Electronic Supplementary Information

A highly efficient and green cascade synthesis of 3-methyl-substituted-4-hydroxy-1-methyl-quinolin-2(1*H*)-ones under solvent- and catalyst-free conditions

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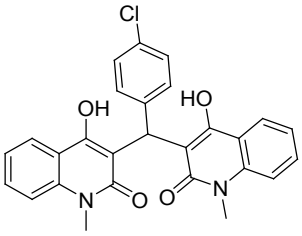
1. Crystallographic Data

Crystallographic data of compound **5b**

Crystal data [CCDC No. 938662]	
Empirical formula	$C_{23}H_{22}N_2O_3$
Formula weight	374.43
Crystal size (mm)	0.3 x 0.2 x 0.1
Crystal system	Monoclinic
Space group	P21/c
a (Å); b (Å); c (Å)	14.0952(13); 10.0541(9); 14.1685(13)
α (˚); β (˚); γ (˚)	90; 111.8180(10); 90
Volume (Å^3)	1864.1(3)
Z	4
Crystal density, g/cm^3	1.334
F(000)	792
Absorption coefficient	0.089
Temperature (T)	296 (2)
Radiation wavelength	0.71073
Radiation type	MoKα
Radiation source	Fine-focus sealed tube
Radiation monochromator	Graphite
h_{min}; k_{min}; l_{min}	-17; -12; -17
h_{max}; k_{max}; l_{max}	17; 12; 17
R-Factor (%)	3.82

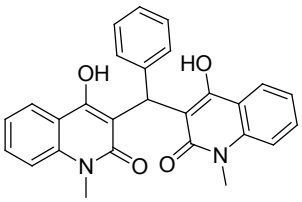
2. Characterization Data

3-((4-chlorophenyl)(4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl)-4-hydroxy-1-methylquinolin-2(1*H*)-one (4a)



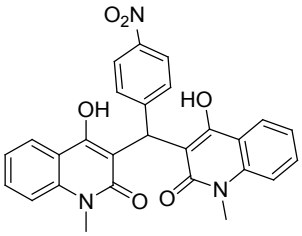
White solid; mp: 175~176 ˚C (lit. 174-175 ˚C)[1]; ^{1}H NMR (400MHz, $CDCl_3$) δ: 3.64 (s, 3H, NCH_3), 3.75 (s, 3H, NCH_3), 6.30 (s, 1H, CH), 7.03 (dt, 2H, J_1 = 1.6Hz, J_2 = 6.4Hz, ArH), 7.13 (dd, 2H, J_1 = 2Hz, J_2 = 6.4Hz, ArH), 7.24-7.27 (m, 2H, ArH), 7.33 (d, 2H, J = 8.4Hz, ArH), 7.52-7.57 (m, 2H, ArH), 8.11 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8Hz, ArH), 8.17 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8Hz, ArH), 12.41 (s, 1H, OH), 12.77 (s, 1H, OH); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 29.0, 29.5, 35.8, 108.4, 110.0, 113.1, 113.2, 116.7, 117.0, 121.6, 123.8, 123.9, 126.9, 127.2, 130.3, 130.4, 135.4, 137.4, 137.5, 160.1, 161.3, 163.8, 165.6; IR (Neat, cm^{-1}): 2568br, 1627, 1556, 1490; Anal. Calcd for $C_{27}H_{21}ClN_2O_4$: C, 68.57; H, 4.48; N, 5.92, Found: C, 68.48; H, 4.54; N, 5.83; MS (ESIMS): 474.1$(M+H)^+$.

4-hydroxy-3-((4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)(phenyl)methyl)-1-methylquinolin-2(1*H*)-one (4b)



White solid; mp: 289~291 ˚C; ^{1}H NMR (400MHz, $CDCl_3$) δ: 3.73 (s, 3H, NCH_3), 3.84 (s, 3H, NCH_3), 6.45 (s, 1H, CH), 7.18-7.22 (m, 3H, ArH), 7.25-7.35 (m, 4H, ArH), 7.41-7.44 (m, 2H, ArH), 7.60-7.65 (m, 2H, ArH), 8.20 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8.4 Hz, ArH), 8.26 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8.4 Hz, ArH), 12.47 (s, 1H, OH), 12.86 (s, 1H, OH); ^{13}C NMR (100.6 MHz, DMSO-d_6) δ: 30.2, 36.6, 115.4, 116.9, 122.8, 123.6, 125.7, 126.2, 128.1, 131.7, 137.6, 138.1, 160.1, 163.2; IR (Neat, cm^{-1}): 2569br, 1627, 1551, 1496; Anal. Calcd for $C_{27}H_{22}N_2O_4$: C, 73.96; H, 5.06; N, 6.39, Found: C, 74.02; H, 4.97; N, 6.31; MS (ESIMS): 439.1$(M+H)^+$.

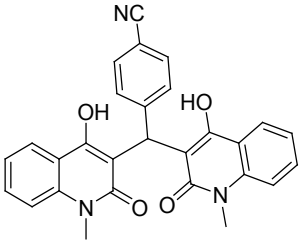
4-hydroxy-3-((4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)(4-nitrophenyl)methyl)-1-methylquinolin-2(1*H*)-one (4c)



White solid; mp: 292~294 ˚C; ^{1}H NMR (400MHz, $CDCl_3$) δ: 3.73 (s, 3H, NCH_3), 3.85 (s, 3H, NCH_3), 6.46 (s, 1H, CH), 7.34-7.38 (m, 4H, ArH), 7.45 (d, 2H, J = 8.4 Hz, ArH), 7.64-7.69 (m, 2H, ArH), 8.11-8.15 (m, 2H, ArH), 8.19 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8 Hz, ArH), 8.26 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8 Hz, ArH), 12.51 (s, 1H,

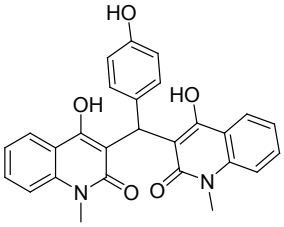
OH), 12.82 (s, 1H, OH); ^{13}C NMR (100.6 MHz, DMSO-d_6) δ: 30.2, 37.2, 94.4, 109.6, 115.4, 116.8, 122.9, 123.2, 123.7, 127.8, 131.9, 138.2, 145.7, 146.7, 156.4, 160.8; IR (Neat, cm^{-1}): 2567br, 1626, 1560, 1545, 1498, 1344; Anal. Calcd for $C_{27}H_{21}N_3O_6$: C, 67.07; H, 4.38; N, 8.69, Found: C, 67.18; H, 4.29; N, 8.56; MS (ESIMS): 484.2(M+H)$^+$.

4-(bis(4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl)benzonitrile (4d)



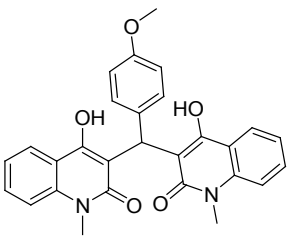
White solid; mp: 290~292 ˚C; ^{1}H NMR (400MHz, MeOD+DMSO-d_6) δ: 3.76 (s, 6H, NCH_3), 6.36 (s, 1H, CH), 7.29-7.31 (m, 2H, ArH), 7.39 (t, 2H, J = 7.2 Hz, ArH), 7.65-7.68 (m, 4H, ArH), 7.11-7.75 (m, 2H, ArH), 8.10 (d, 2H, J = 8 Hz, ArH); ^{13}C NMR (100.6 MHz, MeOD+DMSO-d_6) δ: 28.2, 29.6, 36.7, 108.6, 114.9, 116.7, 118.6, 121.2, 122.5, 123.5, 127.3, 131.5, 131.6, 132.7, 138.2, 143.9, 146.3, 154.4, 164.8; IR (Neat, cm^{-1}): 2564br, 2224, 1630, 1603, 1542, 1498; Anal. Calcd for $C_{28}H_{21}N_3O_4$: C, 72.56; H, 4.57; N, 9.07, Found: C, 72.61; H, 4.54; N, 9.13.

4-hydroxy-3-((4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)(4-hydroxyphenyl)methyl)-1-methylquinolin-2(1*H*)-one (4e)



White solid; mp: 208~210 ˚C; ^{1}H NMR (400MHz, DMSO-d_6) δ: 3.73 (s, 6H, NCH_3), 6.20 (s, 1H, CH), 6.65-6.67 (m, 2H, ArH), 6.86 (d, 2H, J = 8.4 Hz, ArH), 7.34 (t, 2H, J = 7.6 Hz, ArH), 7.67-7.74 (m, 4H, ArH), 8.08 (s, 2H, ArH), 9.22 (s, 1H, OH), 12.49 (s, 1H, OH), 12.88 (s, 1H, OH); ^{13}C NMR (100.6 MHz, DMSO-d_6) δ: 30.1, 30.3, 35.9, 107.7, 110.1, 110.8, 114.9, 115.3, 116.8, 122.7, 123.6, 127.2, 127.3, 131.5, 138.1, 142.3, 155.3, 162.3, 165.8; IR (Neat, cm^{-1}): 2570br, 1636, 1546, 1491; Anal. Calcd for $C_{27}H_{22}N_2O_5$: C, 71.35; H, 4.88; N, 6.16, Found: C, 71.28; H, 4.93; N, 6.28.

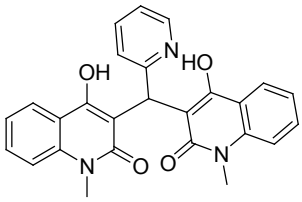
4-hydroxy-3-((4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)(4-methoxyphenyl)methyl)-1-methylquinolin-2(1*H*)-one (4f)



White solid; mp: 236~237 ˚C; ^{1}H NMR (400MHz, DMSO-d_6) δ: 3.70 (s, 9H, NCH_3 & -OCH_3), 6.23 (s, 1H, CH), 6.79-6.82 (m, 2H, ArH), 6.97 (d, 2H, J = 8.4 Hz, ArH), 7.40 (t, 2H, J = 7.6 Hz, ArH), 7.67-7.76 (m, 4H, ArH), 8.07 (s, 2H, ArH), 12.78 (brs, 2H, OH); ^{13}C NMR (100.6 MHz, DMSO-d_6) δ: 30.0, 30.3, 35.9, 38.8, 54.9, 113.4,

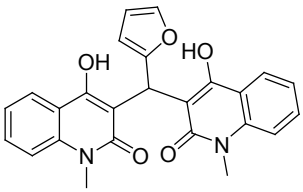
115.4, 116.9, 122.8, 123.6, 127.3, 129.2, 131.6, 138.1, 142.9, 157.3, 162.4, 162.5; IR (Neat, cm^{-1}): 2566br, 1631, 1545, 1493; Anal. Calcd for $C_{28}H_{24}N_2O_5$: C, 71.78; H, 5.16; N, 5.98, Found: C, 71.66; H, 5.23; N, 5.87; ESIMS: 469.9$(M+H)^+$.

4-hydroxy-3-((4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)(pyridin-2-yl)methyl)-1-methylquinolin-2(1*H*)-one (4g)



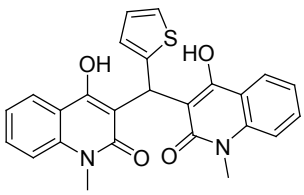
White solid; mp: 267~268 ˚C; ^{1}H NMR (400MHz, $CDCl_3$) δ: 3.74 (s, 6H, NCH_3), 6.49 (s, 1H, CH), 7.10-7.13 (m, 1H, ArH), 7.25 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8 Hz, ArH), 7.30 (tt, 2H, J_1 = 0.8 Hz, J_2 = 8 Hz, ArH), 7.40 (d, 2H, J = 8.4 Hz, ArH), 7.57-7.62 (m, 3H, ArH), 8.21 (dd, 2H, 1.6 Hz, J_2 = 8 Hz, ArH), 8.51-8.52 (m, 1H, ArH), 12.71 (brs, 2H, OH); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 30.3, 40.3, 110.6, 114.2, 118.1, 121.1, 121.4, 122.5, 124.9, 131.1, 136.2, 138.6, 149.0, 158.1, 161.5, 165.9; IR (Neat, cm^{-1}): 2563br, 1629, 1550, 1487; Anal. Calcd for $C_{26}H_{21}N_3O_4$: C, 71.06; H, 4.82; N, 9.56, Found: C, 71.15; H, 4.77; N, 9.42; ESIMS: 440.8$(M+H)^+$.

3-(furan-2-yl(4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl)-4-hydroxy-1-methylquinolin-2(1*H*)-one (4h)



White solid; mp: 240~241 ˚C; ^{1}H NMR (400MHz, DMSO-d_6) δ: 3.73 (s, 6H, NCH_3), 6.08-6.09 (m, 1H, ArH), 6.20 (s, 1H, CH), 6.38-6.39 (m, 1H, ArH), 7.40 (t, 2H, J = 7.6 Hz, ArH), 7.49 (s, 1H, ArH), 7.63-7.75 (m, 4H, ArH), 8.07 (dd, 2H, J_1 = 1.6 Hz, J_2 = 8 Hz, ArH), 12.49 (s, 1H, OH), 12.85 (s, 1H, OH); ^{13}C NMR (100.6 MHz, DMSO-d_6) δ: 30.06, 30.08, 32.7, 106.3, 110.3, 115.4, 116.8, 122.8, 123.6, 131.7, 138.1, 141.4, 150.9, 156.2, 160.2; IR (Neat, cm^{-1}): 2566br, 1633, 1532, 1499; Anal. Calcd for $C_{25}H_{20}N_2O_5$: C, 70.08; H, 4.71; N, 6.54, Found: C, 69.96; H, 4.63; N, 6.43; ESIMS: 429.9 $(M+H)^+$.

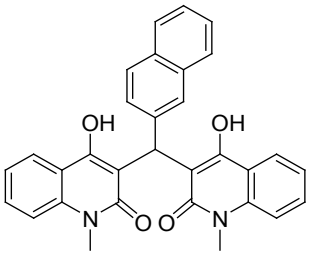
4-hydroxy-3-((4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)(thiophen-2-yl)methyl)-1-methylquinolin-2(1*H*)-one (4i)



White solid; mp: 263~264 ˚C; ^{1}H NMR (400MHz, DMSO-d_6+ MeOD) δ: 3.77 (s, 6H, NCH_3), 6.43 (s, 1H, CH), 6.73-6.74 (m, 1H, ArH), 6.91-6.93 (m, 1H, ArH), 7.25-7.27 (m, 1H, ArH), 7.41 (t, 2H, J = 7.6 Hz, ArH), 7.66 (d, 2H, J = 8.4 Hz, ArH), 7.72-7.76 (m, 2H, ArH), 8.14 (d, 2H, J = 7.6 Hz, ArH); ^{13}C NMR (100.6 MHz, MeOD+DMSO-d_6) δ: 29.3, 30.07, 33.3, 103.6, 105.9, 114.7, 121.6, 122.4, 125.4, 126.0, 131.2, 138.1, 142.7, 147.7,

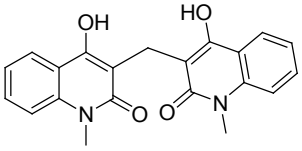
148.3, 156.1, 164.2; IR (Neat, cm^{-1}): 2567br, 1634, 1533, 1498; Anal. Calcd for $C_{25}H_{20}N_2O_4S$: C, 67.55; H, 4.54; N, 6.30, Found: C, 67.46; H, 4.49; N, 6.39.

