

Supporting Information

Hydrophobically directed, Catalyst-free, multi-component synthesis of functionalized 3, 4-dihydroquinazolin-2(1H)-ones

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General methods

Analytical thin-layer chromatography was performed on silica gel 60 F-254 plates and visualized by UV light or ninhydrin stain. Flash column chromatography was performed using silica gel (60, particle size 40-63 nm). IR spectra were recorded on FT-IR spectrometer. ^1H NMR spectra were recorded at 300, 400 and 500 MHz and ^{13}C NMR spectra at 75, 100 and 125 MHz. The chemical shifts for ^1H NMR and ^{13}C NMR were referenced to TMS via residual solvent signals (^1H , CDCl_3 at 7.26 ppm; ^{13}C , CDCl_3 at 77.36 ppm; ^1H , $\text{DMSO}-d_6$ at 2.45 ppm; ^{13}C , $\text{DMSO}-d_6$ at 39.43 ppm, ^1H). Accurate mass values were determined on a mass spectrometer equipped with an electro spray or electron impact ion source and 7-T hybrid ion trap (LTQ) or TOF detector, respectively. All reactions were performed in sealed Pyrex microwave-transparent process vials designed for 0.5–2 mL reaction volumes. Reagents were purchased at the highest commercial quality and were used without further purification. Solvents used for extraction and silica gel chromatography (EtOAc, hexanes, *n*-pentane and dichloromethane) were used without purification or removal of water.

General Experimental

Preparation of methyl (2-formylphenyl)carbamate (1a)

Prepared according to the literature procedure.²⁰ Spectral data were in agreement with reported values.

Preparation of N-1 position of *o*-formyl carbamates

Prepared according to the literature procedure.¹⁵ Spectral data were in agreement with reported values.

General procedure for the preparation of compounds **4** or **6** or **8**

A mixture of o-formyl carbamate **1** (0.55 mmol), amine **2** (0.60 mmol), and 1H-indole **3** (0.55 mmol) or 2-naphthol **6** (0.55 mmol) in 2 mL H₂O was heated to 130 °C for 8h in a closed vessel. After completion of the reaction (TLC), the solid was filtered off, washed with a small amount of Et-OH to yield the pure products **4** or **6** or **8**. Among them, products **4a-4c**, **4h-4i**, **4r-4s**, **6a-6j** were purified by short column chromatography on a silica gel column using EtOAc–hexane mixture as the eluent.

X-ray Crystallography data

Data Collection

A white block crystal of C₂₃H₁₈FN₃O having approximate dimensions of 0.350 x 0.330 x 0.310 mm was mounted on a glass fiber. All measurements were made on a Rigaku SCX mini diffractometer using graphite monochromated Mo-K α radiation.

The crystal-to-detector distance was 52.00 mm. Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

$$a = 9.0737(6) \text{ \AA}$$

$$b = 18.081(1) \text{ \AA}$$

$$b = 111.185(4)^\circ$$

$$c = 12.2682(7) \text{ \AA}$$

$$V = 1876.7(2) \text{ \AA}^3$$

For $Z = 4$ and F.W. = 371.41, the calculated density is 1.314 g/cm³. The reflection conditions of:

$$h0l: l = 2n$$

$$0k0: k = 2n$$

uniquely determine the space group to be:

$$P21/c \text{ (\#14)}$$

The data were collected at a temperature of 20 ± 1 °C to a maximum 2θ value of 55.0°. A total of 540 oscillation images were collected. A sweep of data was done using ω oscillations from -120.0 to 60.0° in 1.0° steps. The exposure rate was 10.0 [sec./°]. The detector swing angle was -30.80°. A second sweep was performed using ω oscillations from -120.0 to 60.0° in 1.0° steps. The exposure rate was 10.0 [sec./°]. The detector swing angle was -30.80°. Another sweep was performed using ω oscillations from -120.0 to 60.0° in 1.0° steps. The exposure rate was 10.0 [sec./°]. The detector swing angle was -30.80°. The crystal-to-detector distance was 52.00 mm. Readout was performed in the 0.146 mm pixel mode.

Data Reduction

Of the 18720 reflections that were collected, 4287 were unique ($R_{int} = 0.0517$); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku).

The linear absorption coefficient, μ , for Mo-K α radiation is 0.891 cm⁻¹. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.579 to 0.973. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods² and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically and the rest were refined using the riding model. The final cycle of full-matrix least-squares refinement³ on F^2 was based on 4287 observed reflections and 257 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \sum |F_o| - |F_c| / \sum |F_o| = 0.0546$$

$$wR2 = [\sum (w(F_o^2 - F_c^2))^2 / \sum w(F_o^2)^2]^{1/2} = 0.1792$$

The standard deviation of an observation of unit weight⁴ was 1.06. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.22 and -0.27 e-/Å³, respectively.

Neutral atom scattering factors were taken from Cromer and Waber⁵. Anomalous dispersion effects were included in F_{calc}⁶; the values for D_f' and D_f" were those of Creagh and McAuley⁷. The values for the mass attenuation coefficients are those of Creagh and Hubbell⁸. All calculations were performed using the CrystalStructure⁹ crystallographic software package except for refinement, which was performed using SHELXL-97¹⁰.

References

(1) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000. J.W. Pflugrath (1999) Acta Cryst. D55, 1718-1725.

(2) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(3) Least Squares function minimized: (SHELXL97)

$\sum w(F_o^2 - F_c^2)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$$[\sum w(F_o^2 - F_c^2)^2 / (N_o - N_v)]^{1/2}$$

where: N_o = number of observations

N_v = number of variables

- (5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).
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- (7) Creagh, D. C. & McAuley, W.J. ; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).
- (8) Creagh, D. C. & Hubbell, J.H.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
- (9) CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.
- (10) SHELX97: Sheldrick, G.M. (2008). *Acta Cryst.* A64, 112-122.

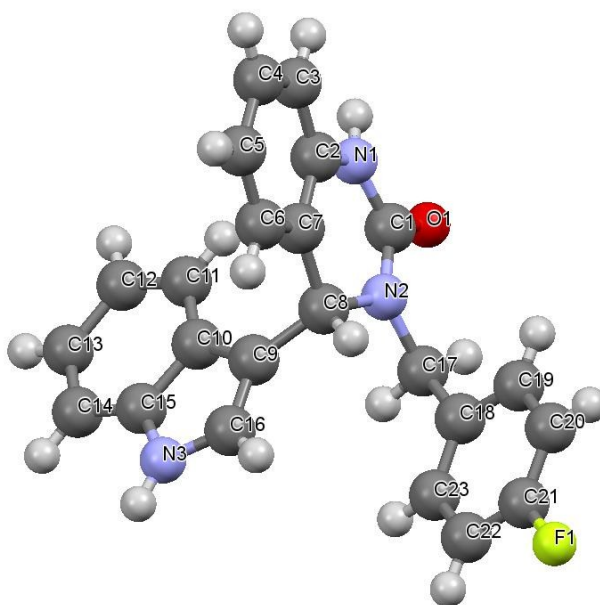


Fig 1. X-ray crystal structure of **4g**

Spectral data of all compounds

3-benzyl-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4a)

Isolated as a white solid; m.p. 232-234 °C; IR (KBr) cm^{-1} : 3301, 3206, 3116, 3051, 2922, 1651, 1607, 1465, 745; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 10.26 (s, 1H), 8.87 (s, 1H), 7.55-7.46 (m, 2H), 7.41-7.36 (m, 1H), 7.32-7.24 (m, 4H), 7.20-6.96 (m, 4H), 6.91-6.82 (m, 2H), 6.77-6.70 (m, 1H), 5.66 (s, 1H), 5.39 (d, $J = 15.2$ Hz, 1H), 3.76 (d, $J = 15.2$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 153.24, 136.75, 136.34, 127.79, 127.14, 127.03, 126.46, 126.14, 124.36, 122.80, 121.02, 120.69, 120.53, 118.69, 118.39, 115.33, 113.20, 111.09, 54.19, 45.90; HRMS (ESI) calc. For $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ 354.16107, found 368.16009.

4-(1H-indol-3-yl)-3-(4-methylbenzyl)-3,4-dihydroquinazolin-2(1H)-one (4b)

Isolated as a white solid; m.p. 224-226 °C; IR (KBr) cm^{-1} : 3437, 3189, 3050, 2913, 1656, 1605, 1465, 744; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 9.71 (s, 1H), 8.51 (s, 1H), 7.55 (d, $J = 7.9$ Hz, 1H), 7.37 (d, $J = 8.1$ Hz, 1H), 7.21-6.98 (m, 8H), 6.90-6.70 (m, 3H), 5.67 (s, 1H), 5.39 (d, $J = 15.1$ Hz, 1H), 3.71 (d, $J = 15.2$ Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 152.97, 136.19, 135.72, 135.19, 133.46, 128.26, 127.00, 126.78, 125.92, 124.18, 122.58, 120.78, 120.42, 118.45, 118.20, 115.20, 112.98, 110.91, 53.81, 45.36, 20.18; HRMS (ESI) calc. For $\text{C}_{24}\text{H}_{22}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ 368.1766, found 368.1757.

4-(1H-indol-3-yl)-3-(4-methoxybenzyl)-3,4-dihydroquinazolin-2(1H)-one (4c)

Isolated as a white solid; m.p. 128-130 °C; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 10.34 (s, 1H), 8.55 (s, 1H), 7.54 (d, $J = 7.9$ Hz, 1H), 7.38 (d, $J = 8.1$ Hz, 1H), 7.23-6.97 (m, 6H), 6.89-6.79 (m, 5H), 5.65 (s, 1H), 5.33 (d, $J = 14.9$ Hz, 1H), 3.79 (s, 3H), 3.66 (d, $J = 15.1$ Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 157.35, 152.26, 135.75, 134.82, 128.07, 127.83, 126.30, 125.45, 123.60, 122.20, 122.13, 120.25, 119.86, 117.90,

117.72, 117.14, 114.70, 112.55, 110.56, 110.49, 53.79, 53.25, 44.98; HRMS (ESI) calc. For $C_{24}H_{22}N_3O_2$ $[M + H]^+$ 384.1719, found 384.1706.

3-(2-chlorobenzyl)-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4d)

Isolated as a white solid; m.p. 220-222 °C; IR (KBr) cm^{-1} : 3450, 3192, 3118, 3052, 2913, 1658, 1603, 1467, 751; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.24 (s, 1H), 9.02 (s, 1H), 7.53 (d, $J = 7.9$ Hz, 1H), 7.40-7.30 (m, 3H), 7.23-6.88 (m, 8H), 6.81-6.73 (m, 1H), 5.70 (s, 1H), 5.21 (d, $J = 16.4$ Hz, 1H), 4.16 (d, $J = 16.6$ Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 153.48, 136.46, 135.37, 134.27, 132.60, 128.81, 127.85, 127.64, 127.26, 126.35, 126.23, 124.38, 122.91, 121.15, 121.00, 118.87, 118.54, 115.51, 113.45, 111.15, 55.48, 44.36; HRMS (ESI) calc. For $C_{23}H_{19}ClN_3O$ $[M + H]^+$ 388.1224, found 388.1211.

3-(2-bromobenzyl)-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4e)

Isolated as a white solid; m.p. 127-129 °C; IR (KBr) cm^{-1} : 3406, 3256, 3052, 2920, 1654, 1602, 1462, 745; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.37 (s, 1H), 9.02 (s, 1H), 7.59-7.44 (m, 2H), 7.41-7.35 (m, 2H), 7.23-6.85 (m, 8H), 6.80-6.70 (m, 1H), 5.66 (s, 1H), 5.26 (d, $J = 15.4$ Hz, 1H), 3.78 (d, $J = 15.4$ Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 153.39, 139.60, 136.48, 135.20, 130.16, 129.61, 129.51, 127.31, 126.37, 125.98, 124.47, 123.01, 121.88, 121.28, 121.04, 120.50, 118.96, 118.49, 115.28, 113.40, 111.23, 54.82, 45.89; HRMS (ESI) calc. For $C_{23}H_{19}BrN_3O$ $[M + H]^+$ 432.0793, found 432.0706.

3-(3-bromobenzyl)-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4f)

Isolated as a white solid; m.p. 99-101 °C; IR (KBr) cm^{-1} : 3216, 3053, 2918, 1658, 1602, 1463, 745; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.32 (s, 1H), 9.05 (s, 1H), 7.54-7.50 (m, 2H), 7.40-6.90 (m, 10H), 7.23-6.85 (m, 8H), 6.80-6.70 (m, 1H), 5.70 (s, 1H), 5.16 (d, $J = 16.8$ Hz, 1H), 4.12 (d, $J = 16.6$ Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 153.48, 136.51, 135.81, 132.15, 127.98, 127.82, 127.34, 127.02, 126.28, 124.44, 123.02, 122.63,

121.20, 120.10, 120.64, 118.93, 118.60, 115.47, 113.50, 111.21, 55.53, 46.94; HRMS (ESI) calc. For $C_{19}H_{17}N_3O$ $[M + H]^+$ 432.0726, found 432.0706.

3-(4-fluorobenzyl)-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4g)

Isolated as a white solid; m.p. 216-218 °C; IR (KBr) cm^{-1} : 3259, 3054, 2923, 1652, 1607, 1464, 741; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.40 (s, 1H), 9.07 (s, 1H), 7.51 (d, J = 7.9 Hz, 1H), 7.38 (d, J = 8.1 Hz, 1H), 7.28-6.93 (m, 8H), 6.92-6.88 (m, 1H), 6.77-6.69 (m, 1H), 5.64 (s, 1H), 5.29 (d, J = 15.2 Hz, 1H), 3.77 (d, J = 15.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 162.75, 159.51, 153.21, 136.34, 135.21, 132.61, 128.88, 128.78, 127.04, 126.12, 124.32, 122.75, 121.03, 120.73, 120.45, 118.70, 118.33, 115.24, 114.61, 114.32, 113.19, 111.07, 54.29, 45.35; HRMS (ESI) calc. For $C_{23}H_{19}FN_3O$ $[M + H]^+$ 372.1516, found 372.1506.

4-(1H-indol-3-yl)-3-(4-(trifluoromethoxy)benzyl)-3,4-dihydroquinazolin-2(1H)-one (4h)

Isolated as a white solid; m.p. 185-187 °C; IR (KBr) cm^{-1} : 3312, 3199, 3053, 2921, 1658, 1607, 1464, 1259, 1164, 745; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.32 (s, 1H), 9.07 (s, 1H), 7.54-7.50 (m, 1H), 7.45-7.18 (m, 6H), 7.14-7.04 (m, 2H), 6.80-6.72 (m, 1H), 5.67 (s, 1H), 5.18 (d, J = 16.2 Hz, 1H), 4.13 (d, J = 16.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$ +DMSO- d_6) δ : 153.46, 146.83, 136.62, 135.39, 129.72, 128.84, 127.85, 127.36, 126.55, 126.37, 124.40, 123.02, 122.94, 121.30, 121.12, 120.56, 119.91, 118.97, 118.72, 188.14, 115.57, 113.50, 111.30, 111.22, 55.60, 41.28; HRMS (ESI) calc. For $C_{24}H_{18}F_3N_3O_2$ $[M + H]^+$ 438.1428, found 438.1423.

4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4i)

Isolated as a white solid; m.p. 252-254 °C; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.18 (s, 1H), 8.60 (s, 1H), 7.51 (d, J = 7.9 Hz, 1H), 7.40 (d, J = 8.3 Hz, 1H), 7.19 (d, J = 2.4 Hz, 1H), 7.17-7.08 (m, 2H), 7.03-6.96 (m, 1H), 6.91-6.84 (m, 2H), 6.82-6.75 (m, 1H), 5.97 (s, 1H), 5.64 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 154.89, 136.60, 136.17, 127.45,

126.16, 124.75, 123.06, 121.32, 121.26, 121.09, 118.95, 118.81, 116.32, 113.69, 112.25, 50.98; ESI-MS m/z 264 $[M + H]^+$; HRMS (ESI) calc. For $C_{16}H_{14}N_3O$ $[M + H]^+$ 264.1138, found 264.1131.

4-(1H-indol-3-yl)-3-methyl-3,4-dihydroquinazolin-2(1H)-one (4j)

Isolated as a white solid; m.p. 234-236 °C; IR (KBr) cm^{-1} : 3202, 3111, 3039, 2917, 1644, 1605, 748; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.28 (s, 1H), 8.76 (s, 1H), 7.54 (d, J = 7.9 Hz, 1H), 7.37 (d, J = 8.1 Hz, 1H), 7.23 (d, J = 2.6 Hz, 1H), 7.14-6.93 (m, 4H), 7.03-6.96 (m, 1H), 6.84 (d, J = 7.9 Hz, 1H), 6.77 (t, J = 7.3 Hz, 1H), 5.97 (s, 1H), 5.75 (s, 1H), 2.90 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 152.12, 135.49, 134.92, 126.09, 125.10, 123.38, 121.91, 119.96, 119.86, 119.58, 117.46, 114.61, 112.21, 110.29, 56.66, 31.05; HRMS (ESI) calc. For $C_{17}H_{16}N_3O$ $[M + H]^+$ 278.1295, found 278.1287.

3-butyl-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4k)

Isolated as a green solid; m.p. 149-151 °C; IR (KBr) cm^{-1} : 3408, 3244, 3054, 2926, 1653, 1604, 1465, 744; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.29 (s, 1H), 8.70 (s, 1H), 7.56 (d, J = 7.9 Hz, 1H), 7.36 (d, J = 8.1 Hz, 1H), 7.23 (d, J = 2.4 Hz, 1H), 7.12-6.96 (m, 4H), 6.86-6.74 (m, 2H), 5.81 (s, 1H), 3.86-3.76 (m, 1H), 2.91-2.81 (m, 1H), 1.65-1.45 (m, 2H), 1.34-1.22 (m, 2H), 0.86 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 152.39, 135.79, 135.21, 126.37, 125.37, 123.80, 121.89, 120.36, 120.32, 119.86, 117.98, 117.84, 115.59, 112.51, 110.56, 54.69, 42.84, 28.12, 18.76, 12.68; HRMS (ESI) calc. For $C_{20}H_{22}N_3O$ $[M + H]^+$ 320.1759, found 320.1757.

4-(1H-indol-3-yl)-3-isopropyl-3,4-dihydroquinazolin-2(1H)-one (4l)

Isolated as a white solid; m.p. 198-200 °C; IR (KBr) cm^{-1} : 3281, 3047, 2967, 1645, 1605, 1453, 755; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.35 (s, 1H), 8.80 (s, 1H), 7.70 (d, J = 7.7 Hz, 1H), 7.34 (d, J = 7.9 Hz, 1H), 7.27 (d, J = 2.6 Hz, 1H), 7.13-6.98 (m, 4H), 6.87-6.74 (m, 2H), 5.84 (s, 1H), 4.47-4.34 (m, 1H), 1.23 (d, J = 6.7 Hz, 3H), 1.02 (d, J = 6.7 Hz, 3H);

^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 153.20, 135.78, 135.19, 126.52, 124.77, 123.79, 122.05, 121.17, 120.56, 120.26, 118.31, 118.11, 118.00, 112.80, 110.82, 52.08, 47.02, 20.00 19.27; HRMS (ESI) calc. For $\text{C}_{19}\text{H}_{20}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ 306.1606, found 306.1600.

