-4-(2-chlorophenyl)-6-(hydroxymethyl)-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2f):



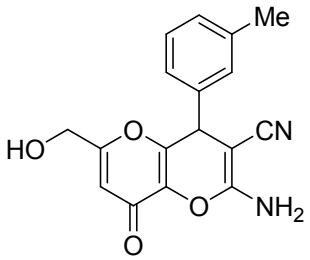
White solid, m.p.216-214 °C; ^1H NMR (300 MHz, $CDCl_3$): δ 7.39 (d, *J* = 7.5 Hz, 1H), 7.31-7.26 (m, 4H), 6.82 (bs, 2H, NH_2), 6.35 (s, 1H), 5.47 (bs, 1H, OH), 5.22 (s, 1H), 4.22 (dd, *J* = 5.4 Hz, *J* = 16 Hz, 1H), 4.14 (dd, *J* = 5.6 Hz, *J* = 16.1 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 195.5, 169.7, 168.4, 159.4, 148.5, 139.9, 136.6, 132.7, 129.9, 129.1, 119.3, 111.5, 59.2, 55.4, 39.8 ppm; IR (KBr): υ 3386, 3274, 3142, 2225, 1652, 925 cm^{-1}; MS (ESI): *m/z* ($[M+H]^+$): 331. HRMS (ESI): *m/z* calcd for $C_{16}H_{12}ClN_2O_4$: 331.0485; found: 331.0482.

2-amino-4-(4-hydroxy-3-methoxyphenyl)-6-(hydroxymethyl)-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2g):



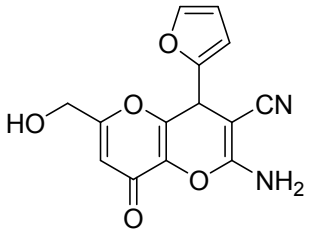
White solid, m.p.226-224 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.84 (s, 1H), 6.97 (bs, 2H, NH_2), 6.77-6.73 (m, 1H), 6.64 (d, *J* = 6.9 Hz, 1H), 6.29 (s, 1H), 5.60 (t, *J* = 6.1 Hz, 1H, OH), 4.56 (s, 1H), 4.22 (dd, *J* = 6.0 Hz, *J* = 15.9 Hz, 1H), 4.15 (dd, *J* = 6.0 Hz, *J* = 15.8 Hz, 1H), 3.80 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 196.9, 169.6, 167.7, 158.8, 158.5, 148.4, 131.5, 128.1, 118.6, 113.5, 110.7, 58.9, 54.4, 53.2, 39.5 ppm; IR (KBr): υ 3382, 3314, 3187, 2842, 2231, 1610, 976 cm^{-1}; MS (ESI): *m/z* ($[M+Na]^+$): 365.

2-amino-6-(hydroxymethyl)-8-oxo-4-m-tolyl-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2h):



White solid, m.p.222-220 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.41 (d, *J* = 7.3 Hz, 1H), 7.32-7.28 (m, 2H), 7.05 (d, *J* = 7.5 Hz, 1H), 6.89 (bs, 2H), 6.31 (s, 1H), 5.43 (bs, 1H, OH), 5.13 (s, 1H), 4.28 (dd, *J* = 5.6 Hz, *J* = 15.7 Hz, 1H), 4.09 (dd, *J* = 5.7 Hz, *J* = 15.8 Hz, 1H), 2.39 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 198.0, 169.0, 167.4, 158.6, 147.9, 139.5, 135.5, 127.9, 126.7, 118.8, 110.4, 58.4, 54.8, 39.0, 28.2 ppm; IR (KBr): υ 3362, 3305, 3216, 2223, 1663, 892 cm^{-1}; MS (ESI): *m/z* ($[M+H]^+$): 311.

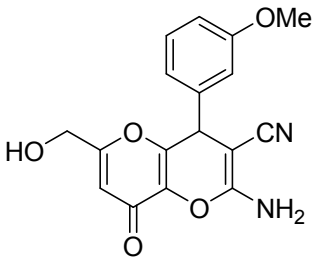
2-amino-4-(furan-2-yl)-6-(hydroxymethyl)-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2i):



White solid, m.p.224-222 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.58-7.51 (m, 3H), 7.41 (d, *J* = 3.5 Hz, 1H), 6.93 (bs, 2H, NH_2), 6.36 (s, 1H), 5.46 (bs, 1H, OH), 4.86 (s, 1H), 4.28 (dd, *J* = 5.7 Hz, *J* = 16.1

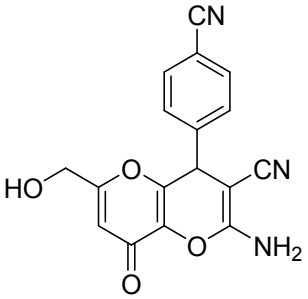
Hz, 1H), 4.18 (dd, J = 5.4 Hz, J = 16 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 195.3, 169.4, 168.6, 159.4, 148.6, 139.9, 129.7, 125.9, 124.1, 119.5, 112.3, 111.5, 59.2, 57.2, 37.8 ppm; IR (KBr): υ 3428, 3367, 3292, 2171, 1631, 894 cm^{-1}; MS (ESI): *m/z* ([M+H]$^+$): 287.

2-amino-6-(hydroxymethyl)-4-(3-methoxyphenyl)-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2j):



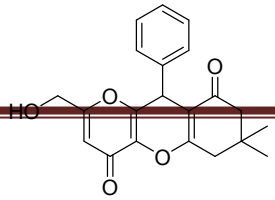
Brown solid, m.p.212-210 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.26-7.14 (m, 3H), 7.01 (s, 1H), 6.53 (bs, 2H, NH_2), 6.33 (s, 1H), 5.40 (bs, 1H, OH), 4.57 (s, 1H), 4.27 (dd, J = 3.5 Hz, J = 16 Hz, 1H), 4.16 (dd, J = 3.3 Hz, J = 16 Hz, 1H), 3.73 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 195.9, 166.9, 158.0, 157.6, 151.2, 147.6, 135.7, 127.3, 117.7, 112.6, 109.8, 58.1, 53.6, 38.7 ppm; IR (KBr): υ 3359, 3286, 3246, 2235, 1696, 958 cm^{-1}; MS (ESI): *m/z* ([M+H]$^+$): 327.

2-amino-4-(4-cyanophenyl)-6-(hydroxymethyl)-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile (2k):



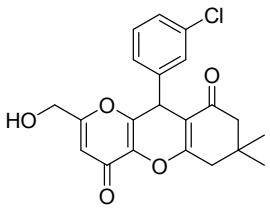
White solid, m.p.216-214 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.46-7.28 (m, 4H), 6.63 (s, 2H, NH_2), 6.38 (s, 1H), 5.43 (bs, 1H, OH), 4.63 (s, 1H), 4.32-4.03 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 197.4, 168.3, 166.3, 158.0, 147.2, 138.9, 134.9, 127.2, 126.2, 126.1, 117.6, 109.7, 57.7, 54.1, 38.9 ppm; IR (KBr): υ 3368, 3325, 3253, 2231, 2217, 1597, 992 cm^{-1}; MS (ESI): *m/z* ([M+H]$^+$): 322. HRMS (ESI): *m/z* calcd for $C_{17}H_{12}NO_4$: 322.0827; found: 322.0825.

2-(hydroxymethyl)-7,7-dimethyl-10-phenyl-7,8-dihydropyrano[3,2-b]chromene-4,9(6H,10H)-dione (3a):



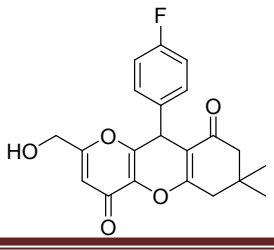
Solid, mp 186–188°C; ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.33–7.16 (m, 5H), 6.37 (s, 1H), 5.48–5.38 (br s, 1H), 4.82 (s, 1H), 4.20 (dd, J = 5.8, 11.7 Hz, 2H), 2.64 (d, J = 5.2 Hz, 2H), 2.20 (d, J = 6.0 Hz, 2H), 1.14 (s, 3H), 1.06 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d6): δ 195.4, 169.6, 168.3, 163.6, 150.9, 140.9, 136.5, 128.5, 127.8, 127.3, 111.4, 111.2, 59.0, 49.6, 37.7, 31.8, 28.2, 26.7; IR (KBr): ν_{max} 3361, 3081, 2955, 2892, 1669, 1624, 1443, 1377, 1284, 1219, 1147, 1076, 991, 953, 712 cm^{-1}; ESI-MS: m/z: 352 (M+). HRMS calcd for $C_{21}H_{20}O_5$: 352.1388, found: 352.1399.

10-(3-chlorophenyl)-2-(hydroxymethyl)-7,7-dimethyl-7,8-dihydropyrano[3,2-b]chromene-4,9(6H,10H)-dione (3b):



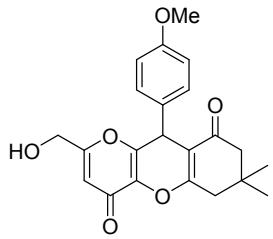
Solid, mp 198–200°C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.35 (d, J = 7.3 Hz, 1H), 7.24–7.15 (m, 3H), 6.38 (s, 1H), 5.36 (s, 1H), 4.30–4.12 (m, 2H), 2.66 (q, J = 17.8 Hz, 2H), 2.20 (q, J = 15.7 Hz, 2H), 1.14 (s, 3H), 1.10 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6): δ 195.2, 169.5, 168.3, 164.2, 150.0, 138.1, 136.7, 132.7, 130.2, 129.5, 129.0, 127.5, 111.4, 110.6, 59.0, 49.6, 35.1, 31.7, 28.2, 26.8; IR (KBr): ν_{max} 3282, 2954, 2871, 1668, 1633, 1595, 1443, 1376, 1221, 1193, 1145, 1039, 952, 753 cm^{-1}; ESI-MS: m/z: 386 (M+). HRMS calcd for $C_{21}H_{19}O_5Cl$: 386.0999, found: 386.1005.

10-(4-fluorophenyl)-2-(hydroxymethyl)-7,7-dimethyl-7,8-dihydropyrano[3,2-b]chromene-4,9(6H,10H)-dione (3c):



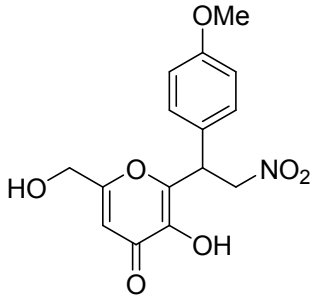
Solid, mp 160–164°C; 1H NMR (500 MHz, DMSO-d_6): δ 7.28–7.20 (m, 2H), 7.03–6.94 (m, 2H), 6.37 (s, 1H), 5.51–5.39 (br s, 1H), 4.29–4.12 (m, 2H), 2.64 (q, J = 17.8 Hz, 2H), 2.20 (q, J = 16.7 Hz, 2H), 1.14 (s, 3H), 1.06 (s, 3H). 13C NMR (75 MHz, DMSO-d_6): δ 195.4, 169.6, 168.3, 163.6, 162.8, 159.6, 150.5, 136.5, 137.1, 137.0, 129.8, 129.7, 115.4, 115.1, 111.4, 111.1, 59.0, 49.6, 37.0, 31.8, 26.8; IR (KBr): ν_{max} 3363, 2960, 2927, 1639, 1600, 1507, 1376, 1221, 1191, 1073, 955, 844 cm^{-1}; ESI-MS: m/z: 370 (M+). HRMS calcd for $C_{21}H_{19}O_5F$: 370.1214, found: 370.1208.

2-(hydroxymethyl)-10-(4-methoxyphenyl)-7,7-dimethyl-7,8-dihydropyrano[3,2-b]chromene-4,9(6H,10H)-dione (3d):



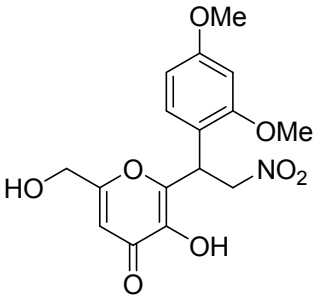
Solid, mp 180–182°C; IR (KBr): ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.14 (d, J = 8.6 Hz, 2H), 6.80 (d, J = 8.4 Hz, 2H), 6.32 (s, 1H), 5.57–5.48 (m, 1H), 4.75 (s, 1H), 4.29–4.11 (m, 2H), 3.74 (s, 3H), 2.63 (d, J = 3.4 Hz, 2H), 2.19 (d, J = 10.0 Hz, 2H), 1.13 (s, 3H), 1.05 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d6): δ 195.9, 170.2, 168.8, 163.9, 158.9, 151.7, 136.9, 133.5, 129.4, 114.4, 111.8, 59.6, 55.5, 50.2, 37.3, 32.3, 28.8, 27.2; ν_{max} 3361, 2955, 1670, 1628, 1512, 1445, 1376, 1261, 1219, 1183, 1075, 952, 824, 777 cm^{-1}; ESI-MS: m/z: 382 (M+). HRMS calcd for $C_{22}H_{22}O_6$: 382.1414, found: 382.1419.

3-hydroxy-6-(hydroxymethyl)-2-(1-(4-methoxyphenyl)-2-nitroethyl)-4H-pyran-4-one (4b):



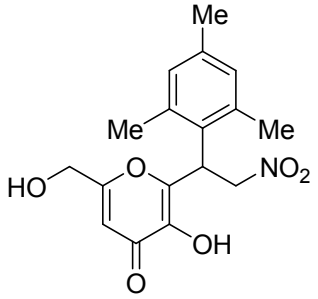
Semi solid; ^{1}H NMR (300 MHz, $CDCl_3$+ DMSO-d_6): δ 8.7 (bs, 1H, OH_{vinyl}), 7.30 (d, *J* = 8.5 Hz, 2H), 6.83 (d, *J* = 8.4 Hz, 2H), 6.30 (s, 1H), 5.52 (bs, 1H, OH_{ali}), 5.16 (dd, *J* = 8.2, *J* = 13.2 Hz, 1H), 5.03-4.94 (m, 2H), 4.31(d, *J* = 6.0 Hz, 2H), 3.6 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$+ DMSO-d_6): δ 173.3, 166.6, 158.3, 146.5, 141.1, 128.1, 126.7, 113.4, 108.3, 74.7, 59.3, 54.2, 40.8 ;MS (ESI): *m/z* ([M+H]$^+$): 322; HRMS (ESI): *m/z* calcd for $C_{15}H_{16}NO_7$: 322.0927; found: 322.0925.

2-(1-(2,4-dimethoxyphenyl)-2-nitroethyl)-3-hydroxy-6-(hydroxymethyl)-4H-pyran-4-one (4d):



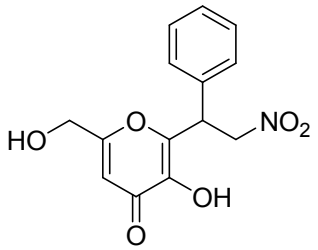
Semi solid; ^{1}H NMR (300 MHz, $CDCl_3$+ DMSO-d_6): δ 8.6 (bs, 1H, OH_{vinyl}), 6.90-6.72 (m, 4H), 6.36 (s, 1H), 5.56 (bs, 1H, OH_{ali}), 5.39 (dd, *J* = 5.6, *J* = 9.6 Hz, 1H), 5.19-5.13 (m, 1H), 4.85-.76 (m, 1H), 4.33 (s, 2H), 3.84 (s, 3H), 3.71 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$+ DMSO-d_6): δ 174.6, 167.9, 159.6, 156.8, 148.0, 142.4, 129.4, 128.0, 114.7, 109.5, 76.0, 60.6, 58.7, 55.5, 42.0 ; MS (ESI): *m/z* ([M+H]$^+$): 352; HRMS (ESI): *m/z* calcd for $C_{16}H_{18}NO_8$: 352.1032; found: 352.1035.

3-hydroxy-6-(hydroxymethyl)-2-(1-mesityl-2-nitroethyl)-4H-pyran-4-one (4e):



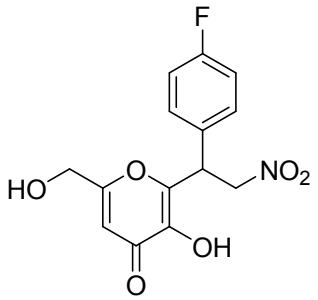
Semi solid; ^{1}H NMR (300 MHz, $CDCl_3$+ DMSO-d_6): δ 8.6 (bs, 1H, OH_{vinyl}), 6.78 (s, 2H), 6.34 (s, 1H), 5.57-5.27 (m, 3H), 4.70 (dd, *J* = 5.2, *J* = 13.8 Hz, 1H, OH_{ali}), 4.26 (septet, *J* = 5.9, *J* = 15.4 Hz, 1H), 2.30 (s, 6H), 2.21 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$+ DMSO-d_6): δ 173.2, 166.9, 145.9, 141.9, 136.9, 136.3, 129.8, 128.7, 108.4, 72.9, 59.7, 38.2, 20.16, 20.11; MS (ESI): *m/z* ([M+H]$^+$): 334.

3-hydroxy-6-(hydroxymethyl)-2-(2-nitro-1-phenylethyl)-4H-pyran-4-one (4a):



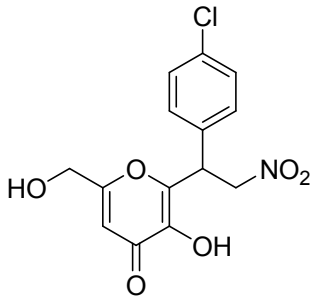
Semi solid; ^{1}H NMR (300 MHz, $CDCl_3$+ DMSO-d_6): δ 8.7 (bs, 1H, OH_{vinyl}), 7.38-7.17 (m, 5H), 6.30 (s, 1H), 5.51 (bs, 1H, OH_{ali}), 5.11-4.89 (m, 3H), 4.31 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$+ DMSO-d_6): δ 173.0, 166.2, 145.7, 141.2, 134.8, 127.8, 126.9, 126.7, 108.1, 74.4, 59.0, 41.2; MS (ESI): *m/z* ([M+H]$^+$): 292; HRMS (ESI): *m/z* calcd for $C_{14}H_{14}NO_6$: 292.0821; found: 292.0820.

2-(1-(4-fluorophenyl)-2-nitroethyl)-3-hydroxy-6-(hydroxymethyl)-4H-pyran-4-one (4c):



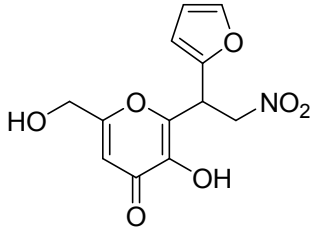
Semi solid; ^{1}H NMR (300 MHz, $CDCl_3$+ DMSO-d_6): δ 8.5 (bs, 1H, OH_{vinyl}), 7.54 (d, *J* = 5.4, 2H), 7.40 (d, *J* = 5.4 Hz, 2H), 6.32 (s, 1H), 5.42 (bs, 1H, OH_{ali}), 5.2-4.88 (m, 3H), 4.31 (d, *J* = 6.0 Hz, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$+ DMSO-d_6): δ 173.4, 166.6, 146.2, 141.7, 135.3, 128.3, 127.4, 127.2, 108.5, 74.8, 54.4, 41.6; MS (ESI): *m/z* ([M+H]$^+$): 310.