4-hydroxy-3-((4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)(naphthalen-2-yl)methyl)-1-methylquinolin-2(1*H*)-one (4j)



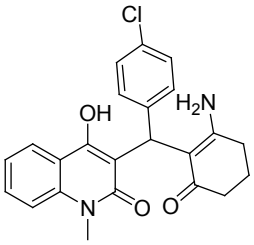
White solid; mp: 303~304 ˚C; ^{1}H NMR (400MHz, $CDCl_3$) δ: 3.65 (s, 3H, NCH_3), 3.79 (s, 3H, NCH_3), 6.52 (s, 1H, CH), 7.23-7.32 (m, 5H, ArH), 7.36-7.39 (m, 2H, ArH), 7.54-7.71 (m, 6H, ArH), 8.16 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8 Hz, ArH), 8.21 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8 Hz, ArH), 12.45 (s, 1H, OH), 12.81 (s, 1H, OH); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 30.1, 30.6, 37.5, 109.7, 111.6, 114.2, 114.3, 117.8, 118.2, 122.6, 122.7, 124.8, 124.9, 125.0, 125.2, 125.3, 125.7, 127.5, 127.7, 127.9, 131.2, 131.3, 132.1, 133.5, 135.4, 138.5, 138.6, 161.3, 162.2, 165.0, 166.8; IR (Neat, cm^{-1}): 2569br, 1631, 1539, 1472; Anal. Calcd for $C_{31}H_{24}N_2O_4$: C, 76.21; H, 4.95; N, 5.73, Found: C, 76.10; H, 4.82; N, 5.66; ESIMS: 489.2 $(M+H)^+$.

4-hydroxy-3-((4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl)-1-methylquinolin-2(1*H*)-one (4k)



White solid; mp: 293~294 ˚C; ^{1}H NMR (400MHz, $CDCl_3$) δ: 3.72 (s, 6H, NCH_3), 3.96 (s, 2H, CH_2), 7.19-7.25 (m, 2H, ArH), 7.31 (d, 2H, J = 8.4 Hz, ArH), 7.49-7.54 (m, 2H, ArH), 8.11 (dd, 2H, J_1 = 1.6 Hz, J_2 = 8 Hz, ArH), 12.44 (s, 2H, OH); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 20.0, 28.7, 29.1, 108.1, 113.1, 116.6, 121.5, 123.4, 129.9, 137.3, 159.6, 165.2; IR (Neat, cm^{-1}): 2563br, 1630, 1537, 1483; Anal. Calcd for $C_{21}H_{18}N_2O_4$: C, 69.60; H, 5.01; N, 7.73, Found: C, 69.51; H, 5.14; N, 7.68; ESIMS: 363.2 $(M+H)^+$.

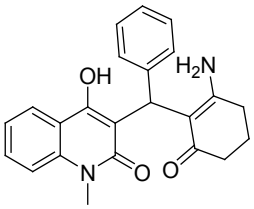
3-((2-amino-6-oxocyclohex-1-enyl)(4-chlorophenyl)methyl)-4-hydroxy-1-methylquinolin-2(1*H*)-one (5a)



White solid; mp: 266~267 ˚C; ^{1}H NMR (400MHz, DMSO-d_6) δ: 1.85-1.92 (m, 2H), 2.24-2.35 (m, 2H), 2.43-2.46 (m, 2H), 3.69 (s, 3H, NCH_3), 5.72 (s, 1H, CH), 7.04-7.07 (m, 2H, ArH), 7.23-7.32 (m, 3H, ArH), 7.57 (d, 1H, J = 8 Hz, ArH), 7.64-7.69 (m, 1H, ArH), 7.93-7.97 (m, 2H, ArH), 8.35 (s, 1H, ArH), 13.7 (s, 1H, OH); ^{13}C NMR (100.6 MHz, DMSO-d_6) δ: 20.3, 29.4, 29.9, 34.7, 35.7, 108.7, 109.2, 114.7, 121.9, 123.7, 127.7, 128.2, 129.6, 131.1, 138.4, 159.9, 164.7, 171.2, 195.5; IR (Neat, cm^{-1}): 3224, 3069, 1693,

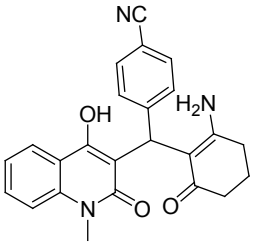
1561, 1489; Anal. Calcd for $C_{23}H_{21}ClN_2O_3$: C, 67.56; H, 5.18; N, 6.85, Found: C, 67.49; H, 5.03; N, 6.78; ESIMS: 409.2 $(M+H)^+$.

3-((2-amino-6-oxocyclohex-1-enyl)(phenyl)methyl)-4-hydroxy-1-methylquinolin-2(1*H*)-one ($S_3$5b)



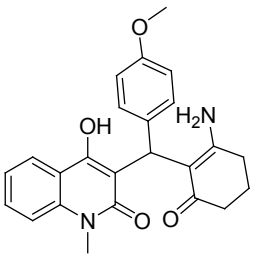
White solid; mp: 250~251 ˚C; ^{1}H NMR (400MHz, DMSO-d_6+MeOD) δ: 1.91-1.97 (m, 2H), 2.29-2.38 (m, 2H), 2.50-2.67 (m, 2H), 3.74 (s, 3H, NCH_3), 5.82 (s, 1H, CH), 7.07-7.13 (m, 3H, ArH), 7.19-7.23 (m, 2H, ArH), 7.29-7.32 (m, 1H, ArH), 7.56 (d, 1H, J = 8.4 Hz, ArH), 7.64-7.69 (m, 1H, ArH), 8.00-8.04 (m, 1H, ArH); ^{13}C NMR (100.6 MHz, DMSO-d_6+MeOD) δ: 20.2, 29.1, 29.3, 35.1, 37.8, 108.6, 109.2, 116.8, 121.6, 123.5, 124.7, 126.0, 127.5, 130.7, 138.2, 139.6, 160.0 164.8, 170.5, 195.6; IR (Neat, cm^{-1}): 3226, 3066, 1691, 1564, 1492; Anal. Calcd for $C_{23}H_{22}N_2O_3$: C, 73.78; H, 5.92; N, 7.48, Found: C, 73.59; H, 5.86; N, 7.59; ESIMS: 375.2 $(M+H)^+$.

4-((2-amino-6-oxocyclohex-1-enyl)(4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl)benzonitrile (5d)



White solid; mp: 258~259 ˚C; ^{1}H NMR (400MHz, $CDCl_3$) δ: 1.93-1.99 (m, 2H), 2.23-2.29 (m, 2H), 2.42-2.49 (m, 2H), 3.70 (s, 3H, NCH_3), 4.97 (s, 1H, NH), 5.88 (s, 1H, CH), 7.19-7.22 (m, 2H, ArH), 7.31 (d, 1H, J = 8.4 Hz, ArH), 7.44-7.59 (m, 4H, ArH), 8.08 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8 Hz, ArH), 8.83 (s, 1H, NH), 12.83 (s, 1H, OH); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 13.1, 20.1, 21.6, 29.1, 30.0, 30.9, 35.4, 36.1, 107.9, 108.1, 109.5, 112.8, 116.7, 121.3, 123.9, 126.4, 130.2, 130.9, 137.8, 144.6, 160.0, 164.7, 168.1, 196.2; IR (Neat, cm^{-1}): 3226, 3061, 2224, 1690, 1558, 1490; Anal. Calcd for $C_{24}H_{21}N_3O_3$: C, 72.16; H, 5.30; N, 10.52, Found: C, 72.08; H, 5.21; N, 10.41; ESIMS: 400.1$(M+H)^+$.

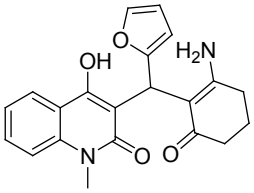
3-((2-amino-6-oxocyclohex-1-enyl)(4-methoxyphenyl)methyl)-4-hydroxy-1-methylquinolin-2(1*H*)-one (5f)



White solid; mp: 251~252 ˚C; ^{1}H NMR (400MHz, $CDCl_3$) δ: 1.89-1.98 (m, 2H), 2.19-2.27 (m, 2H), 2.41-2.45 (m, 2H), 3.68 (s, 6H, -OCH_3 & NCH_3), 4.97 (s, 1H, NH), 5.82 (s, 1H, , CH, ArH), 6.69-6.72 (m, 2H), 7.00 (d, 2H, J = 8.4 Hz, ArH), 7.17-7.30 (m, 3H, ArH), 7.48-7.53 (m, 1H, ArH), 8.09-8.11 (m, 1H, ArH), 8.80 (s, 1H, NH), 13.03 (s, 1H, OH); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 19.8, 28.7, 29.2, 30.1, 34.4, 35.2, 54.2, 109.1,

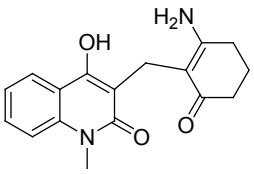
110.4, 112.4, 112.6, 116.9, 120.9, 123.9, 126.5, 129.7, 130.1, 137.7, 156.3, 159.9, 164.9, 167.5, 196.2; IR (Neat, cm^{-1}): 3227, 3062, 1694, 1559, 1483; Anal. Calcd for $C_{24}H_{24}N_2O_4$: C, 71.27; H, 5.98; N, 6.93, Found: C, 71.36; H, 6.09; N, 6.77; ESIMS: 405.0 $(M+H)^+$.

3-((2-amino-6-oxocyclohex-1-enyl)(furan-2-yl)methyl)-4-hydroxy-1-methylquinolin-2(1*H*)-one (5h)



White solid; mp: 239~241 °C; ^{1}H NMR (400MHz, $CDCl_3$) δ: 1.87-1.97 (m, 2H), 2.18-2.25 (m, 2H), 2.38-2.41 (m, 2H), 3.67 (s, 3H, N*CH*$_3$), 4.88 (s, 1H, NH), 5.78 (s, 1H, ArH), 5.92 (s, 1H, CH), 6.20 (s, 1H, ArH), 7.17-7.34 (m, 2H, ArH), 7.48-7.55 (m, 1H, ArH), 8.11-8.16 (m, 1H, ArH), 8.64 (s, 1H, NH), 13.06 (s, 1H, OH); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 13.1, 19.7, 21.6, 28.6, 28.7, 29.9, 31.2, 104.1, 109.2, 112.7, 121.7, 123.9, 129.9, 137.7, 139.7, 151.9, 160.1, 196.4; IR (Neat, cm^{-1}): 3226, 3072, 1681, 1625, 1598; Anal. Calcd for $C_{21}H_{20}N_2O_4$: C, 69.22; H, 5.53; N, 7.69, Found: C, 69.34; H, 5.48; N, 7.57; ESIMS: 365.2$(M+H)^+$.

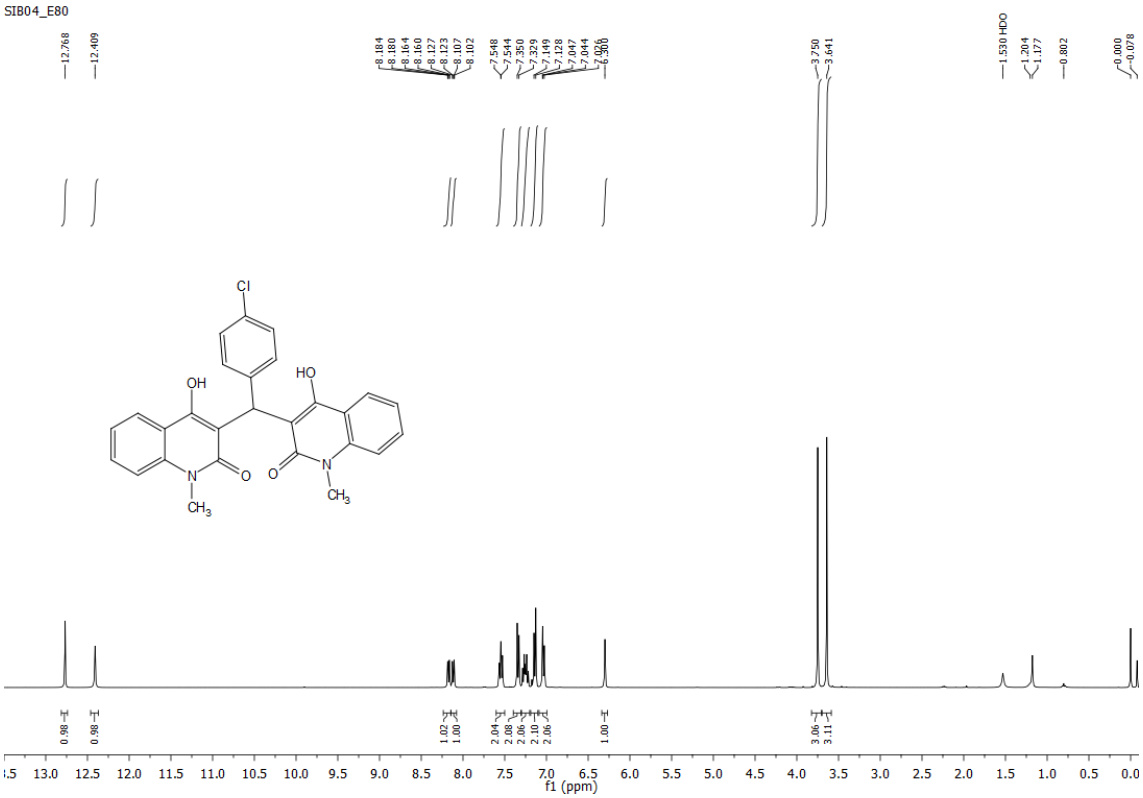
3-((2-amino-6-oxocyclohex-1-enyl)methyl)-4-hydroxy-1-methylquinolin-2(1*H*)-one ($S_3$5k)



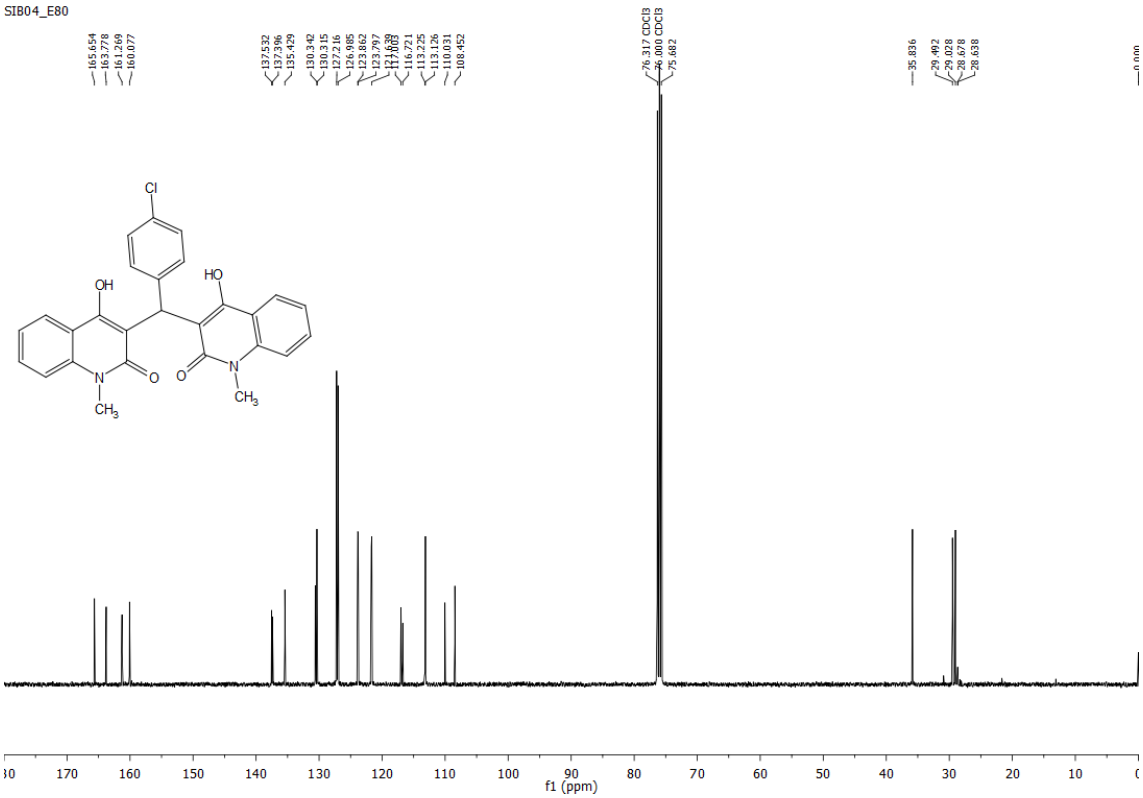
White solid; mp: 241~242 °C; ^{1}H NMR (400MHz, DMSO-d_6+MeOD) δ: 1.77-1.95 (m, 2H), 2.30 (t, 2H, J = 6.4 Hz) 2.45 (t, 2H, J = 6.4 Hz), 3.51 (s, 2H, CH_2), 3.67 (s, 3H, N*CH*$_3$), 7.25-7.29 (m, 1H, ArH), 7.50 (d, 1H, J = 8.8 Hz, ArH) 7.57-7.62 (m, 1H, ArH), 8.00 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8 Hz, ArH); ^{13}C NMR (100.6 MHz, DMSO-d_6+MeOD) δ: 18.6, 20.5, 28.3, 28.7, 34.1, 37.6, 37.8, 38.2, 101.0, 106.7, 108.9, 113.9, 116.4, 121.4, 123.0, 130.2, 133.9, 137.9, 164.4, 169.1, 196.1; IR (Neat, cm^{-1}): 3226, 3050, 1685, 1570, 1479; Anal. Calcd for $C_{17}H_{18}N_2O_3$: C, 68.44; H, 6.08; N, 9.39, Found: C, 68.36; H, 5.95; N, 9.44; ESIMS: 298.9 $(M+H)^+$.