3-cyclopropyl-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4m)

Isolated as a white solid; m.p. 226-228 °C; IR (KBr) cm^{-1} : 3225, 3054, 2916, 1653, 1602, 1443, 739; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 10.25 (s, 1H), 8.95 (s, 1H), 7.69 (d, $J = 7.9$ Hz, 1H), 7.35 (d, $J = 7.9$ Hz, 1H), 7.14-6.99 (m, 5H), 6.90-6.79 (m, 2H), 5.78 (s, 1H), 2.47-2.37 (m, 1H), 1.04-0.65 (m, 4H); ^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 155.01, 136.07, 135.38, 127.51, 125.51, 124.98, 122.49, 122.23, 121.02, 118.83, 118.27, 115.73, 113.38, 111.10, 56.26, 27.70, 9.97, 5.59; HRMS (ESI) calc. For $\text{C}_{19}\text{H}_{18}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ 304.1450, found 304.1444.

3-cyclohexyl-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4n)

Isolated as a white solid; m.p. 228-230 °C; IR (KBr) cm^{-1} : 3436, 3193, 3057, 2923, 1662, 1601, 1451, 747; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 10.11 (s, 1H), 8.53 (s, 1H), 7.73 (d, $J = 7.7$ Hz, 1H), 7.34 (d, $J = 7.5$ Hz, 1H), 7.25(d, $J = 2.2$ Hz, 1H), 7.19-6.99 (m, 4H), 6.84-6.76 (m, 2H), 5.85 (s, 1H), 4.18-4.05 (m, 1H), 1.90-1.49 (m, 7H), 1.08-0.81 (m, 3H); ^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 136.08, 135.46, 126.95, 124.17, 122.83, 121.33, 121.02, 120.87, 118.78, 118.57, 118.26, 113.25, 111.18, 55.38, 52.17, 30.80, 29.95, 29.09, 25.61, 25.57, 24.94; HRMS (ESI) calc. For $\text{C}_{22}\text{H}_{24}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ 346.1920, found 346.1913.

3-(furan-2-ylmethyl)-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4o)

Isolated as a white solid; m.p. 140-142 °C; IR (KBr) cm^{-1} : 3306, 3201, 3116, 3050, 2913, 1654, 1607, 1460, 746; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 10.13 (s, 1H), 8.77 (s, 1H), 7.54 (d, $J = 7.7$ Hz, 1H), 7.42-7.37 (m, 2H), 7.27 (d, $J = 2.4$ Hz, 1H), 7.16-6.96 (m, 3H), 6.94-6.81 (m, 2H), 6.78-6.70 (m, 1H), 6.35-6.29 (m, 1H), 6.27-6.21 (m, 1H), 5.82 (s, 1H), 5.26 (d, $J = 15.4$ Hz, 1H), 3.83 (d, $J = 15.6$ Hz, 1H); ^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$)

δ : 150.72, 141.72, 136.61, 135.33, 127.36, 126.50, 124.22, 13.33, 121.41, 121.15, 120.83, 119.10, 118.75, 115.45, 113.46, 111.29, 109.82, 108.09, 54.75, 39.48; HRMS (ESI) calc. For $C_{21}H_{17}N_3O_2$ $[M + H]^+$ 344.13928, found 344.13935.

4-(1H-indol-3-yl)-3-(pyridin-2-ylmethyl)-3,4-dihydroquinazolin-2(1H)-one (4p)

Isolated as a white solid; m.p. 152-154 °C; IR (KBr) cm^{-1} : 3306, 3203, 3117, 3051, 2918, 1655, 1608, 1464, 746; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 10.24 (s, 1H), 8.97 (s, 1H), 8.51 (d, $J = 4.3$ Hz, 1H), 7.62-7.51 (m, 2H), 7.31-7.26 (m, 2H), 7.21-7.04 (m, 4H), 6.99-6.87 (m, 3H), 6.79-6.72 (m, 1H), 5.85 (s, 1H), 5.24 (d, $J = 16.2$ Hz, 1H), 4.14 (d, $J = 16.0$ Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 156.60, 152.32, 147.72, 135.81, 135.27, 135.00, 126.42, 125.56, 123.66, 122.63, 120.72, 120.26, 120.13, 199.99, 119.92, 117.93, 117.84, 114.56, 112.62, 110.49, 54.96, 47.61; HRMS (ESI) calc. For $C_{22}H_{19}N_4O$ $[M + H]^+$ 355.15489, found 355.15534.

3-benzyl-4-(2-methyl-1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4q)

Isolated as a white solid; m.p. 168-170 °C; IR (KBr) cm^{-1} : 3316, 3201, 3050, 2917, 1654, 1606, 1466, 753; 1H NMR (500 MHz, $CDCl_3$ +DMSO- d_6) δ : 9.61 (s, 1H), 8.45 (s, 1H), 7.42-7.38 (m, 1H), 7.30-7.18 (m, 6H), 7.08-7.01 (m, 2H), 6.96-6.92 (m, 1H), 6.82 (d, $J = 8.5$ Hz, 1H), 6.71-6.64 (m, 2H), 5.76 (s, 1H), 5.38 (d, $J = 15.4$ Hz, 1H), 3.63 (d, $J = 15.4$ Hz, 1H), 2.20 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 152.62, 136.45, 135.04, 134.68, 132.50, 127.97, 126.66, 126.55, 125.98, 125.83, 125.31, 120.18, 119.94, 119.67, 118.00, 117.26, 112.62, 110.37, 109.67, 52.55, 45.27, 10.37; HRMS (ESI) calc. For $C_{24}H_{21}N_3O$ $[M + H]^+$ 339.1492, found 339.1480.

3-benzyl-4-(5-methyl-1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4r)

Isolated as a white solid; m.p. 191-193 °C; IR (KBr) cm^{-1} : 3286, 3035, 2921, 1642, 1607, 1464, 748; 1H NMR (400 MHz, $CDCl_3$) δ : 8.12 (s, 1H), 7.34-7.23 (m, 7H), 7.13-7.06 (m, 2H), 7.03-7.00 (m, 1H), 6.91-6.87 (m, 1H), 6.82-6.75 (m, 2H), 5.69 (s, 1H), 5.45 (d, $J = 15.4$

Hz, 1H), 3.79 (d, $J = 15.5$ Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 152.67, 136.32, 134.81, 134.11, 127.28, 126.82, 126.54, 125.96, 125.50, 124.07, 122.44, 122.09, 120.17, 117.26, 114.16, 112.72, 110.39, 53.63, 45.38, 20.43; HRMS (ESI) calc. For $\text{C}_{24}\text{H}_{22}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ 368.17645, found 368.17574.

3-benzyl-4-(5-methoxy-1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4s)

Isolated as a white solid; m.p. 138-140 °C; IR (KBr) cm^{-1} : 3218, 3052, 2923, 1656, 1603, 1459, 752; ^1H NMR (300 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 10.19 (s, 1H), 9.12 (s, 1H), 7.37-7.23 (m, 6H), 7.20-7.15 (m, 1H), 7.12-7.02 (m, 1H), 7.00-6.95 (m, 1H), 6.93-6.83 (m, 2H), 6.82-6.73 (m, 2H), 5.61 (s, 1H), 5.38 (d, $J = 15.4$ Hz, 1H), 3.89-3.66 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ : 154.45, 154.28, 137.10, 135.37, 134.44, 131.62, 129.72, 128.96, 128.56, 128.04, 127.96, 127.31, 126.93, 125.73, 123.63, 122.10, 121.14, 116.56, 113.75, 112.07, 100.95, 55.63, 54.54, 46.94; HRMS (ESI) calc. For $\text{C}_{24}\text{H}_{21}\text{N}_3\text{O}_2$ $[\text{M} + \text{H}]^+$ 384.17108, found 384.18323.

3-benzyl-4-(5-bromo-1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4t)

Isolated as a white solid; m.p. 236-238 °C; IR (KBr) cm^{-1} : 3226, 3036, 2894, 1639, 1605, 1465, 748; ^1H NMR (500 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 10.54 (s, 1H), 8.95 (s, 1H), 7.58 (s, 1H), 7.33-7.16 (m, 8H), 7.08 (t, $J = 7.6$ Hz, 1H), 6.90 (d, $J = 8.0$ Hz, 1H), 6.83 (d, $J = 7.7$ Hz, 1H), 6.75 (t, $J = 7.4$ Hz, 1H), 5.60 (s, 1H), 5.37 (d, $J = 15.4$ Hz, 1H), 3.73 (d, $J = 15.2$ Hz, 1H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 152.76, 136.37, 135.12, 134.82, 127.73, 127.52, 126.94, 126.83, 126.23, 125.81, 125.76, 124.03, 123.44, 120.47, 119.87, 114.83, 113.04, 112.55, 111.49, 53.75, 45.67; HRMS (ESI) calc. For $\text{C}_{23}\text{H}_{18}\text{BrN}_3\text{O}$ $[\text{M} + \text{H}]^+$ 339.1492, found 339.1480.

3-benzyl-4-(5-nitro-1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4u)

Isolated as a yellow solid; m.p. 265-267 °C; IR (KBr) cm^{-1} : 3393, 3201, 3125, 3064, 2920, 1661, 1602, 1331, 745; ^1H NMR (300 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 11.25 (s, 1H), 9.23 (s,

1H), 8.01 (dd, $J = 9.0, 2.0$ Hz, 1H), 7.51-7.41 (m, 2H), 7.36-7.23 (m, 6H), 7.15-7.06 (m, 1H), 7.01-6.93 (m, 1H), 6.89-6.73 (m, 2H), 5.67 (s, 1H), 5.38 (d, $J = 15.4$ Hz, 1H), 3.76 (d, $J = 15.4$ Hz, 1H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 152.35, 139.93, 139.03, 136.04, 134.96, 127.25, 126.84, 126.49, 125.97, 125.89, 125.47, 122.95, 120.25, 119.27, 117.51, 115.84, 115.07, 112.92, 110.84, 53.34, 45.60; HRMS (ESI) calc. For $\text{C}_{23}\text{H}_{18}\text{N}_4\text{O}_3$ $[\text{M} + \text{H}]^+$ 399.14925, found 399.14802.

3-benzyl-4-(7-methyl-1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4v)

Isolated as a white solid; m.p. 222-224 °C; IR (KBr) cm^{-1} : 3419, 3192, 3052, 2915, 1661, 1603, 1463, 756; ^1H NMR (300 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 10.27 (s, 1H), 8.98 (s, 1H), 7.30-7.10 (m, 7H), 7.03-6.92 (m, 1H), 6.89-6.72 (m, 4H), 6.71-6.58 (m, 1H), 5.56 (s, 1H), 5.28 (d, $J = 15.2$ Hz, 1H), 3.66 (d, $J = 15.2$ Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 152.04, 136.10, 135.02, 134.60, 126.98, 126.16, 125.62, 125.25, 123.05, 121.89, 120.61, 119.72, 119.60, 117.95, 115.01, 114.83, 112.35, 53.52, 44.96, 15.39; HRMS (ESI) calc. For $\text{C}_{24}\text{H}_{21}\text{N}_3\text{O}$ $[\text{M} + \text{Na}]^+$ 390.15815, found 390.15768.

3-benzyl-4-(1H-indol-3-yl)-1-methyl-3,4-dihydroquinazolin-2(1H)-one (4w)

Isolated as a white solid; m.p. 188-190 °C; IR (KBr) cm^{-1} : 3286, 3029, 2923, 1635, 1598, 1458, 757; ^1H NMR (400 MHz, CDCl_3) δ : 8.20 (s, 1H), 7.48-7.45 (m, 1H), 7.36-7.15 (m, 8H), 7.10-7.05 (m, 2H), 7.01-6.92 (m, 2H), 6.86 (td, $J = 7.4, 0.8$ Hz, 1H), 5.66 (s, 1H), 5.45 (d, $J = 15.4$ Hz, 1H), 3.88 (d, $J = 15.4$ Hz, 1H), 3.53 (s, 3H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 152.28, 136.48, 135.60, 127.13, 126.68, 126.25, 125.80, 125.26, 123.57, 122.09, 121.98, 120.39, 120.20, 119.95, 117.18, 113.95, 111.53, 110.53, 110.61, 53.06, 46.80, 29.01; HRMS (ESI) calc. For $\text{C}_{24}\text{H}_{21}\text{N}_3\text{O}$ $[\text{M} + \text{Na}]^+$ 390.15828, found 390.15768.

1-allyl-3-benzyl-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4x)

Isolated as a white solid; m.p. 198-200 °C; ¹H NMR (500 MHz, CDCl₃) δ: 8.31 (s, 1H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.35-7.23 (m, 6H), 7.21-7.13 (m, 3H), 7.10-7.04 (m, 2H), 7.01-6.97 (m, 1H), 6.94-6.91 (m, 1H), 6.83 (td, *J* = 7.3, 0.7 Hz, 1H), 6.07-5.98 (m, 1H), 5.66 (s, 1H), 5.48 (d, *J* = 15.4 Hz, 1H), 5.33-5.24 (m, 2H), 4.82-4.66 (m, 2H), 3.86 (d, *J* = 15.4 Hz, 1H); ¹³C NMR (75 MHz, CDCl₃+DMSO-*d*₆) δ: 152.79, 136.36, 135.86, 135.72, 132.36, 127.41, 126.66, 126.53, 126.09, 125.75, 123.91, 122.25, 122.20, 120.69, 120.53, 118.19, 117.53, 115.25, 114.37, 112.57, 110.84, 53.27, 47.04, 44.31; HRMS (ESI) calc. For C₂₆H₂₃N₃O [M + H]⁺ 394.17641, found 394.17574.

1,3-dibenzyl-4-(1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4y)

Isolated as a white solid; m.p. 101-103 °C; IR (KBr) cm⁻¹: 3408, 3268, 3028, 2922, 1637, 1600, 1451, 745; ¹H NMR (400 MHz, CDCl₃) δ: 8.19 (s, 1H), 7.54-7.45 (m, 1H), 7.42-7.23 (m, 11H), 7.22-7.16 (m, 1H), 7.12-6.95 (m, 4H), 6.88-6.77 (m, 2H), 5.72 (s, 1H), 5.53 (d, *J* = 15.4 Hz, 1H), 5.46-5.25 (m, 2H), 3.91 (d, *J* = 15.2 Hz, 1H); ¹³C NMR (75 MHz, CDCl₃+DMSO-*d*₆) δ: 152.86, 136.62, 136.26, 135.74, 135.59, 127.27, 126.49, 126.30, 125.91, 125.74, 125.61, 125.31, 123.69, 122.20, 121.91, 120.49, 120.34, 118.01, 117.40, 114.20, 112.39, 110.62, 53.28, 46.99, 45.28; HRMS (ESI) calc. For C₃₀H₂₅N₃O [M + Na]⁺ 466.18990, found 466.18998.

3-benzyl-4-(1-methyl-1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4z)

Isolated as a white solid; m.p. 157-159 °C; ¹H NMR (400 MHz, CDCl₃) δ: 7.99 (s, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.35-7.28 (m, 5H), 7.12-7.04 (m, 1H), 7.02 (s, 1H), 6.94-6.89 (m, 1H), 6.82-6.75 (m, 2H), 5.72 (s, 1H), 5.44 (d, *J* = 15.4 Hz, 1H), 3.85 (d, *J* = 15.4 Hz, 1H), 3.74 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ: 154.49, 137.26, 137.22, 135.37, 128.54, 127.94, 127.33, 127.23, 126.73, 125.88, 121.99, 121.96, 121.57, 119.74, 119.26, 115.45, 113.90, 109.45, 54.44, 47.10, 32.79; HRMS (ESI) calc. For C₂₄H₂₁N₃O [M + Na]⁺ 390.15841, found 390.15768.

3-(4-methoxybenzyl)-4-(1-methyl-1H-indol-3-yl)-3,4-dihydroquinazolin-2(1H)-one (4za)

Isolated as a white solid; m.p. 202-204 °C; IR (KBr) cm^{-1} : 3198, 3053, 2918, 1661, 1605, 1462, 1243, 745; ^1H NMR (400 MHz, CDCl_3) δ : 7.60-7.53 (m, 2H), 7.30-7.28 (m, 1H), 7.24-7.19 (m, 3H), 7.09 (t, $J = 7.4$ Hz, 2H), 7.02 (s, 1H), 6.92 (d, $J = 7.3$ Hz, 1H), 6.88-6.83 (m, 2H), 6.81-6.73 (m, 2H), 5.67 (s, 1H), 5.37 (d, $J = 15.1$ Hz, 1H), 3.81-3.73 (m, 7H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 158.27, 153.42, 136.77, 135.34, 128.94, 128.81, 128.72, 127.20, 126.77, 126.13, 125.17, 123.35, 120.87, 119.00, 118.79, 115.07, 113.35, 108.97, 54.68, 53.67, 45.62, 32.24; HRMS (ESI) calc. For $\text{C}_{25}\text{H}_{23}\text{N}_3\text{O}_2$ $[\text{M} + \text{H}]^+$ 398.18738, found 398.18630.

3-benzyl-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6a)

Isolated as a white solid; m.p. 133-135 °C; IR (KBr) cm^{-1} : 3597, 3327, 3061, 2922, 1647, 1605, 1473, 749; ^1H NMR (300 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 9.37 (s, 1H), 8.74-8.57 (m, 1H), 8.00-7.62 (m, 3H), 7.32-6.48 (m, 12H), 5.42-5.00 (m, 1H), 3.61-3.41 (m, 1H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 152.75, 136.67, 129.05, 128.18, 127.69, 127.07, 126.92, 126.55, 125.70, 125.49, 125.33, 122.04, 121.42, 120.31, 119.79, 117.01, 116.74, 112.52, 52.31, 45.93; HRMS (ESI) calc. For $\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_2\text{Na}$ $[\text{M} + \text{Na}]^+$ 403.1410, found 403.1417.

4-(2-hydroxynaphthalen-1-yl)-3-(4-methylbenzyl)-3,4-dihydroquinazolin-2(1H)-one (6b)

Isolated as a white solid; m.p. 122-124 °C; IR (KBr) cm^{-1} : 3215, 3052, 2920, 1651, 1604, 1466, 748; ^1H NMR (400 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 8.90 (s, 1H), 8.07-7.60 (m, 4H), 7.50-7.28 (m, 2H), 7.23-6.90 (m, 6H), 6.77-6.48 (m, 3H), 5.35 (d, $J = 14.7$ Hz, 1H), 3.45 (d, $J = 15.0$ Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 153.22, 135.60, 134.14, 129.63, 129.12, 128.84, 128.43, 128.15, 127.85, 127.08, 126.22, 125.99, 122.73, 122.04, 121.00, 120.53, 120.32, 118.81, 117.25, 112.98, 52.91, 46.31, 45.98, 20.54; HRMS (ESI) calc. For $\text{C}_{26}\text{H}_{23}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 395.1598, found 395.1597.

3-(4-(tert-butyl)benzyl)-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6c)

Isolated as a white solid; m.p. 196-198 °C; IR (KBr) cm^{-1} : 3216, 2957, 1638, 1604, 1496, 1469, 1286, 748; ^1H NMR (300 MHz, CDCl_3 +DMSO- d_6) δ : 9.51-9.31 (m, 1H), 8.78-8.64 (m, 1H), 8.00-7.61 (m, 3H), 7.43-6.47 (m, 12H), 5.38-4.84 (m, 1H), 3.70-3.38 (m, 1H), 1.33-1.24 (m, 9H); ^{13}C NMR (75 MHz, CDCl_3 +DMSO- d_6) δ : 153.18, 148.84, 135.42, 134.24, 133.98, 131.80, 129.67, 129.24, 127.55, 127.11, 126.85, 126.24, 125.97, 125.54, 124.64, 124.24, 122.84, 122.03, 121.93, 121.01, 120.54, 120.35, 118.82, 117.92, 117.24, 113.02, 112.66, 53.26, 46.58, 46.12, 33.80, 30.85, 21.73, 13.54; HRMS (ESI) calc. For $\text{C}_{29}\text{H}_{29}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 437.2211, found 437.2223.