2-(1-(4-chlorophenyl)-2-nitroethyl)-3-hydroxy-6-(hydroxymethyl)-4H-pyran-4-one (4f):



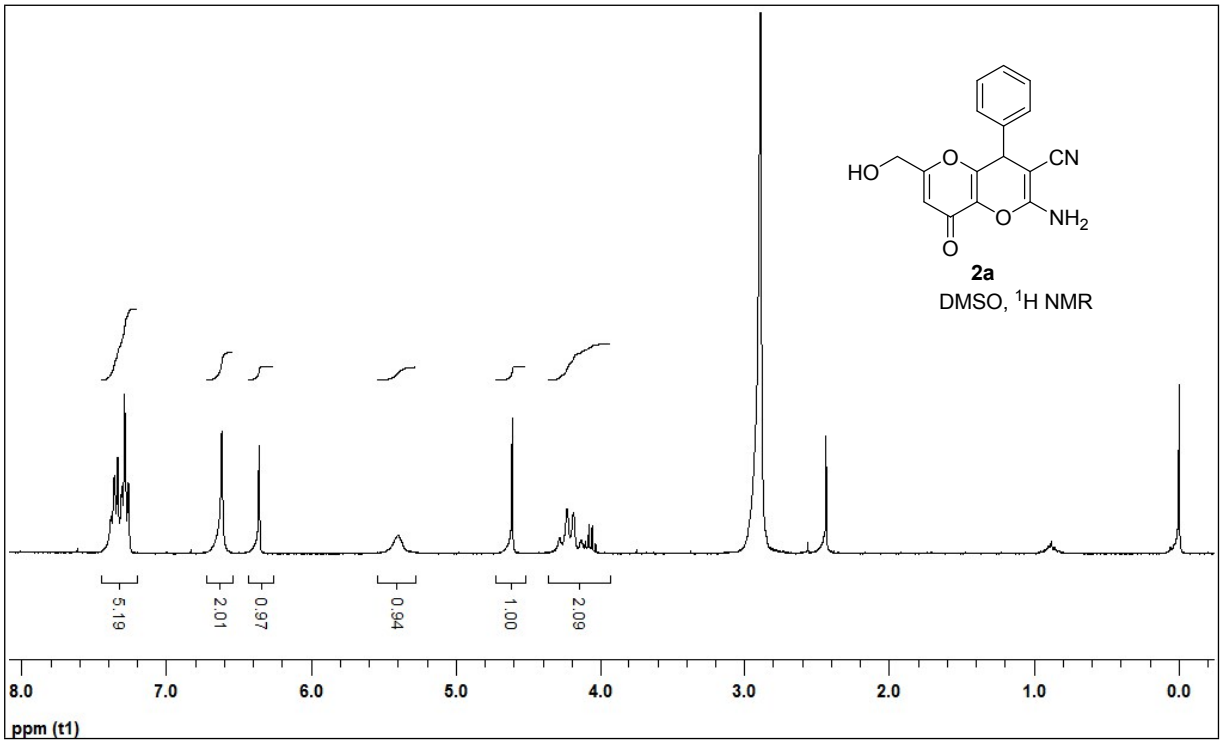
Semi solid; ^{1}H NMR (300 MHz, $CDCl_3$+ DMSO-d_6): δ 8.6 (bs, 1H, OH_{vinyl}), 7.36 (d, *J* = 8.2 Hz, 2H), 6.98 (d, *J* = 8.5 Hz, 2H), 6.28 (s, 1H), 5.60 (bs, 1H, OH_{ali}), 5.23-4,93 (m, 2H), 4.35(d, *J* = 5.6 Hz, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$+ DMSO-d_6): δ 175.0, 164.1, 145.7, 141.2, 134.8, 127.8, 126.9, 108.1, 74.4, 54.1, 41.2; MS (ESI): *m/z* ($[M+H]^+$): 326; HRMS (ESI): *m/z* calcd for $C_{14}H_{13}ClNO_6$: 326.0431; found: 326.0437.

2-(1-(furan-2-yl)-2-nitroethyl)-3-hydroxy-6-(hydroxymethyl)-4H-pyran-4-one (4g):

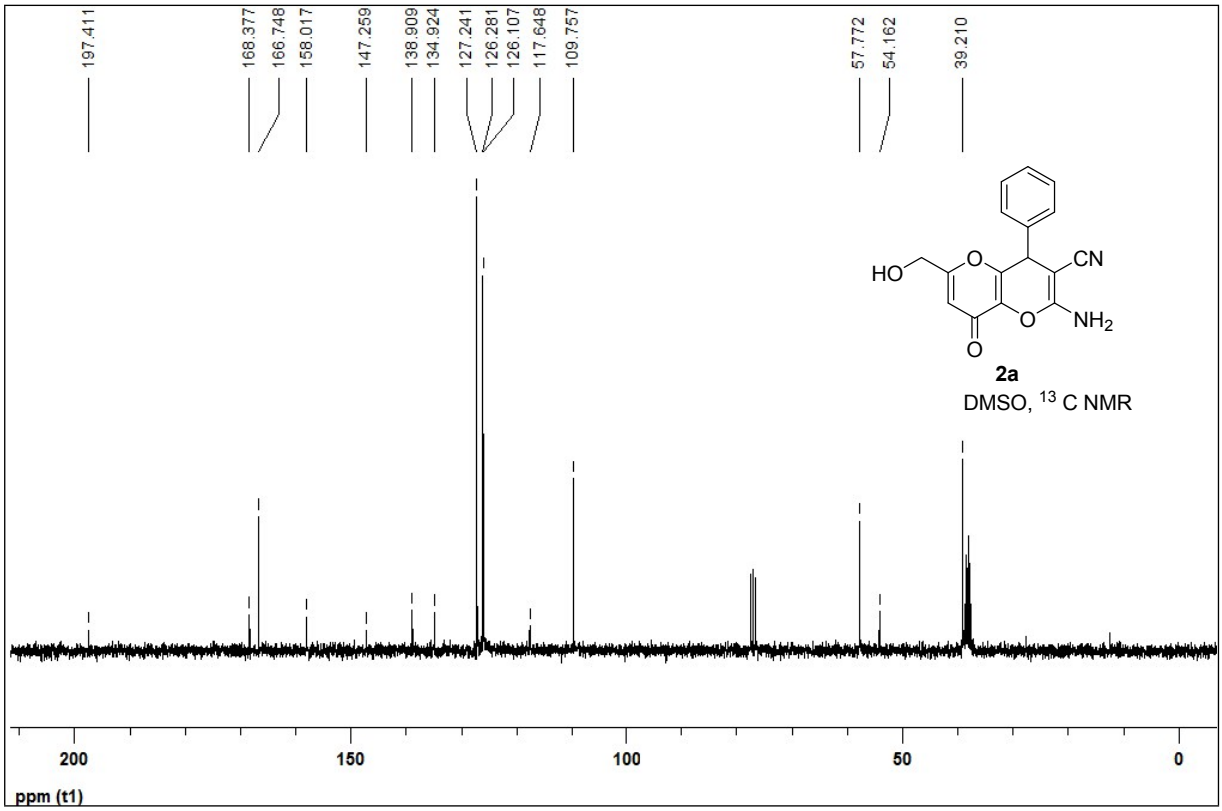


Semi solid; ^{1}H NMR (300 MHz, $CDCl_3$+ DMSO-d_6): δ 8.8 (bs, 1H, OH_{vinyl}), 7.87 (m, 1H), 7.77 (d, *J* = 3.3 Hz, 1H), 7.69 (d, *J* = 3.8 Hz, 1H), 6.77-6.69 (m, 1H), 6.24 (s, 1H), 5.51 (bs, 1H, OH_{ali}), 4.41 (d, *J* = 4.7 Hz, 2H), 4.97 (d, *J* = 5.3 Hz, 2H), 4.31 (d, *J* = 6.0 Hz, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$+ DMSO-d_6): δ 171.2, 166.1, 147.0, 140.6, 126.3, 113.0, 110.5, 74.3, 53.7, 40.3; MS (ESI): *m/z* ($[M+H]^+$): 282.

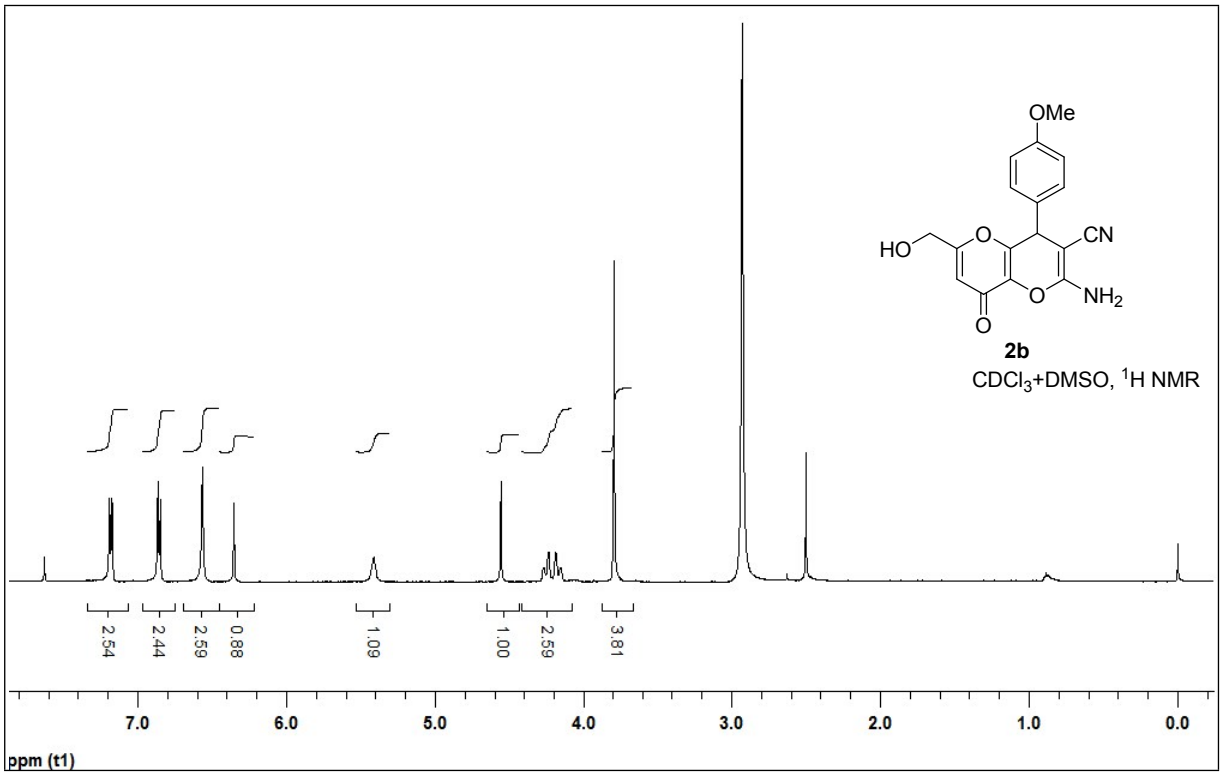
Copies of ^{1}H NMR & ^{13}C NMR spectras:



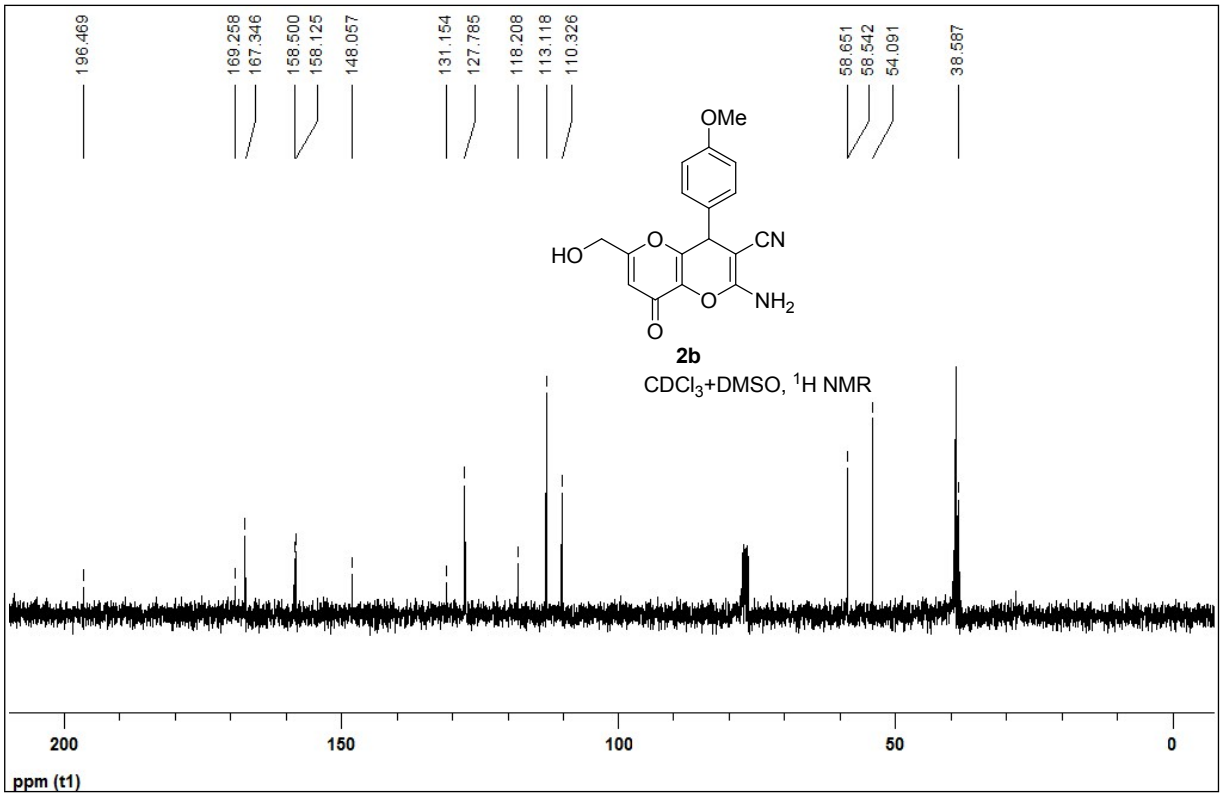
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2a



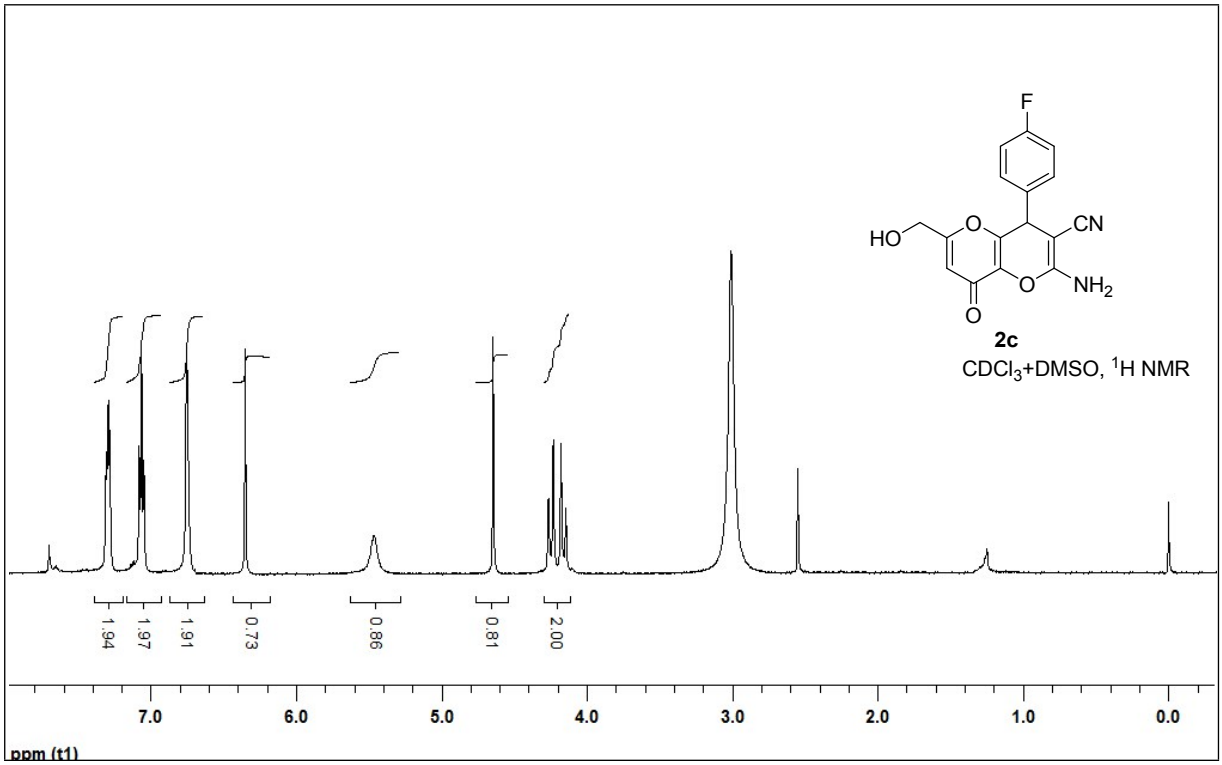
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2a



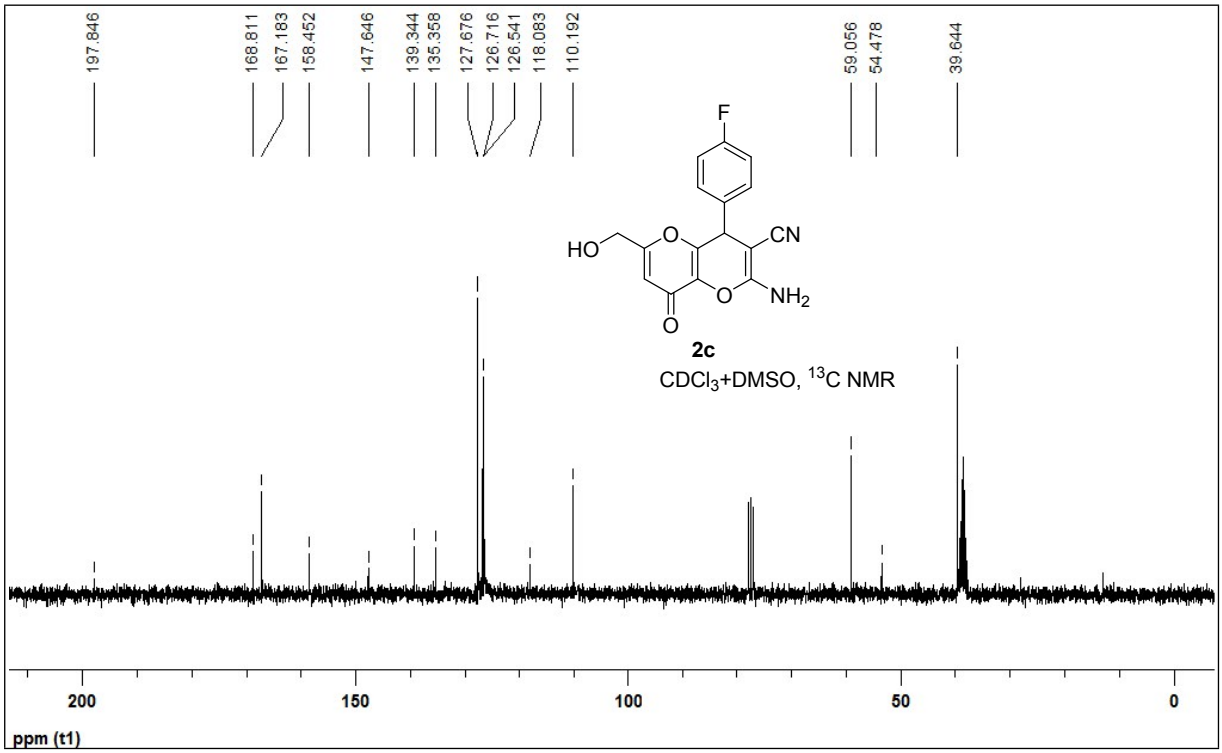
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2b



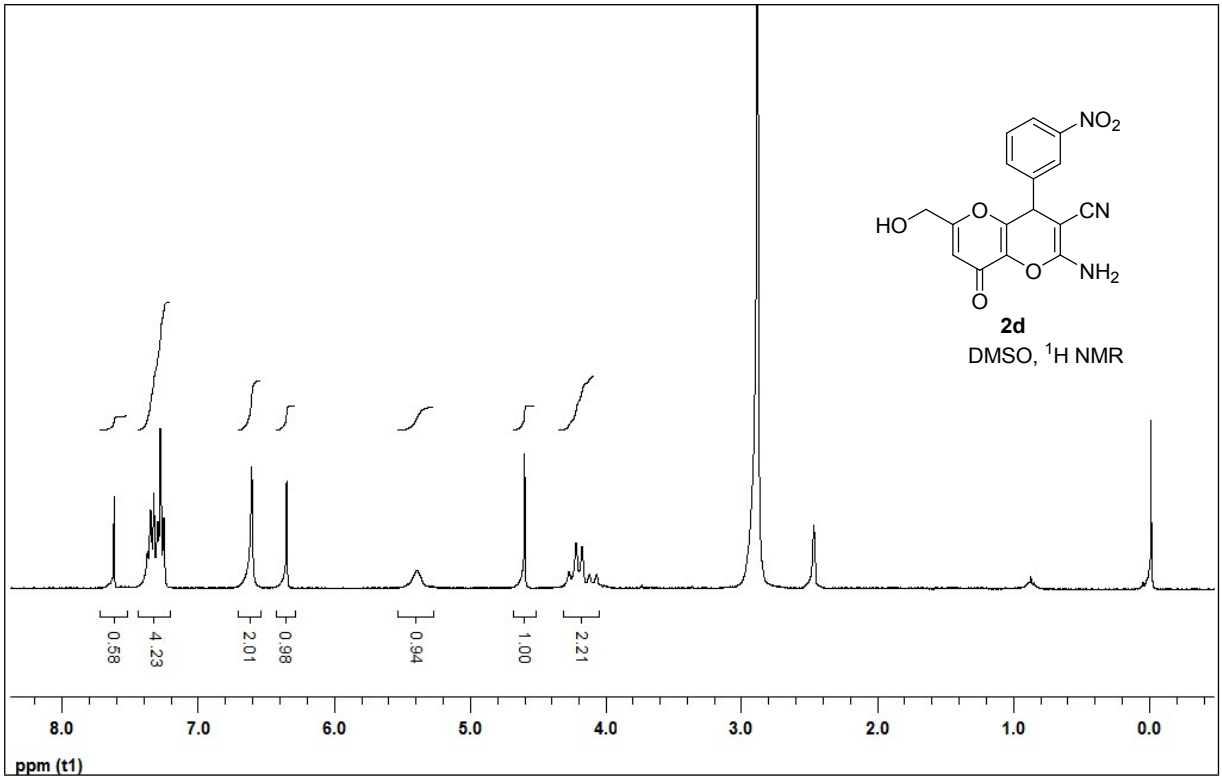
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2b