3. Selected Copies of ^{1}H and ^{13}C NMR spectra

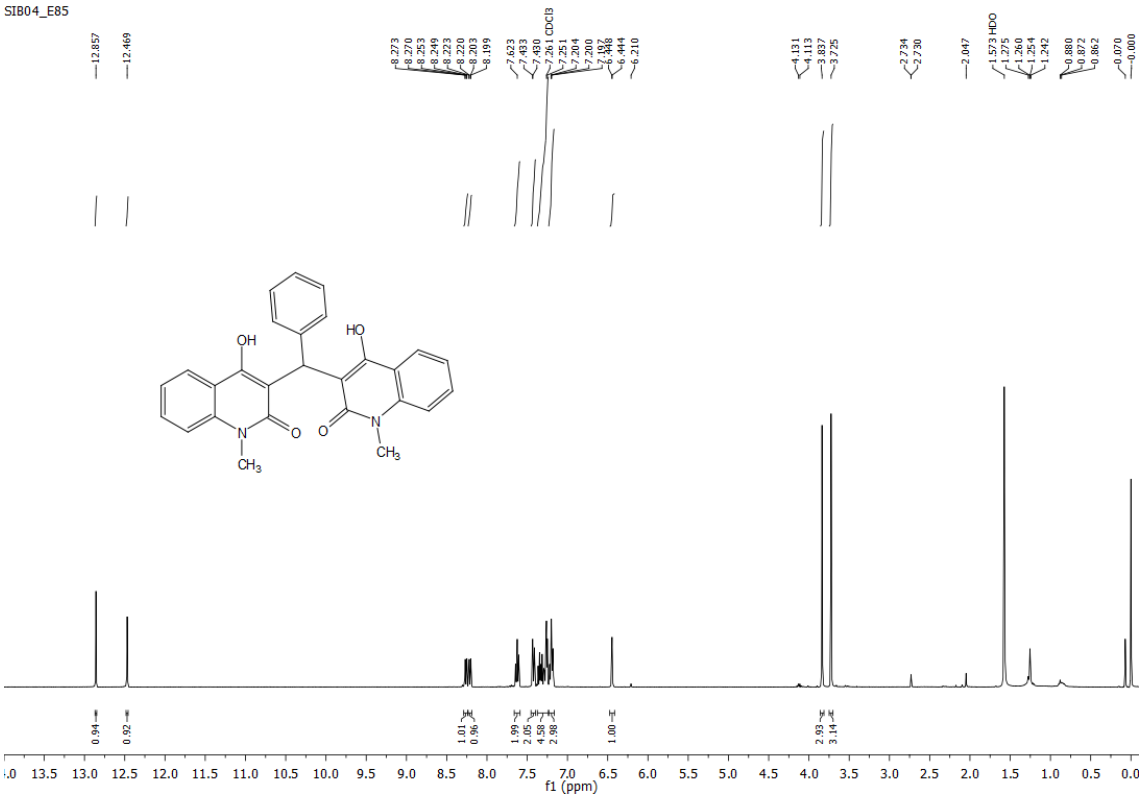
^{1}H NMR of compound 4a



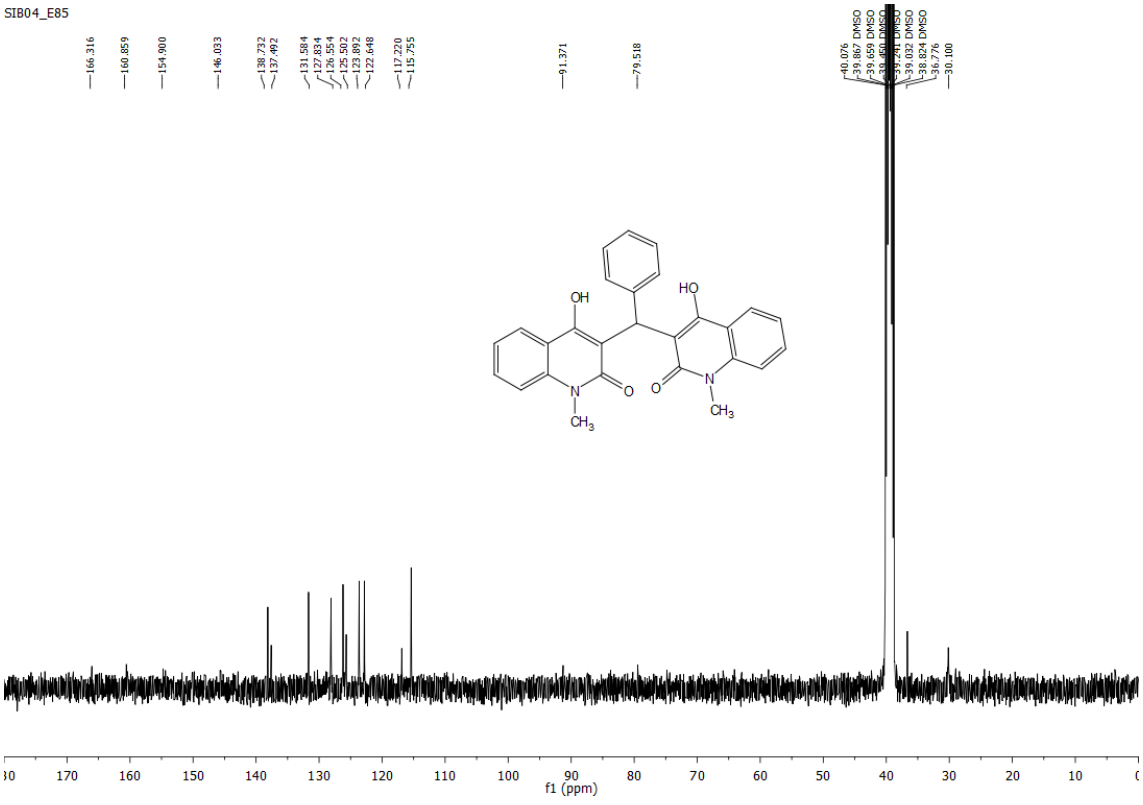
^{13}C NMR of compound 4a



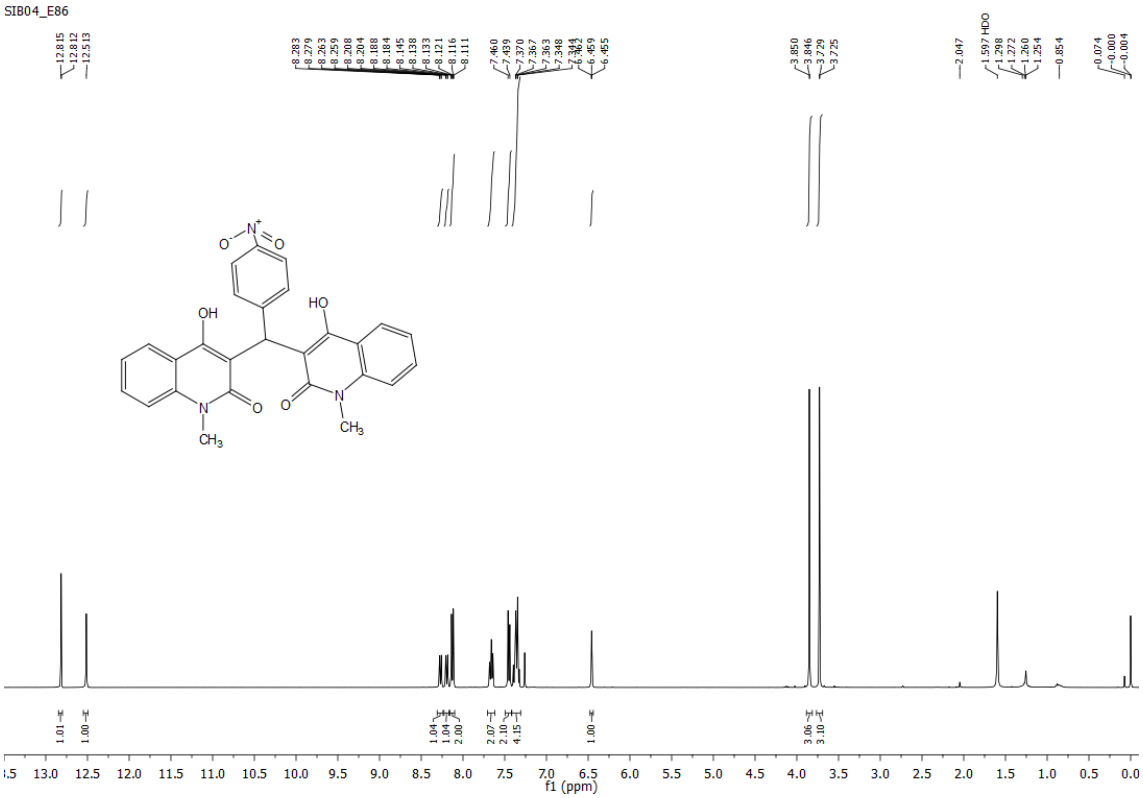
^{1}H NMR of compound 4b



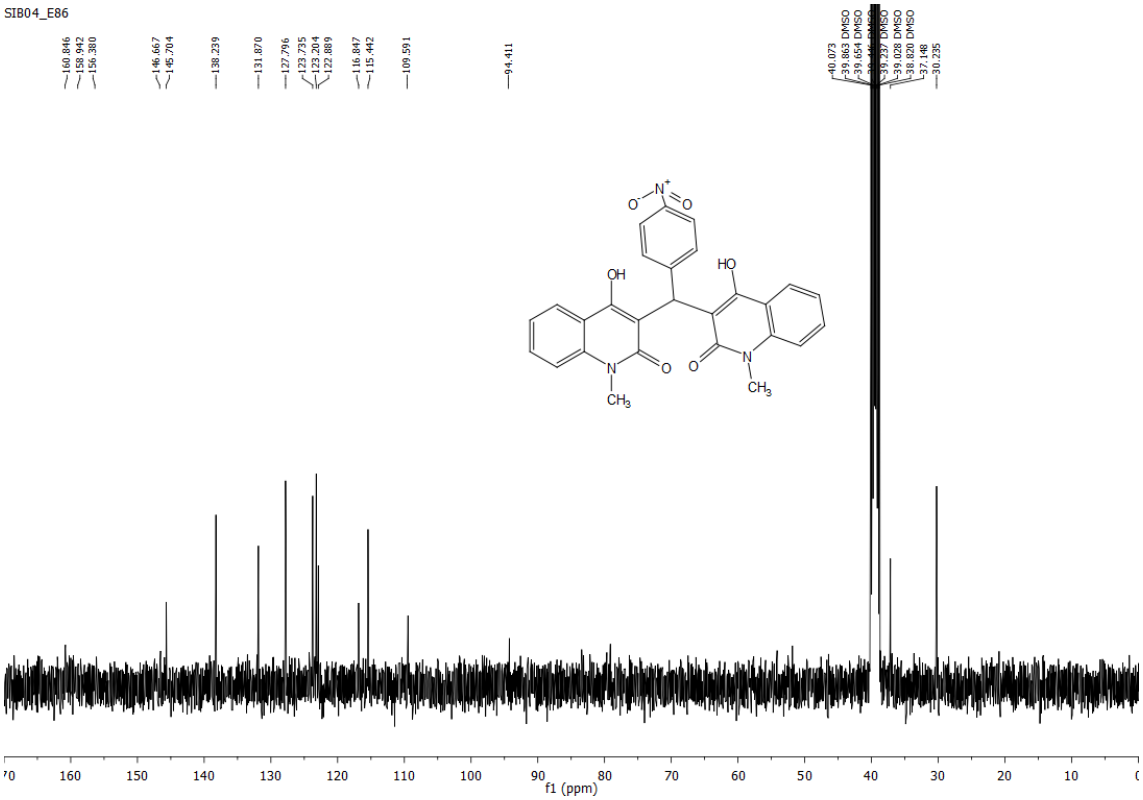
^{13}C NMR of compound 4b



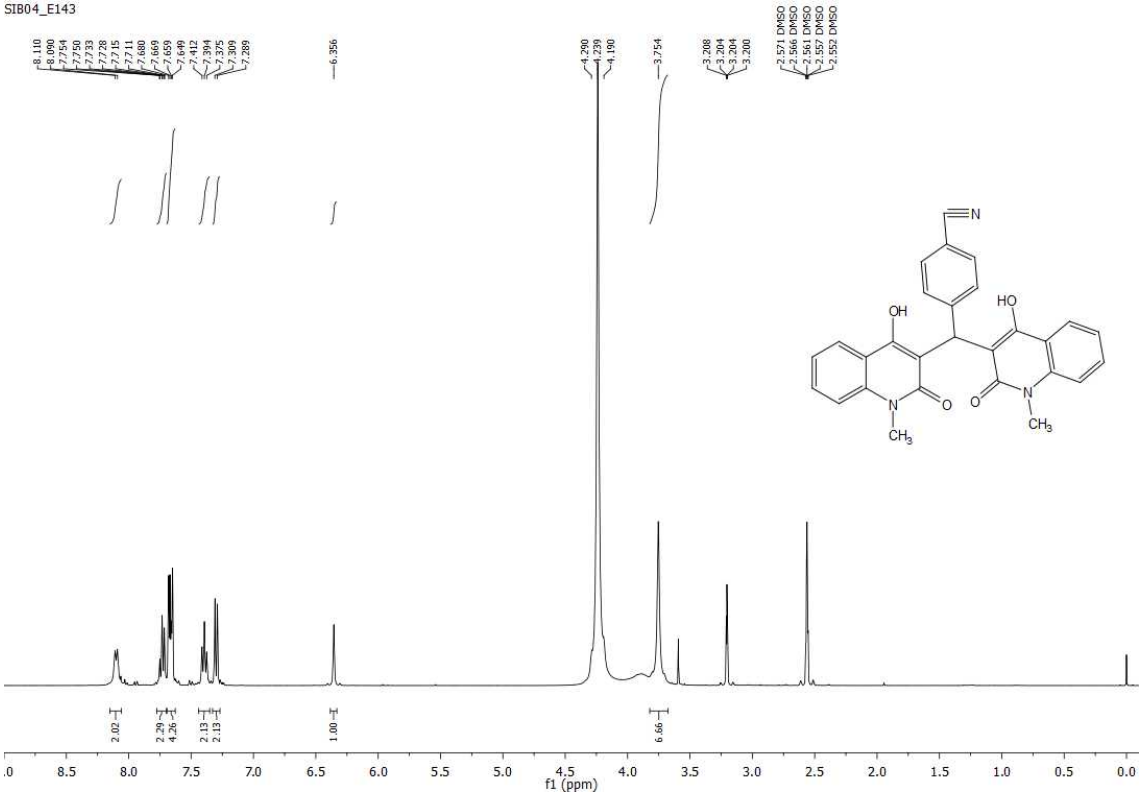