4-(2-hydroxynaphthalen-1-yl)-3-(4-methoxybenzyl)-3,4-dihydroquinazolin-2(1H)-one (6d)

Isolated as a white solid; m.p. 136-138 °C; IR (KBr) cm^{-1} : 3217, 3056, 2925, 1653, 1604, 1511, 1465, 1244, 748; ^1H NMR (500 MHz, CDCl_3) δ : 8.75 (s, 1H), 8.00-7.63 (m, 4H), 7.46-7.32 (m, 1H), 7.20-6.92 (m, 4H), 6.86-6.63 (m, 5H), 6.50 (s, 1H), 5.35 (d, $J = 15.1$ Hz, 1H), 3.79 (s, 3H), 3.45 (d, $J = 14.9$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3 +DMSO- d_6) δ : 157.95, 157.65, 152.99, 135.29, 131.53, 1129.35, 128.98, 128.75, 128.66, 128.54, 127.96, 126.82, 126.61, 126.53, 125.88, 125.66, 122.48, 121.76, 120.63, 120.24, 119.94, 117.33, 117.04, 113.20, 113.02, 112.85, 112.75, 112.57, 112.35, 54.37, 52.48, 45.72; HRMS (ESI) calc. For $\text{C}_{26}\text{H}_{23}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 411.1700, found 411.1703.

4-(2-hydroxynaphthalen-1-yl)-3-(3,4,5-trimethoxybenzyl)-3,4-dihydroquinazolin-2(1H)-one (6e)

Isolated as a white solid; m.p. 142-144 °C; ^1H NMR (500 MHz, CDCl_3) δ : 8.71 (s, 1H), 8.00-7.65 (m, 4H), 7.49-7.31 (m, 2H), 7.11-6.97 (m, 2H), 6.89-6.84 (m, 3H), 6.50-6.18 (m, 2H), 5.27 (d, $J = 13.8$ Hz, 1H), 3.86-3.54 (m, 10H); ^{13}C NMR (100 MHz, CDCl_3) δ : 154.70,

152.97, 137.02, 135.40, 132.97, 132.33, 130.15, 128.84, 128.41, 127.79, 126.97, 126.15, 122.78, 122.00, 121.16, 120.43, 119.08, 118.16, 113.62, 106.59, 105.62, 60.73, 56.10, 55.79, 53.93, 48.14; HRMS (ESI) calc. For $C_{28}H_{27}N_2O_5$ $[M + H]^+$ 471.1907, found 471.1914.

3-(2-bromobenzyl)-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6f)

Isolated as a white solid; m.p. 162-164 °C; IR (KBr) cm^{-1} : 3220, 3056, 2920, 1653, 1603, 1466, 1436, 743; 1H NMR (300 MHz, $CDCl_3$) δ : 8.19-7.86 (m, 1H), 7.80-7.52 (m, 3H), 7.47-6.94 (m, 9H), 6.88-6.52 (m, 4H), 5.36-5.18 (m, 1H), 3.82 (d, J = 15.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 152.98, 135.11, 135.03, 131.15, 130.93, 129.06, 127.71, 127.34, 126.89, 126.61, 126.26, 125.48, 125.29, 121.95, 121.60, 121.34, 120.43, 119.61, 116.66, 116.54, 112.68, 52.67, 46.17; HRMS (ESI) calc. For $C_{25}H_{20}N_2O_2BrNa$ $[M + Na]^+$ 481.0511, found 481.0522.

3-(4-fluorobenzyl)-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6g)

Isolated as a white solid; m.p. 223-225 °C; IR (KBr) cm^{-1} : 3218, 3055, 2921, 1651, 1603, 1510, 1466, 747; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 9.60-9.49 (m, 1H), 9.20-8.56 (m, 1H), 7.93-7.63 (m, 3H), 7.46-6.45 (m, 12H), 5.27-4.85 (m, 1H), 3.66-3.45 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 153.31, 135.41, 133.02, 131.77, 129.72, 129.61, 129.50, 129.38, 128.78, 128.18, 127.13, 126.12, 125.93, 122.77, 122.04, 121.04, 120.50, 117.17, 114.55, 114.11, 113.83, 112.95, 114.31, 52.94, 46.12; HRMS (ESI) calc. For $C_{25}H_{20}N_2O_2F$ $[M + H]^+$ 399.1504, found 399.1504.

4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6h)

Isolated as a white solid; m.p. 193-195 °C; IR (KBr) cm^{-1} : 3769, 3413, 2923, 2856, 1658, 1389, 1254, 1094, 742; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 9.51 (s, 1H), 8.77 (s, 1H), 7.95 (s, 1H), 7.76-7.66 (m, 2H), 7.28-6.57 (m, 8H), 5.65 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 152.80, 135.98, 131.29, 128.82, 127.51, 126.48, 124.73, 121.30,

120.56, 120.37, 117.27, 112.85, 48.48; HRMS (ESI) calc. For $C_{18}H_{13}N_2O_2$ $[M + H]^+$ 289.0963, found 289.0971.

4-(2-hydroxynaphthalen-1-yl)-3-methyl-3,4-dihydroquinazolin-2(1H)-one (6i)

Isolated as a white solid; m.p. 222-224 °C; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 9.62-9.35 (m, 1H), 8.84-8.61 (m, 1H), 7.89-7.54 (m, 3H), 7.37-6.97 (m, 4H), 6.89-6.60 (m, 4H), 2.70 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 153.24, 136.52, 131.54, 129.50, 128.68, 128.09, 127.06, 125.83, 122.59, 121.97, 120.87, 120.48, 117.21, 116.95, 112.91, 55.07, 31.12; HRMS (ESI) calc. For $C_{19}H_{15}N_2O_2$ $[M + H]^+$ 303.1125, found 303.1128.

3-ethyl-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6j)

Isolated as a white solid; m.p. 174-176 °C; IR (KBr) cm^{-1} : 3218, 1643, 1603, 1469, 747; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 9.61-9.20 (m, 1H), 8.57-8.40 (m, 1H), 7.96-7.77 (m, 1H), 7.72-7.55 (m, 2H), 7.38-7.10 (m, 3H), 7.07-6.89 (m, 2H), 6.82-6.61 (m, 3H), 3.73-3.56 (m, 1H), 2.78-2.68 (m, 1H), 1.01 (t, $J = 6.9$ Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 152.57, 151.69, 135.22, 131.01, 128.67, 127.90, 127.41, 126.25, 125.09, 124.87, 122.20, 121.17, 119.85, 116.80, 116.55, 112.09, 51.60, 37.61, 10.78; HRMS (ESI) calc. For $C_{20}H_{16}N_2O_2Na$ $[M + Na]^+$ 339.1098, found 339.1104.

3-butyl-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6k)

Isolated as a yellow solid; m.p. 156-158 °C; IR (KBr) cm^{-1} : 3216, 2955, 2926, 2868, 1642, 1603, 1466, 745; 1H NMR (300 MHz, $CDCl_3$ +DMSO- d_6) δ : 9.61-9.20 (m, 1H), 8.67-8.35 (m, 1H), 7.95-7.55 (m, 3H), 7.41-6.93 (m, 5H), 6.83-6.59 (m, 3H), 3.77-3.51 (m, 1H), 2.65-2.54 (m, 1H), 1.64-1.50 (m, 1H), 1.32-1.12 (m, 3H), 0.77 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO- d_6) δ : 153.34, 153.15, 135.64, 129.64, 128.86, 128.21, 127.14, 126.17, 125.95, 123.10, 122.12, 121.01, 120.79, 117.61, 117.26, 112.89, 52.95, 43.59, 28.10, 19.53, 13.34; HRMS (ESI) calc. For $C_{22}H_{21}N_2O_2$ $[M + H]^+$ 345.1593, found 345.1597.

3-cyclopropyl-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6l)

Isolated as a white solid; m.p. 152-154 °C; IR (KBr) cm^{-1} : 3240, 2926, 2853, 1645, 1603, 1461, 746; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 9.60 (s, 1H), 9.11-8.76 (m, 1H), 8.49-7.49 (m, 3H), 7.37-6.60 (m, 7H), 2.15-1.86 (m, 1H), 0.92-0.62 (m, 3H), 0.40-0.17 (m, 1H); ^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 155.01154.26, 135.81, 132.49, 128.84, 128.14, 127.60, 126.60, 126.24, 125.19, 121.69, 120.80, 120.44, 120.22, 118.71, 118.42, 117.40, 112.71, 55.28, 26.96, 9.55, 8.90, 5.26, 4.96; HRMS (ESI) calc. For $\text{C}_{21}\text{H}_{19}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 331.1436, found 331.1441.

3-cyclohexyl-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6m)

Isolated as a yellow solid; m.p. 155-157 °C; IR (KBr) cm^{-1} : 3240, 2926, 2853, 1645, 1603, 1490, 1461, 1377, 1289, 746; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 9.54-9.32 (m, 1H), 8.40-8.29 (m, 1H), 8.11-7.52 (m, 3H), 7.39-6.58 (m, 7H), 3.85-3.39 (m, 1H), 2.15-0.67 (m, 10H); ^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 154.69, 152.59, 151.69, 135.07, 131.93, 129.13, 128.78, 128.62, 128.34, 128.07, 126.80, 126.58, 125.85, 125.05, 124.97, 123.01, 121.88, 121.64, 121.12, 121.03, 120.65, 120.32, 120.04, 118.70, 117.21, 112.52, 112.27, 57.22, 52.54, 29.79, 29.61, 29.07, 28.96, 25.29, 24.85; HRMS (ESI) calc. For $\text{C}_{24}\text{H}_{23}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 371.1753, found 371.1754.

4-(2-hydroxynaphthalen-1-yl)-1-methyl-3,4-dihydroquinazolin-2(1H)-one (6n)

Isolated as a white solid; m.p. 212-214 °C; ^1H NMR (400 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 9.86 (s, 1H), 7.98-7.67 (m, 3H), 7.37-7.14 (m, 4H), 7.02-6.91 (m, 1H), 6.88-6.68 (m, 2H), 6.64-6.44 (m, 2H), 3.40 (s, 3H); ^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 153.37, 152.69, 137.56, 130.91, 128.51, 127.14, 126.35, 124.15, 120.89, 120.10, 116.82, 112.22, 47.18, 27.99; HRMS (ESI) calc. For $\text{C}_{19}\text{H}_{17}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 305.1276, found 305.1284.

1-hexyl-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6o)

Isolated as a white solid; m.p. 223-225 °C; IR (KBr) cm^{-1} : 3331, 2956, 2928, 2849, 1662, 1467, 746; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$) δ : 9.48 (s, 1H), 7.95 (s, 1H), 7.77-7.66

(m, 2H), 7.38-7.13 (m, 4H), 6.99-6.90 (m, 1H), 6.84-6.69 (m, 2H), 5.69 (s, 1H), 4.11-3.88 (m, 2H), 1.84-1.70 (m, 2H), 1.49-1.33 (m, 6H), 0.92 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 153.72, 137.39, 131.88, 129.80, 128.13, 127.34, 125.77, 122.07, 121.23, 112.44, 41.59, 31.11, 29.09, 26.87, 26.10, 22.11, 13.57; HRMS (ESI) calc. For $\text{C}_{24}\text{H}_{27}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 375.2057, found 375.2067.

1-allyl-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6p)

Isolated as a white solid; m.p. 215-217 °C; IR (KBr) cm^{-1} : 3222, 2924, 1660, 1600, 1469, 1437, 1293, 751; ^1H NMR (300 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 9.47 (s, 1H), 8.05-7.89 (m, 1H), 7.78-7.67 (m, 2H), 7.35-7.10 (m, 4H), 6.98-6.58 (m, 4H), 6.09-5.92 (m, 1H), 5.76 (s, 1H), 5.43-5.19 (m, 2H), 4.80-4.53 (m, 2H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 153.23, 153.03, 136.83, 132.57, 131.25, 128.87, 127.50, 126.44, 124.85, 121.28, 120.46, 117.26, 114.88, 112.37, 47.76, 43.16; HRMS (ESI) calc. For $\text{C}_{21}\text{H}_{19}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 331.1430, found 331.1441.

1-benzyl-4-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinazolin-2(1H)-one (6q)

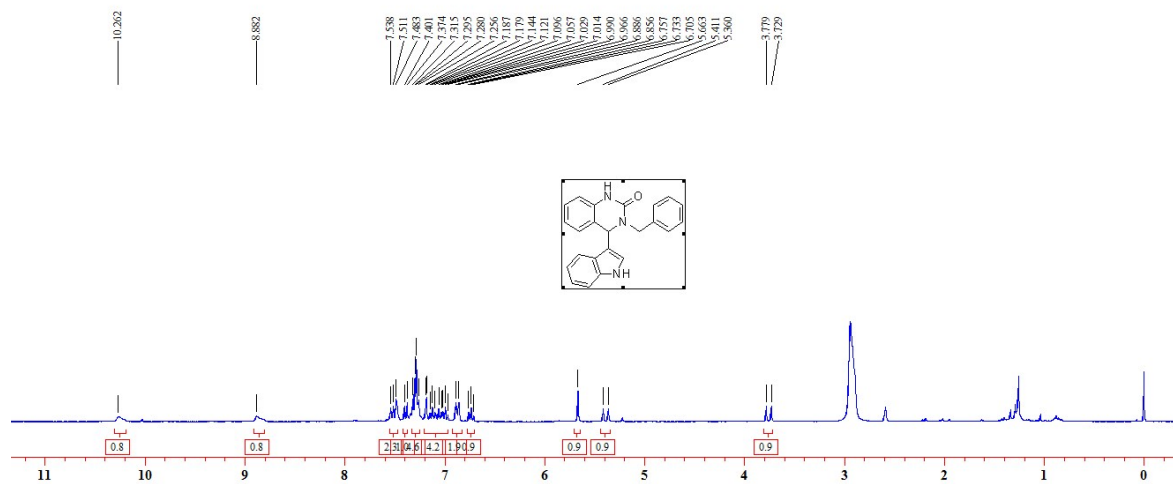
Isolated as a white solid; m.p. 112-114 °C; ^1H NMR (300 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 9.54 (s, 1H), 8.05-7.67 (m, 3H), 7.48-7.19 (m, 7H), 7.08-6.62 (m, 4H), 5.86 (s, 1H), 5.27 (dd, $J = 41.1, 25.1$ Hz, 2H); ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$) δ : 153.60, 137.35, 131.87, 129.52, 128.11, 127.08, 126.35, 126.06, 125.60, 123.42, 121.93, 121.18, 117.93, 113.06, 48.48, 44.91; HRMS (ESI) calc. For $\text{C}_{25}\text{H}_{19}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 379.1439, found 379.1441.

3-benzyl-4-(1H-pyrrol-2-yl)-3,4-dihydroquinazolin-2(1H)-one (8)

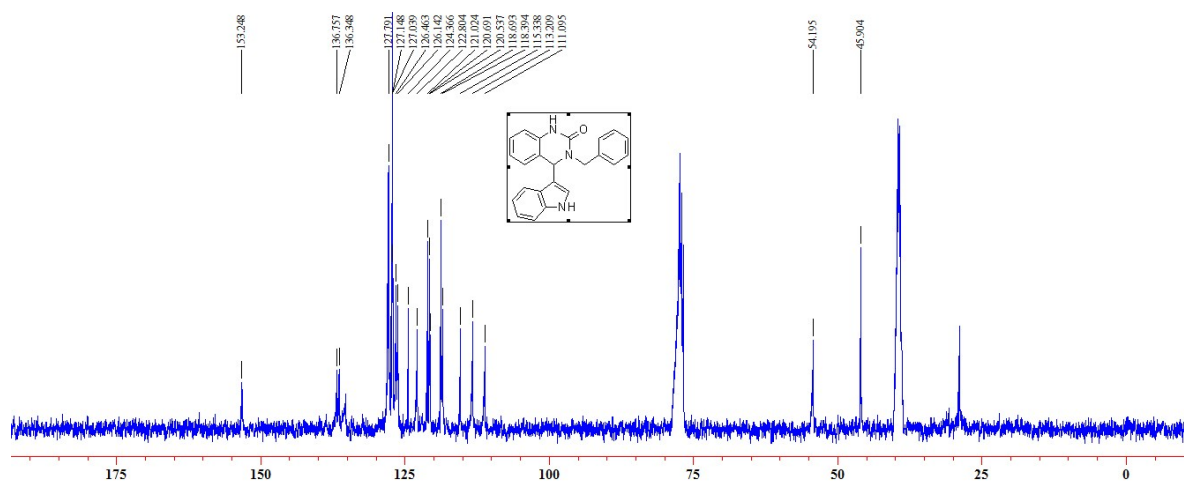
Isolated as a white solid; m.p. 113-115 °C; IR (KBr) cm^{-1} : 3251, 3119, 3056, 2921, 2852, 1654, 1604, 1468; ^1H NMR (500 MHz, CDCl_3) δ : 8.58-8.43 (m, 2H), 7.35-7.23 (m, 5H), 7.12-7.04 (m, 1H), 6.91-6.81 (m, 2H), 6.77-6.72 (m, 1H), 6.64-6.58 (m, 1H), 6.18-6.13 (m, 1H), 6.11-6.07 (m, 1H), 5.42 (s, 1H), 5.26 (d, $J = 15.2$ Hz, 1H), 3.82 (d, $J = 15.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 154.48, 136.64, 135.20, 130.80, 128.59, 128.32, 127.70, 127.32,

127.06, 122.17, 119.82, 119.49, 114.29, 108.20, 107.48, 55.65, 46.88; HRMS (ESI) calc. For $\text{C}_{25}\text{H}_{19}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 379.1439, found 379.1441; HRMS (ESI) calc. For $\text{C}_{19}\text{H}_{17}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ 304.14458, found 304.14444.