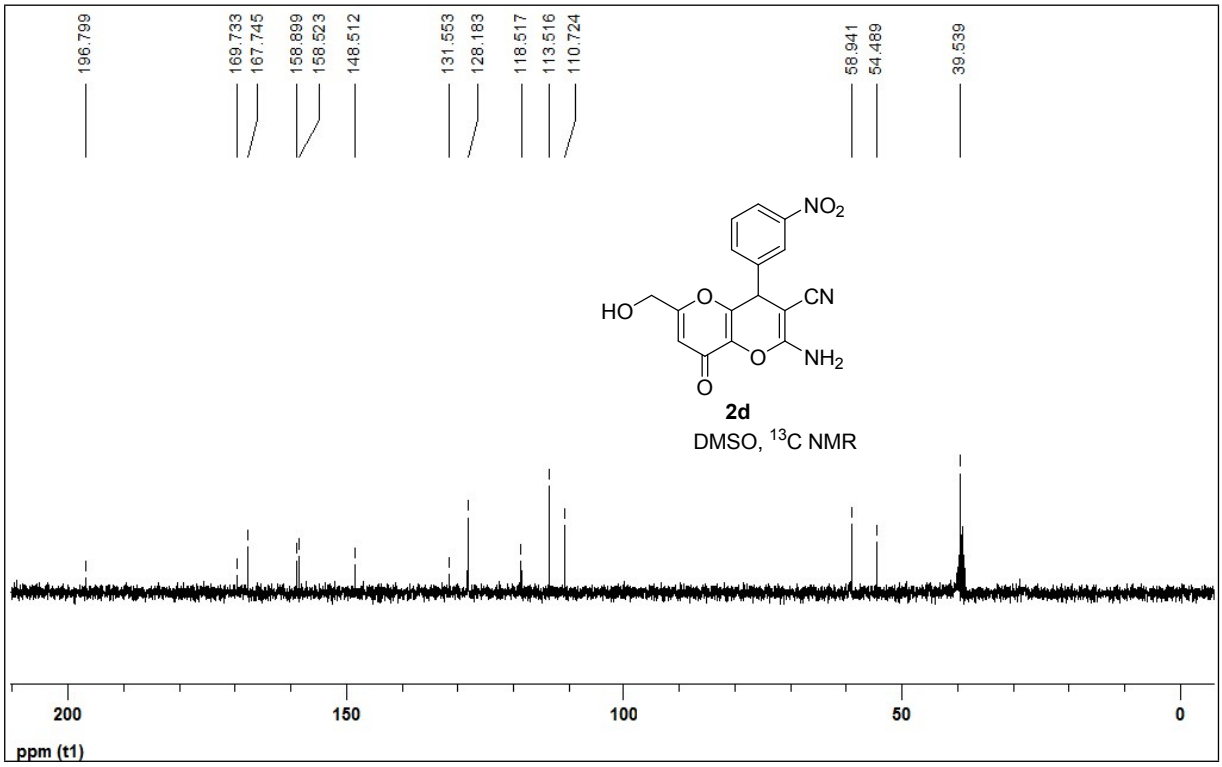
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2c



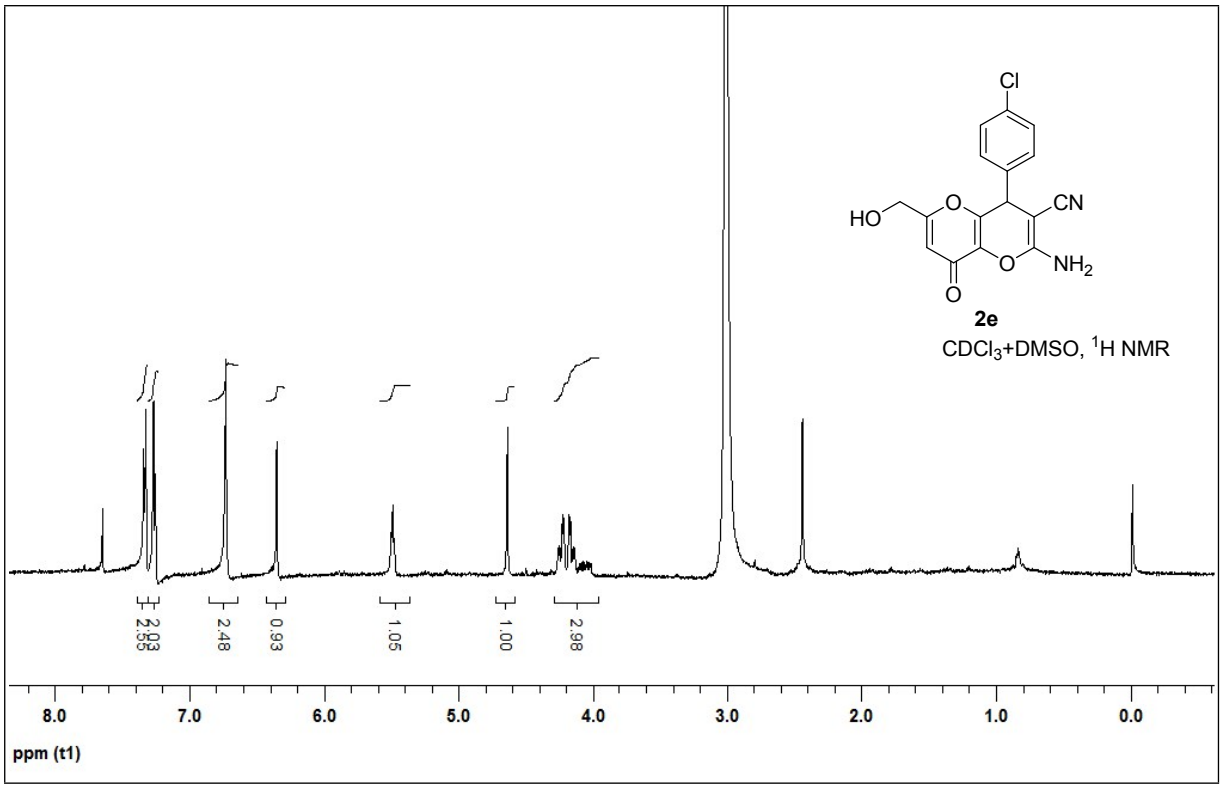
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2c



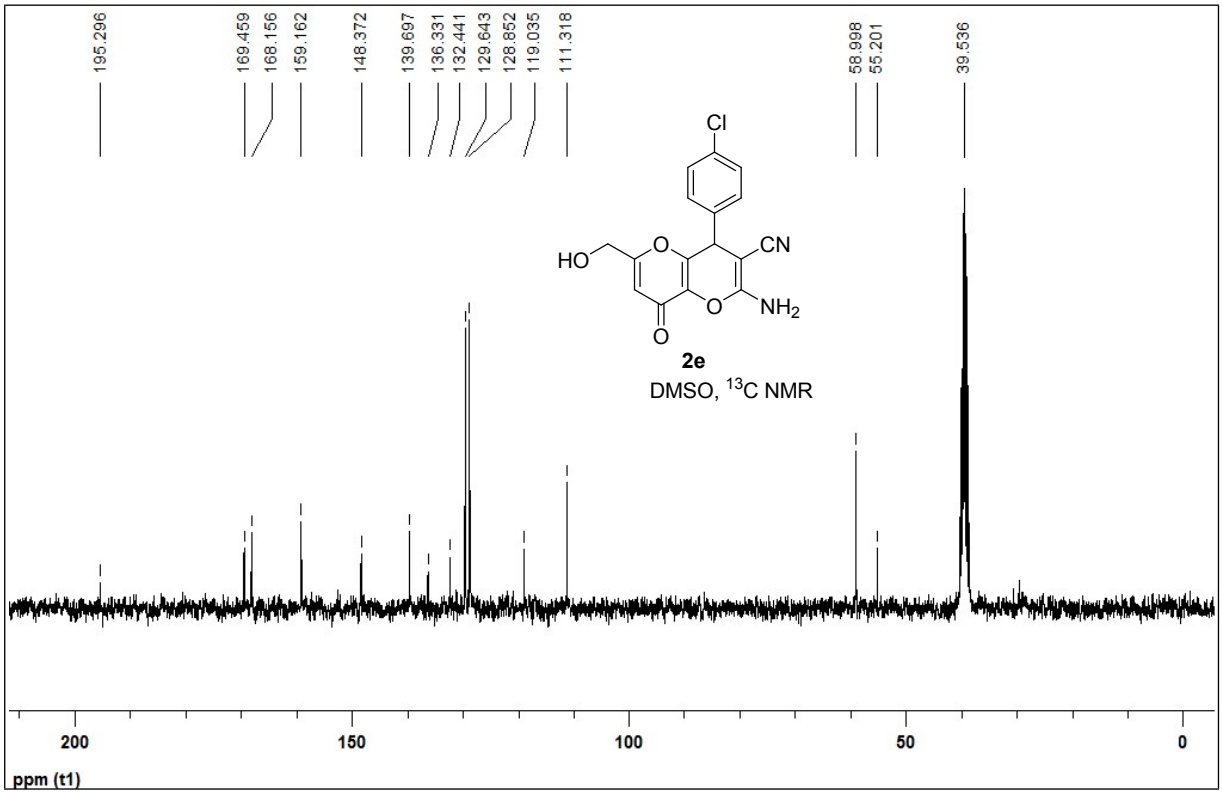
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2d



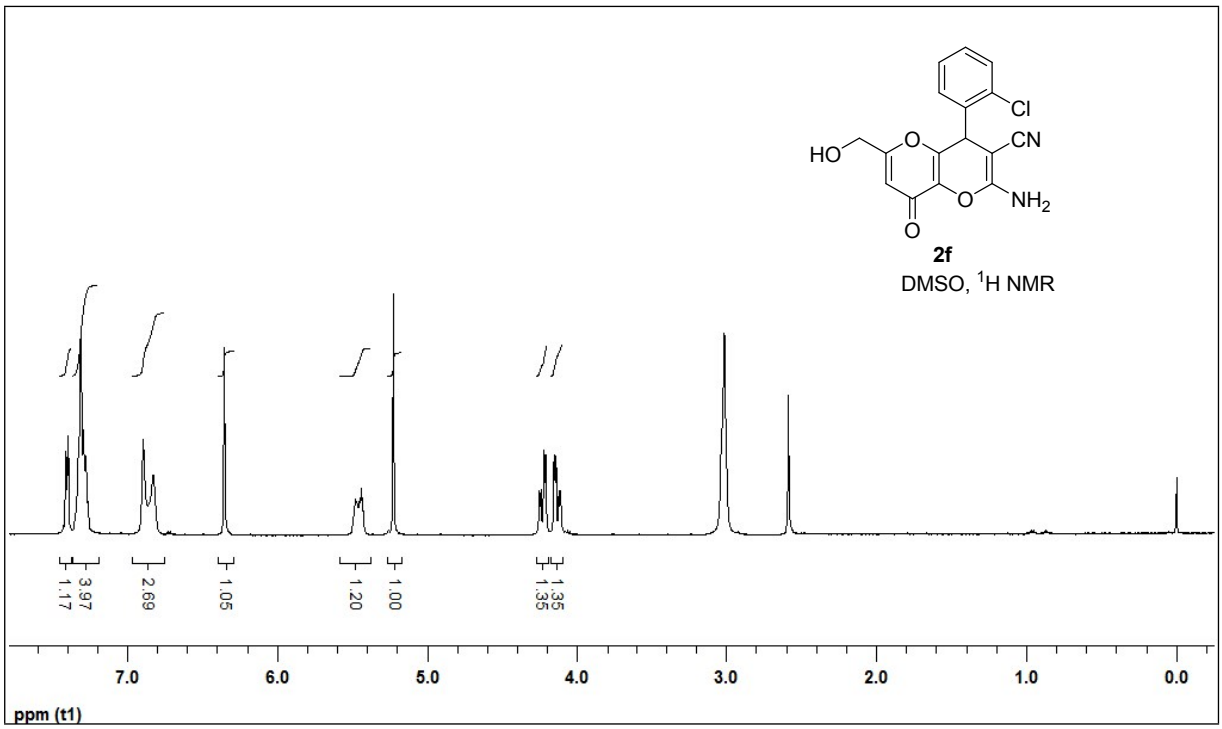
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2d



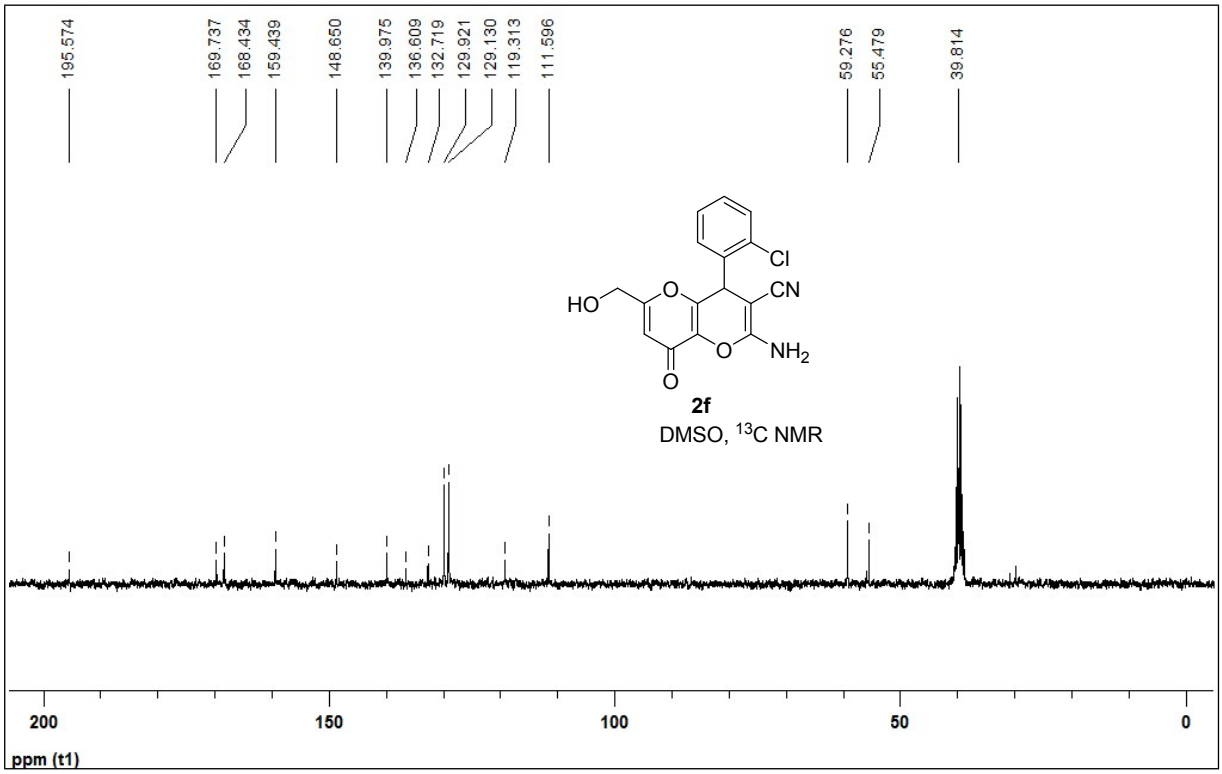
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2e



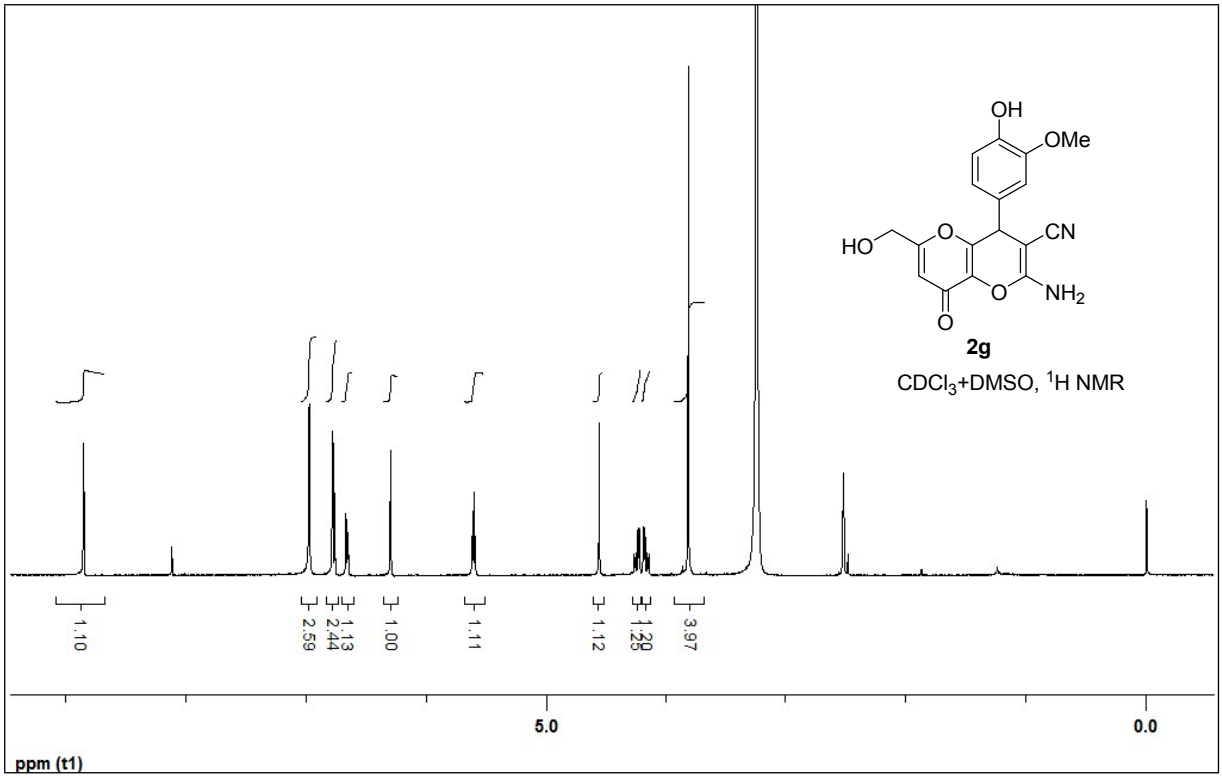
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2e