^{1}H NMR of compound 4c



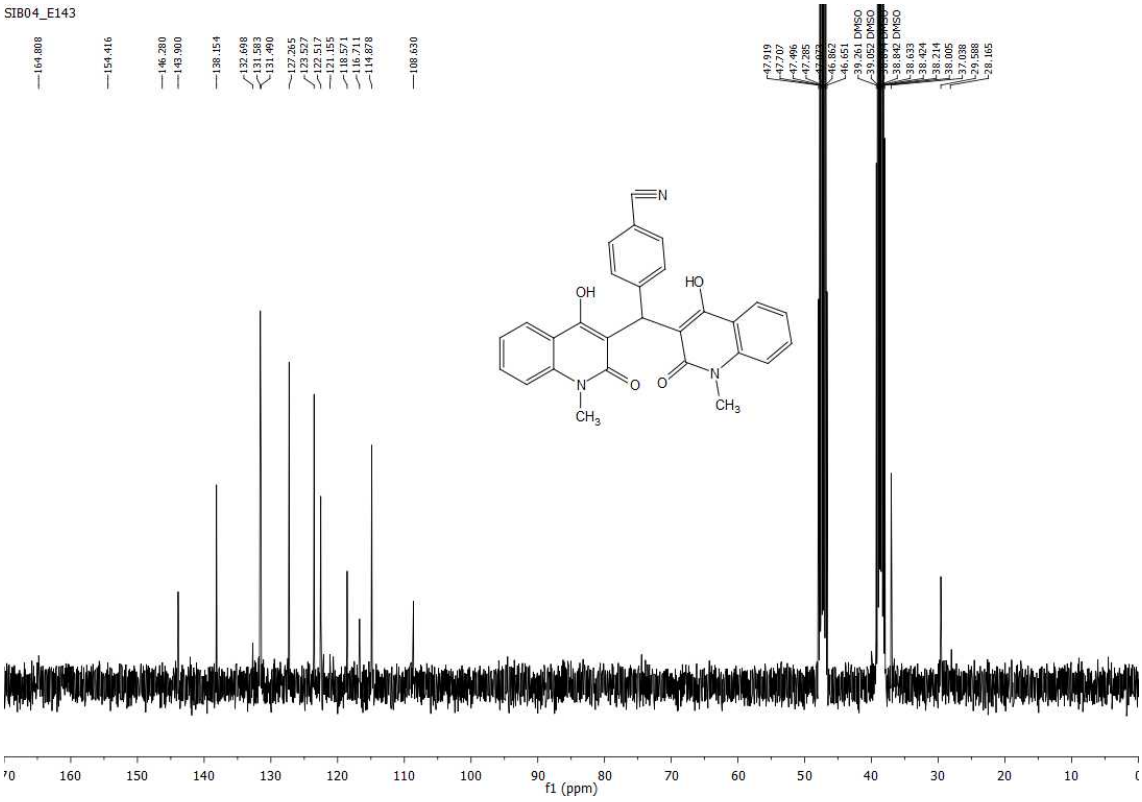
^{13}C NMR of compound 4c



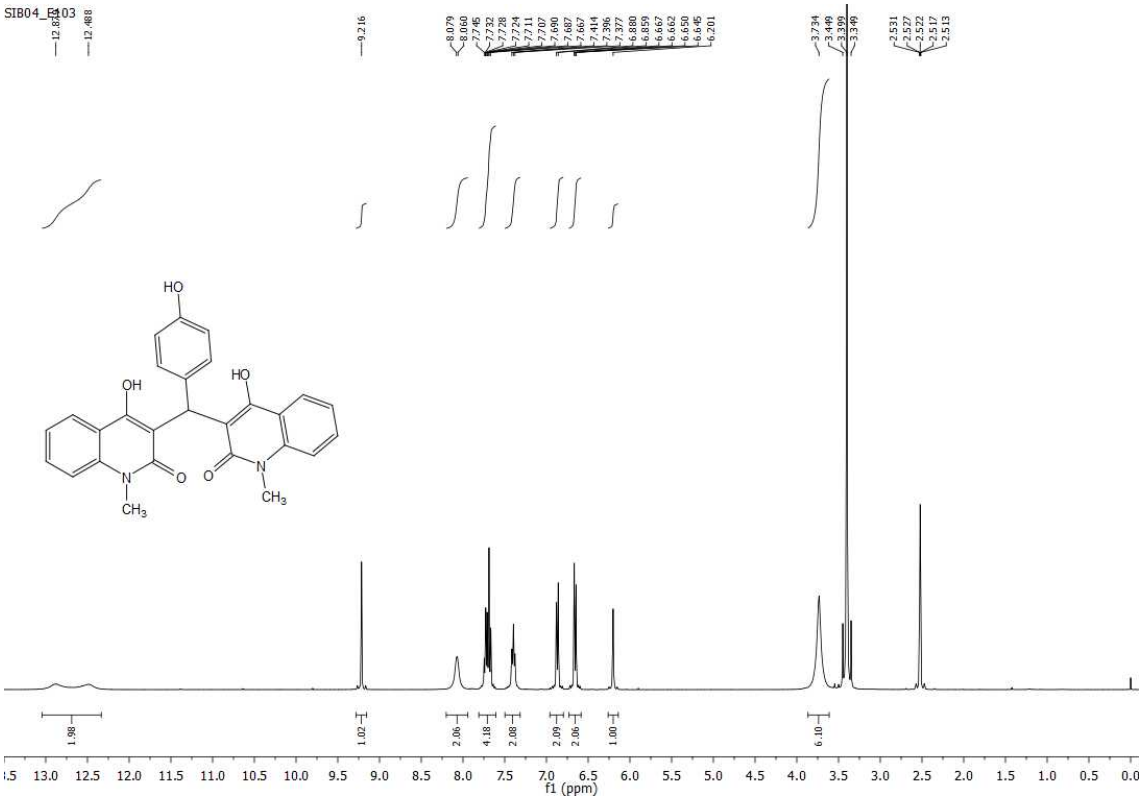
^{1}H NMR of compound 4d



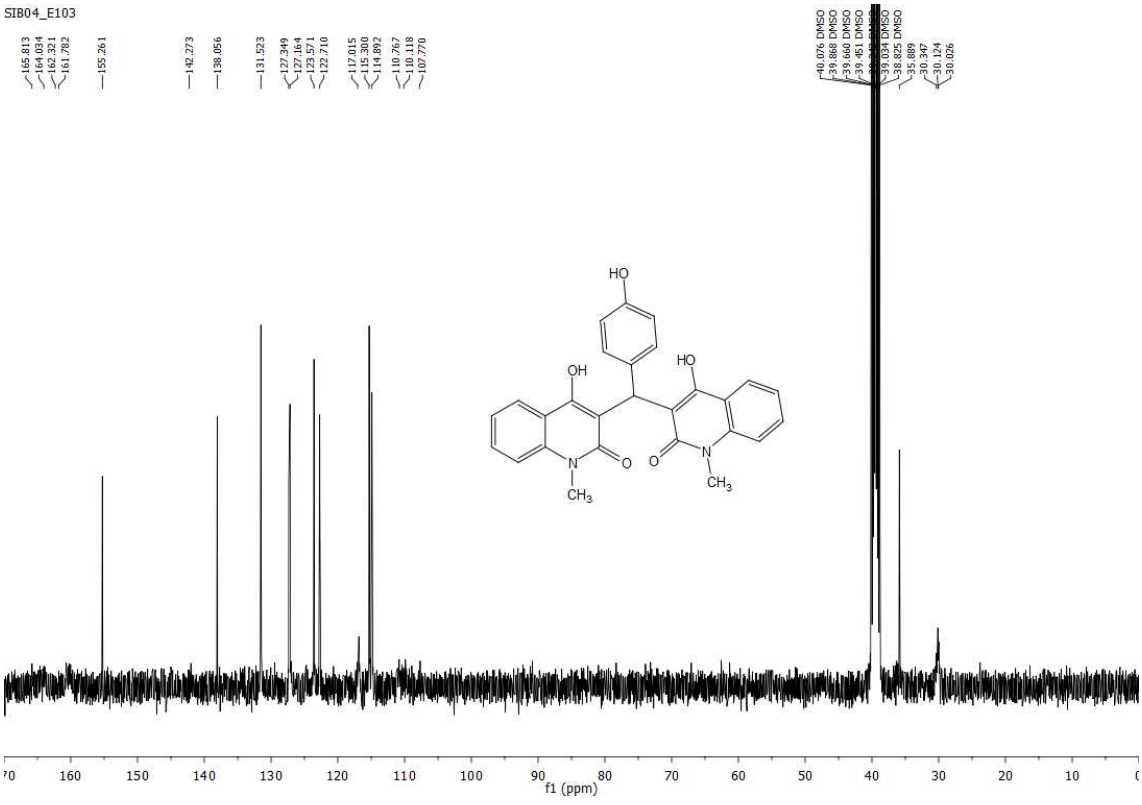
^{13}C NMR of compound 4d



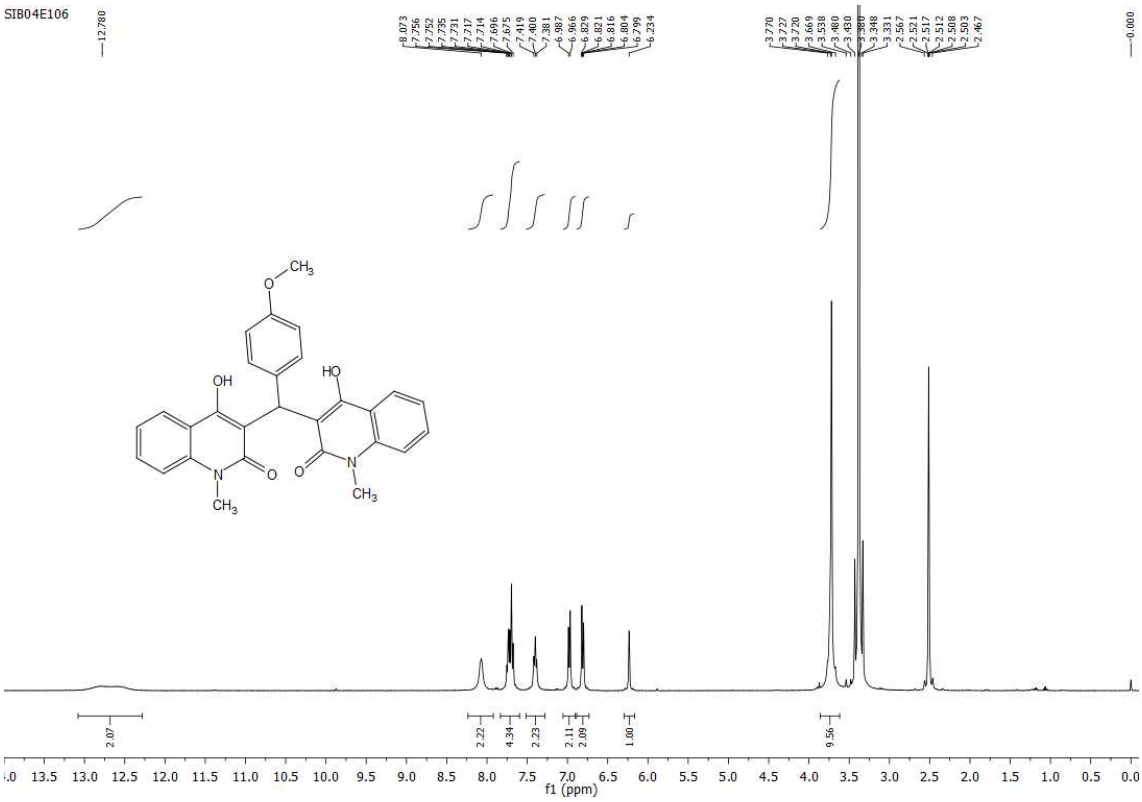
^{1}H NMR of compound 4e



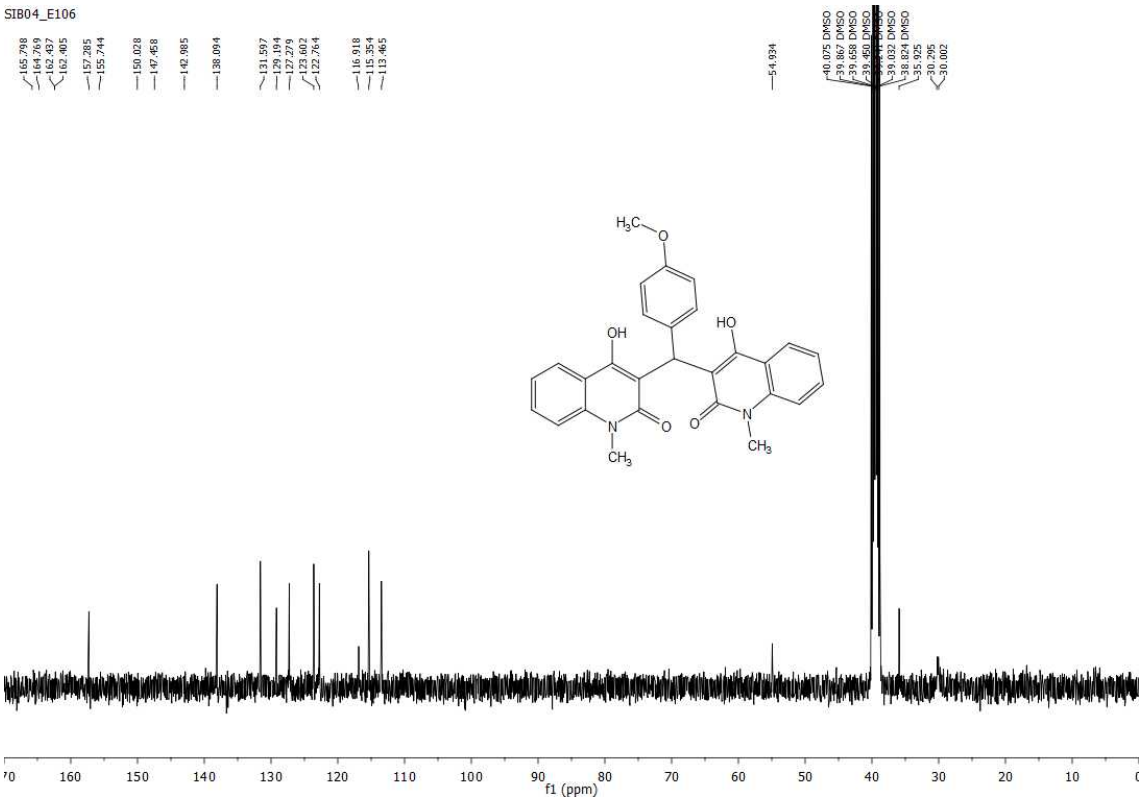