¹H & ¹³C NMR spectra of 4a

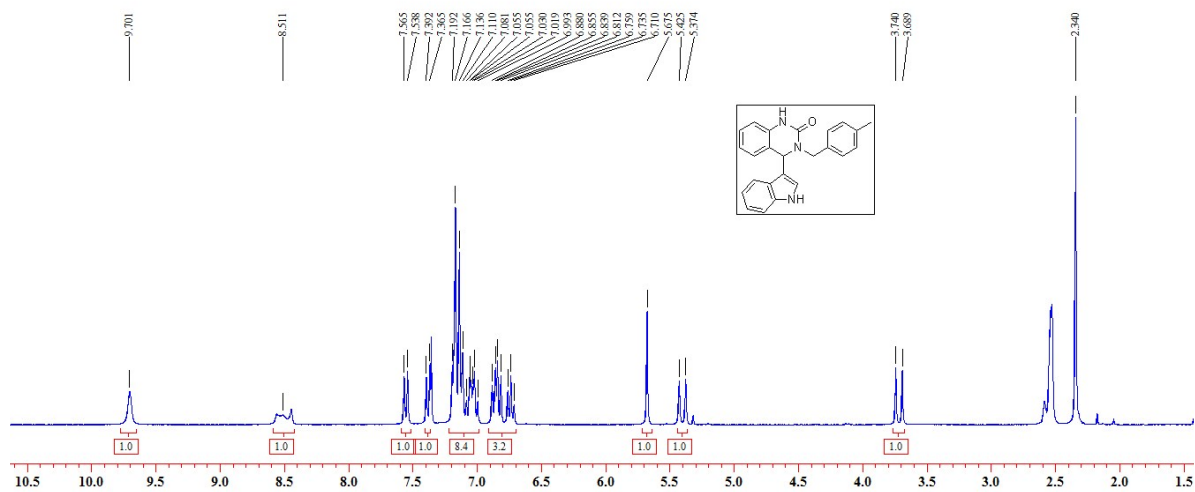


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

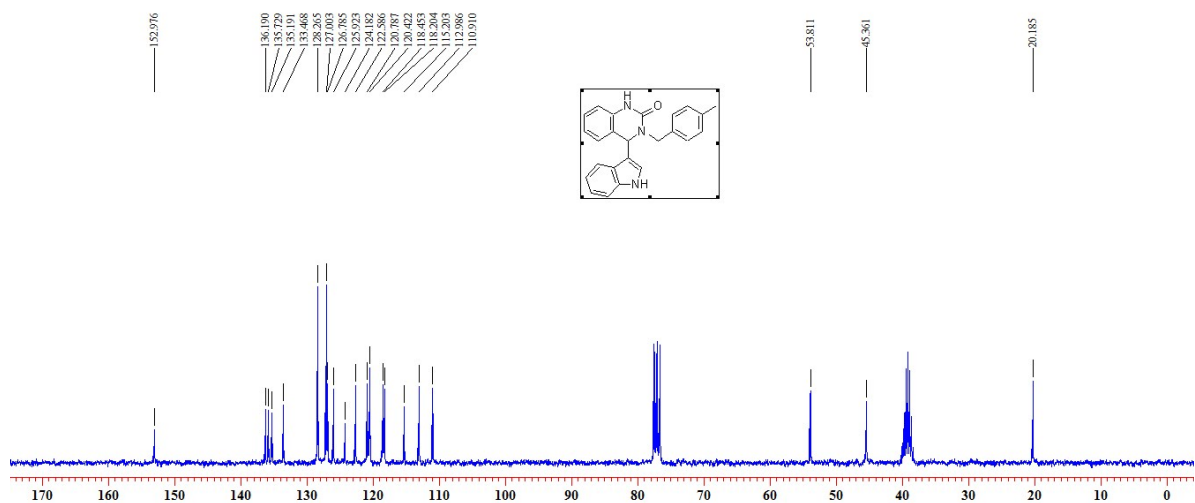


¹³C NMR (100 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4b

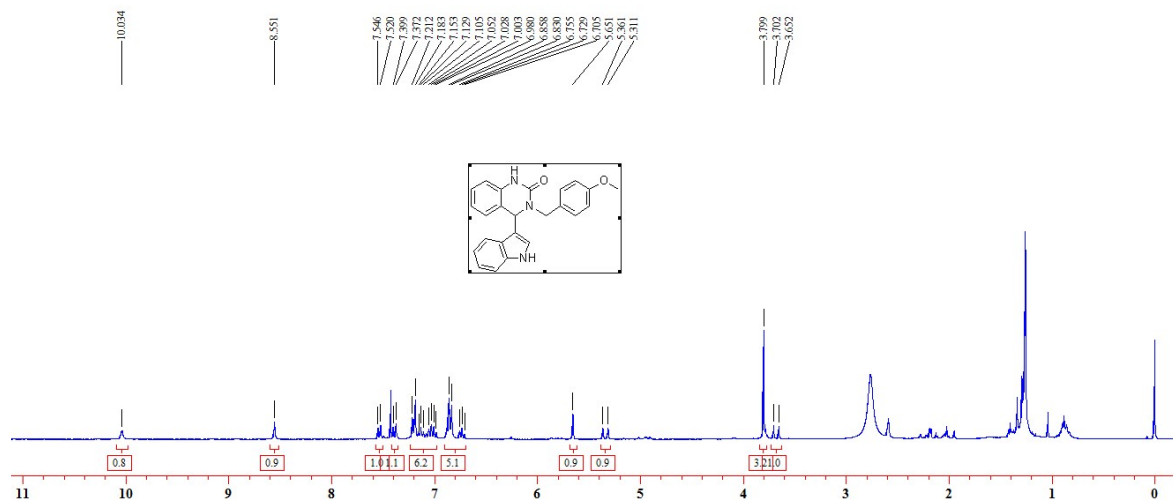


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

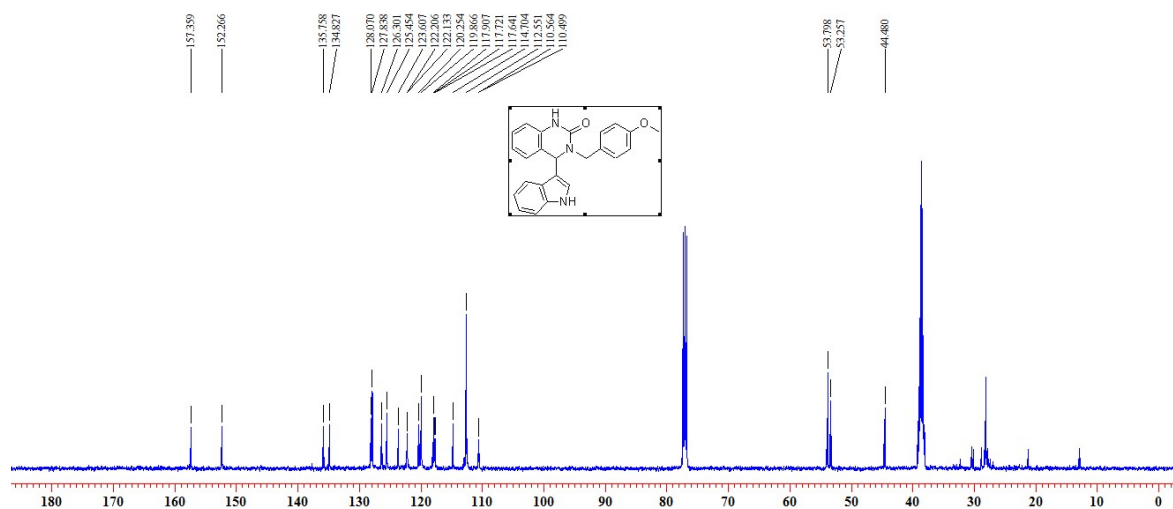


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4c



¹H NMR (300 MHz, CDCl₃+DMSO-d₆)



¹³C NMR (125 MHz, CDCl₃+DMSO-d₆)

Chemical structure of compound 10 is shown in the center of the spectrum. The structure is a complex molecule featuring a central nitrogen atom bonded to a phenyl ring, a benzimidazole ring, and a 2-chlorophenyl ring. The nitrogen atom is also bonded to a carbonyl group (C=O).

Key peaks in the ^{13}C NMR spectrum are labeled with their chemical shifts (ppm):

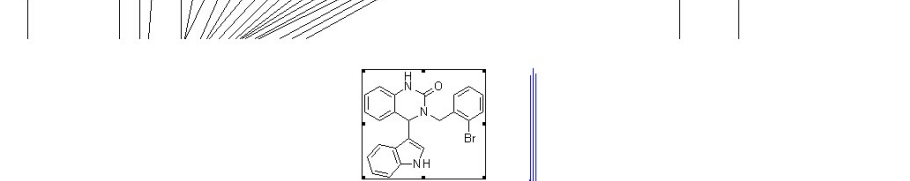
- 153.481
- 136.465
- 135.371
- 134.699
- 132.609
- 128.813
- 127.856
- 127.606
- 126.544
- 126.325
- 124.866
- 122.916
- 121.158
- 121.003
- 118.875
- 118.549
- 115.514
- 113.451
- 111.155
- 77.000 (solvent)
- 55.480
- 44.392

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Chemical structure of compound 10: O=C1N(c2ccccc2)c3ccccc3N1Cc4ccc(Br)cc4

¹H NMR spectrum (CDCl₃):

Chemical Shift (ppm)	Integration
10.379	0.9
9.027	0.9
7.548	1.8
7.535	2.5
7.521	8.0
7.508	1.0
7.495	
7.480	
7.375	
7.356	
7.192	
7.174	
7.115	
7.091	
7.068	
7.045	
6.970	0.9
6.954	0.9
6.908	
6.883	
6.861	
6.840	
6.743	
6.719	
5.666	
5.287	
5.235	
3.808	1.0
3.757	

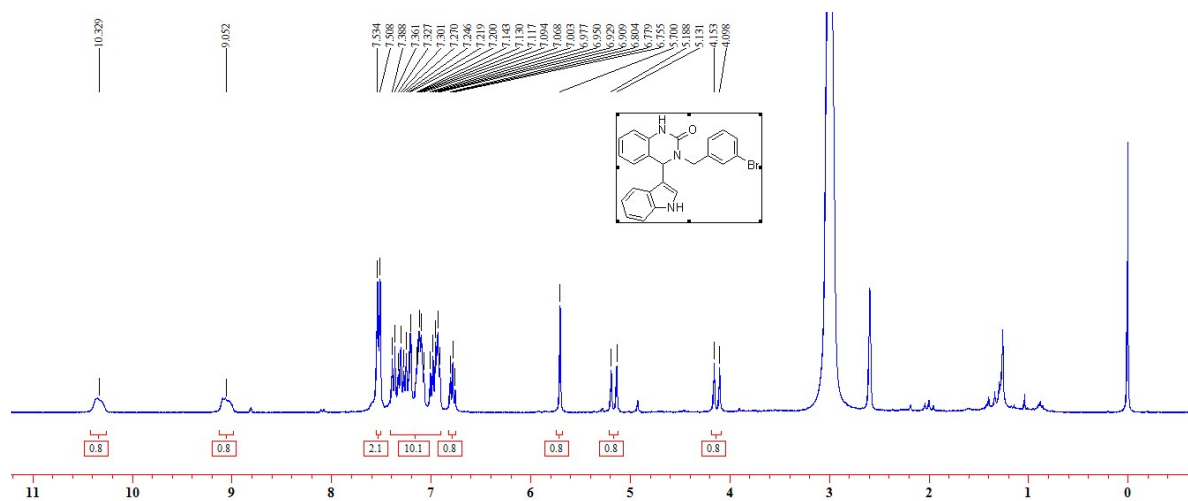


153.393
139.608
136.468
135.200
130.168
129.619
129.517
127.310
126.512
125.982
124.475
123.010
121.881
121.579
121.044
120.598
118.963
118.496
117.588
113.408
111.288
54.821
45.892

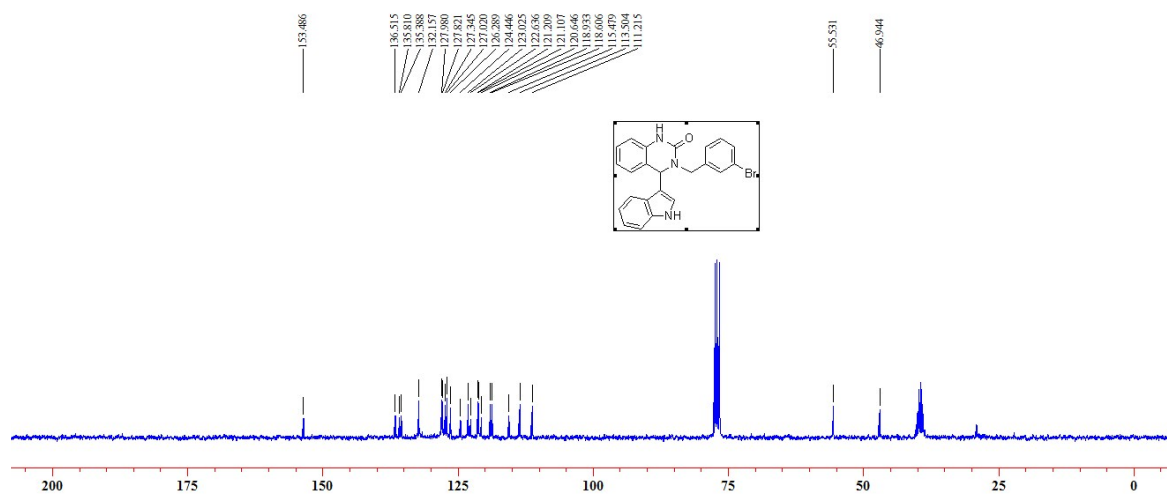
Cc1c[nH]c2c(c1)c3c[nH]c4ccccc34C(=O)N(Cc5ccccc5Br)c5ccccc25

28

¹H & ¹³C NMR spectra of 4f

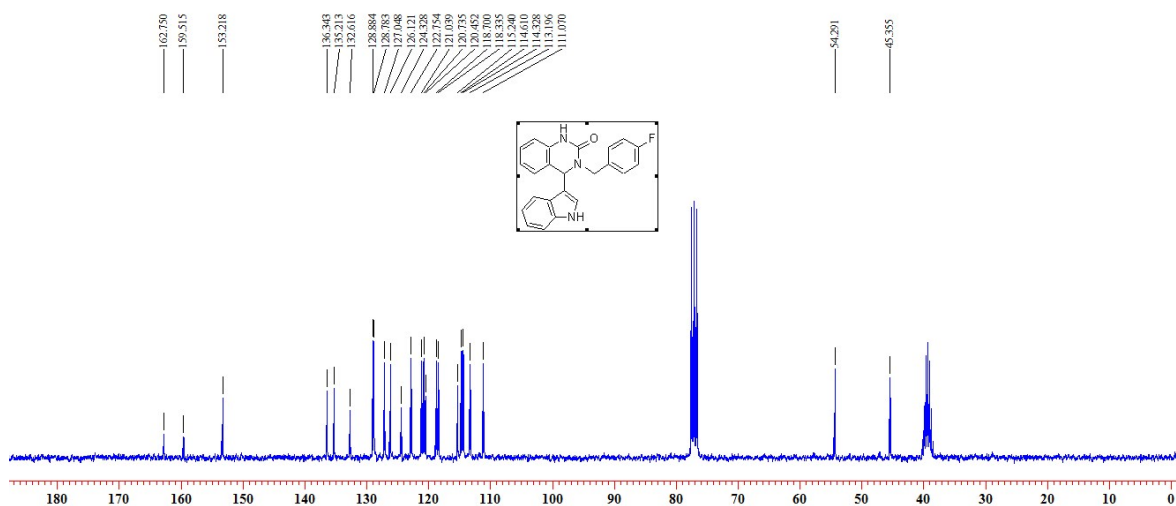
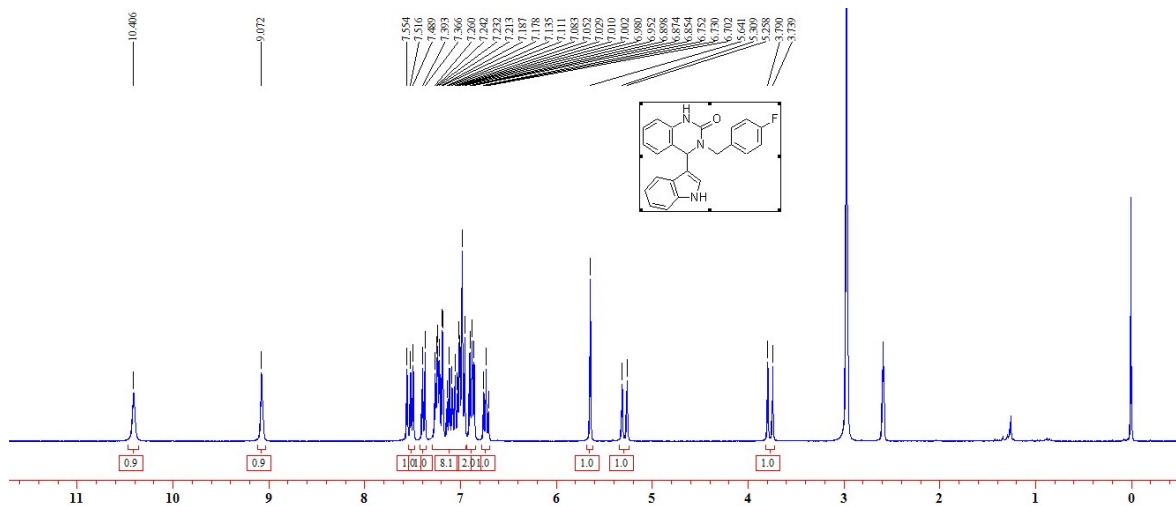