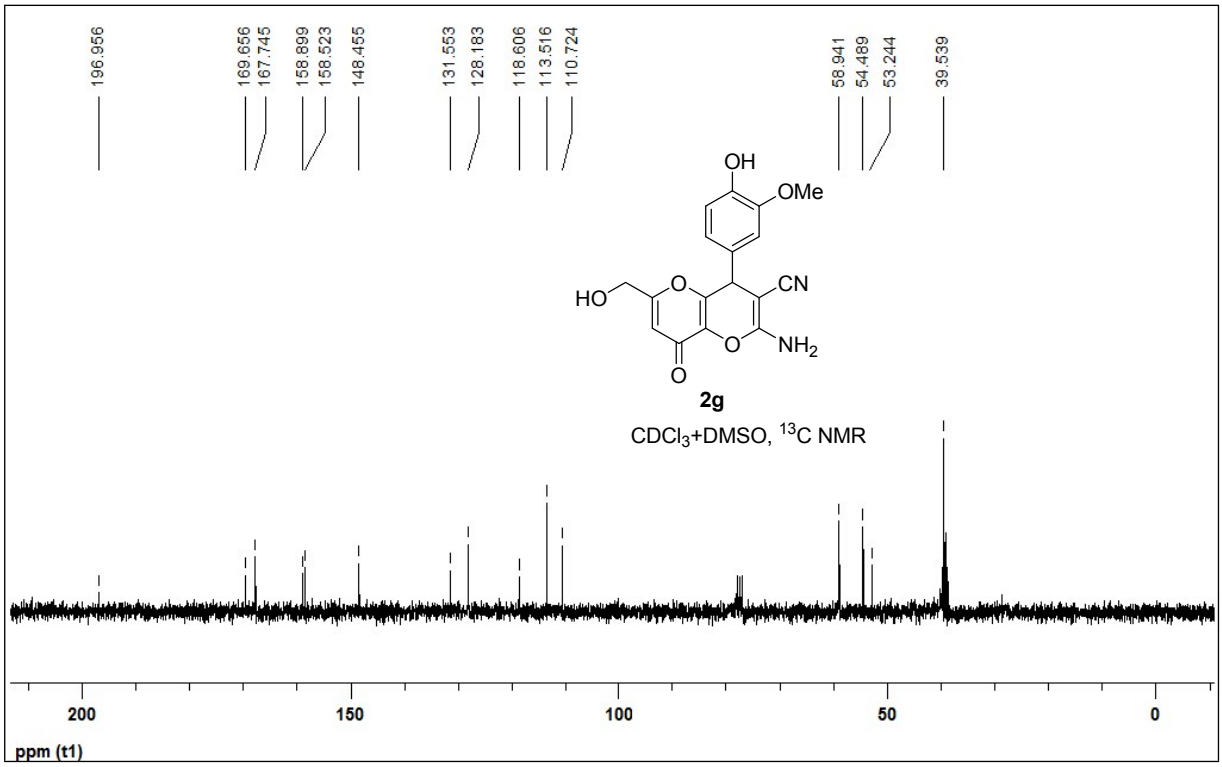
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2f



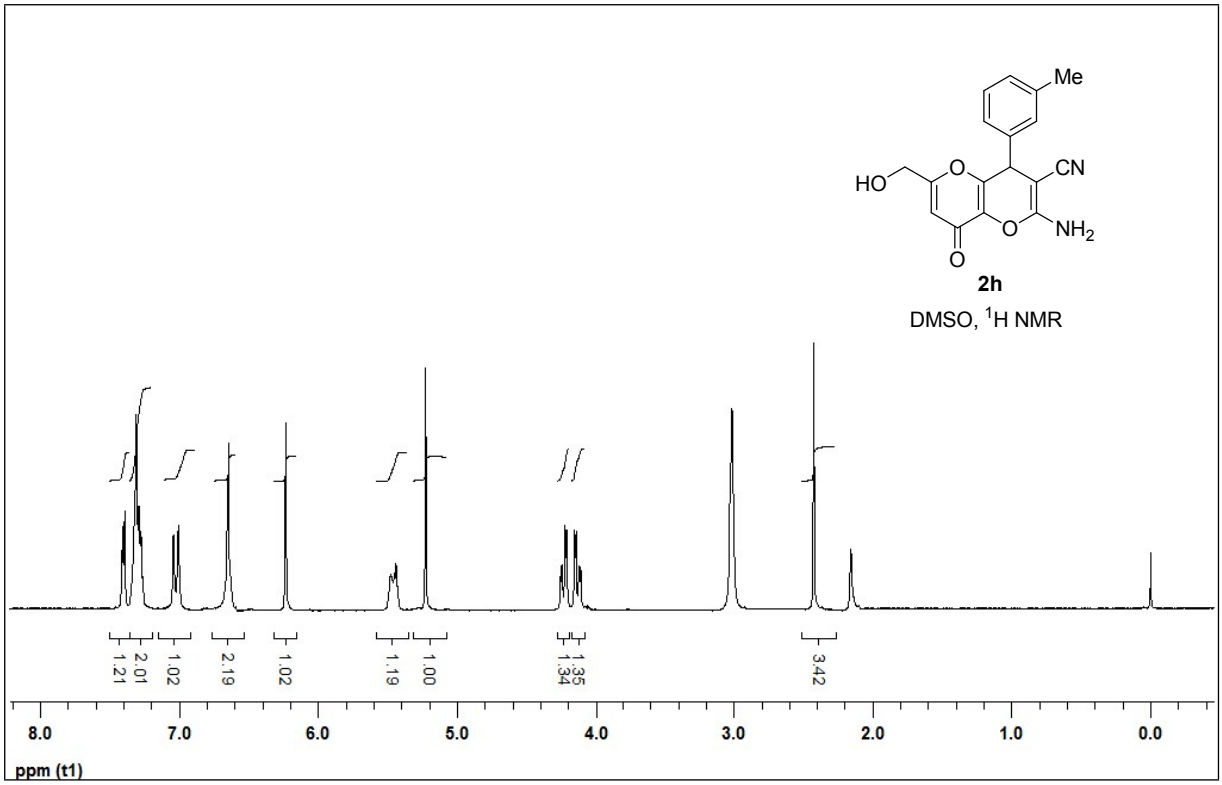
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2f



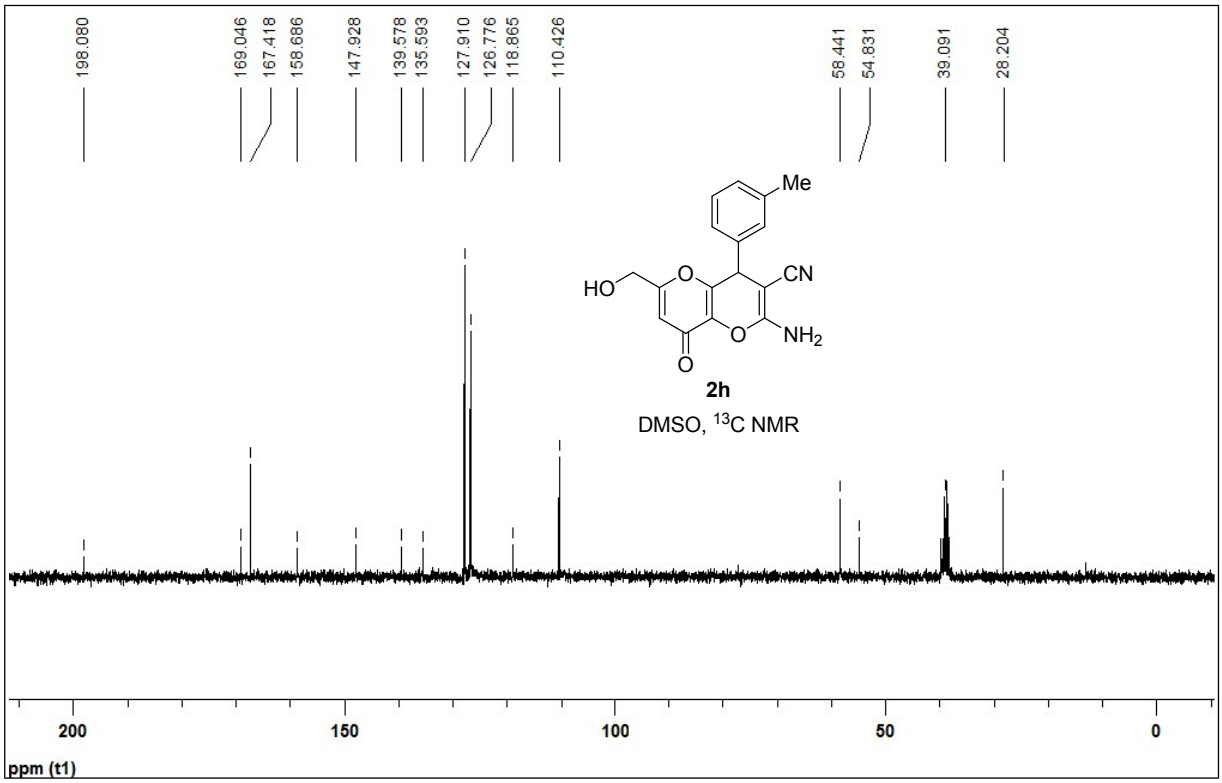
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2g



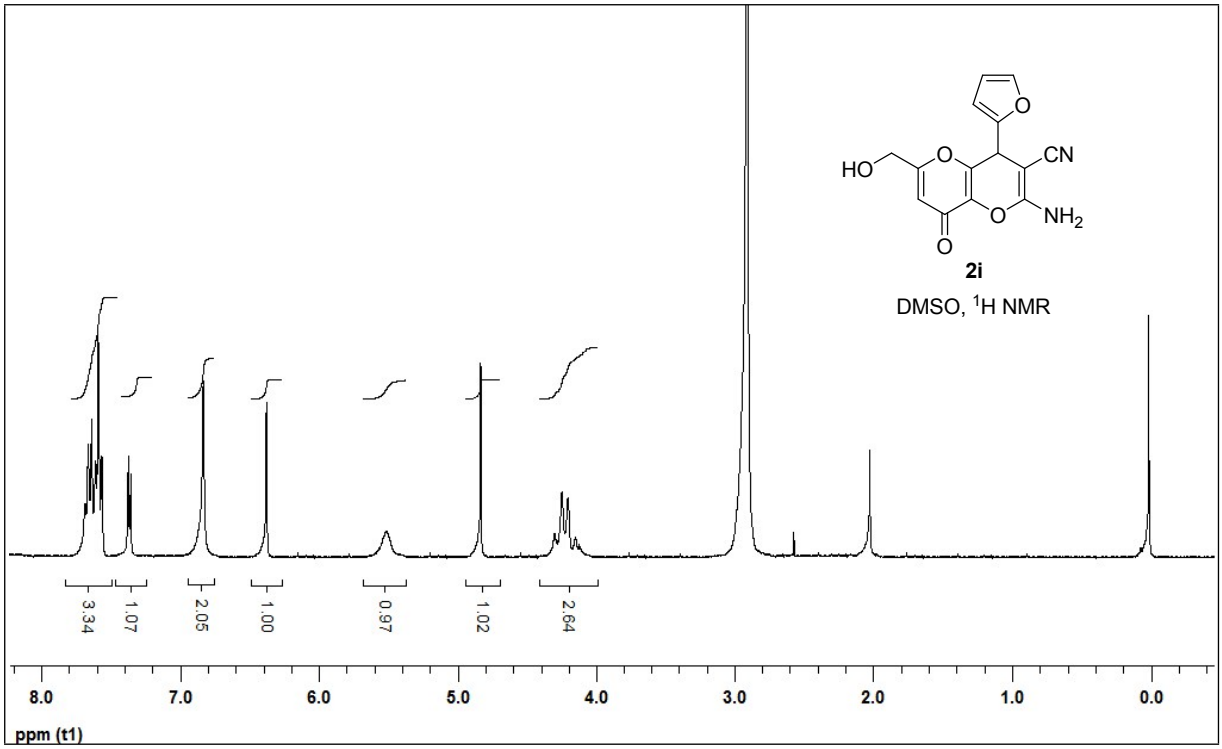
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2g



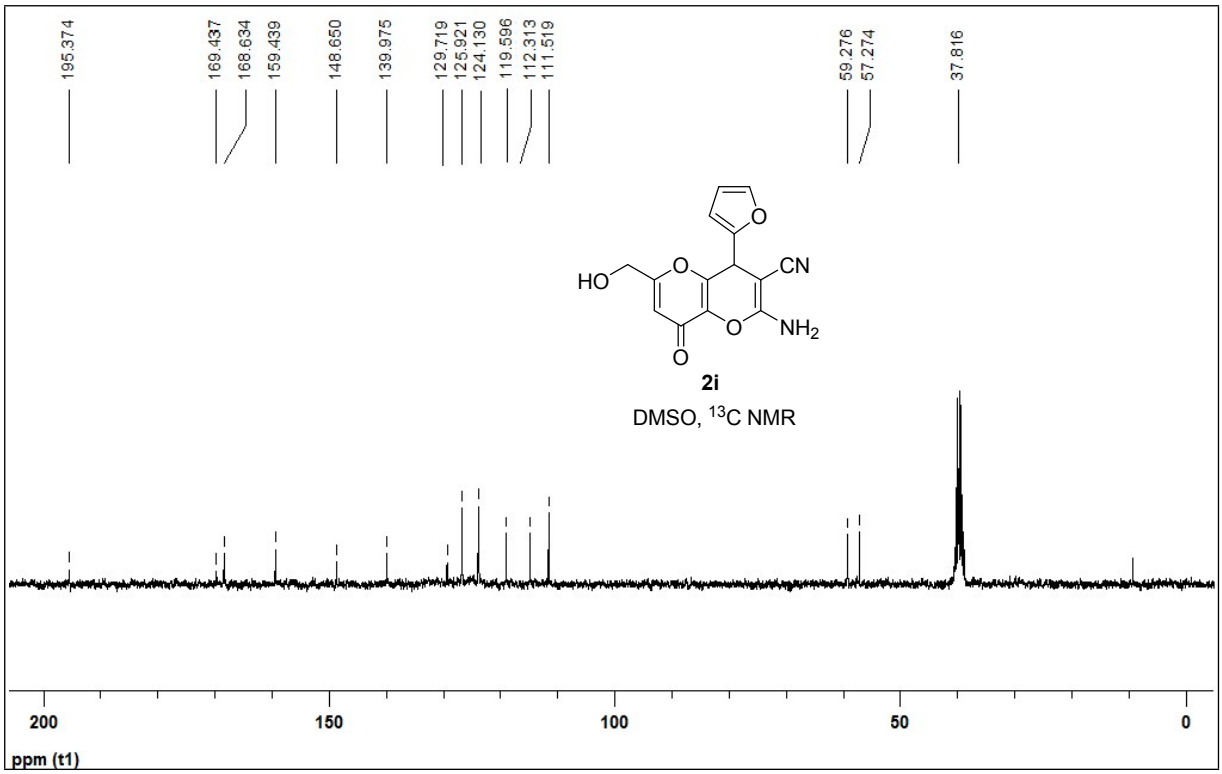
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2h



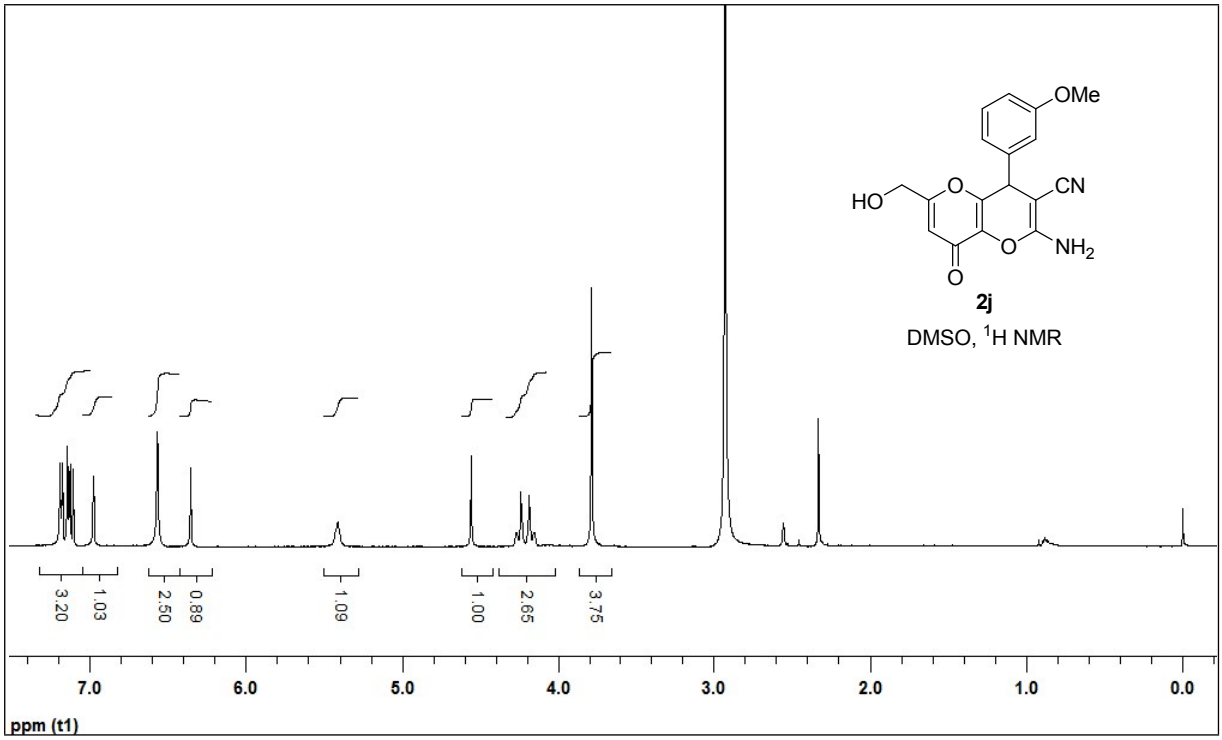
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2h



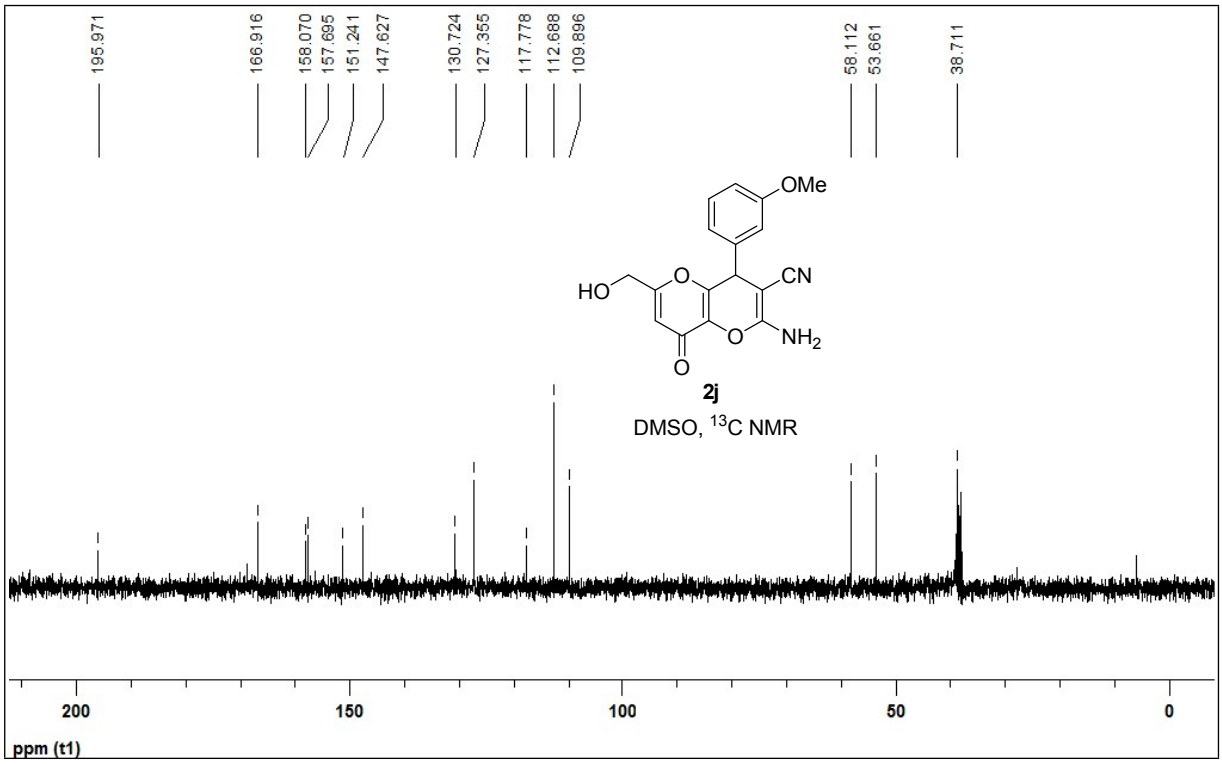
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2i