^{13}C NMR of compound 4e



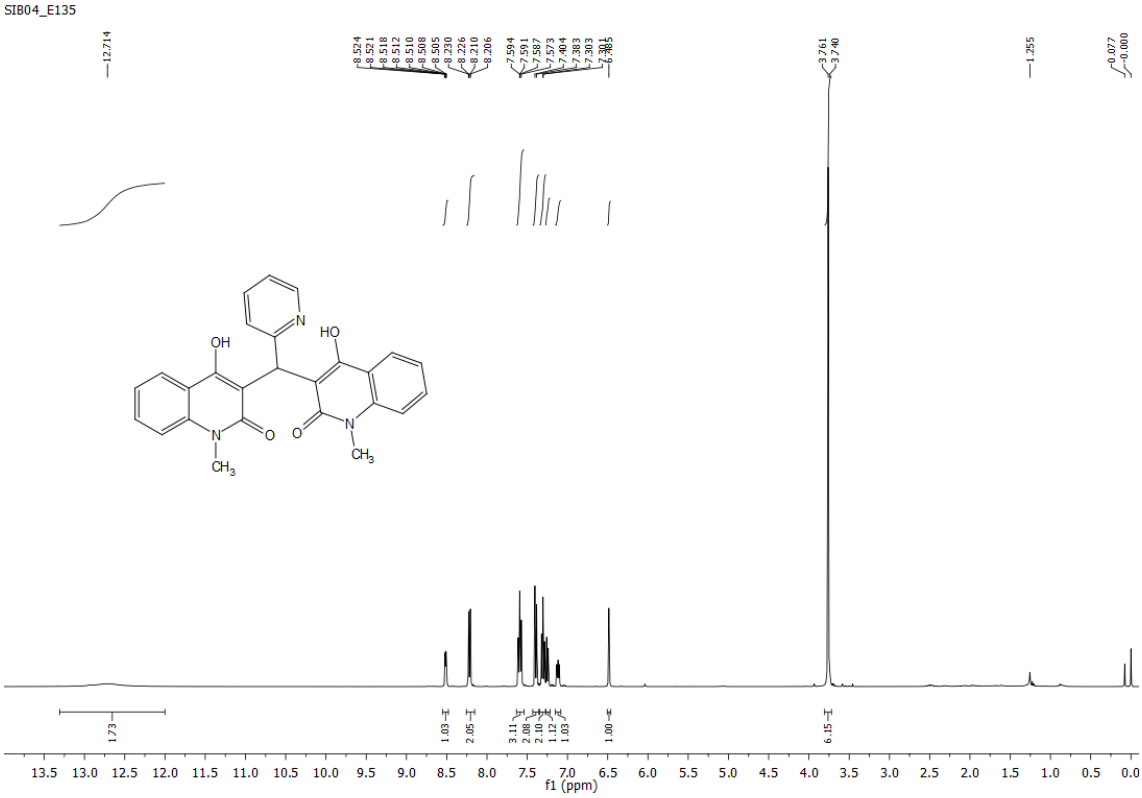
^{1}H NMR of compound 4f



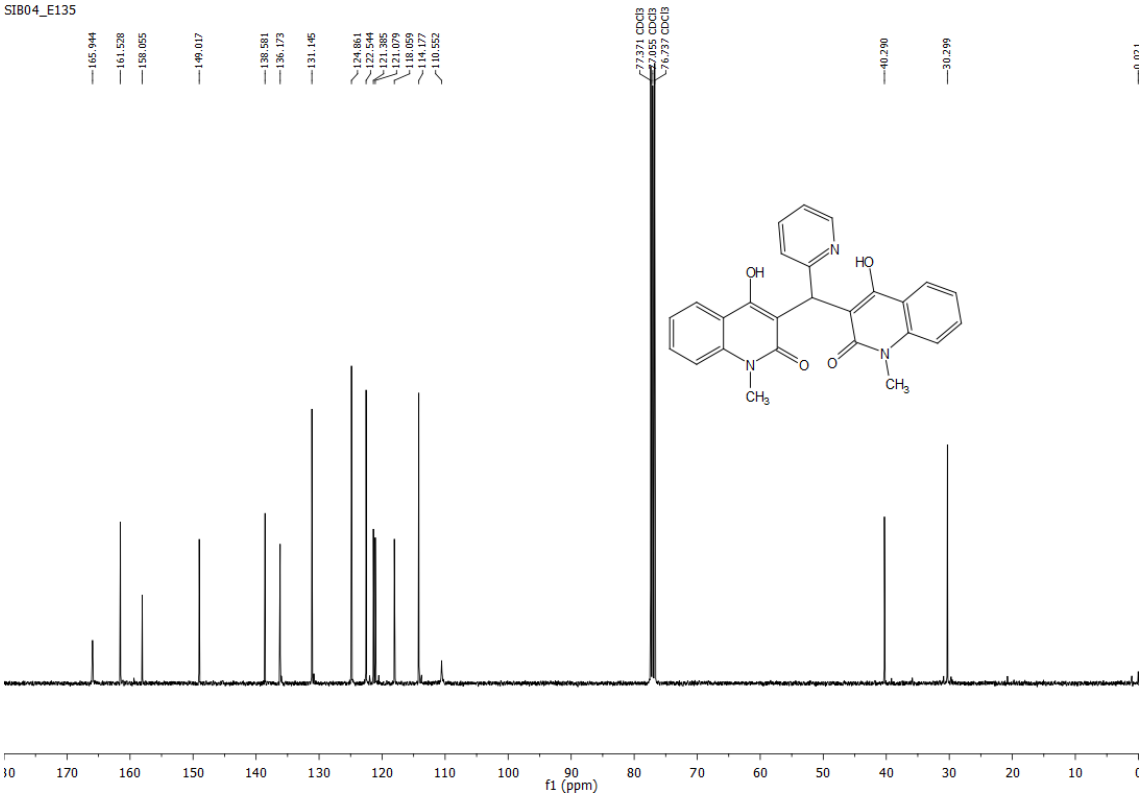
^{13}C NMR of compound 4f



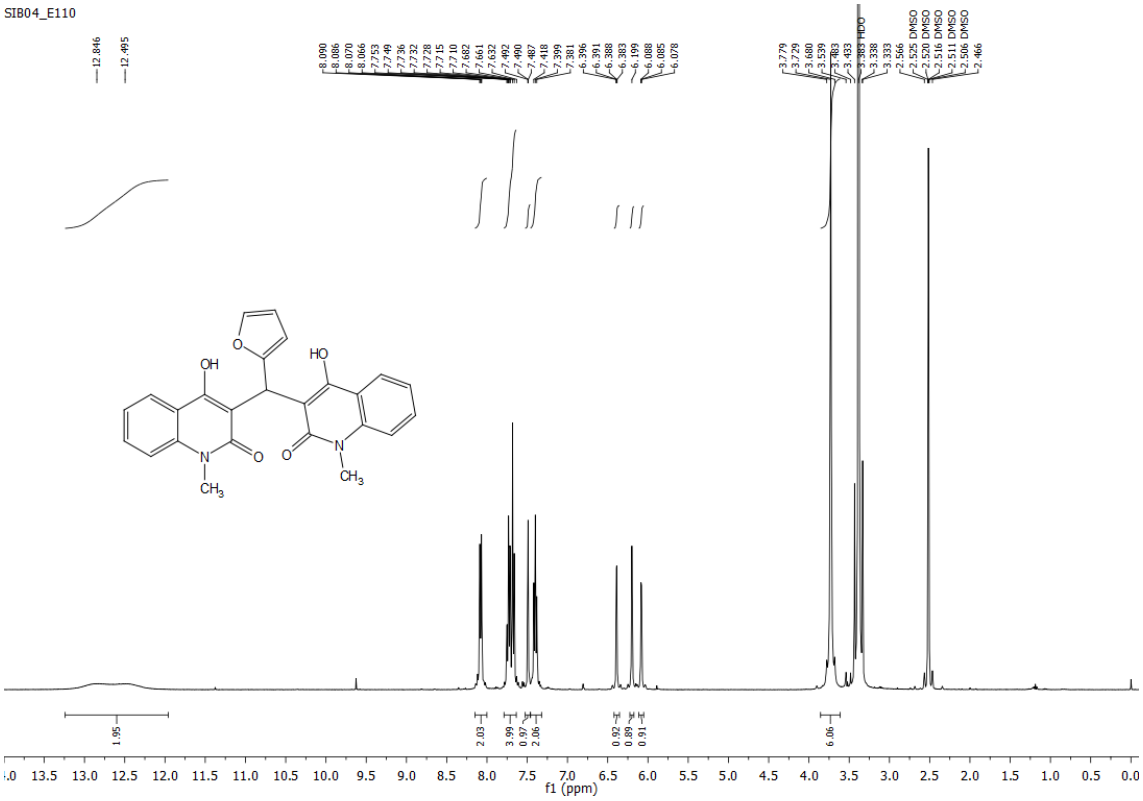
^{1}H NMR of compound 4g



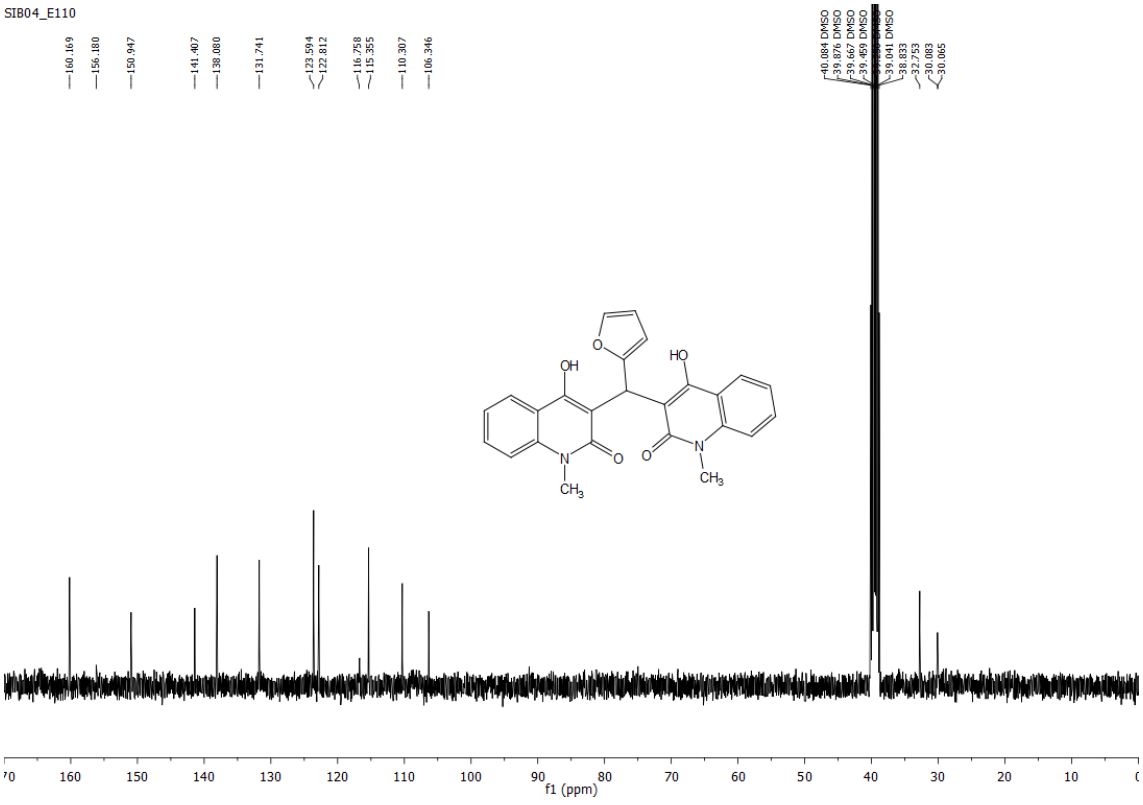
^{1}HNMR of compound 4g



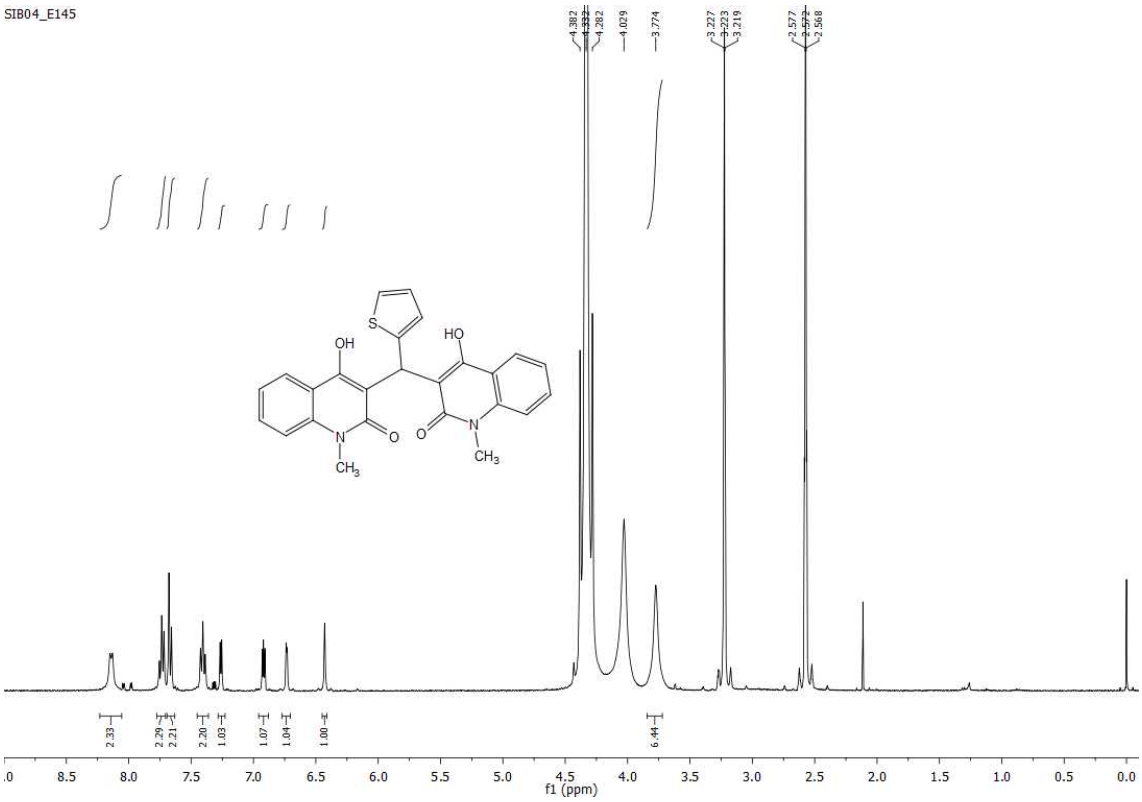
^{1}H NMR of compound 4h