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

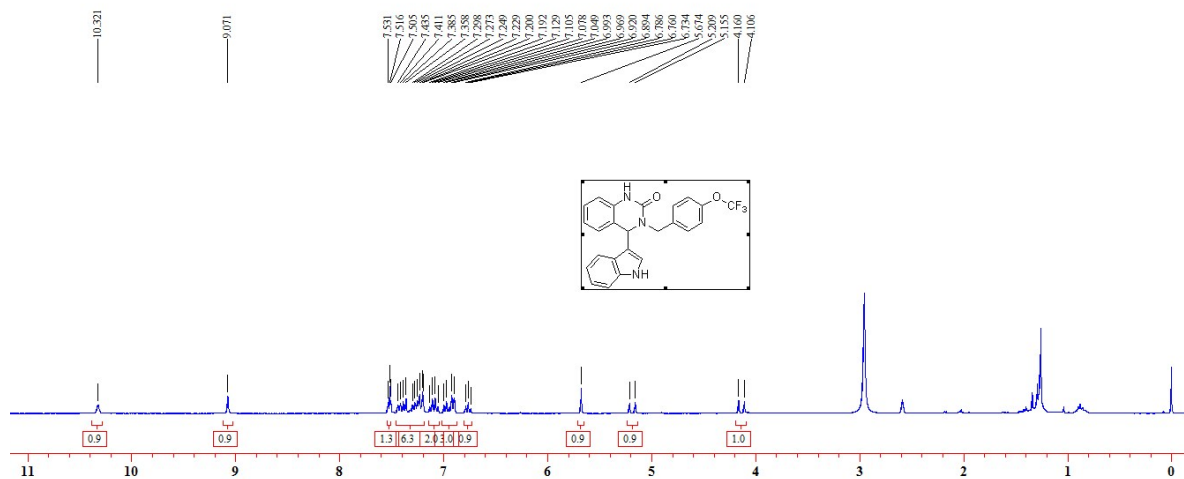


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

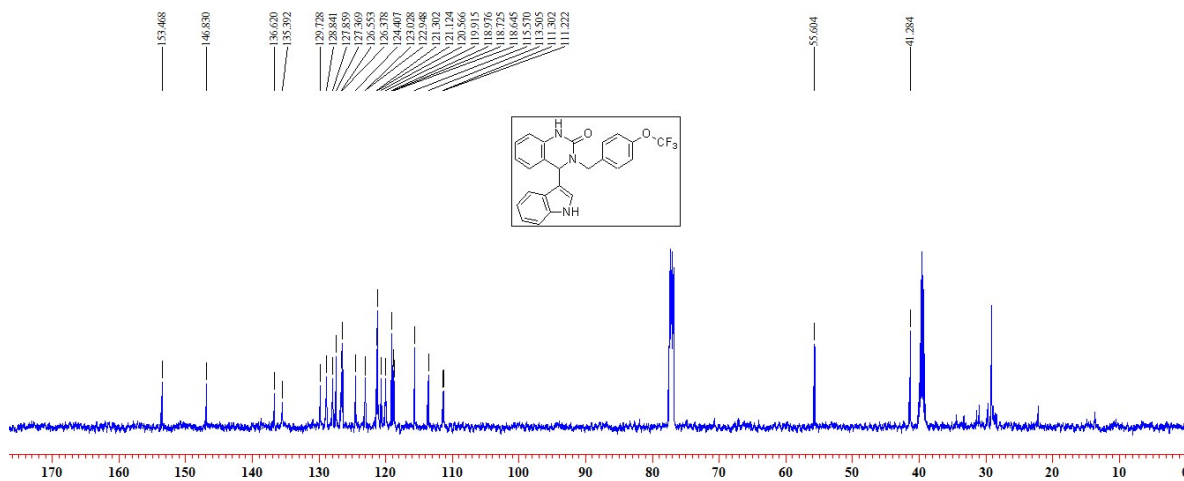
¹H & ¹³C NMR spectra of 4g



¹H & ¹³C NMR spectra of 4h

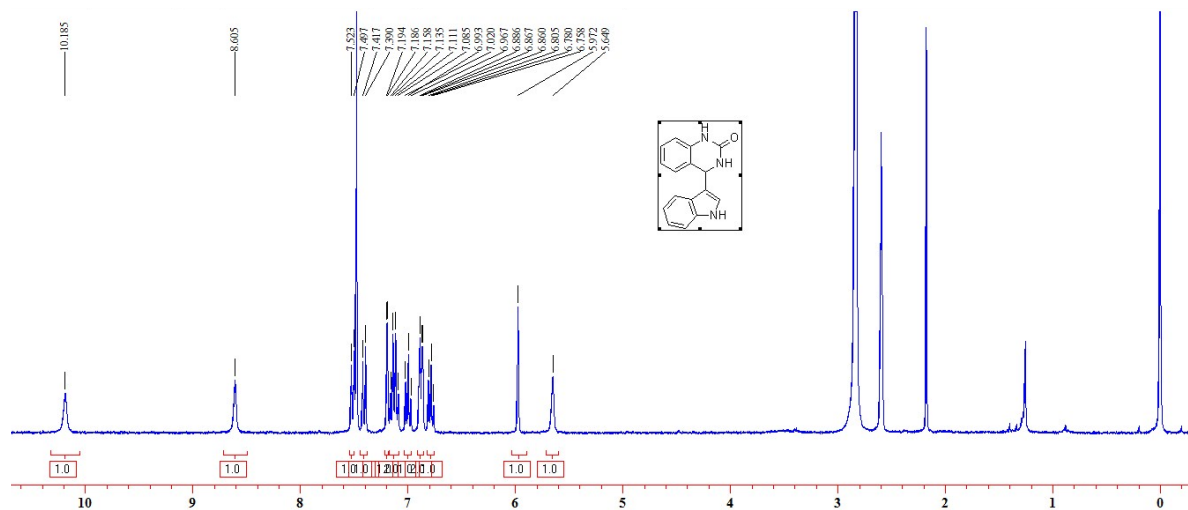


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

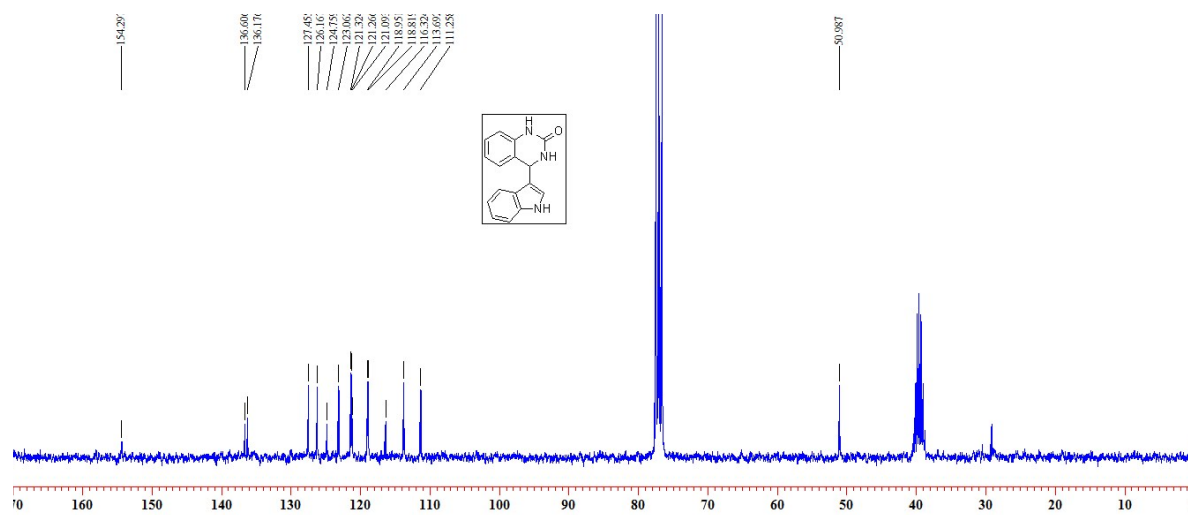


¹³C NMR (125 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4i

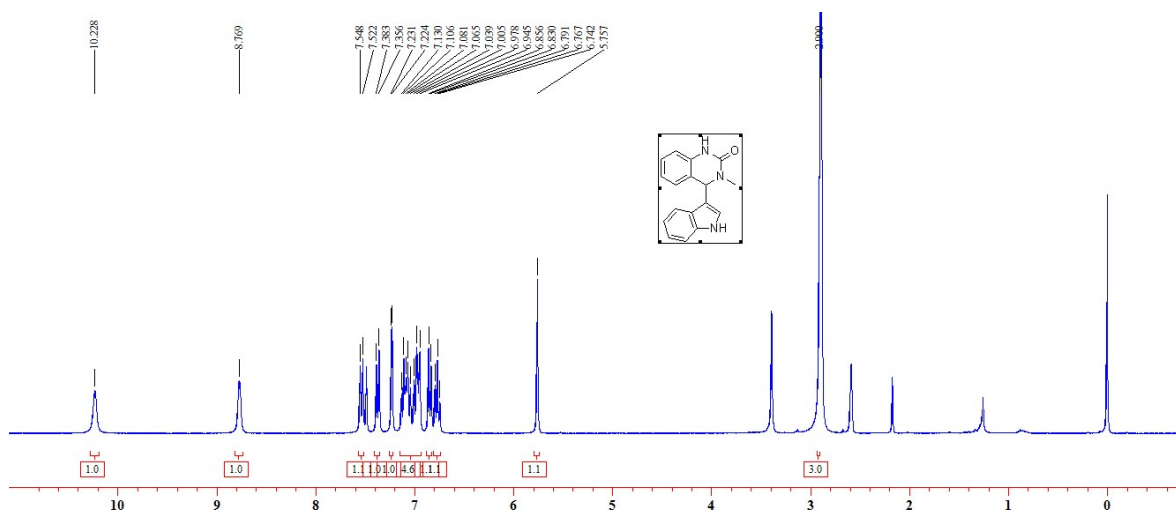


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

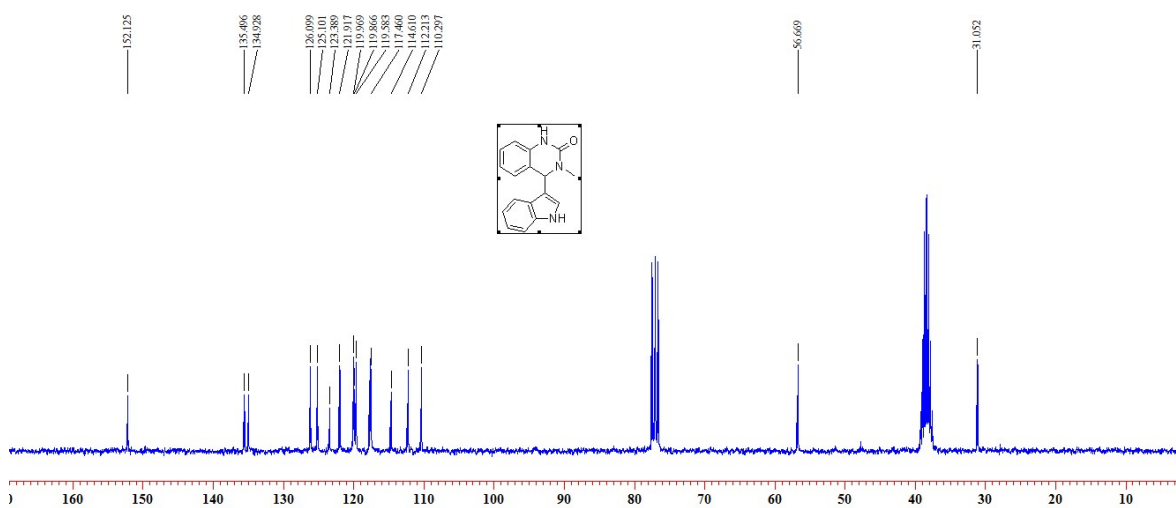


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4j



¹H NMR (300 MHz, CDCl₃+DMSO-d₆)



¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

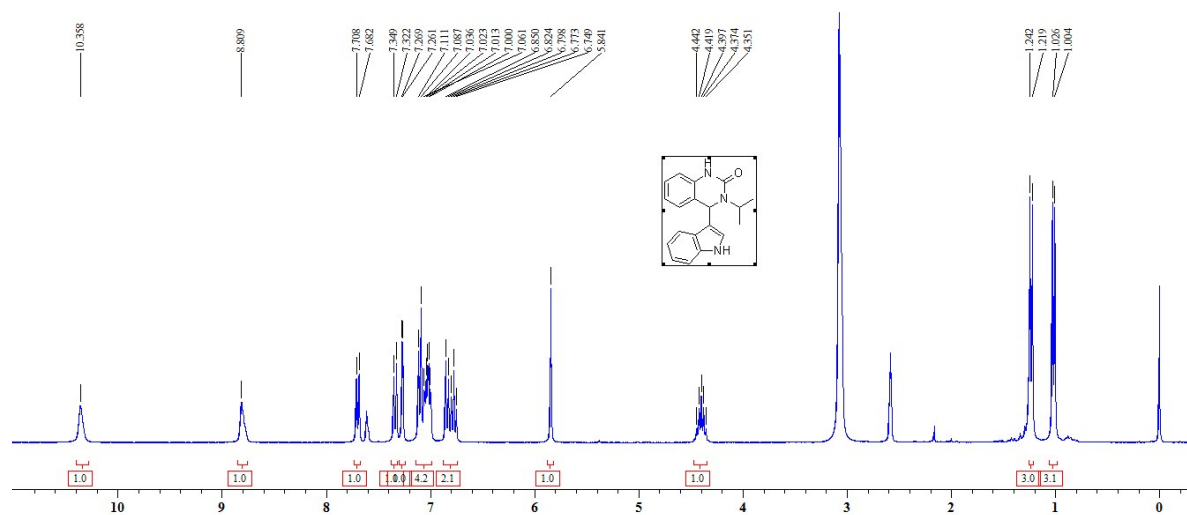
Chemical structure of 1-(2-phenyl-1H-indol-3-yl)-N-phenylmethanimine is shown in the center of the spectrum.

Chemical structure: CCCCN(C(=O)Nc1ccc(cc1)-c2cc3c[nH]c3cc2)c4c[nH]c5ccccc45

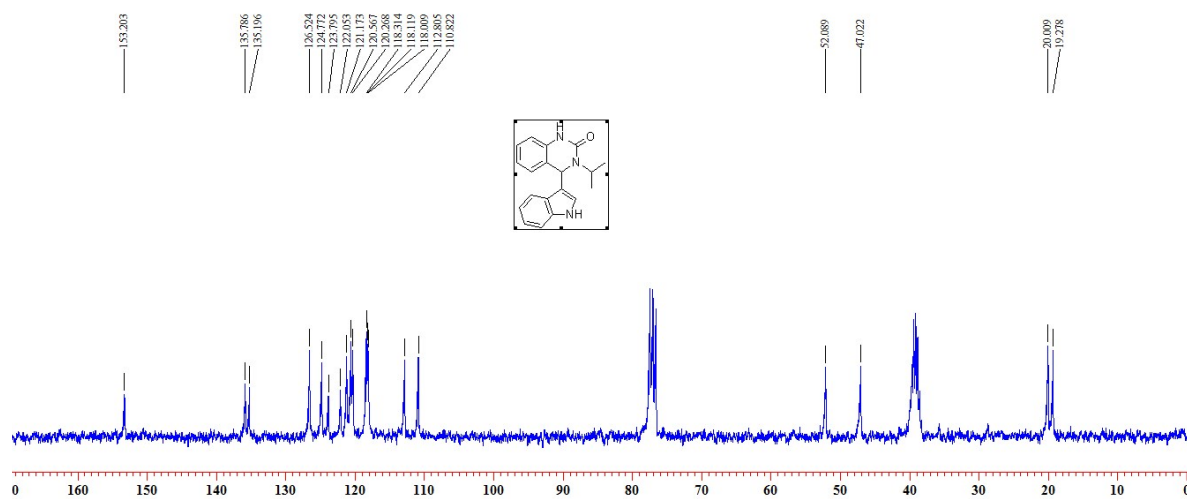
¹³C NMR peaks (ppm): 152.399, 135.796, 135.218, 126.371, 125.372, 123.809, 121.895, 120.369, 119.677, 119.869, 117.985, 117.842, 115.545, 112.113, 110.565, 54.691, 42.845, 28.121, 18.762, 12.683.