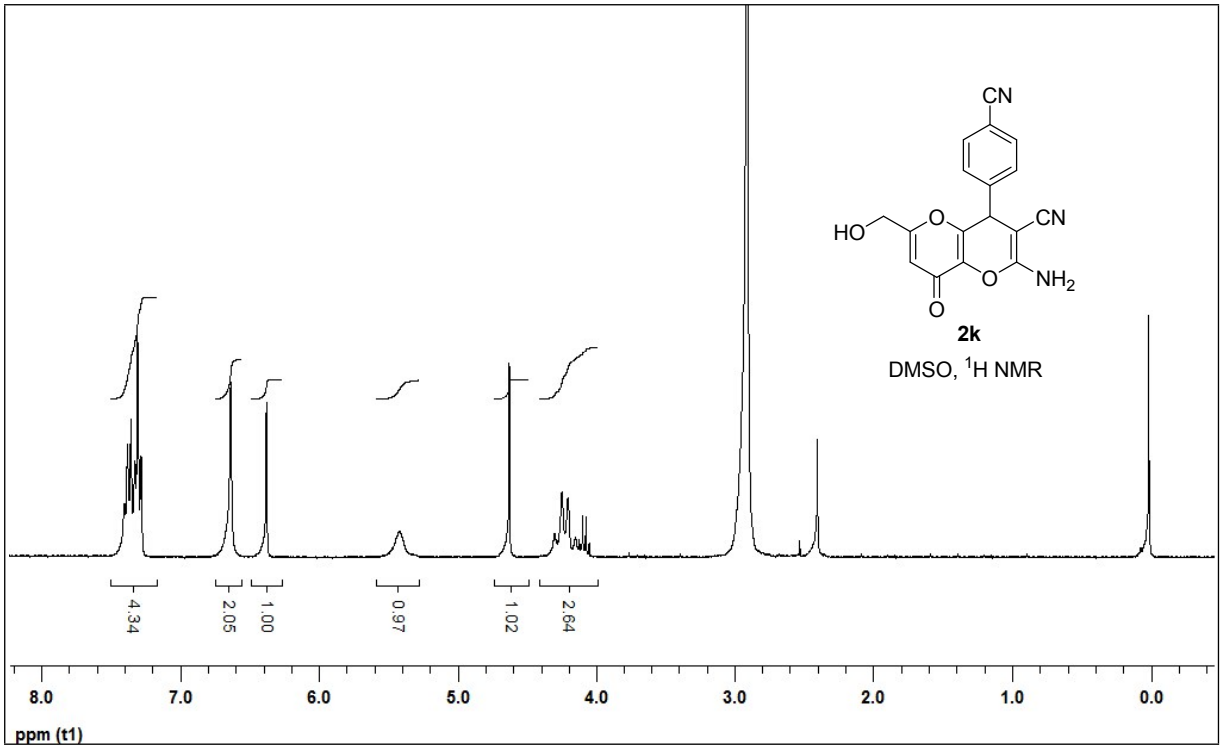
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2i



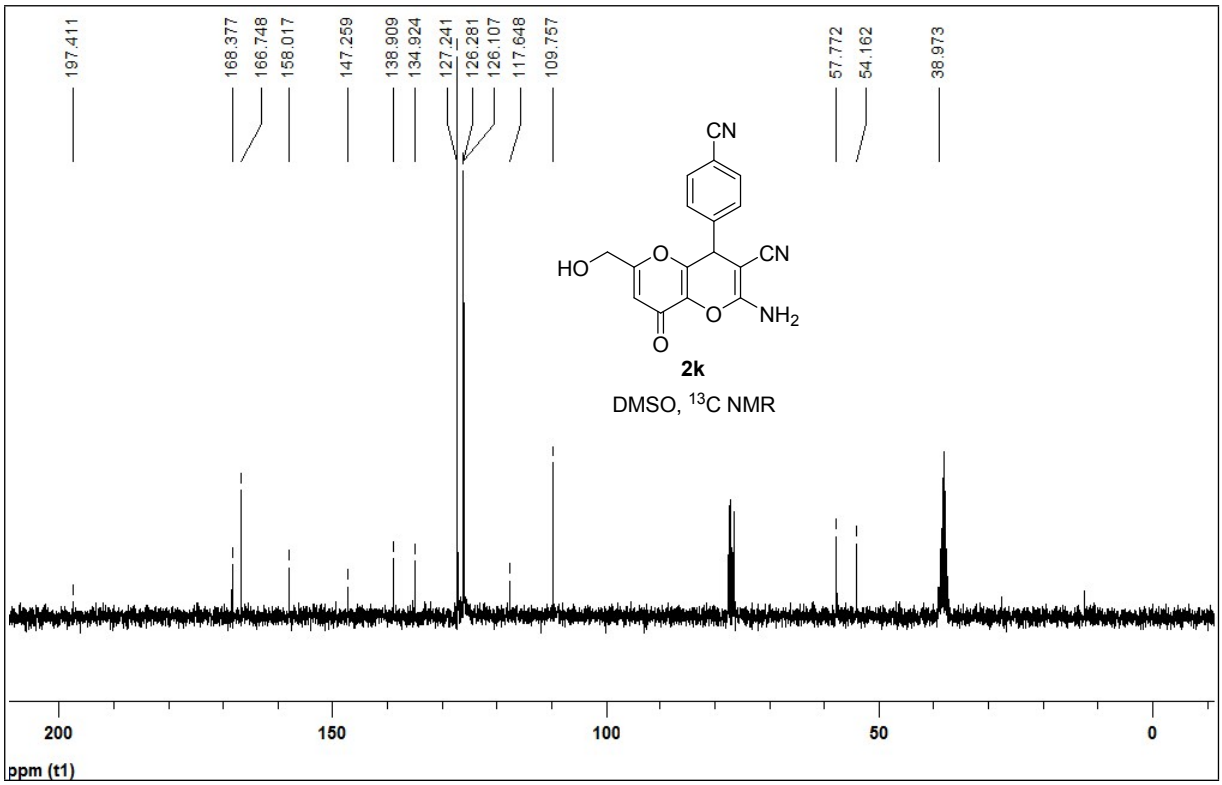
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2j



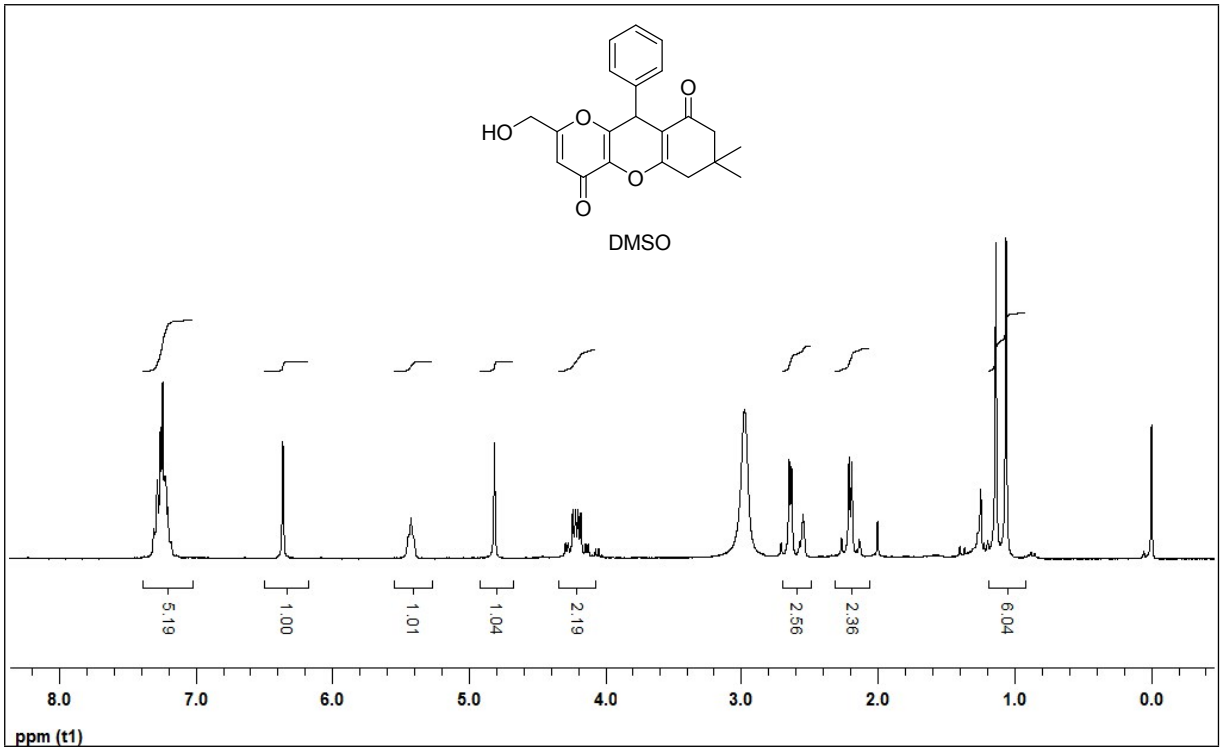
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2j



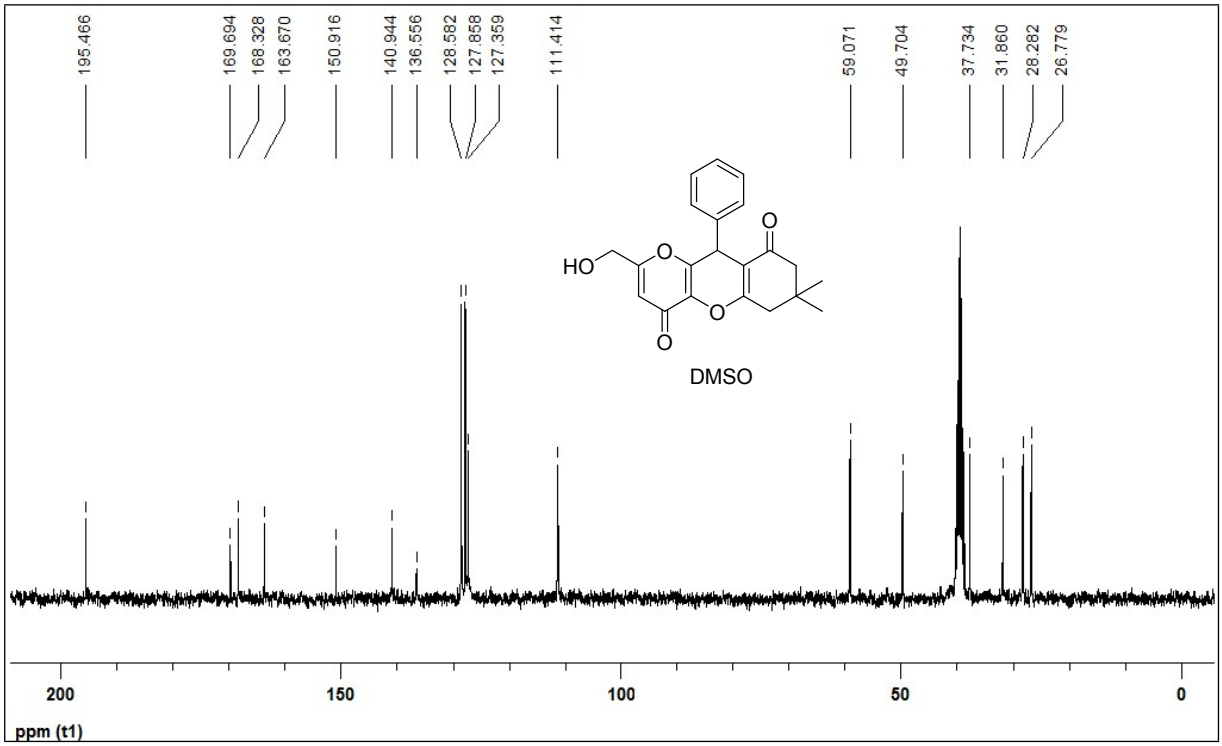
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 2k



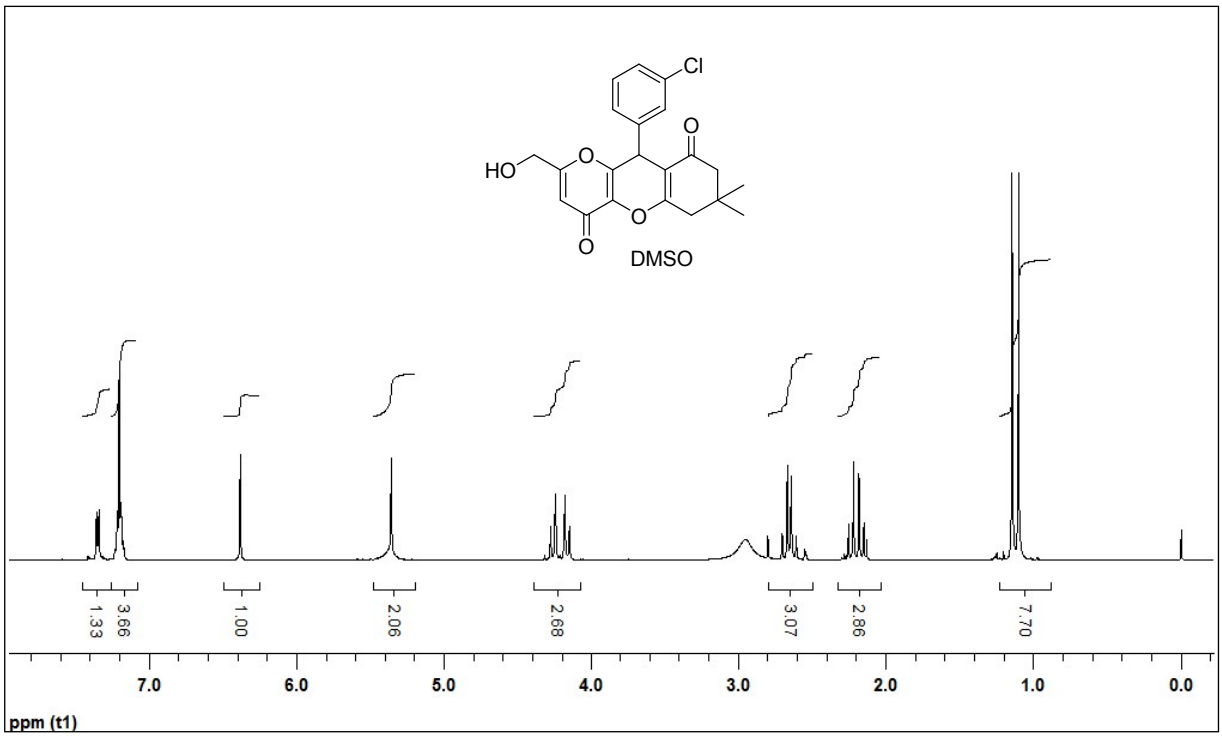
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 2k



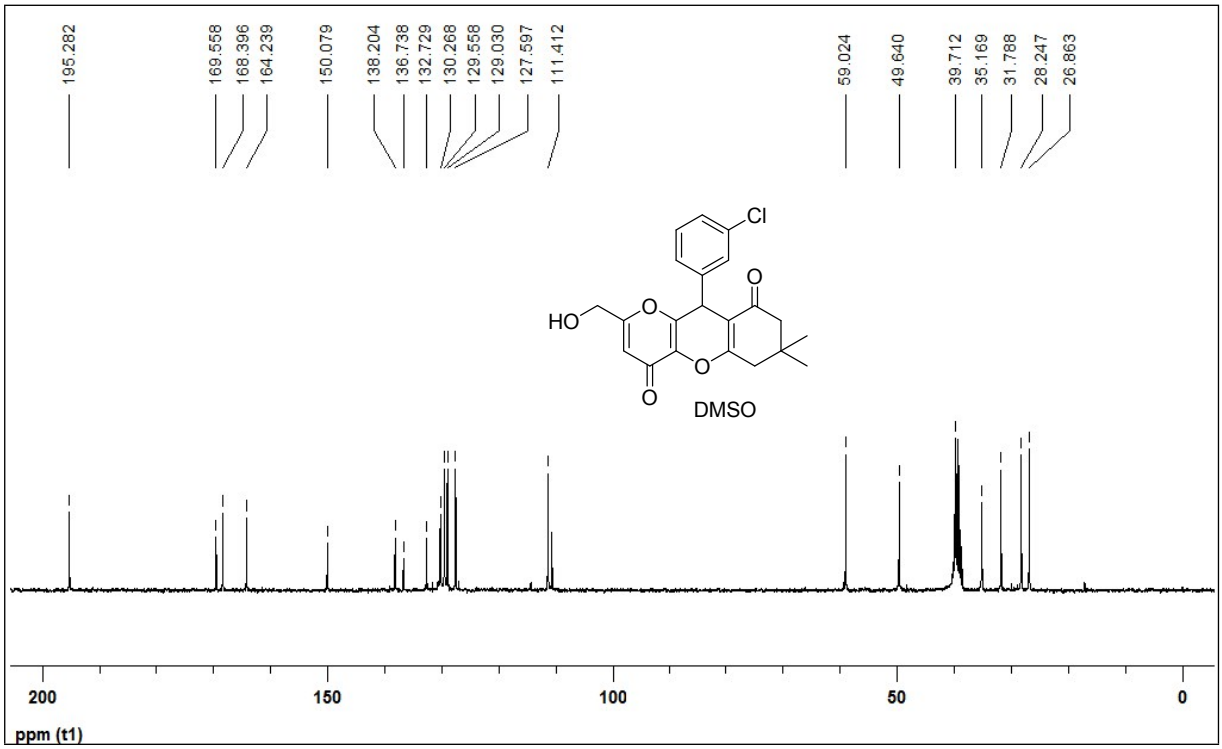
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3a



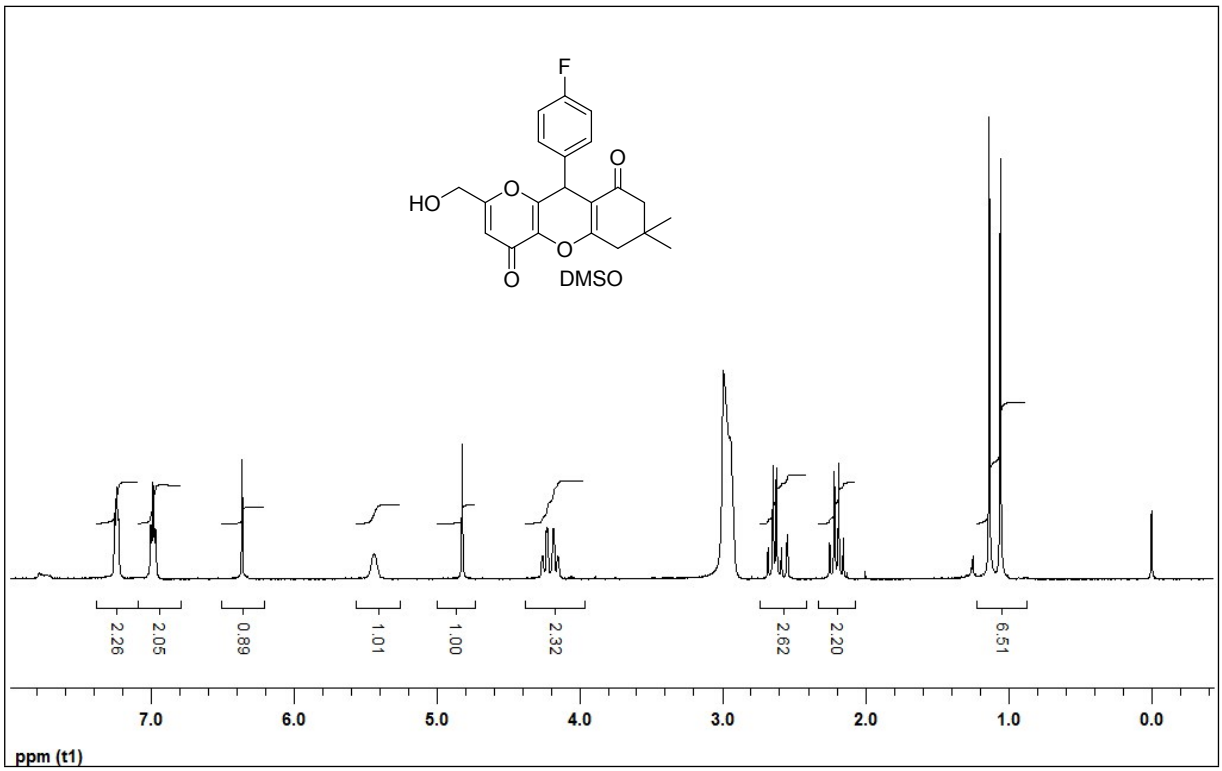
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3a