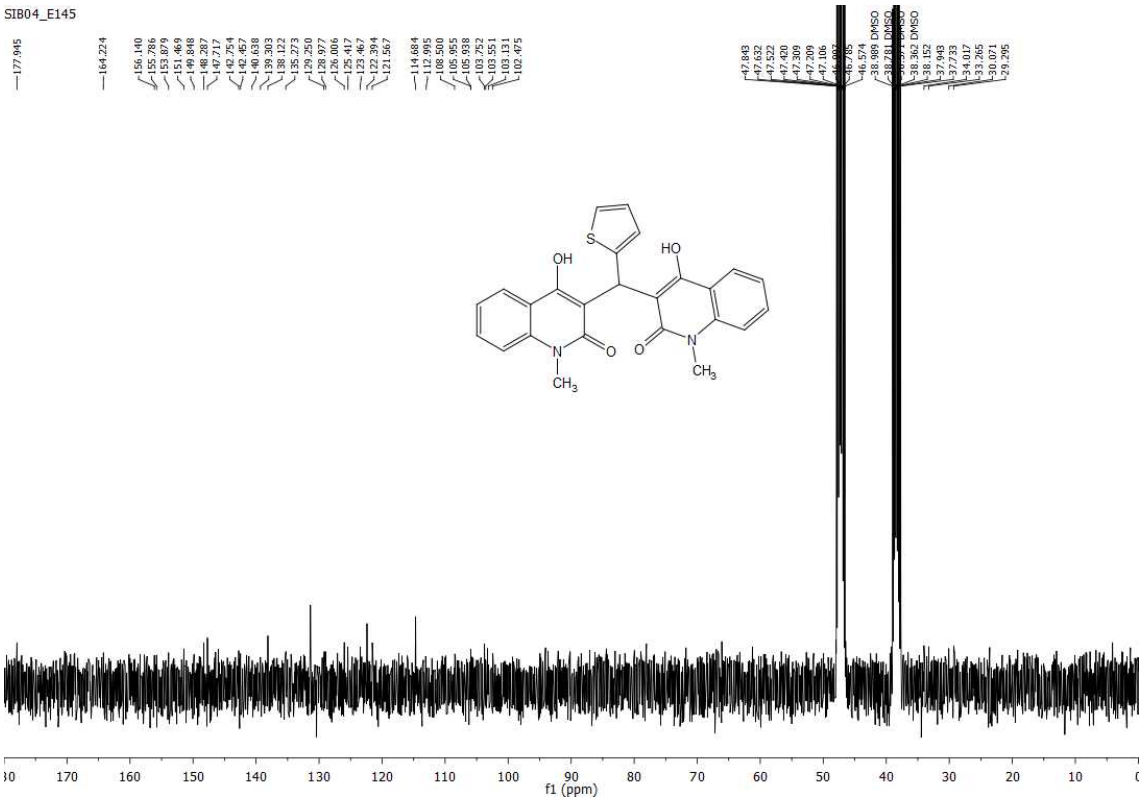
^{13}C NMR of compound 4h



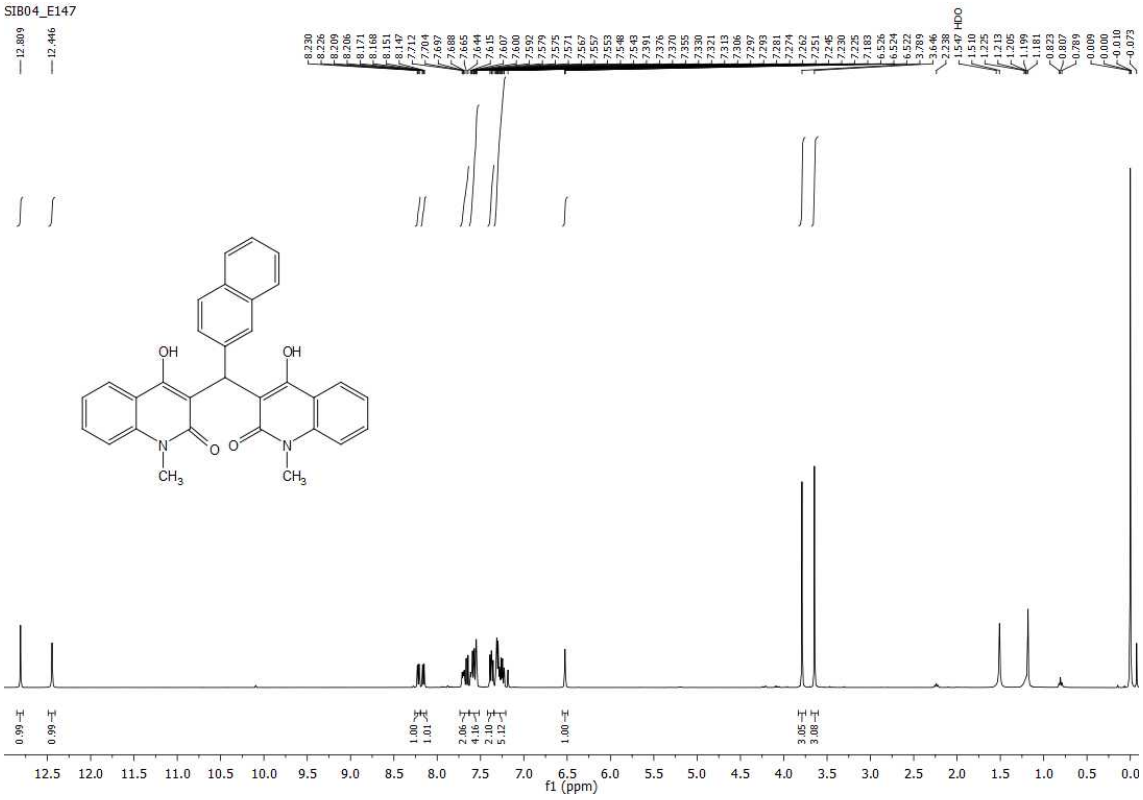
^{1}H NMR of compound 4i



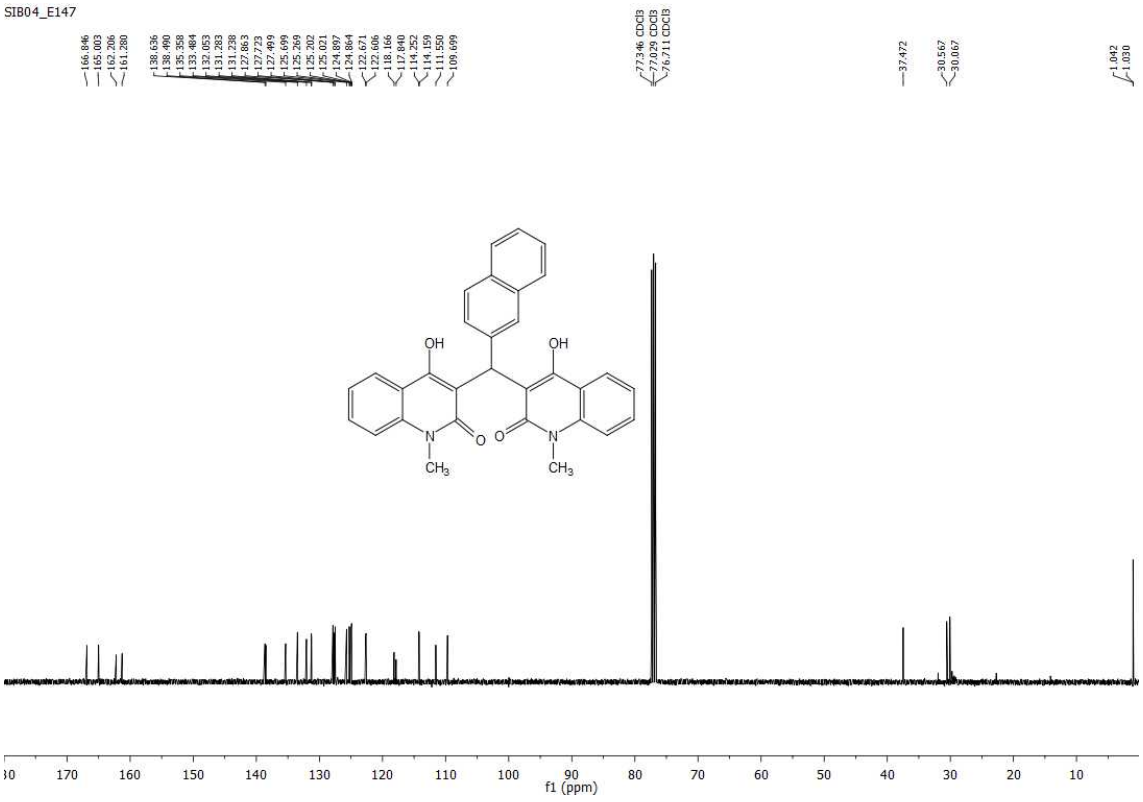
^{13}C NMR of compound 4i



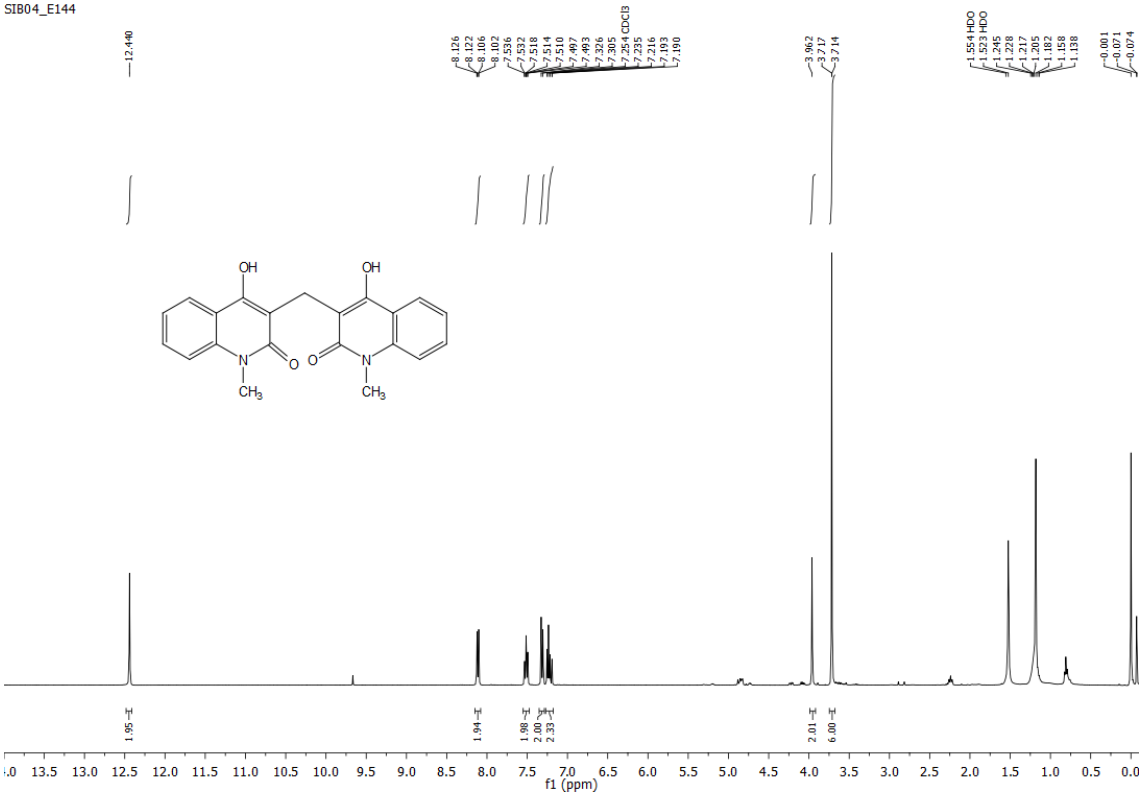
^{1}H NMR of compound 4j



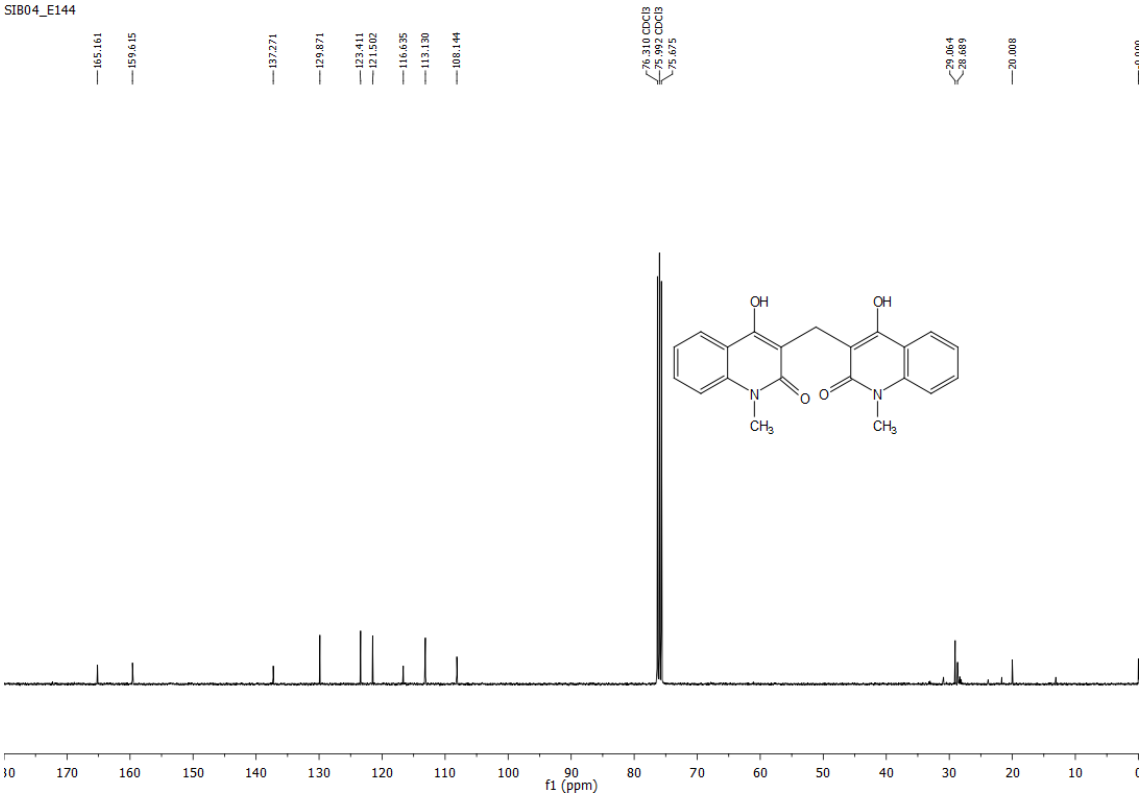
^{1}H NMR of compound 4j