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¹H & ¹³C NMR spectra of 4l

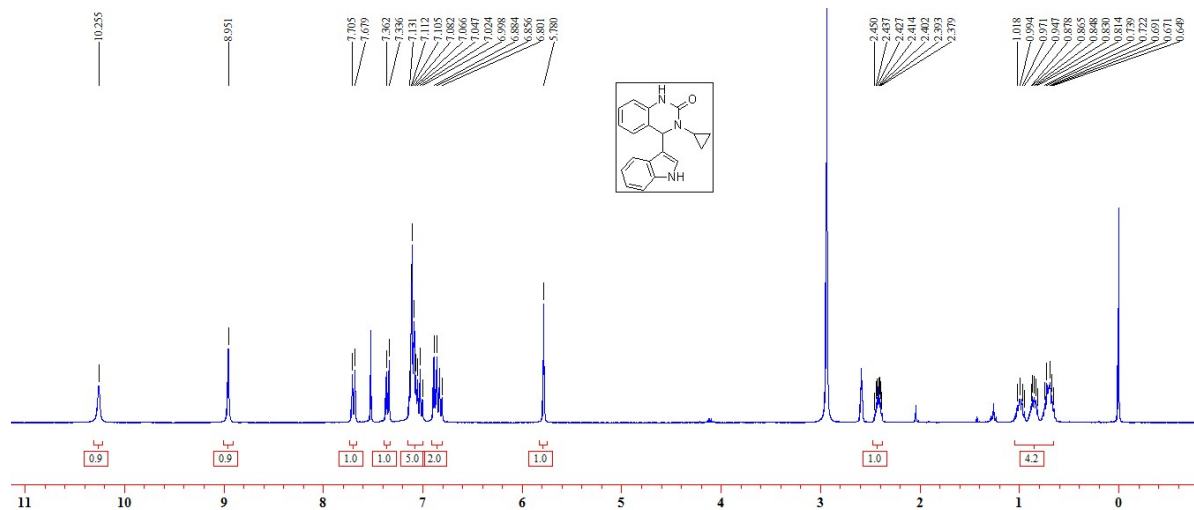


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

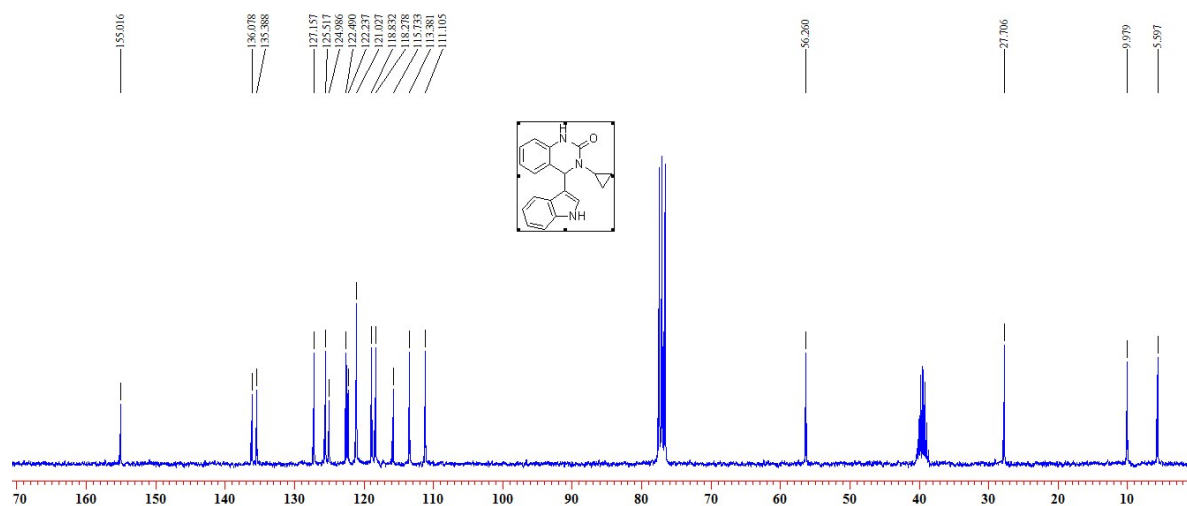


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4m

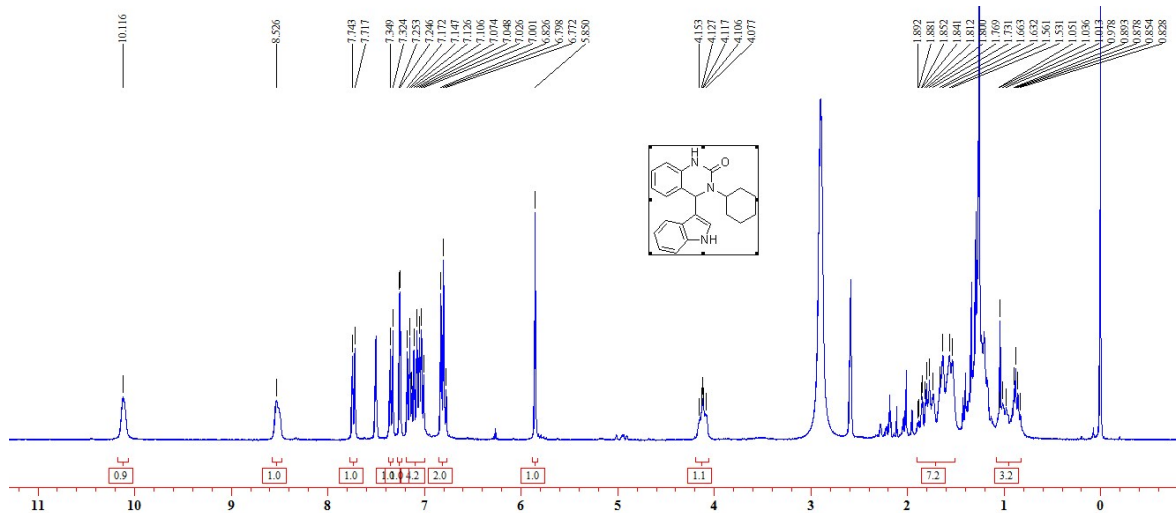


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

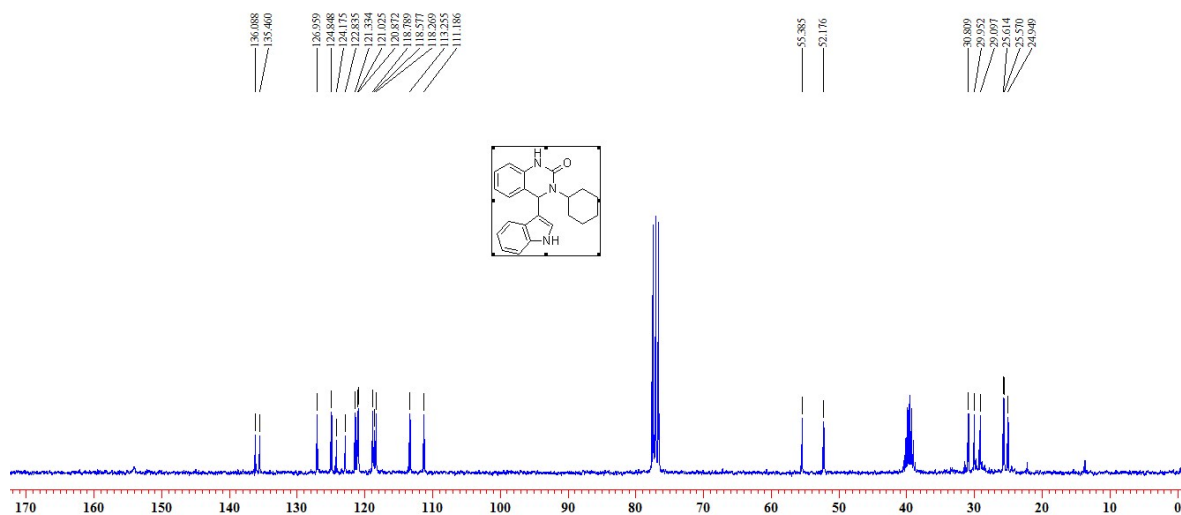


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4n

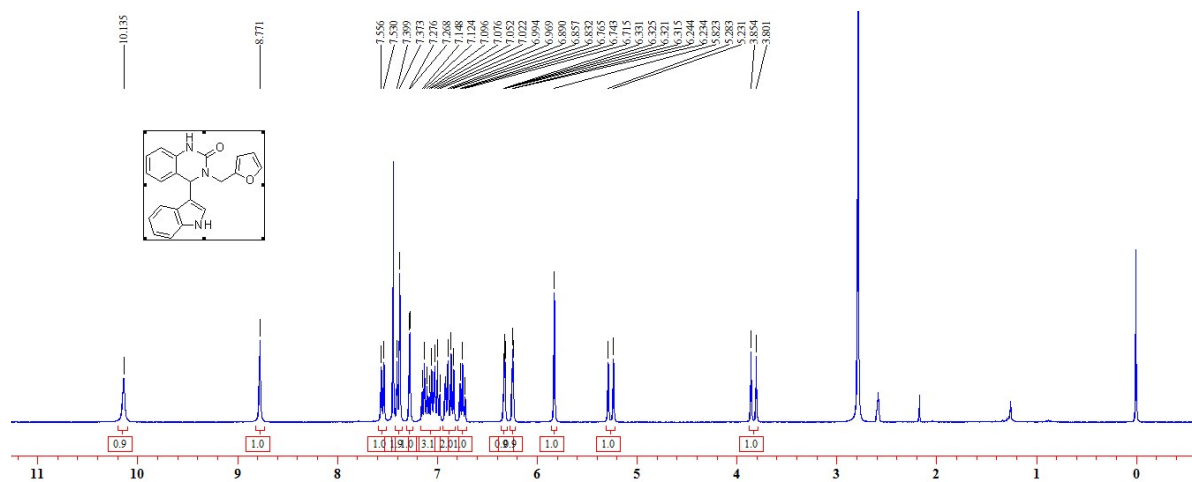


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

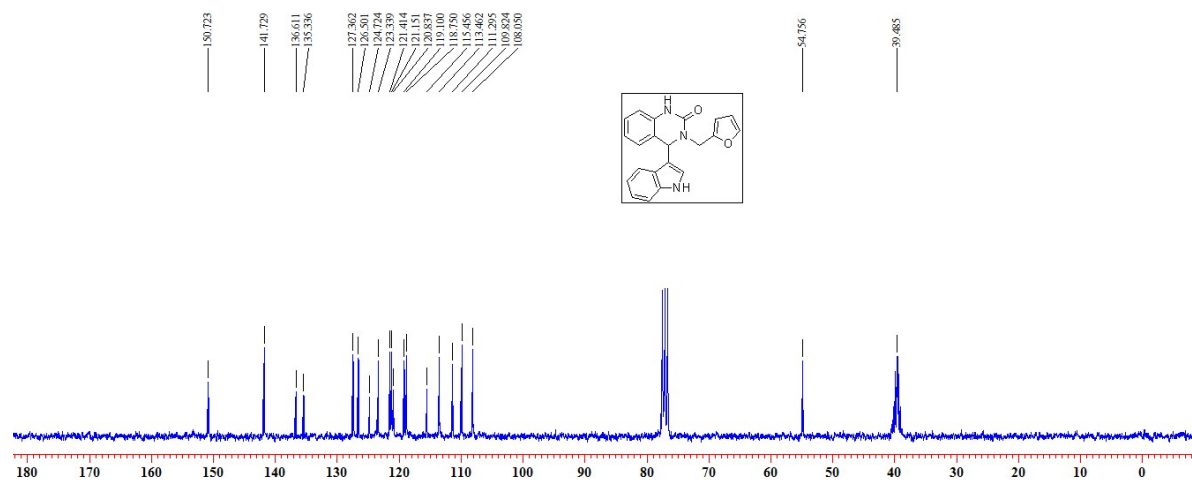


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4o

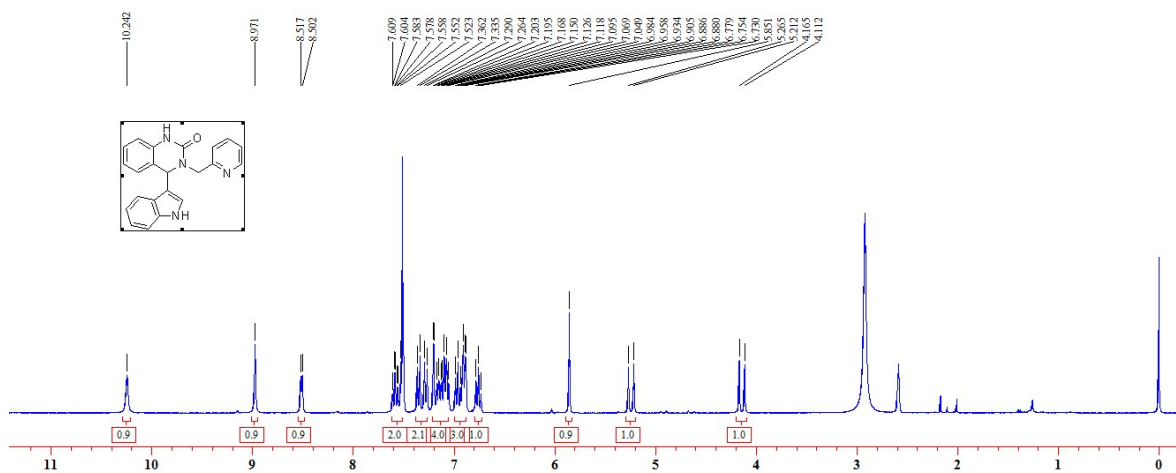


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

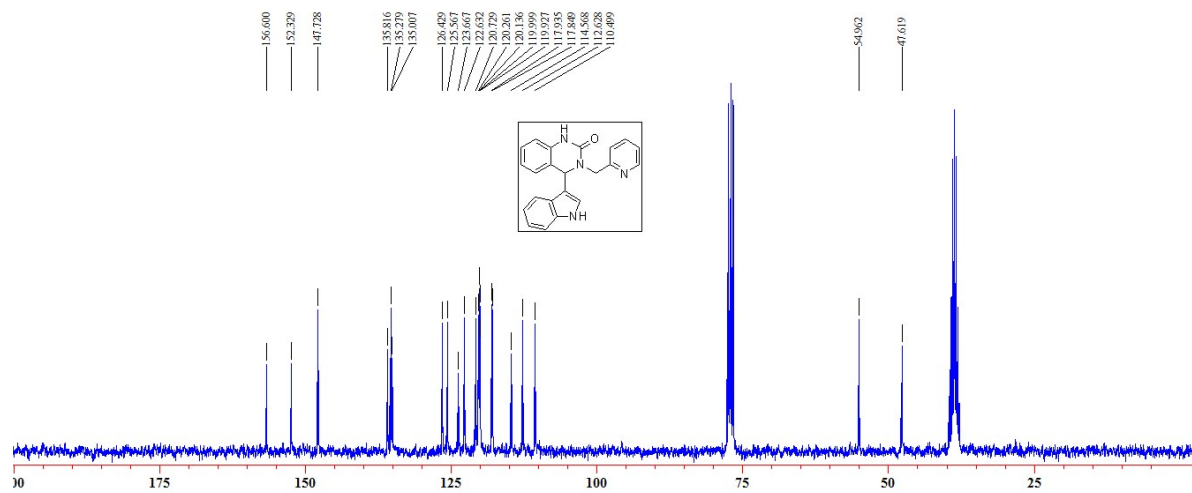


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4p

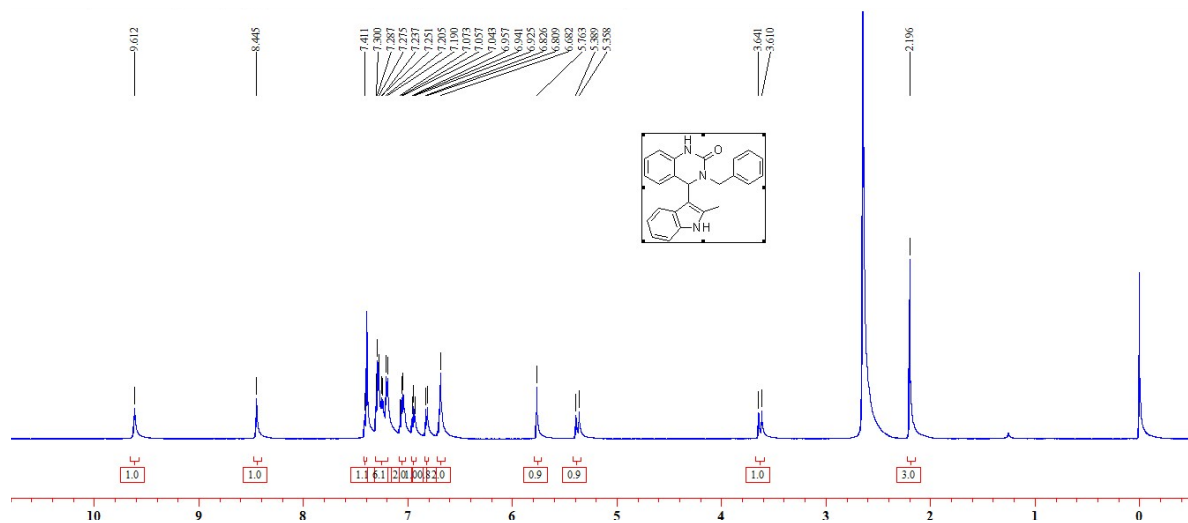


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

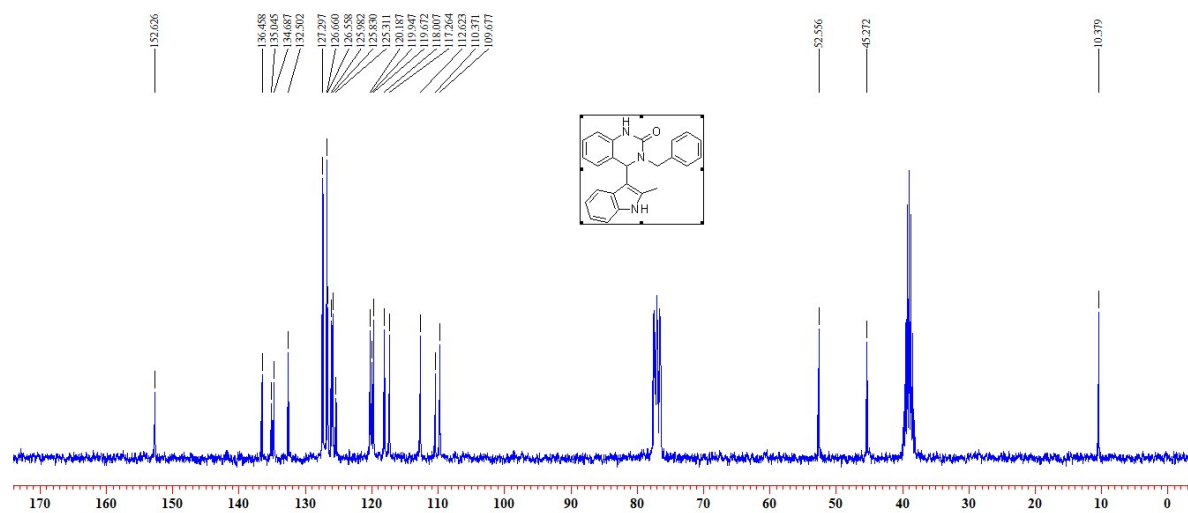


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4q

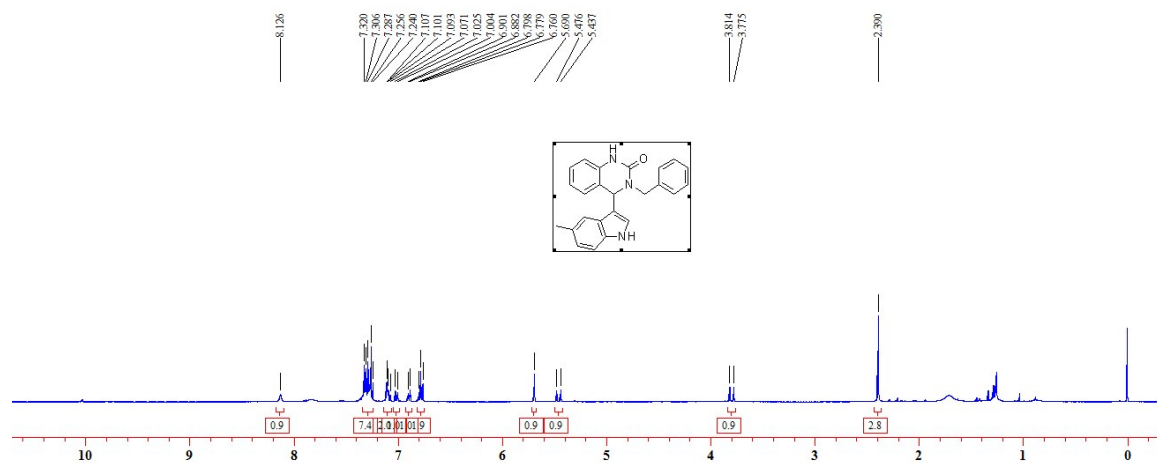


¹H NMR (500 MHz, CDCl₃+DMSO-d₆)

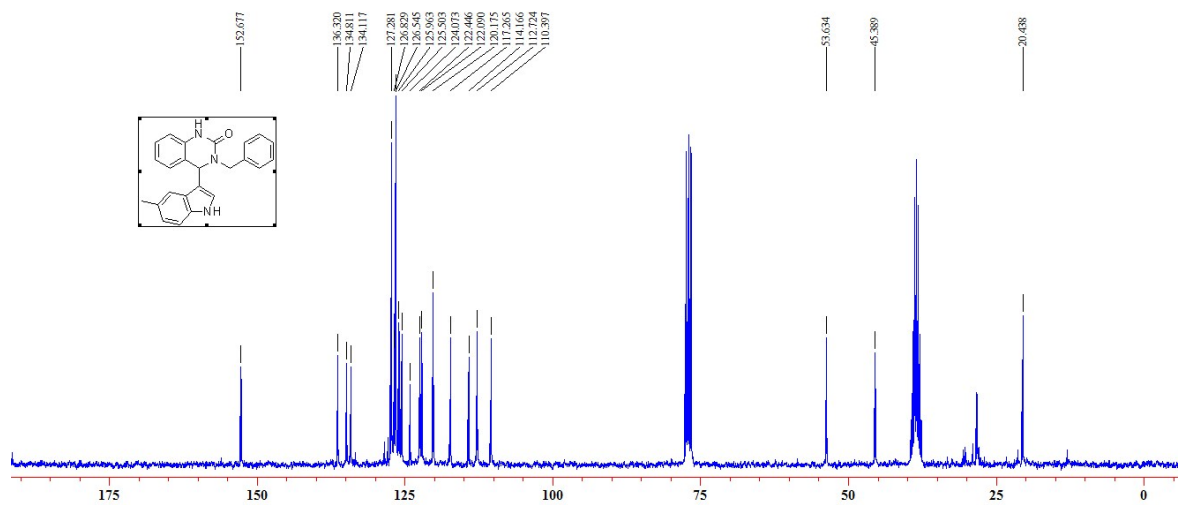


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4r

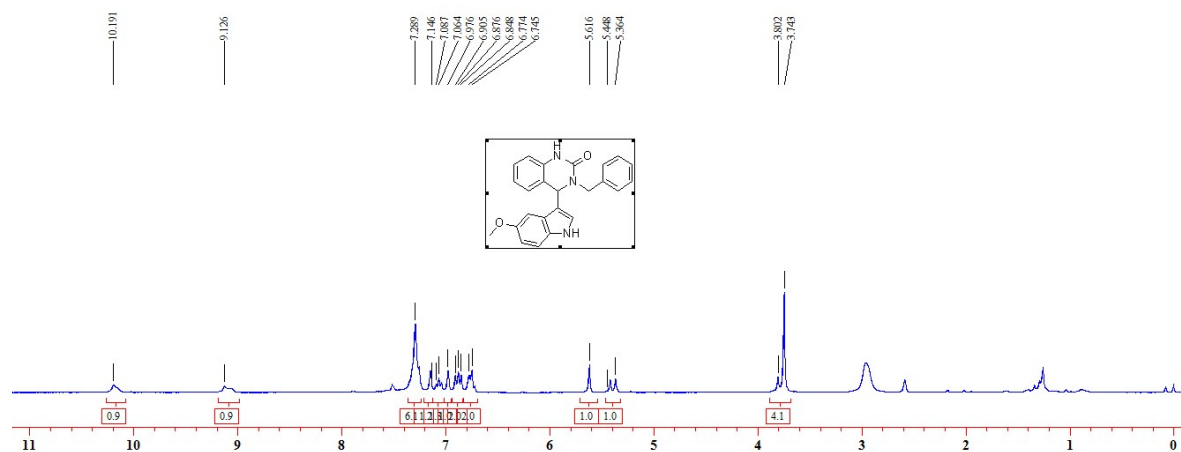


¹H NMR (400 MHz, CDCl₃)