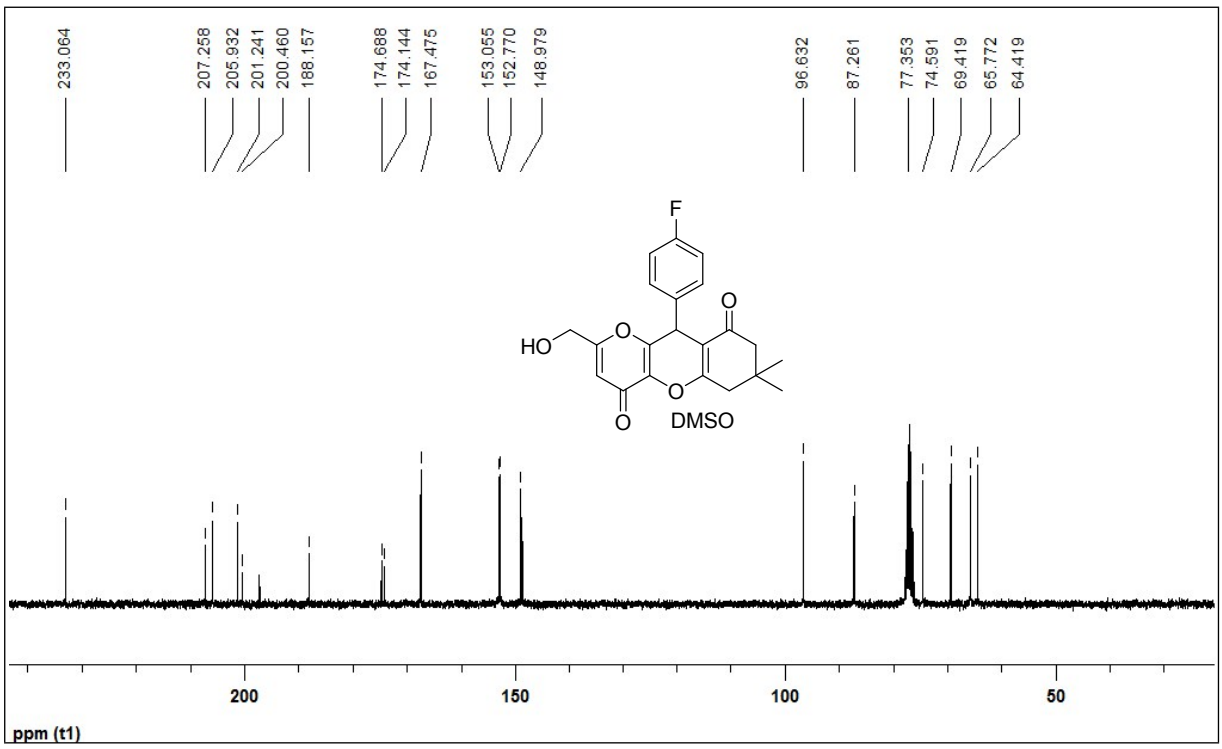
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3b



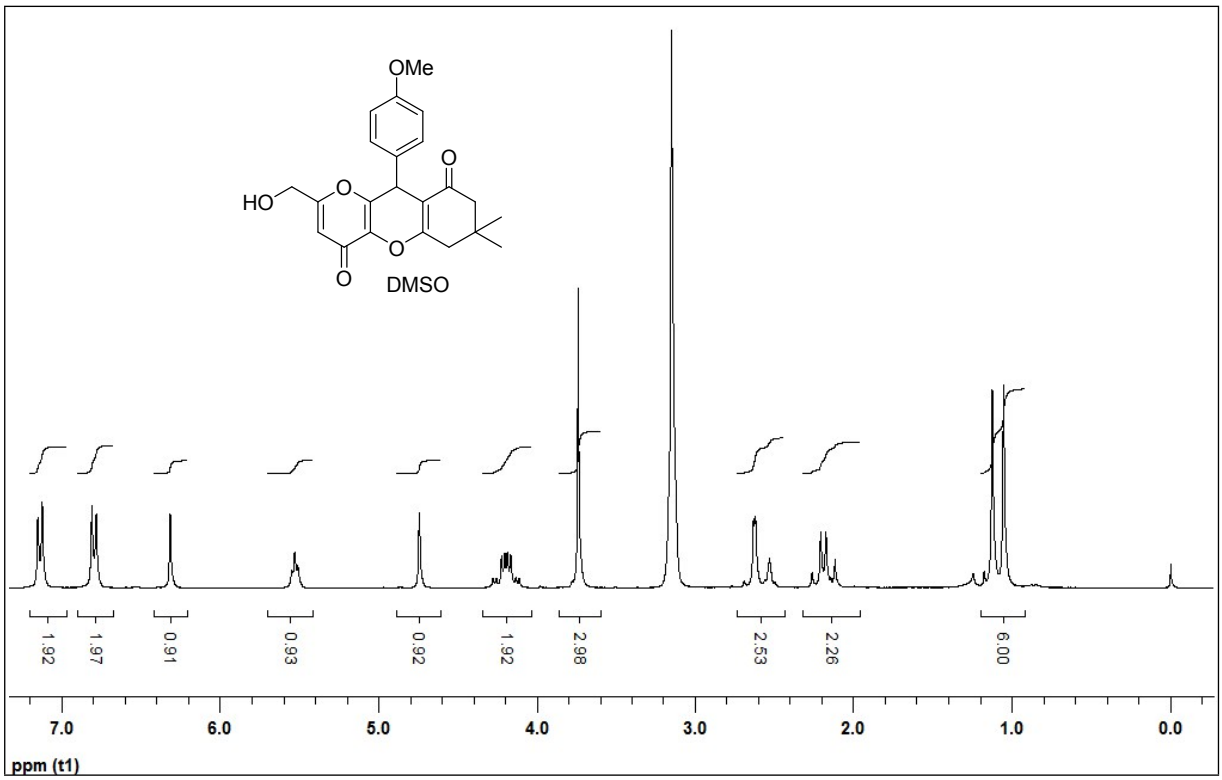
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3b



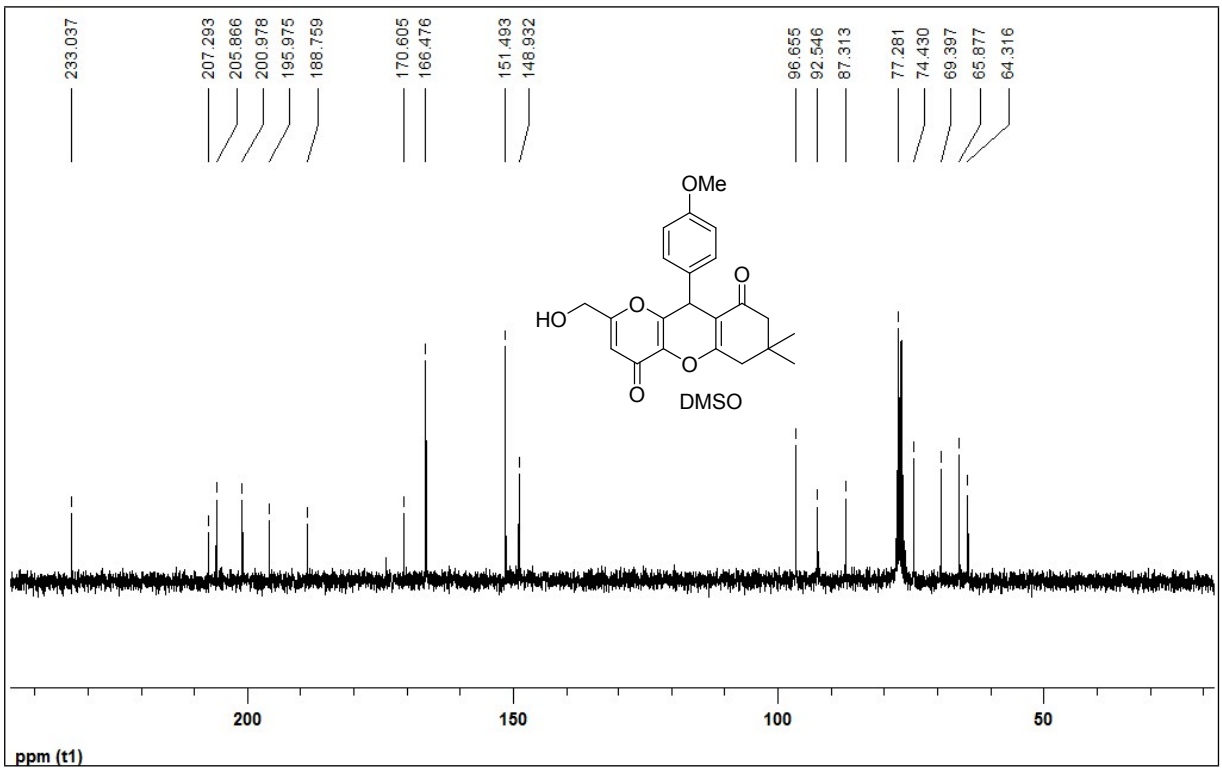
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3c



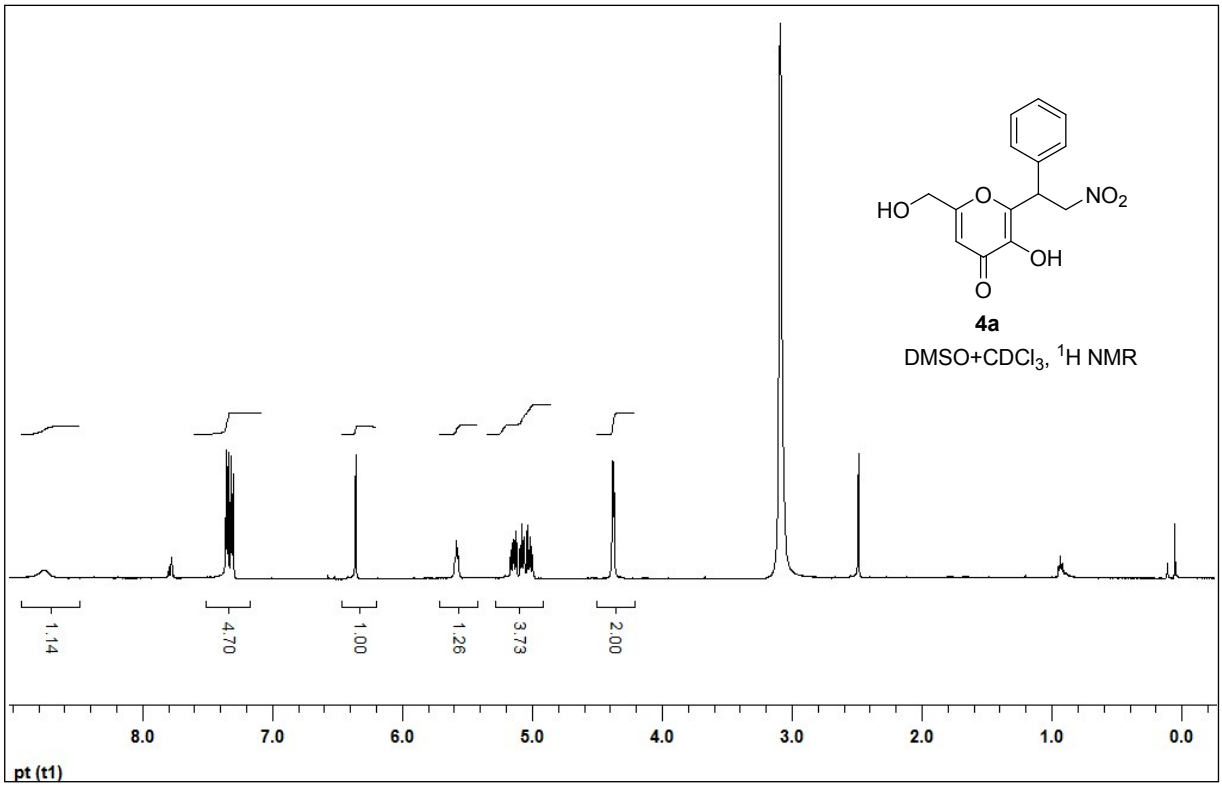
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3c



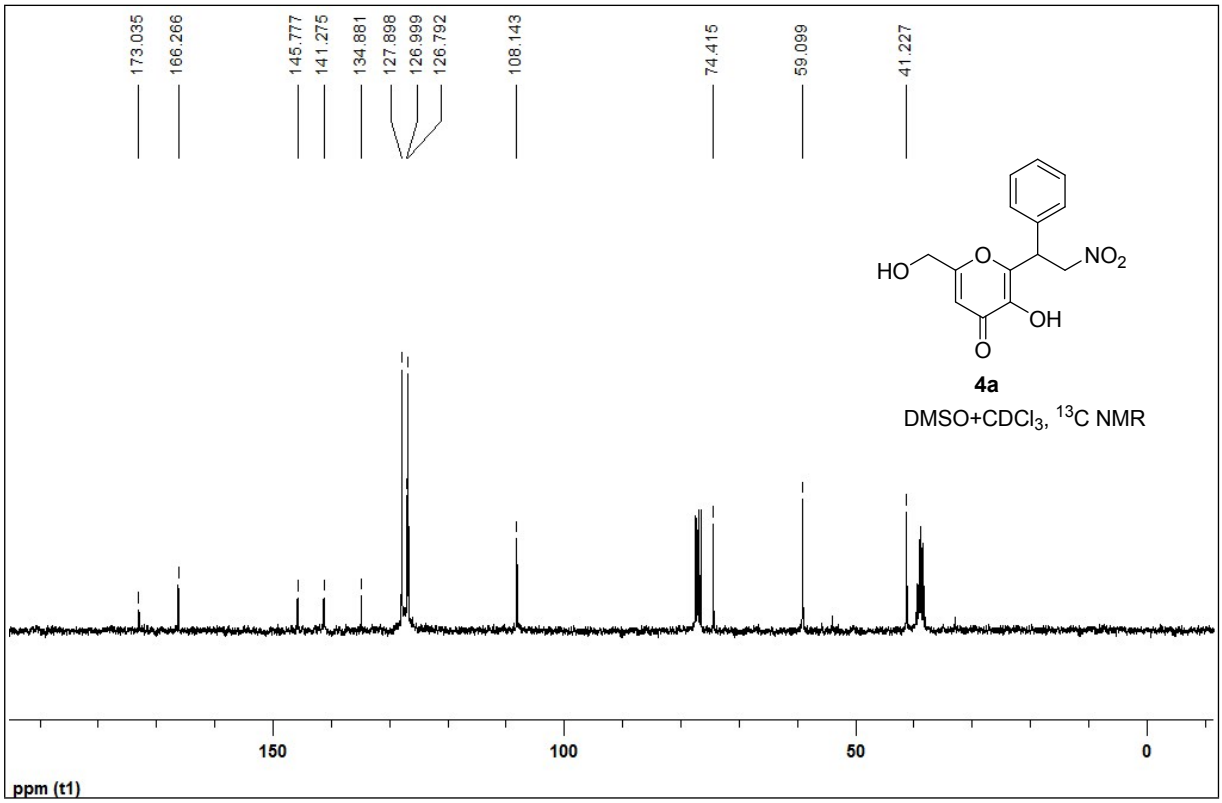
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3d



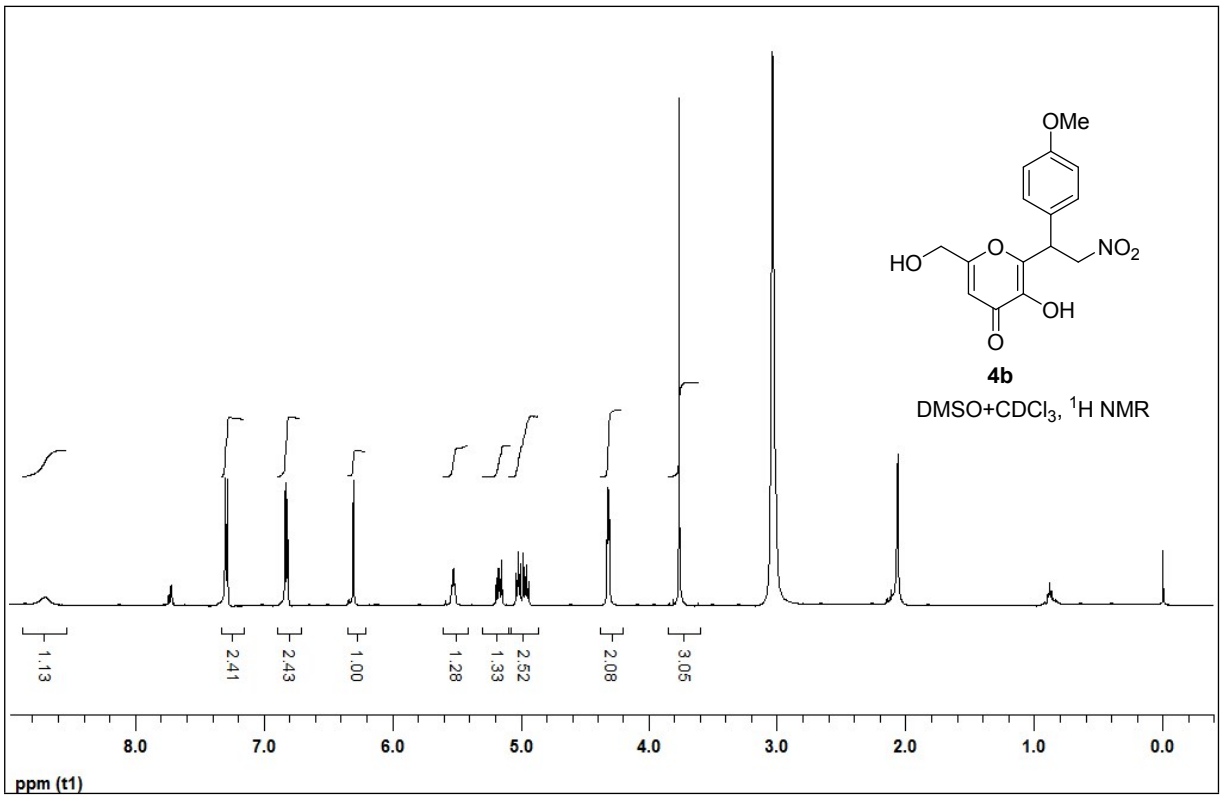
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3d



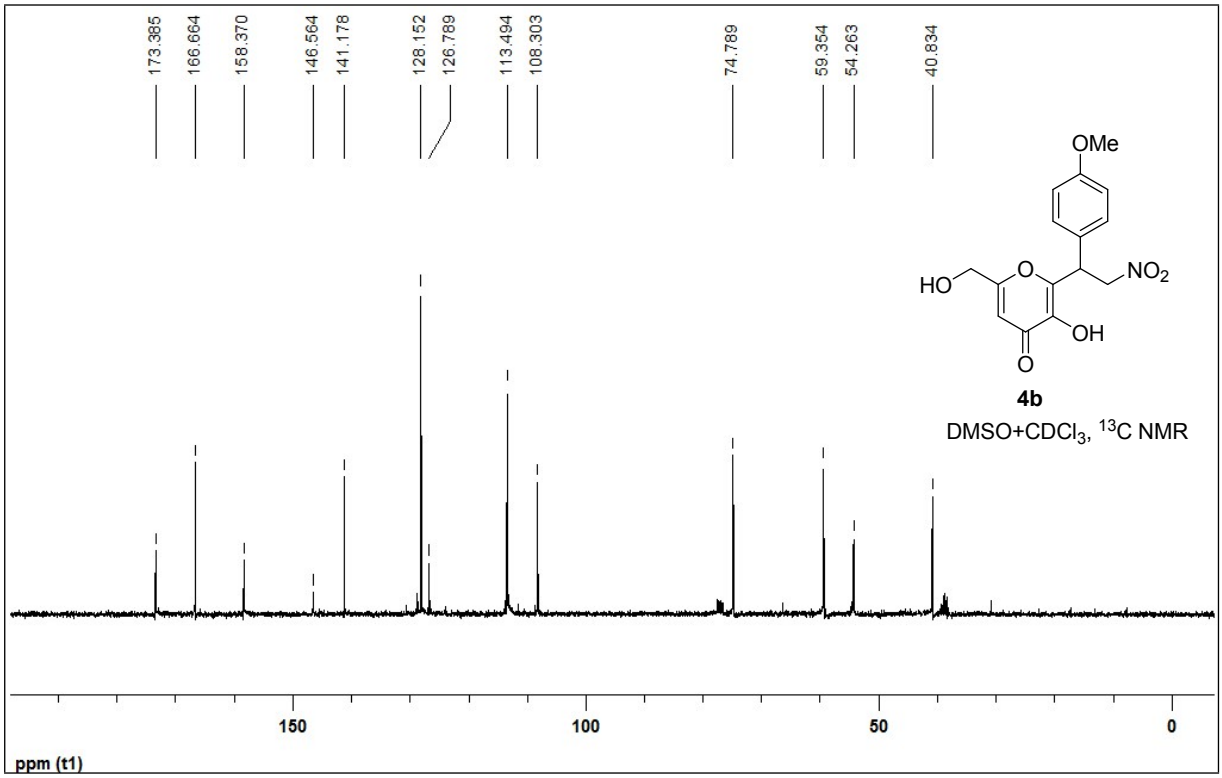
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 4a