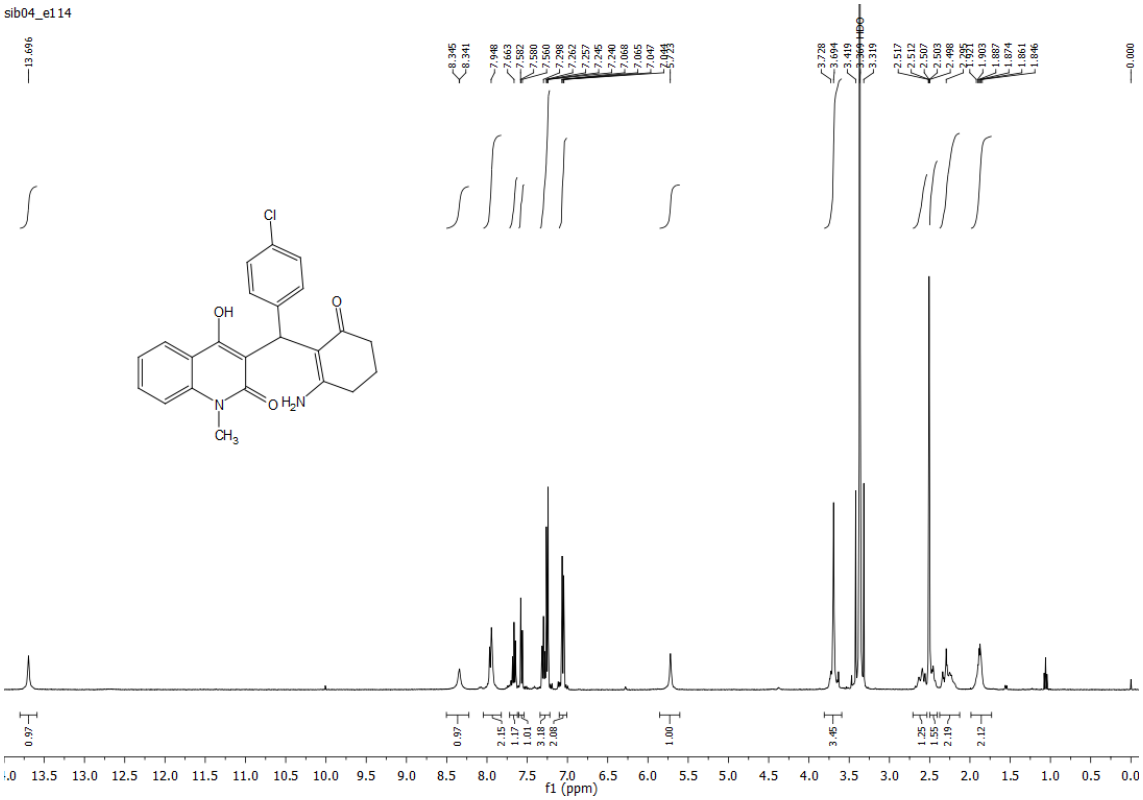
^{1}H NMR of compound 4k



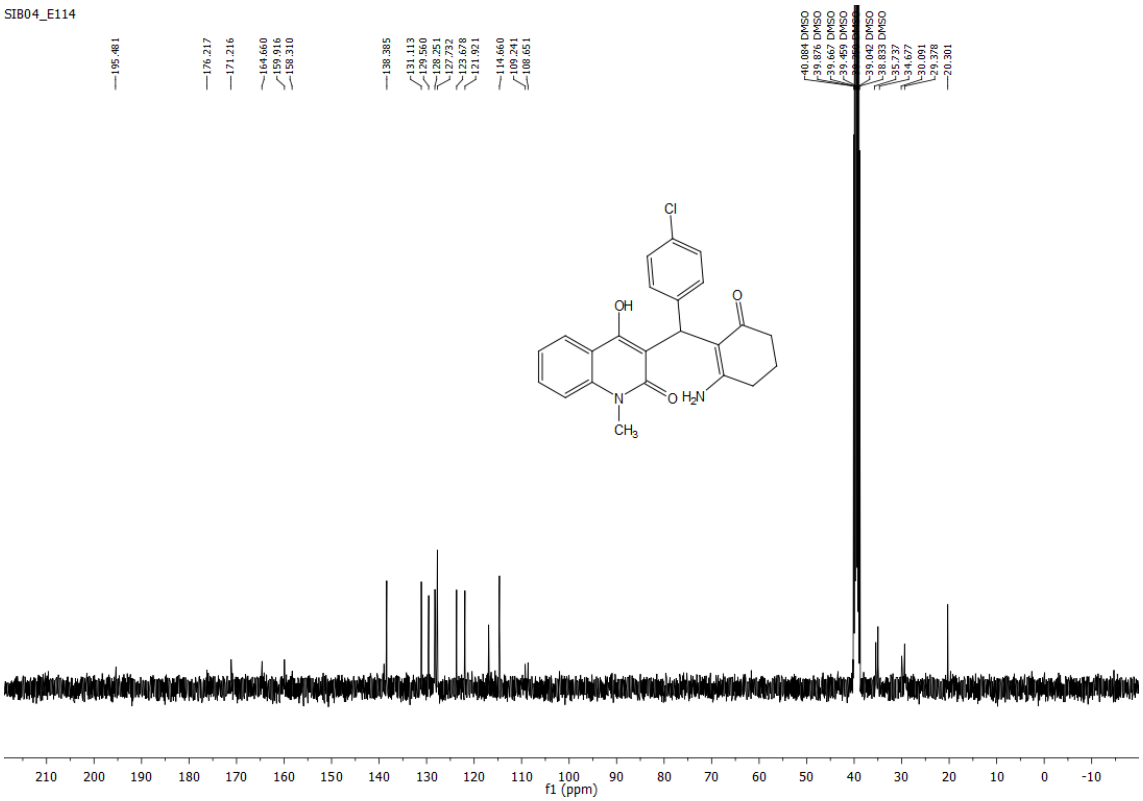
^{13}C NMR of compound 4k



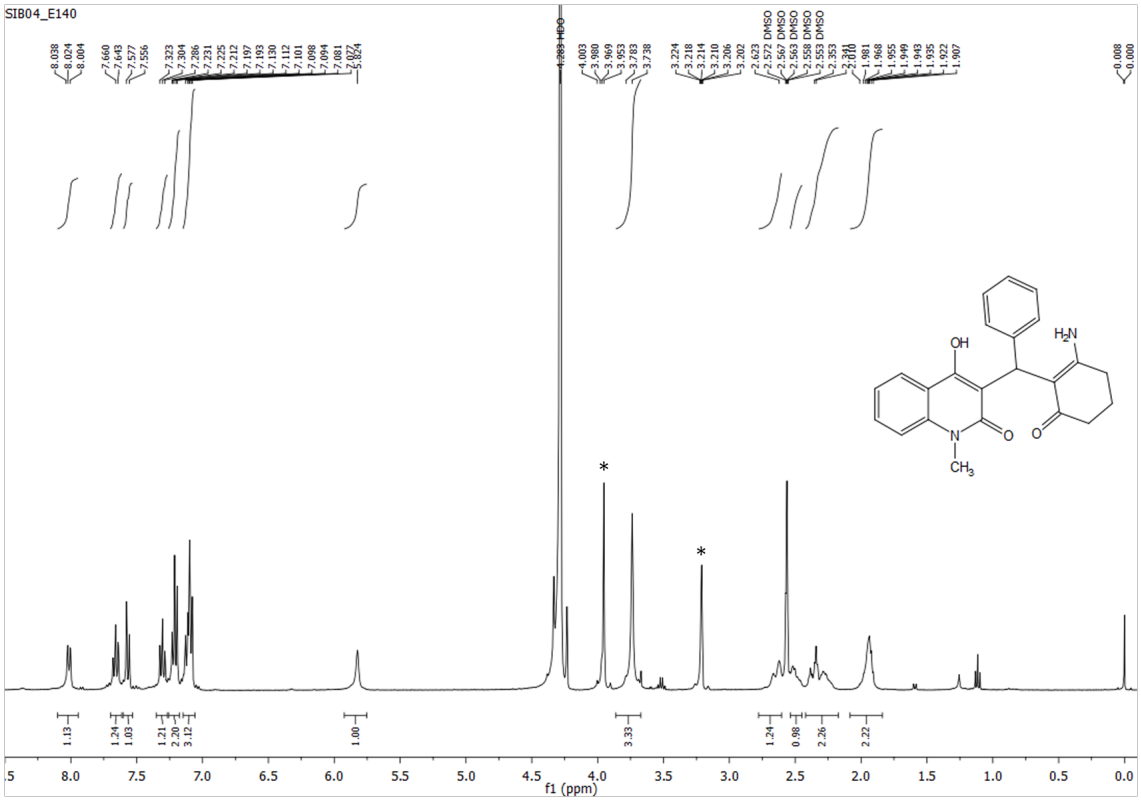
^{1}H NMR of compound 5a



^{13}C NMR of compound 5a

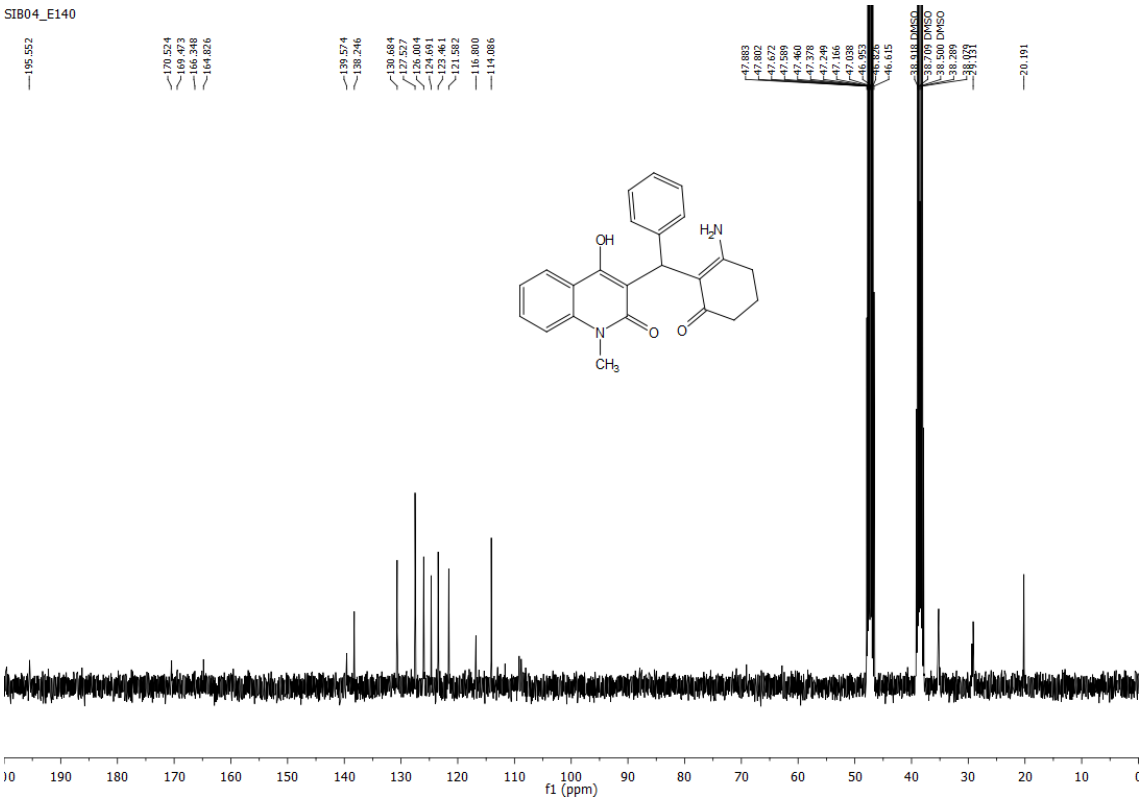


^{1}H NMR of compound 5b

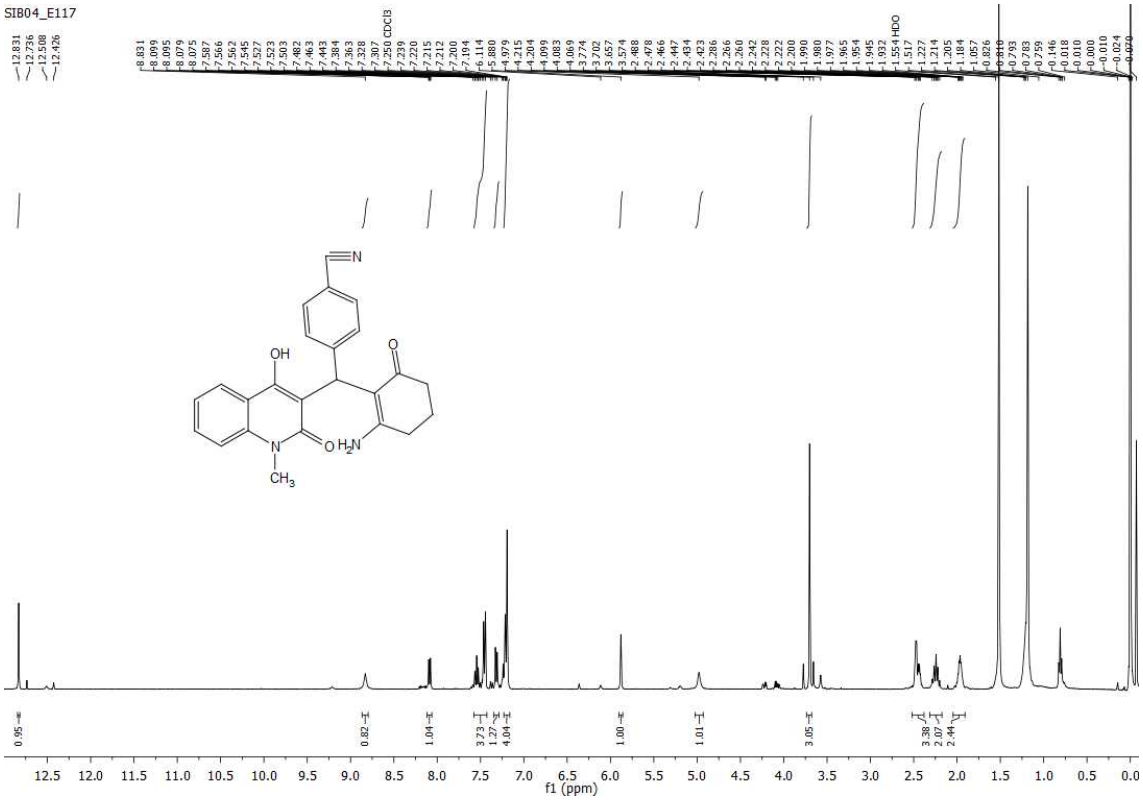


* Peaks Corresponds to MeOH[2]