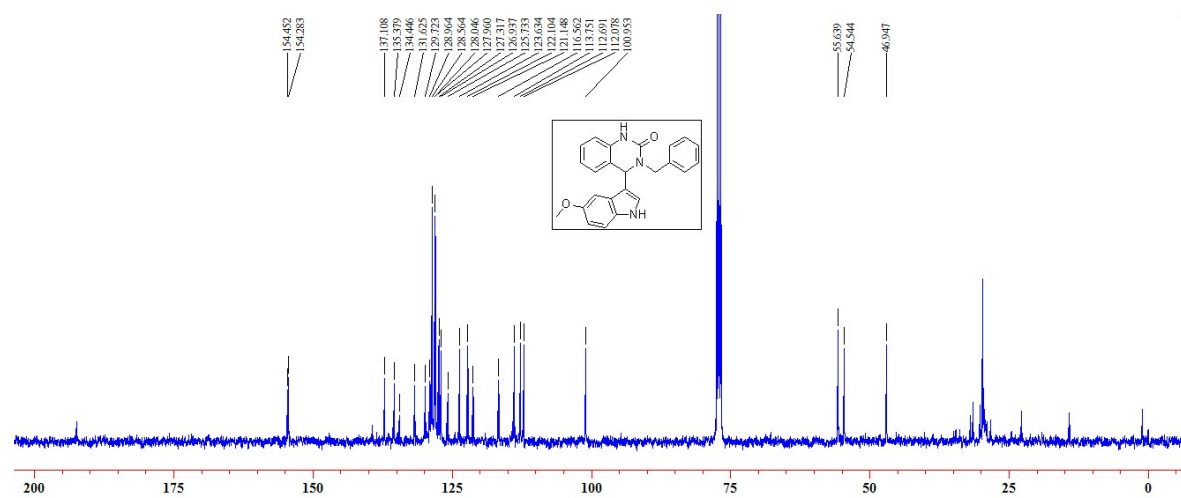


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4s

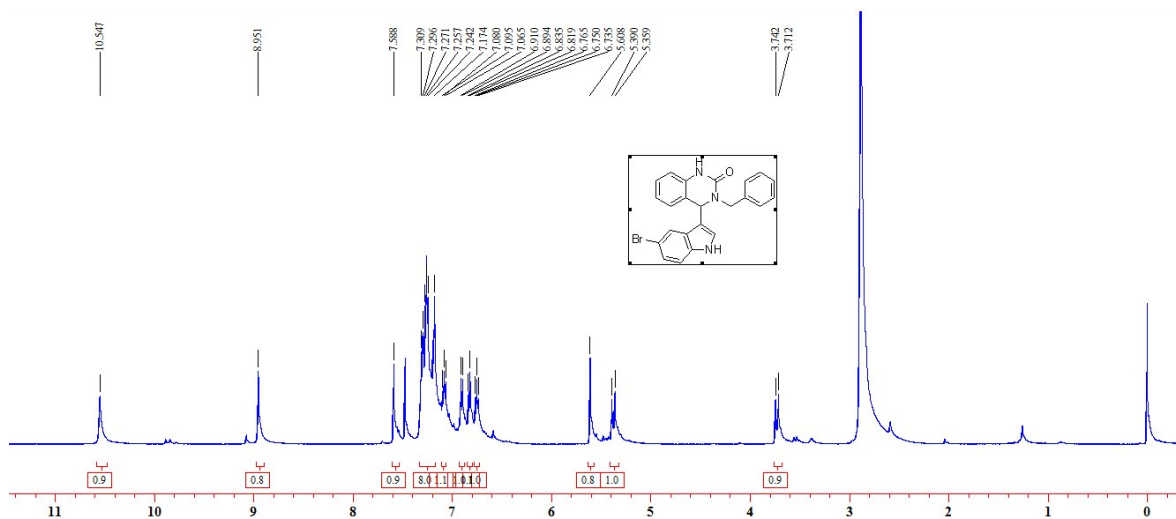


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

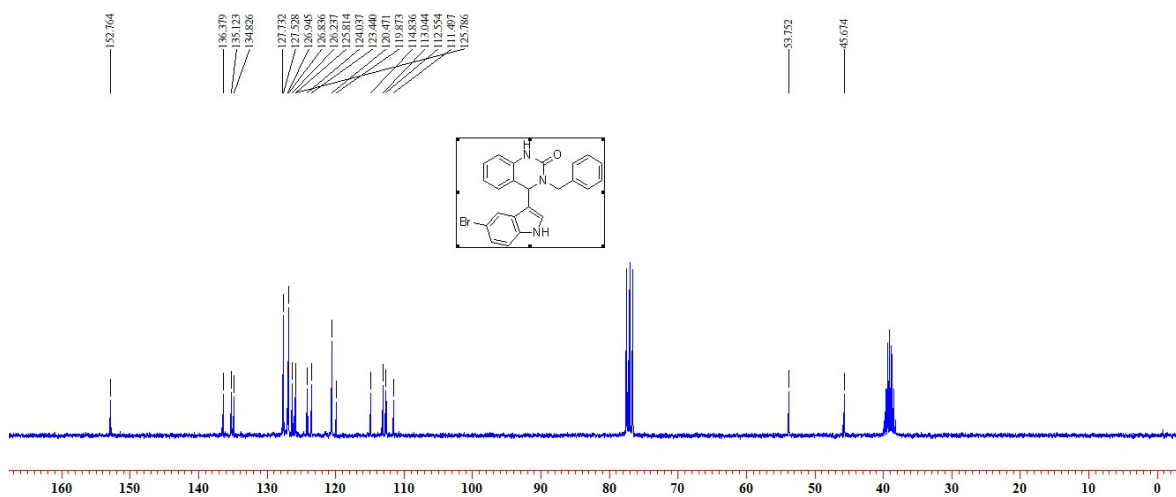


¹³C NMR (100 MHz, CDCl₃)

¹H & ¹³C NMR spectra of 4t

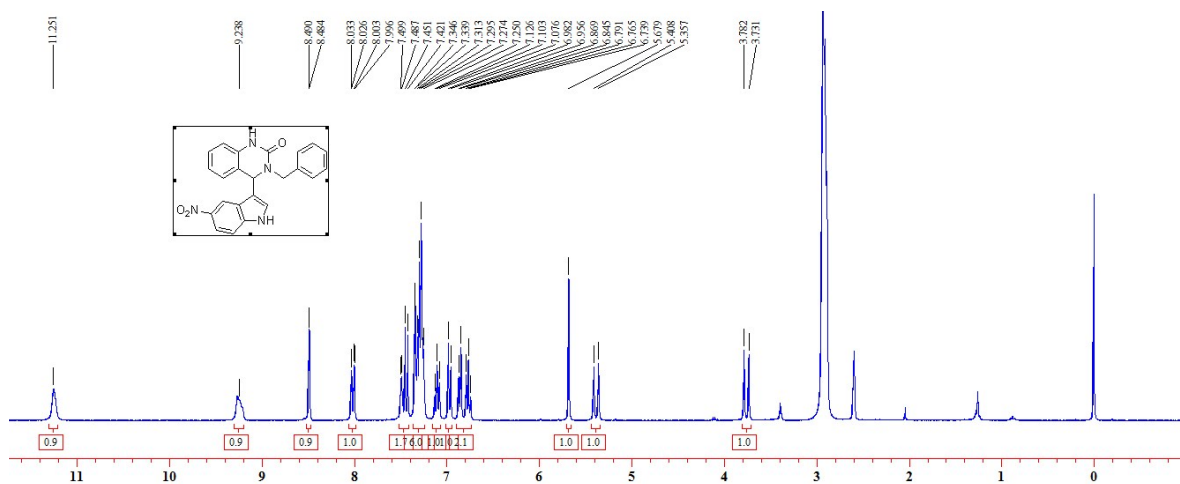
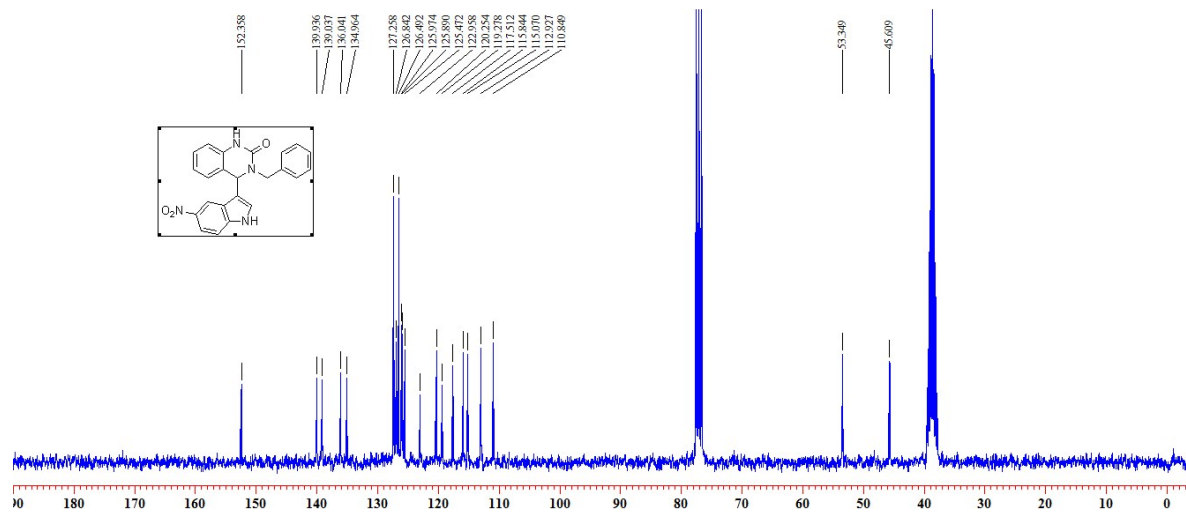


¹H NMR (500 MHz, CDCl₃+DMSO-d₆)

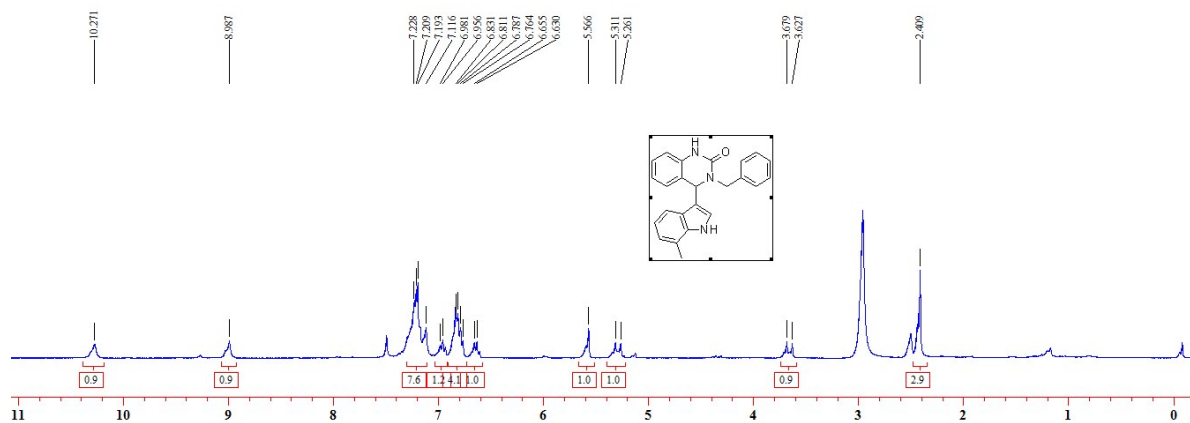


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

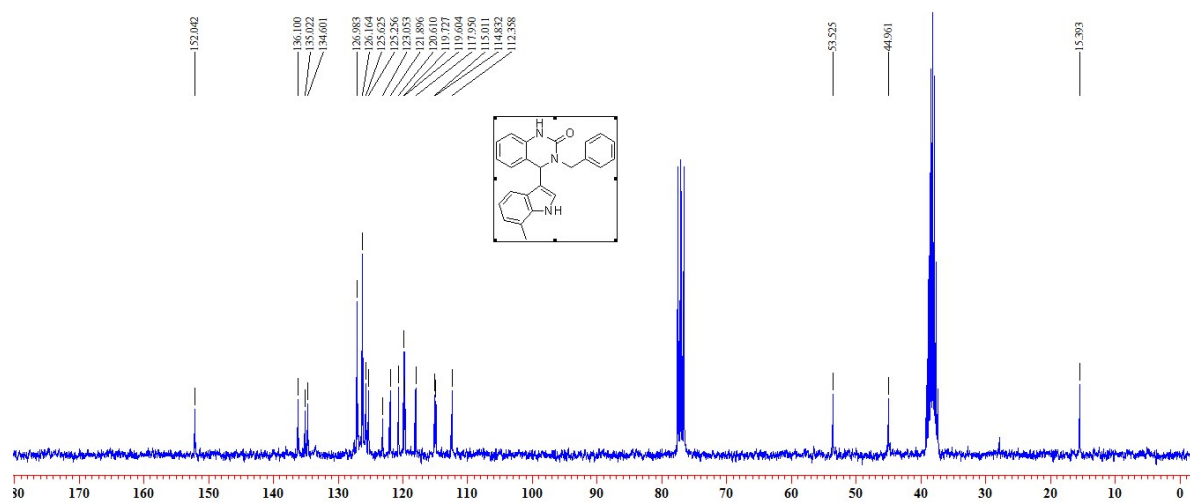
¹H & ¹³C NMR spectra of 4u

¹H NMR (300 MHz, CDCl₃+DMSO-d₆) ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$)

¹H & ¹³C NMR spectra of 4v

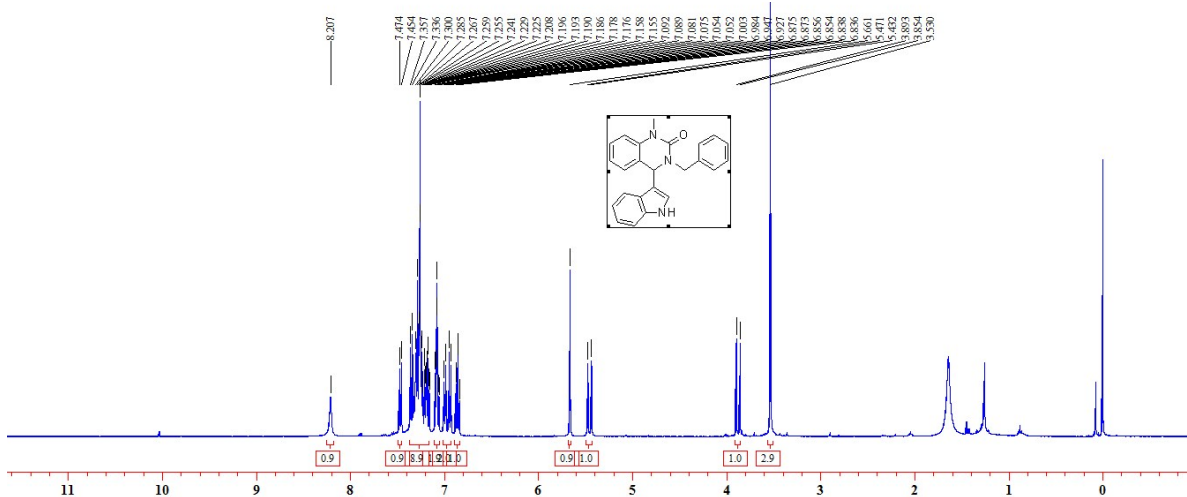
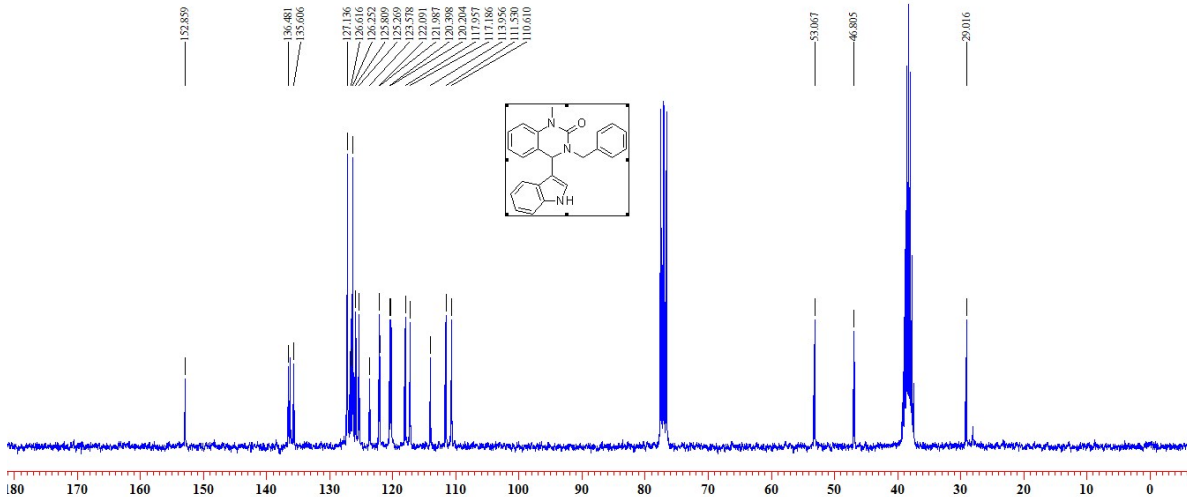


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

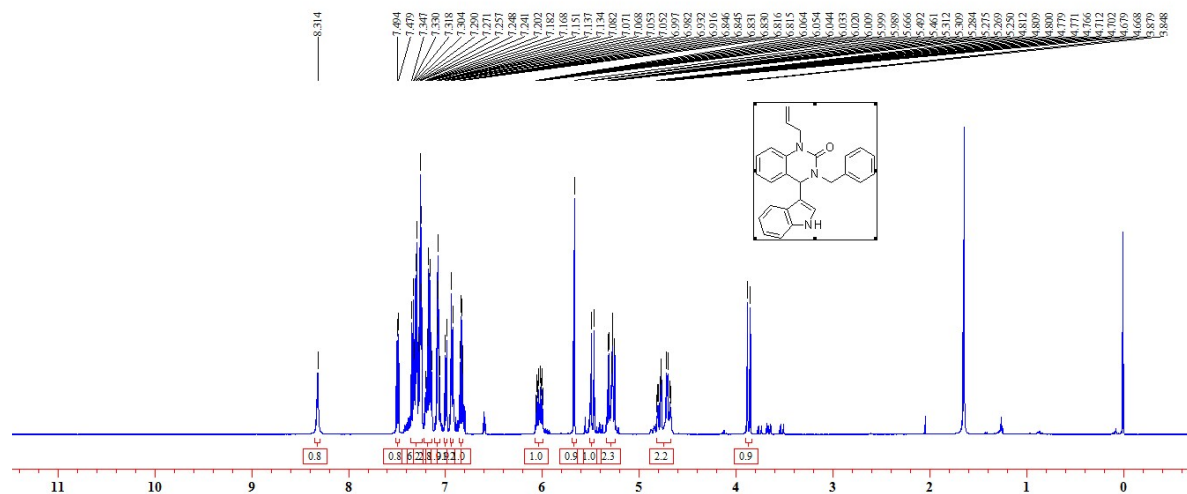


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

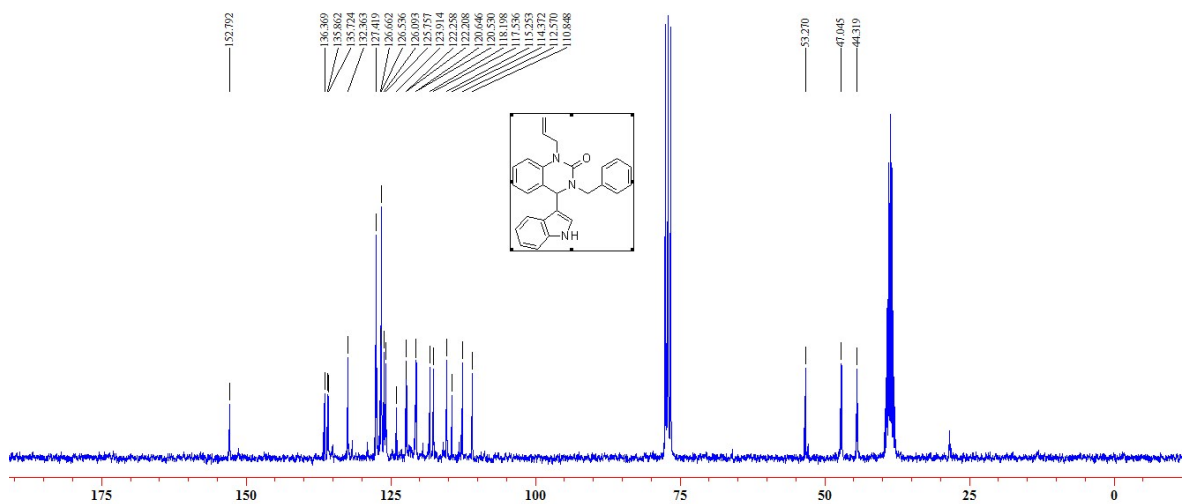
^1H & ^{13}C NMR spectra of 4w

¹H NMR (400 MHz, CDCl₃) ^{13}C NMR (75 MHz, $\text{CDCl}_3 + \text{DMSO-d}_6$)