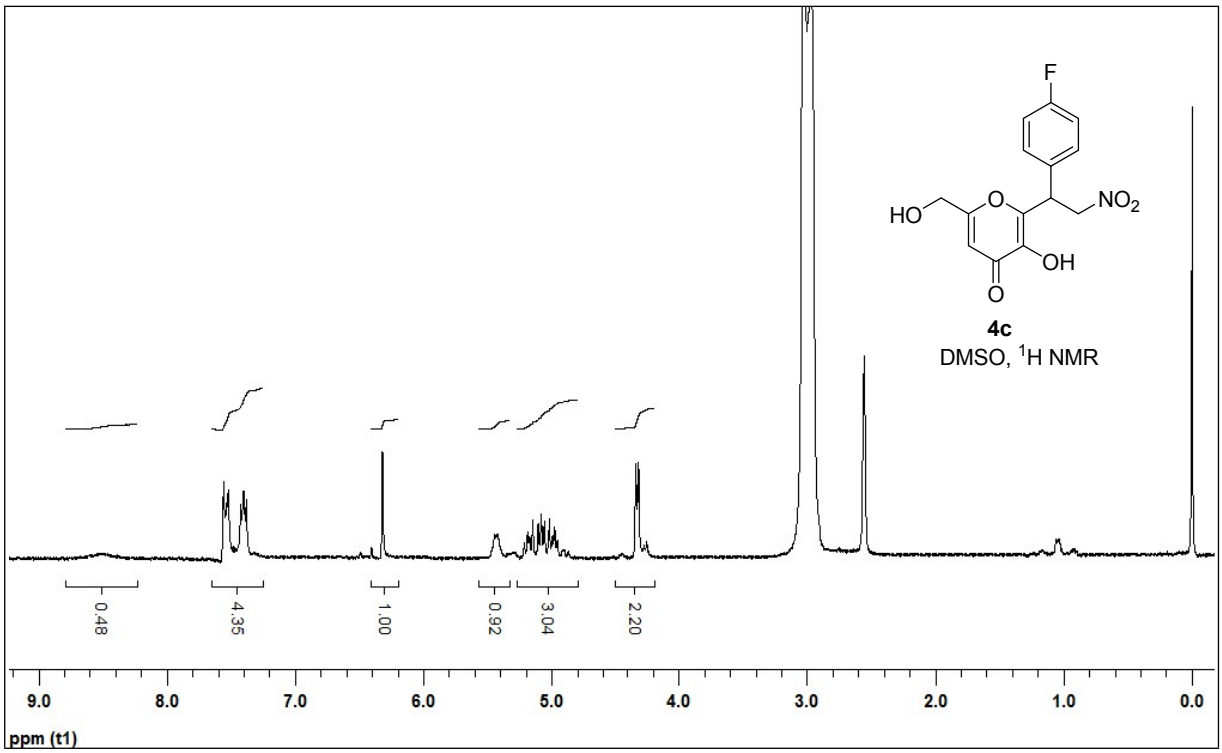
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 4a



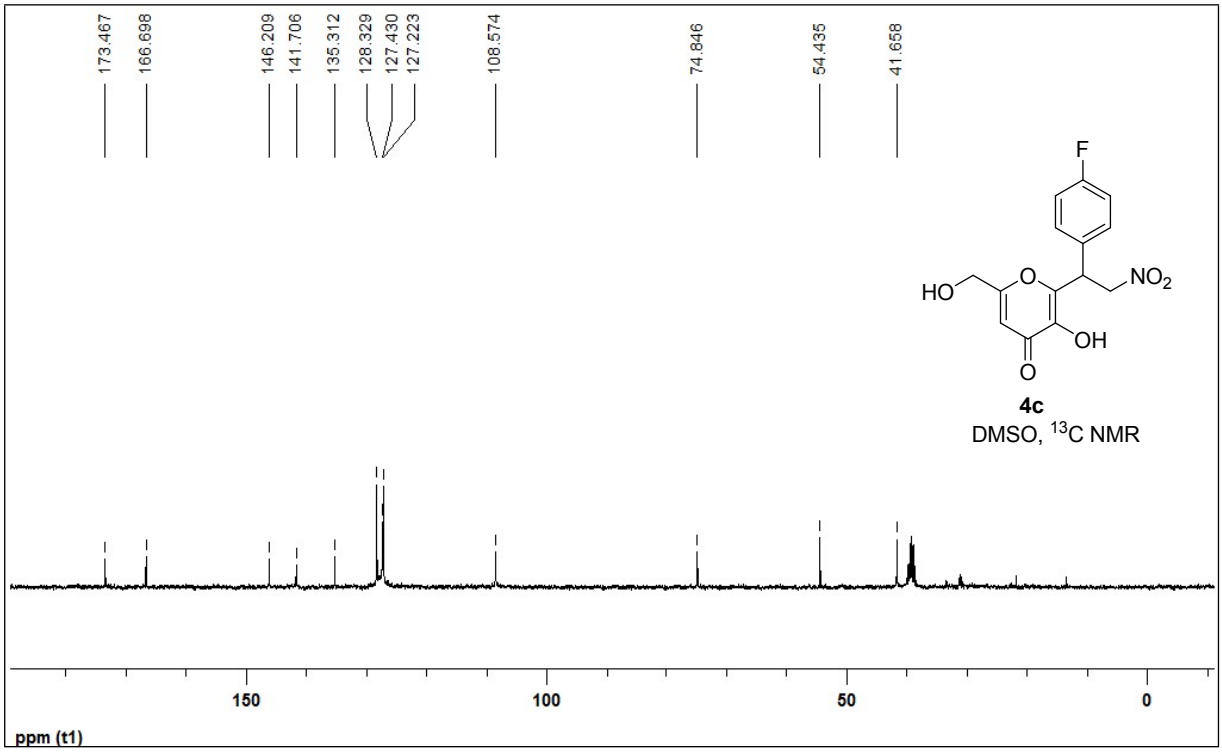
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 4b



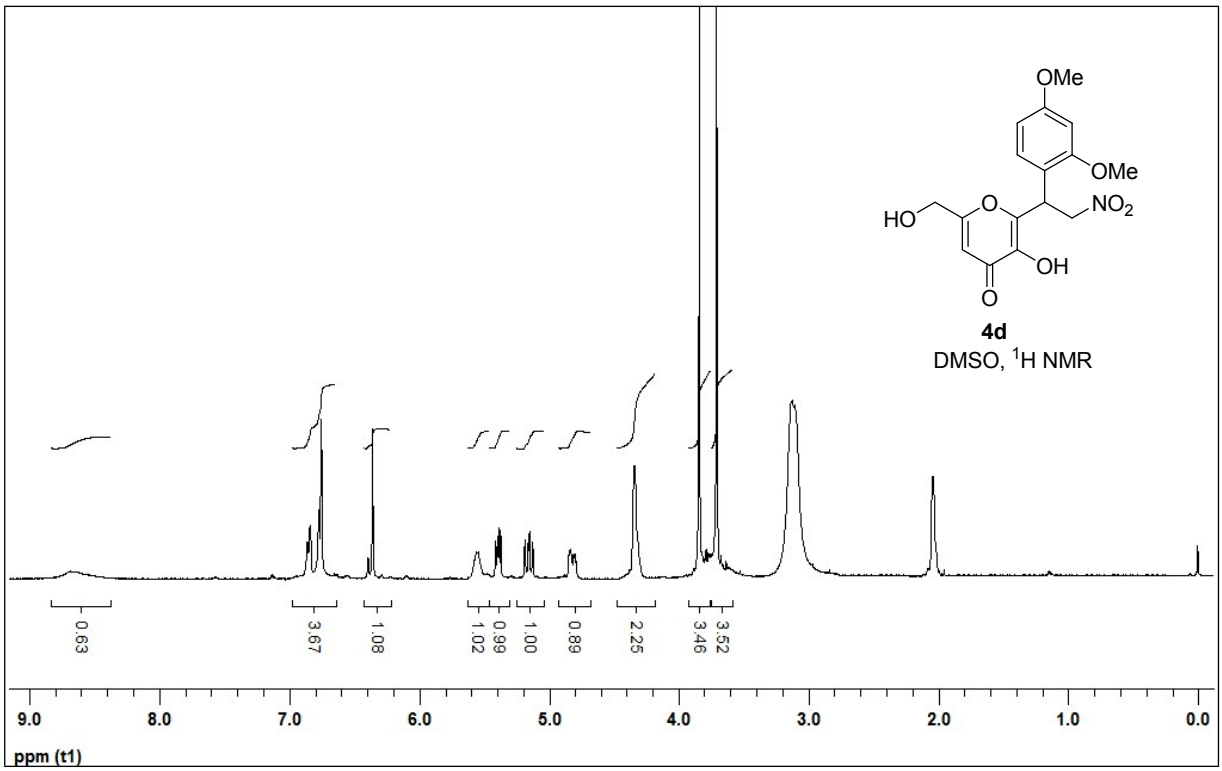
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 4b



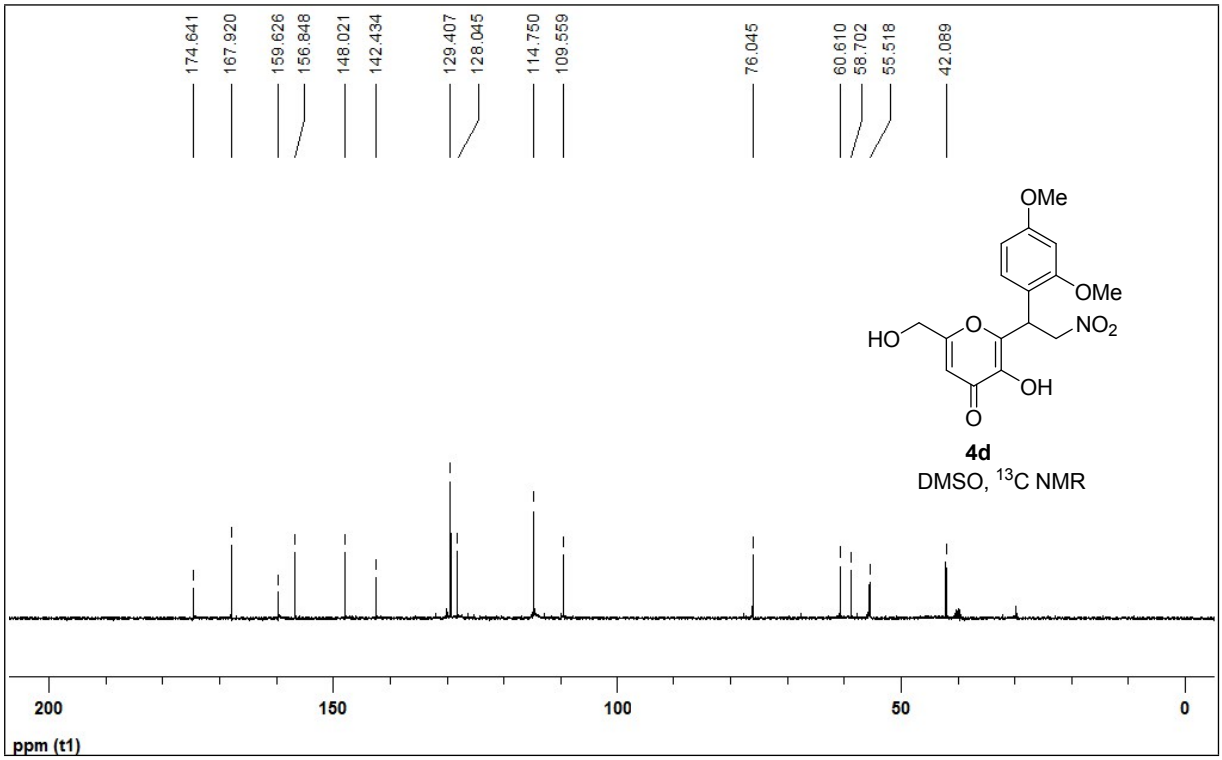
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 4c



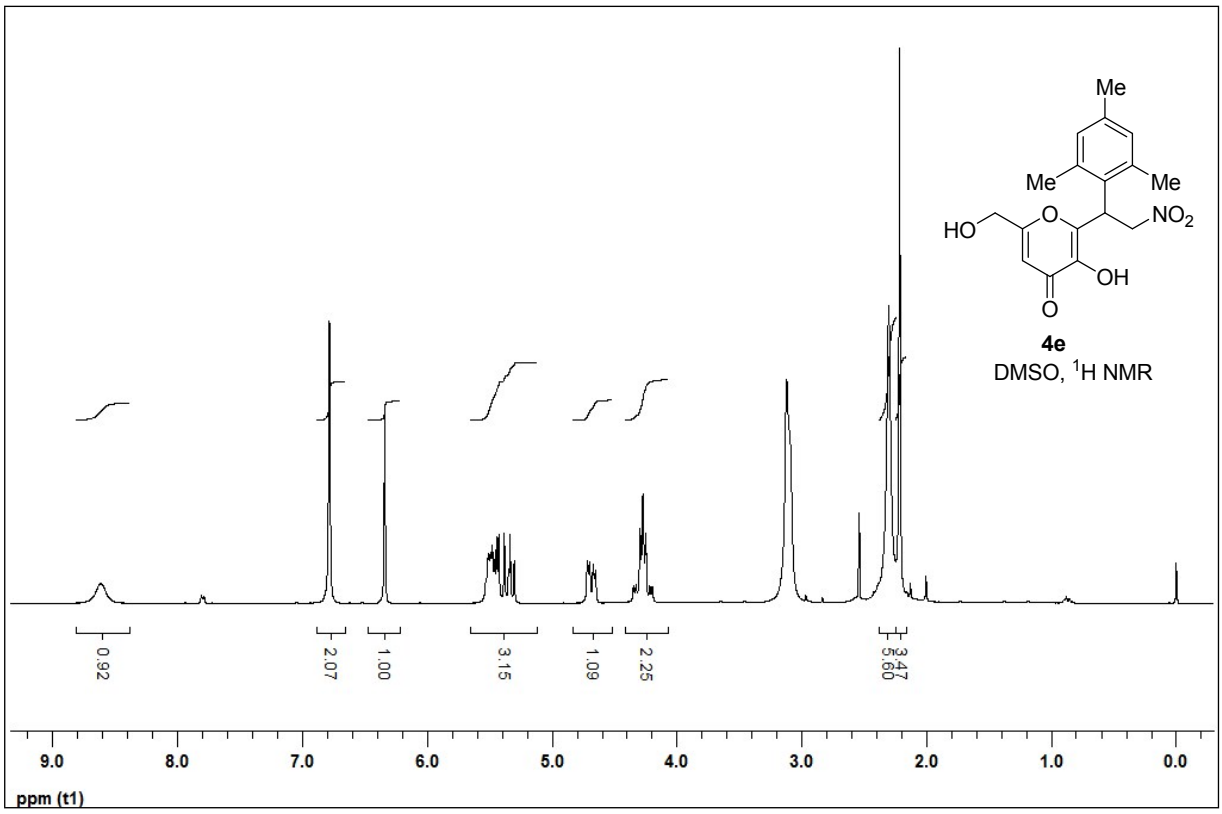
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 4c



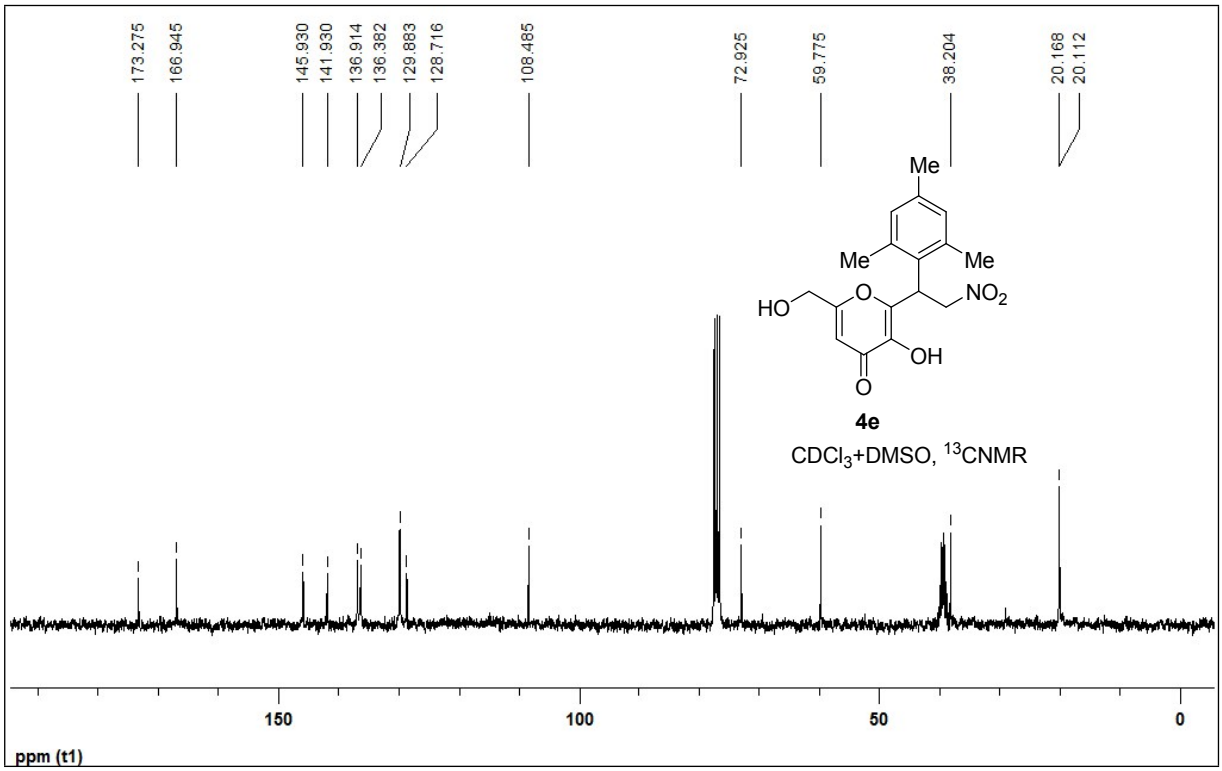
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 4d