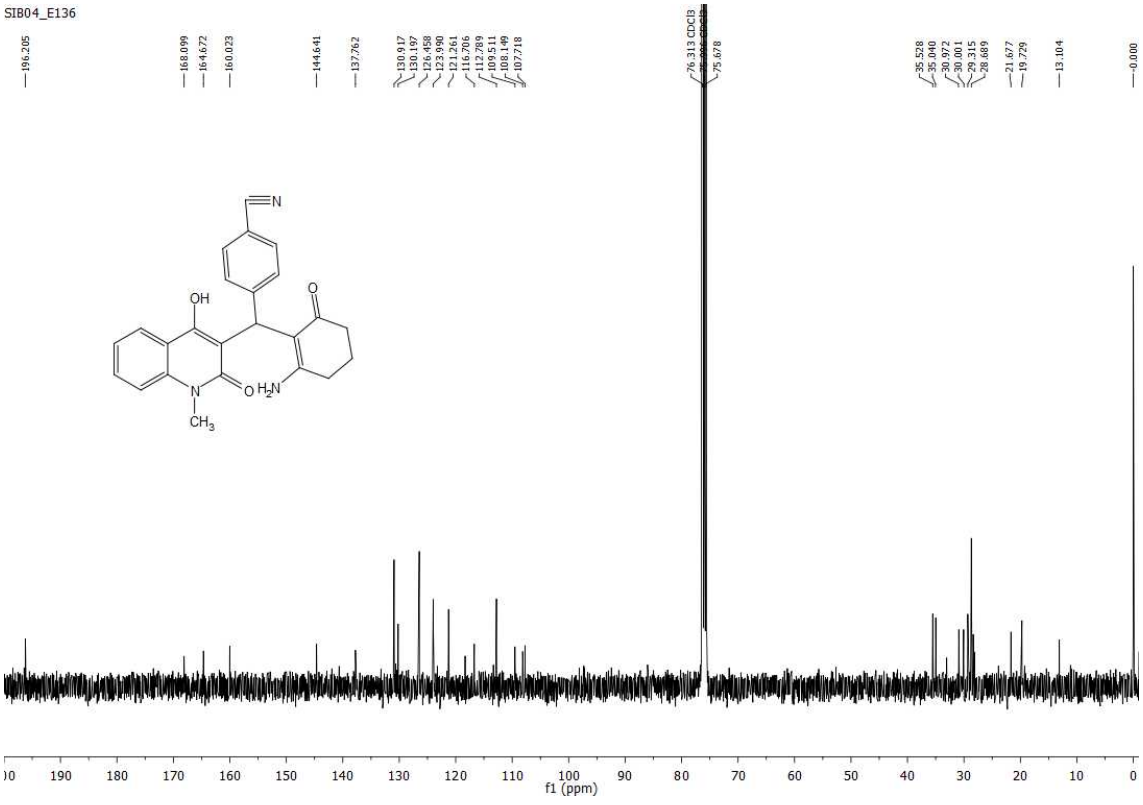
^{13}C NMR of compound 5b



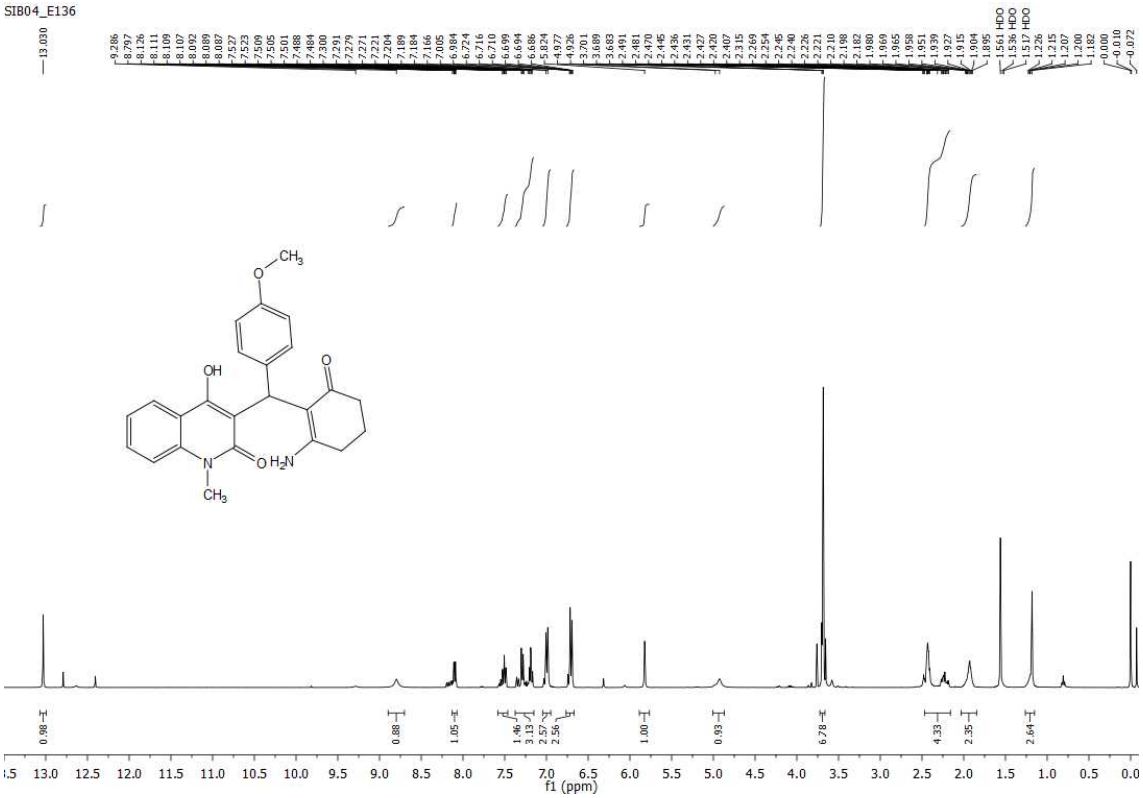
^{1}H NMR of compound 5d



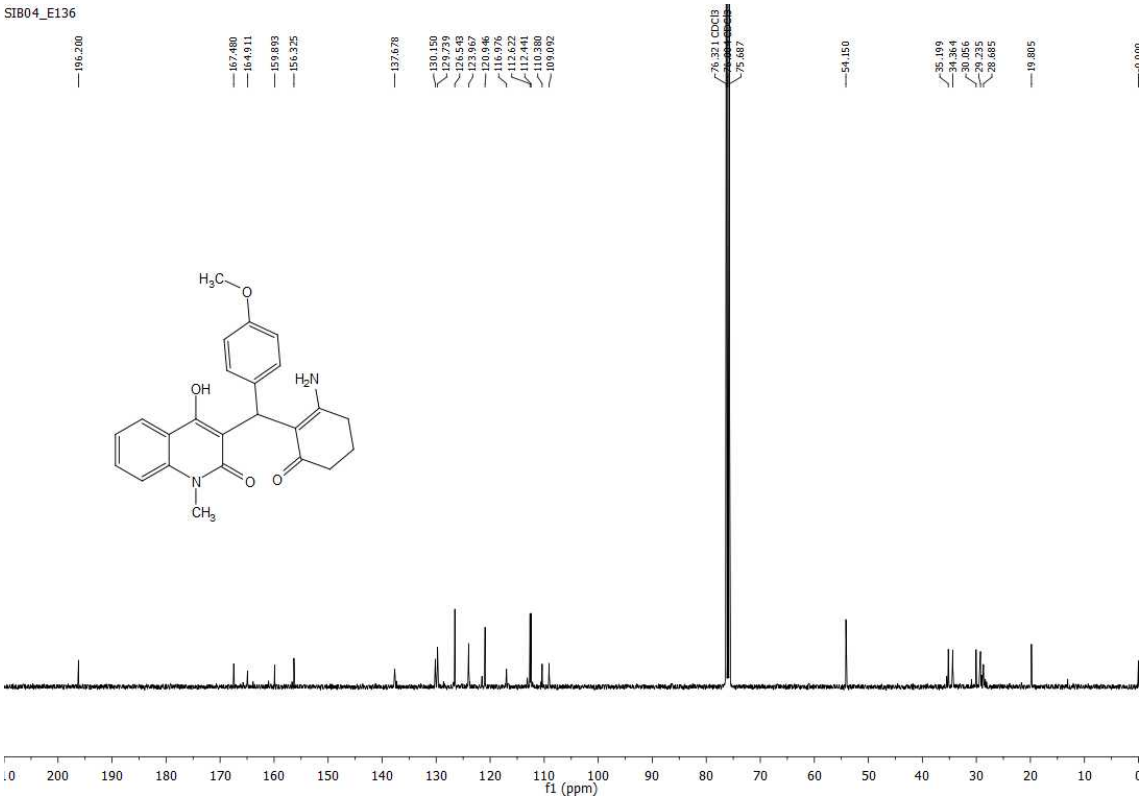
^{13}C NMR of compound 5d



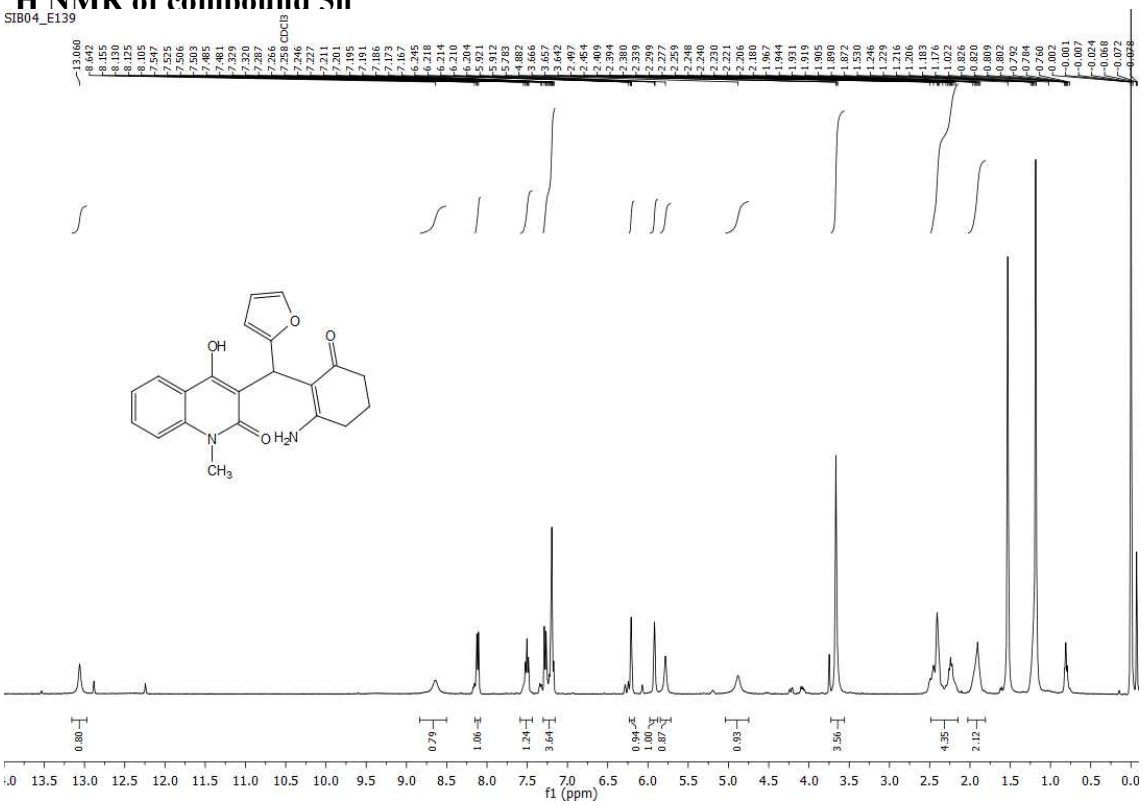
^{1}H NMR of compound 5f



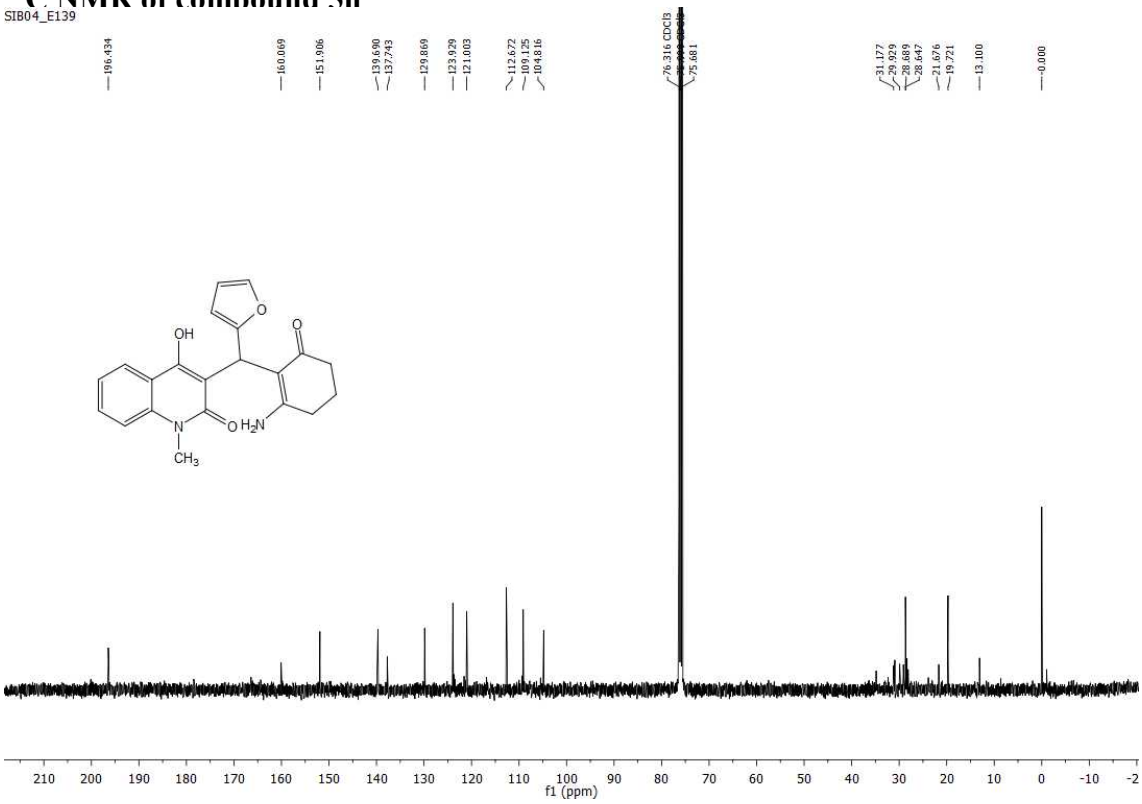
^{13}C NMR of compound 5f



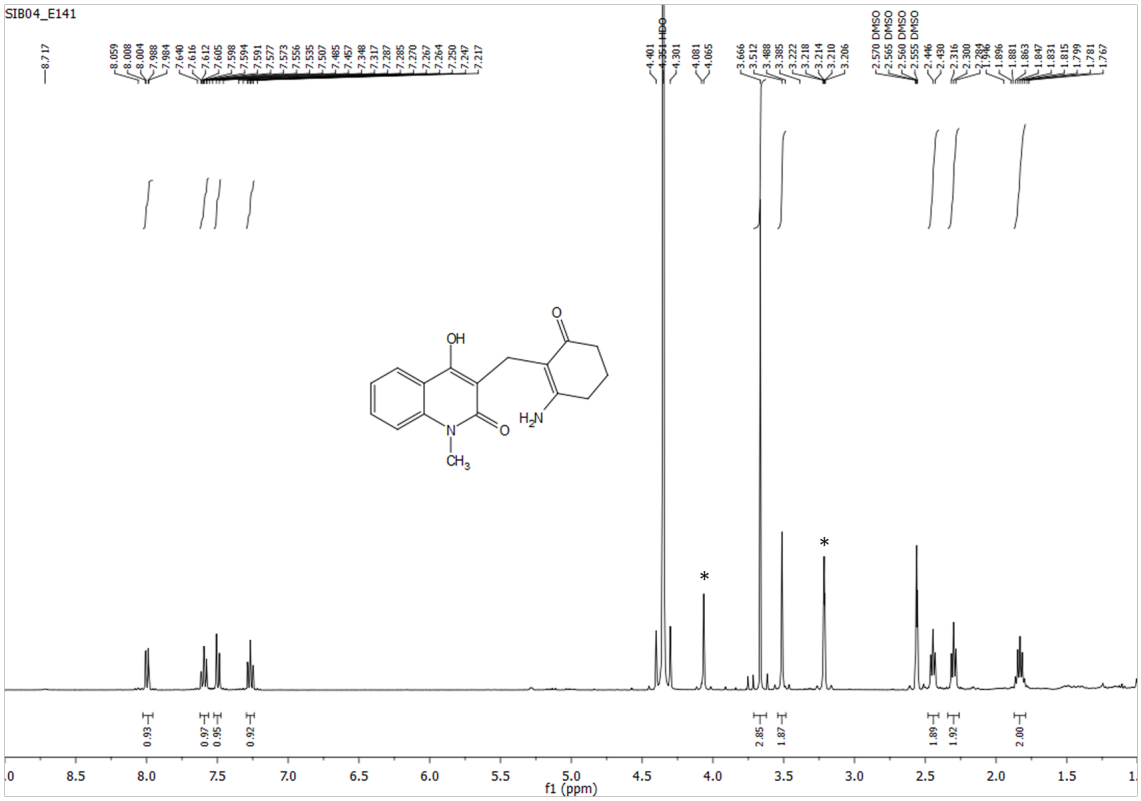
^{1}H NMR of compound 5h



^{13}C NMR of compound 5h

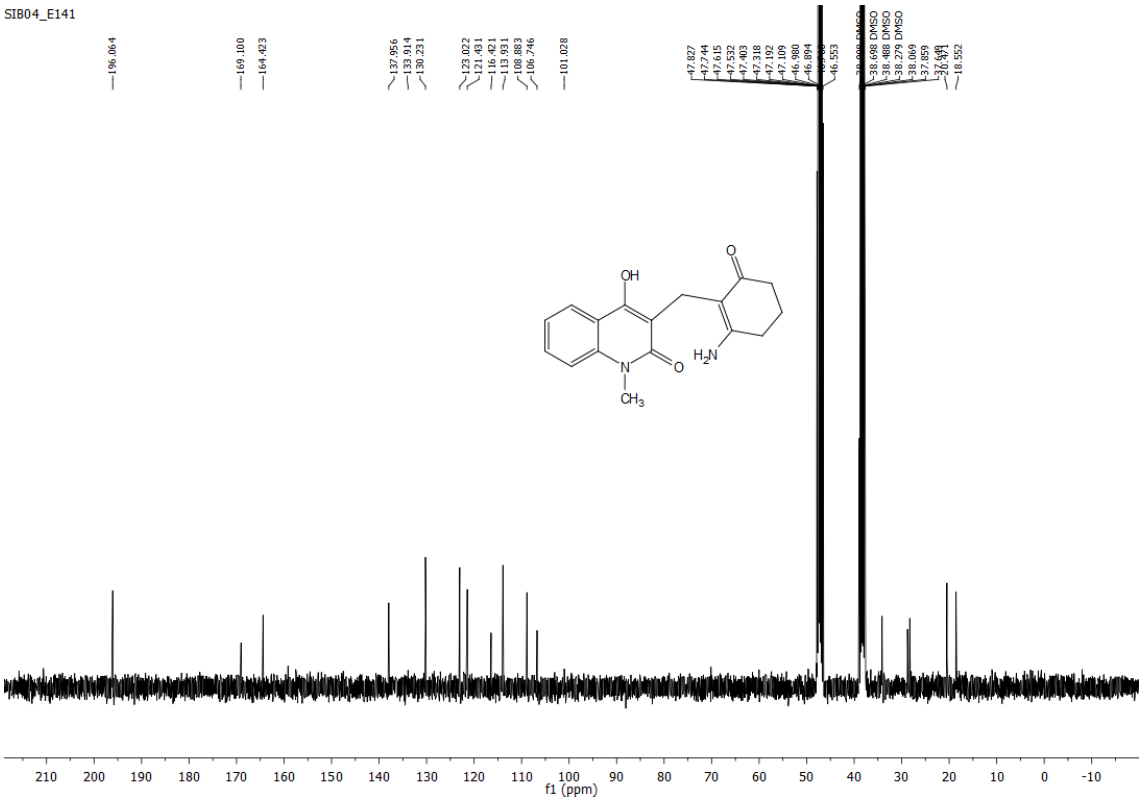


^{1}H NMR of compound 5k



* Peaks Corresponds to MeOH[2]

^{13}C NMR of compound 5k



4. References

1. Grigg, R.; Whitney, S.; Sridharan, V.; Keep, A.; Derrick, A. *Tetrahedron* **2009,** *65*, 7468.

2. Gottlieb, H. E.; Kotlyar, V.; Nudelman, A. *J. Org. Chem.* **1997,** *62,* 7512.