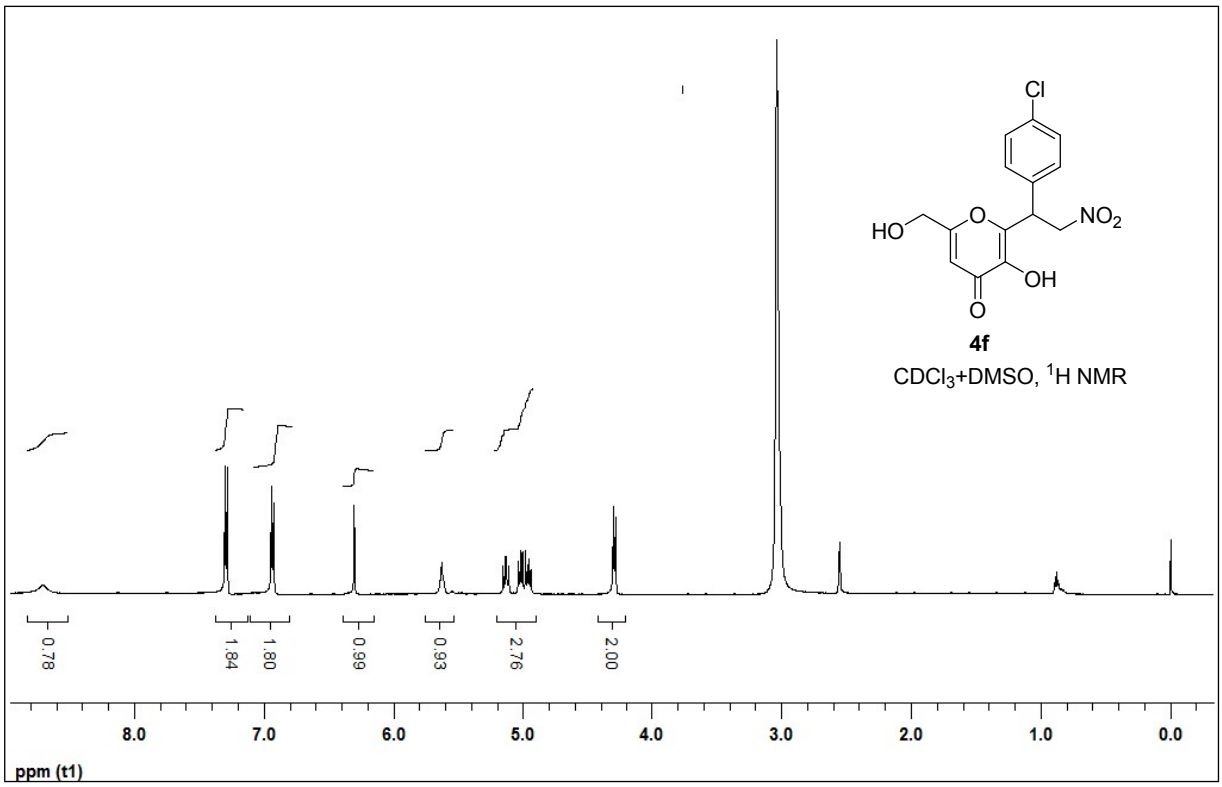
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 4d



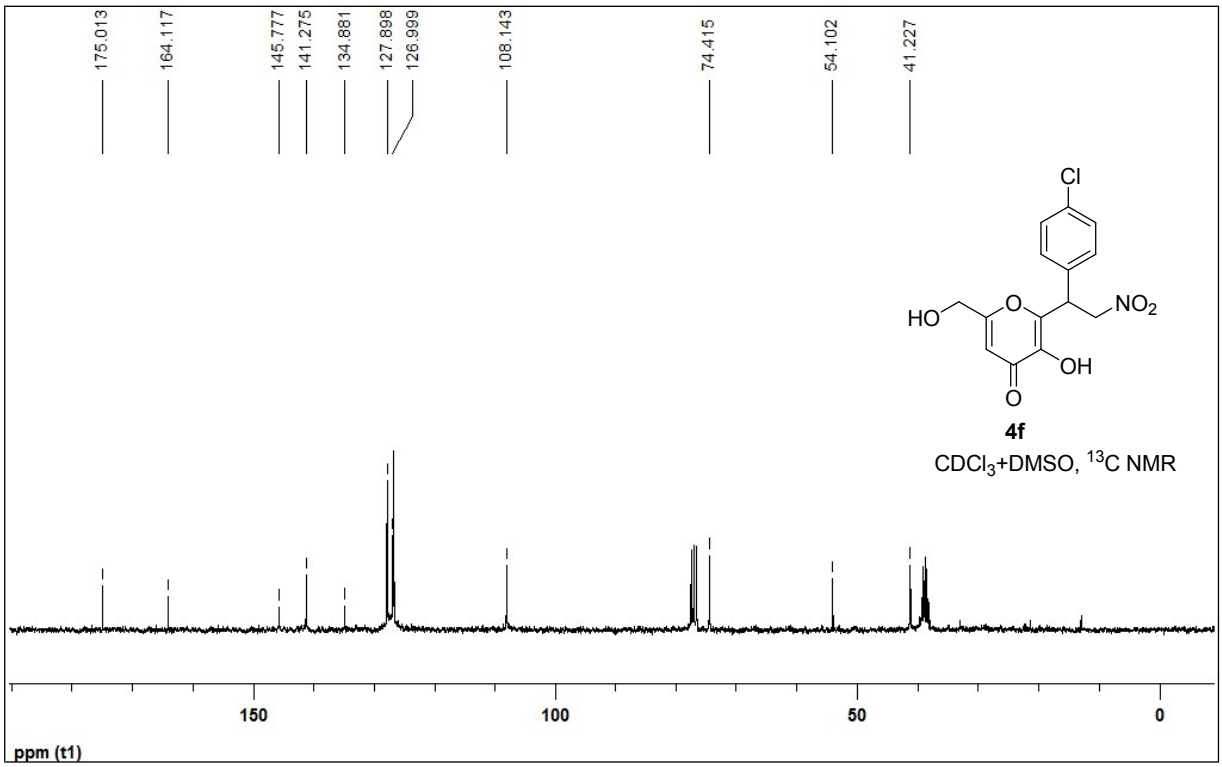
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 4e



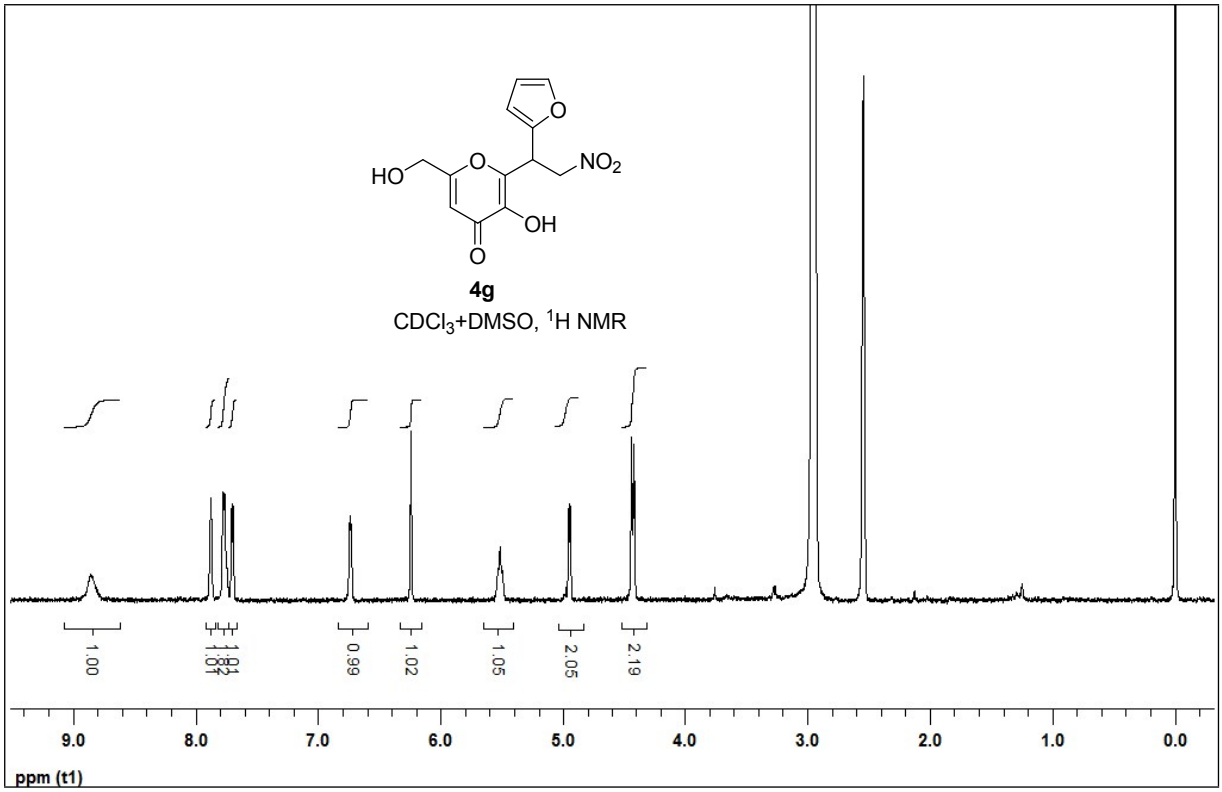
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 4e



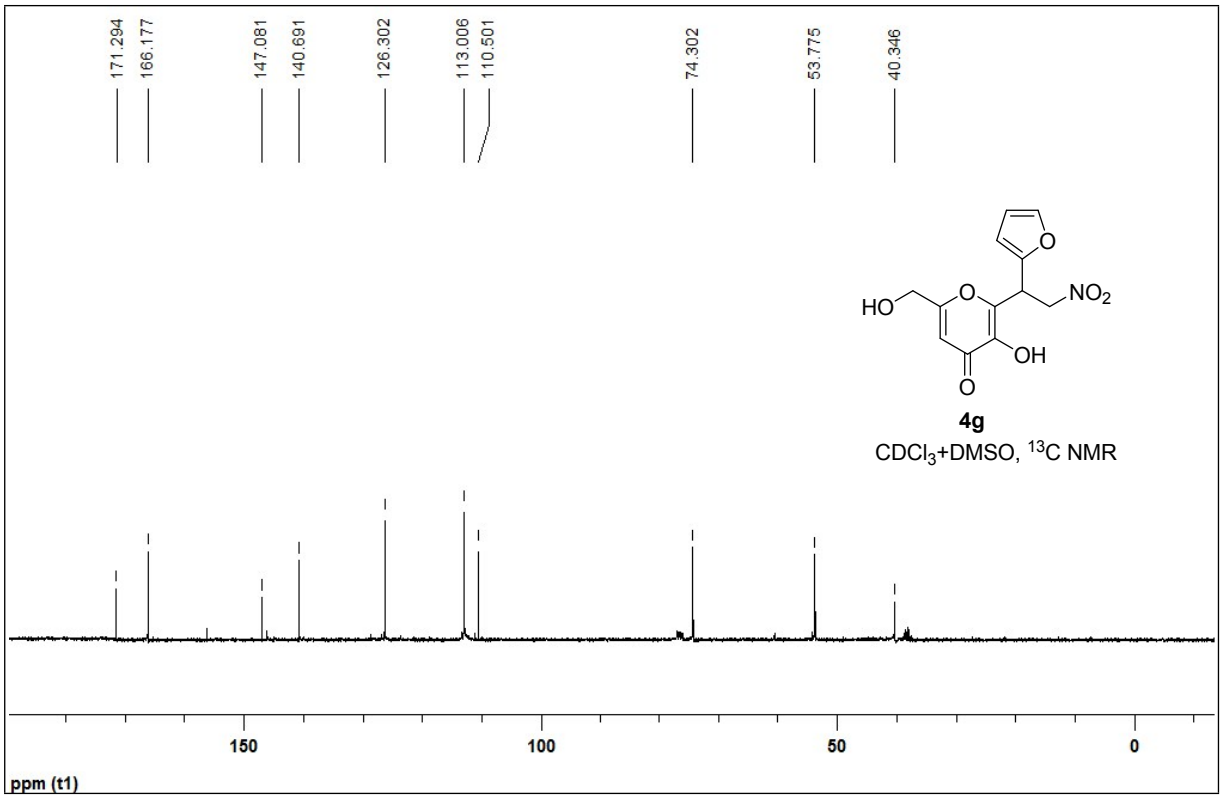
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 4f



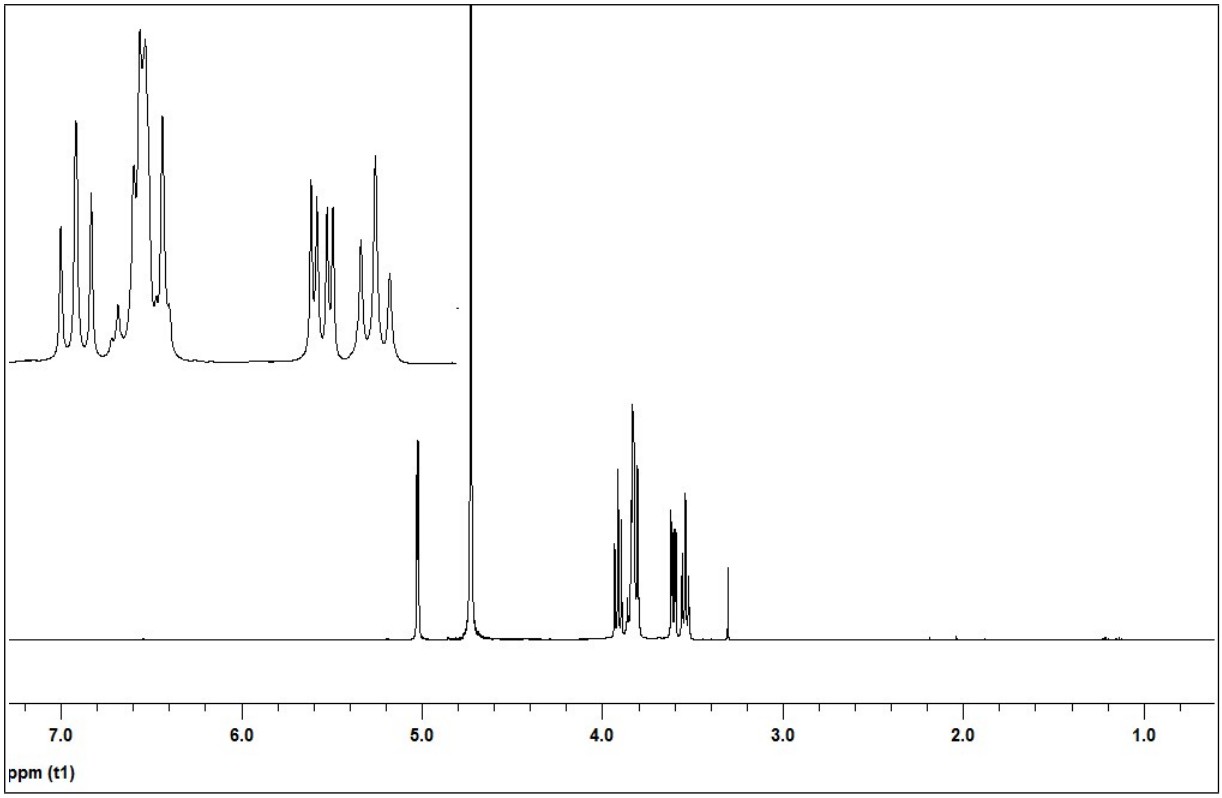
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 4f



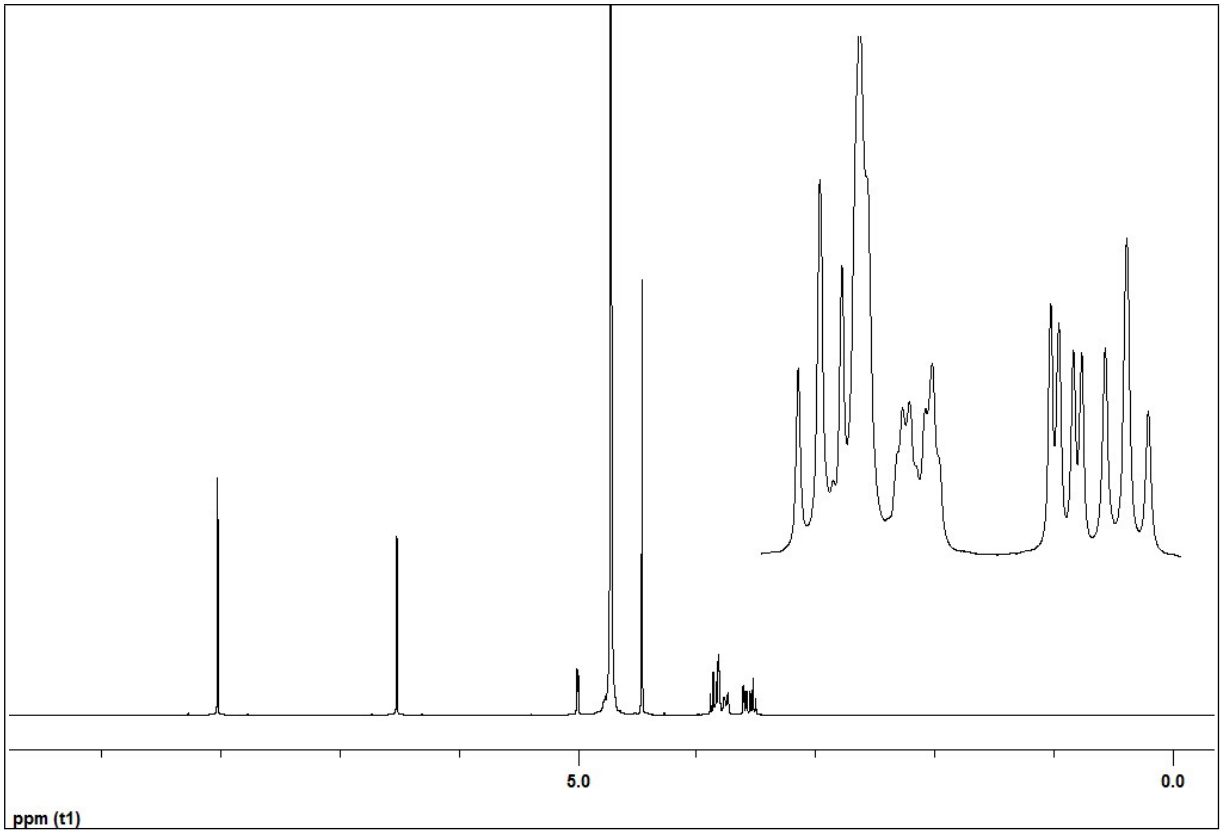
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 4g



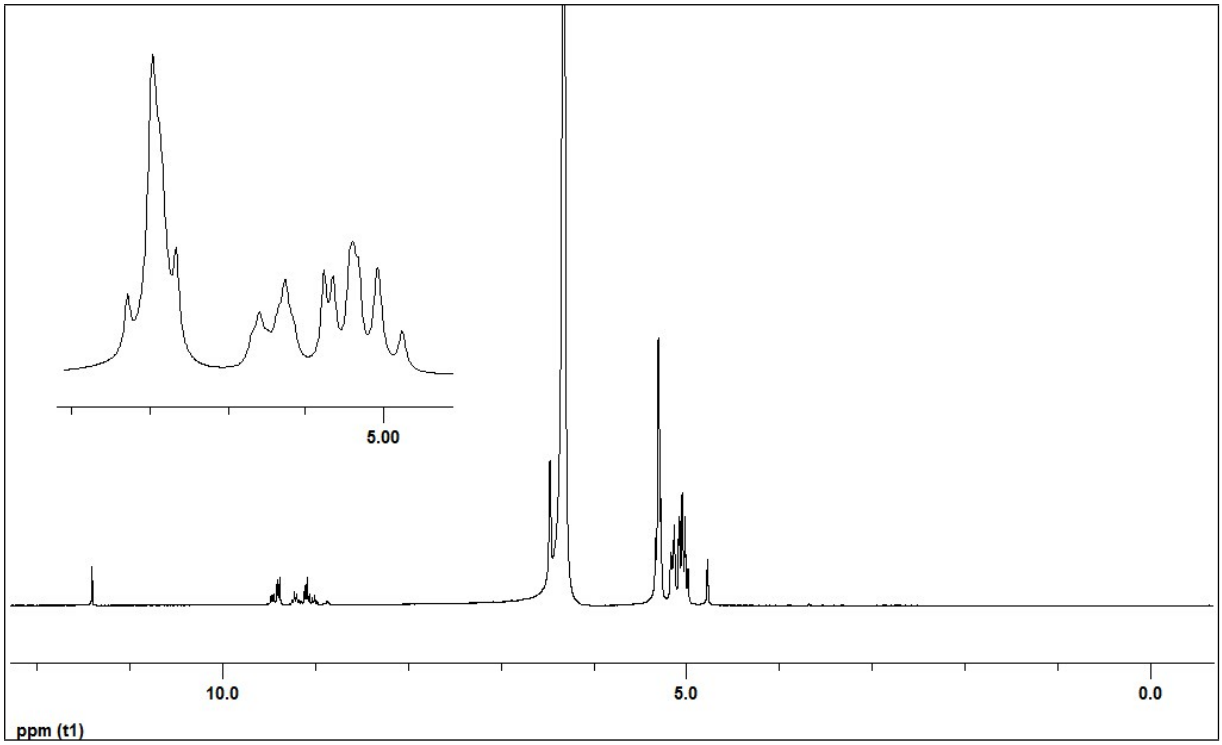
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 4g



^{1}H NMR (500 MHz, D_2O) spectrum of β-CD



^{1}H NMR (500 MHz, D_2O) spectrum of β-CD: Kojic acid inclusion complex



^{1}H NMR (500 MHz, D_2O) spectrum of β-CD: Benzaldehyde complex