¹H & ¹³C NMR spectra of 4x

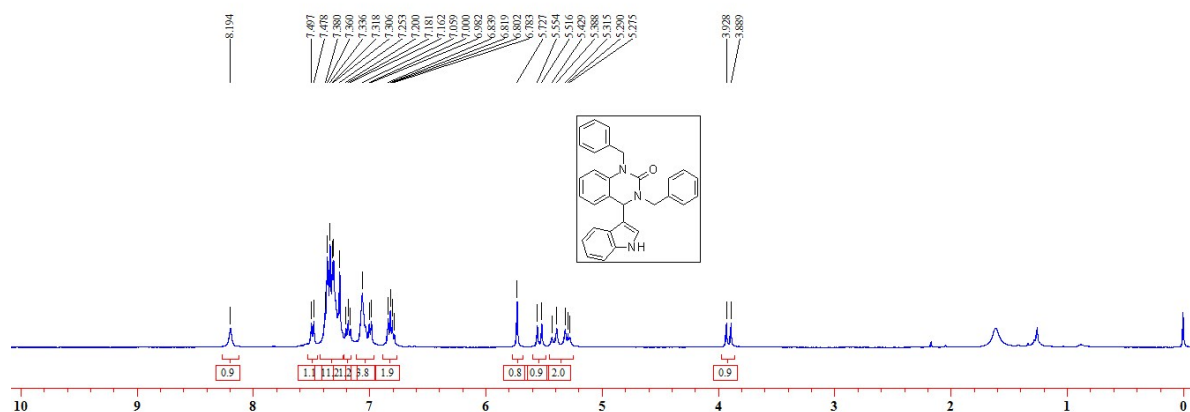


¹H NMR (500 MHz, CDCl₃)

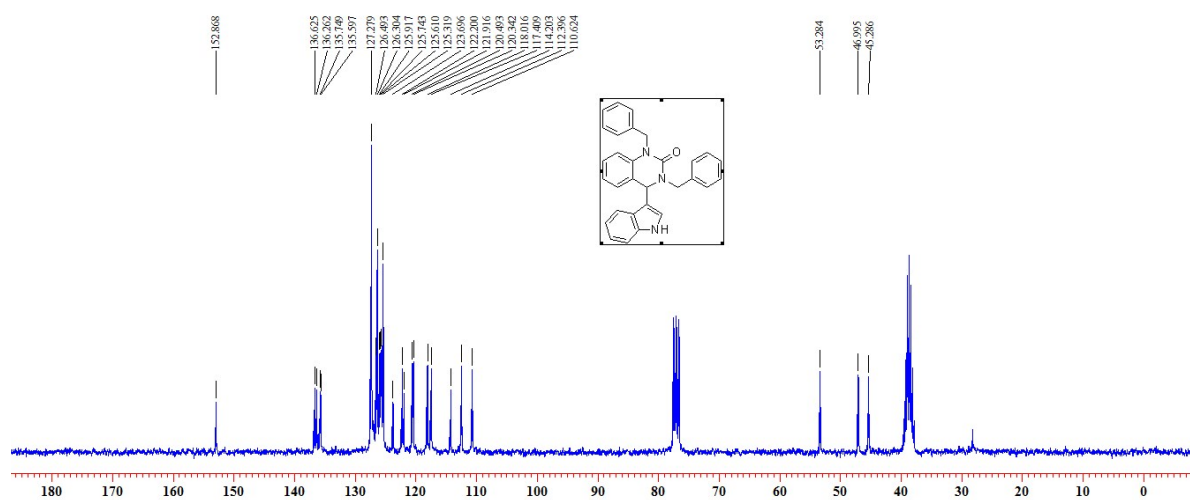


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 4y

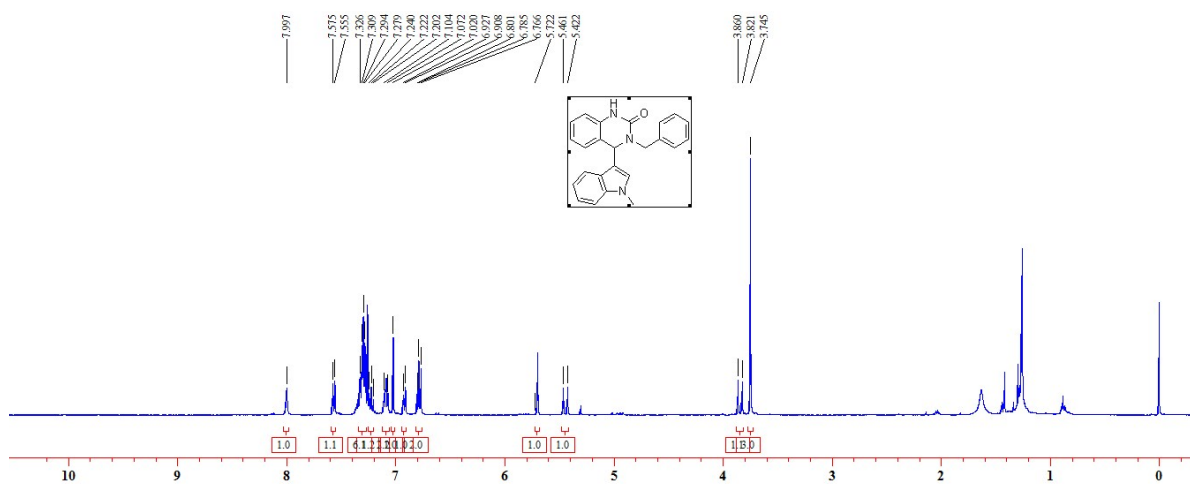
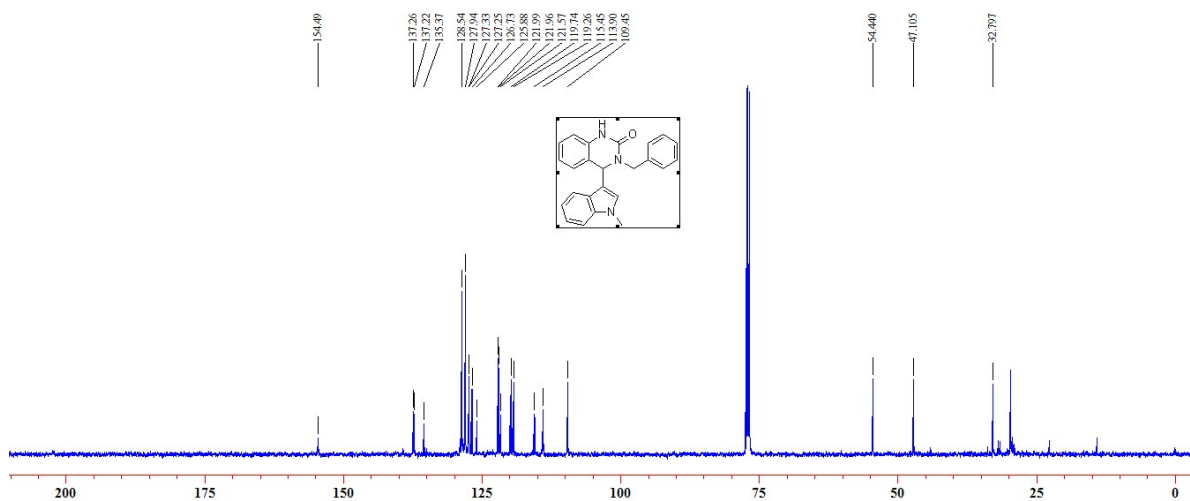


¹H NMR (400 MHz, CDCl₃)

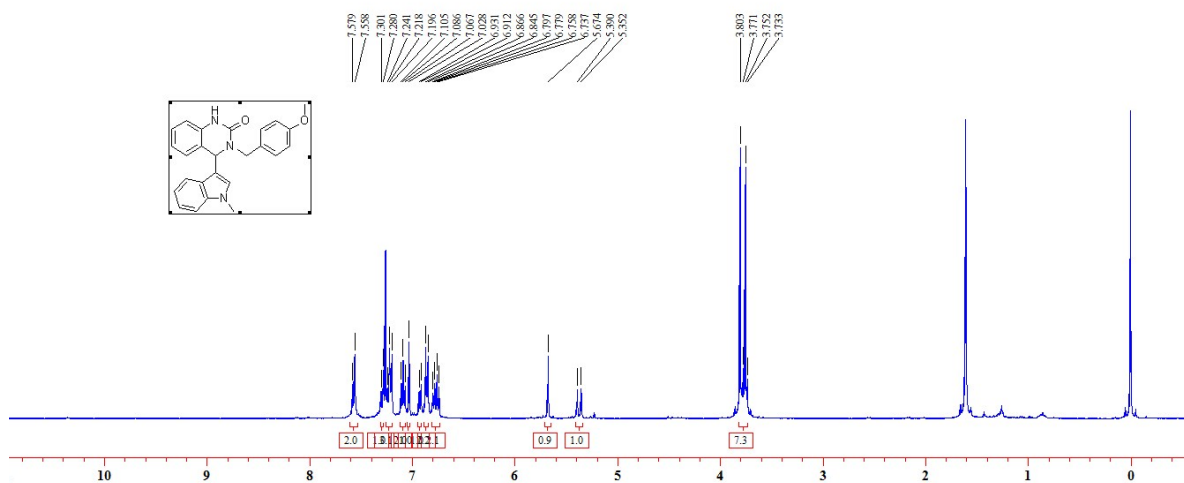


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

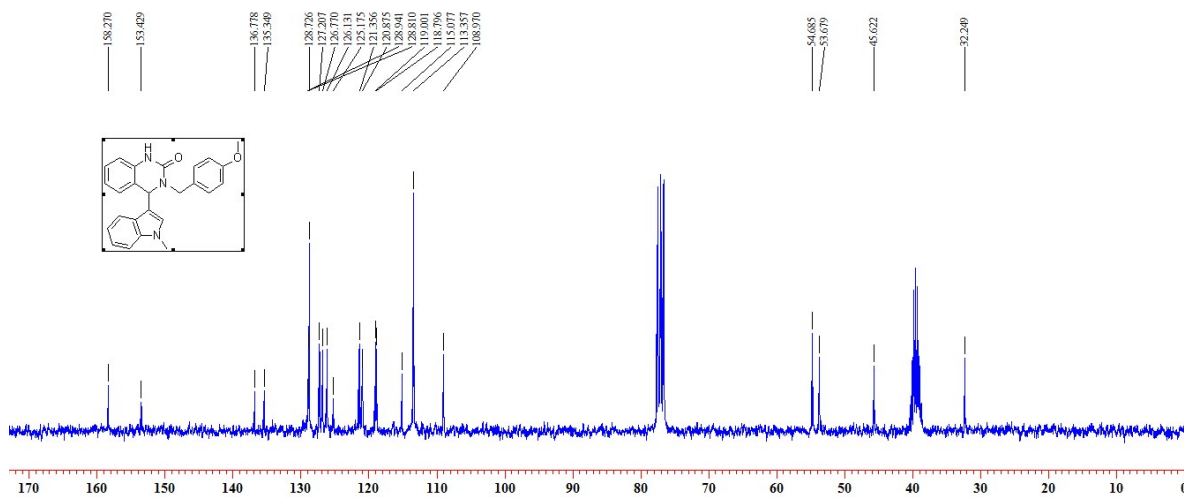
^1H & ^{13}C NMR spectra of 4z

¹H NMR (400 MHz, CDCl₃) ^{13}C NMR (125 MHz, CDCl_3)

¹H & ¹³C NMR spectra of 4za

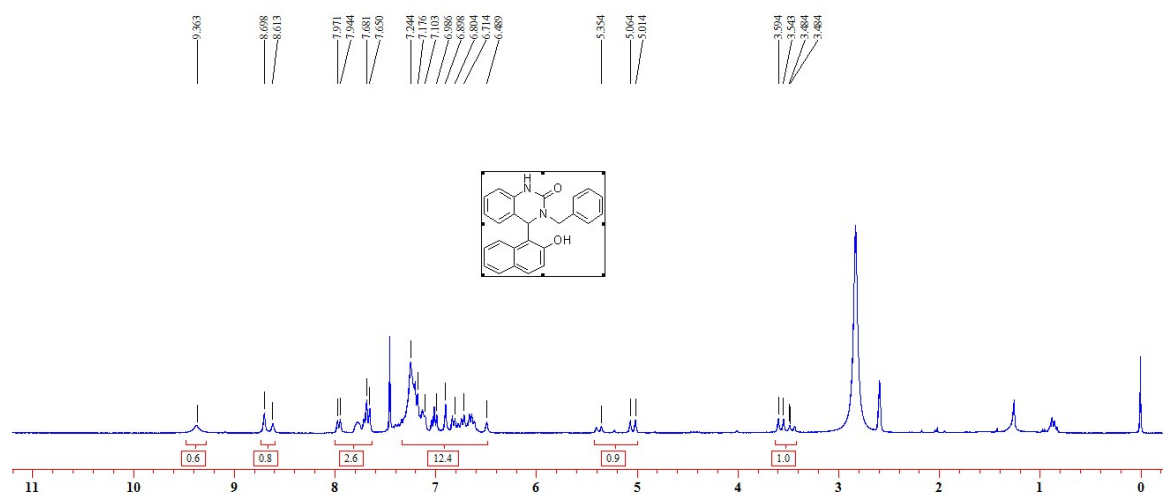


¹H NMR (400 MHz, CDCl₃)

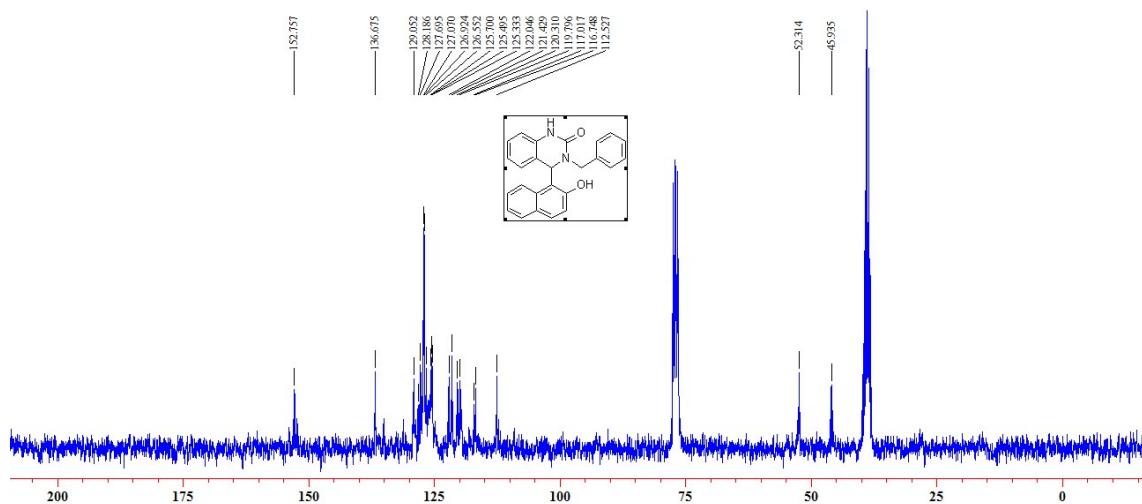


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6a

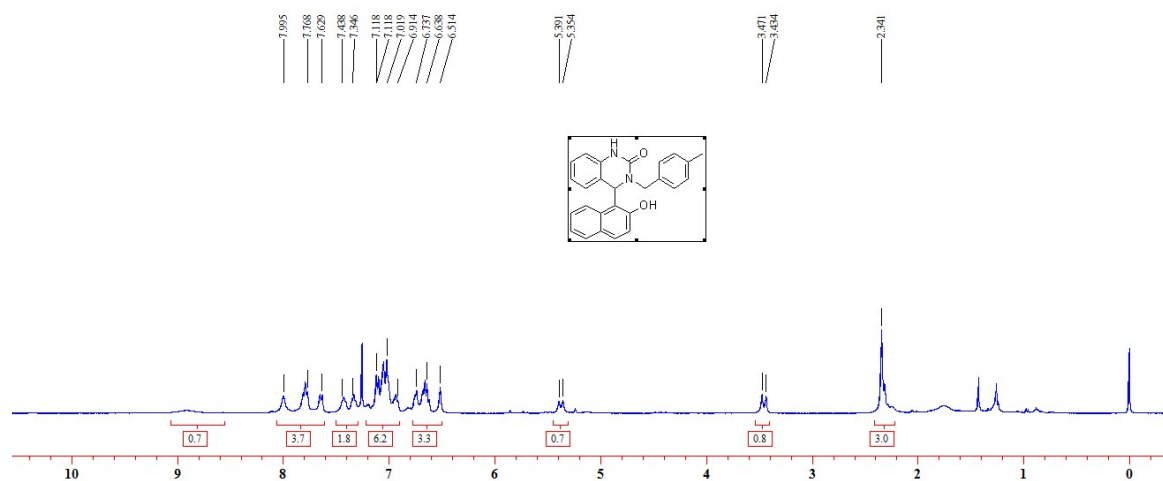


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

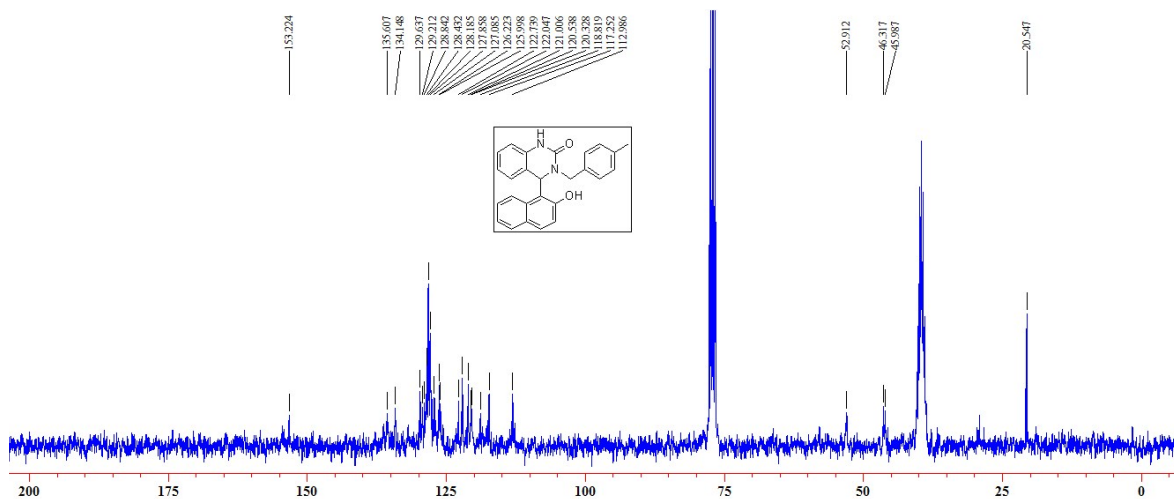


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6b



¹H NMR (400 MHz, CDCl₃+DMSO-d₆)



¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

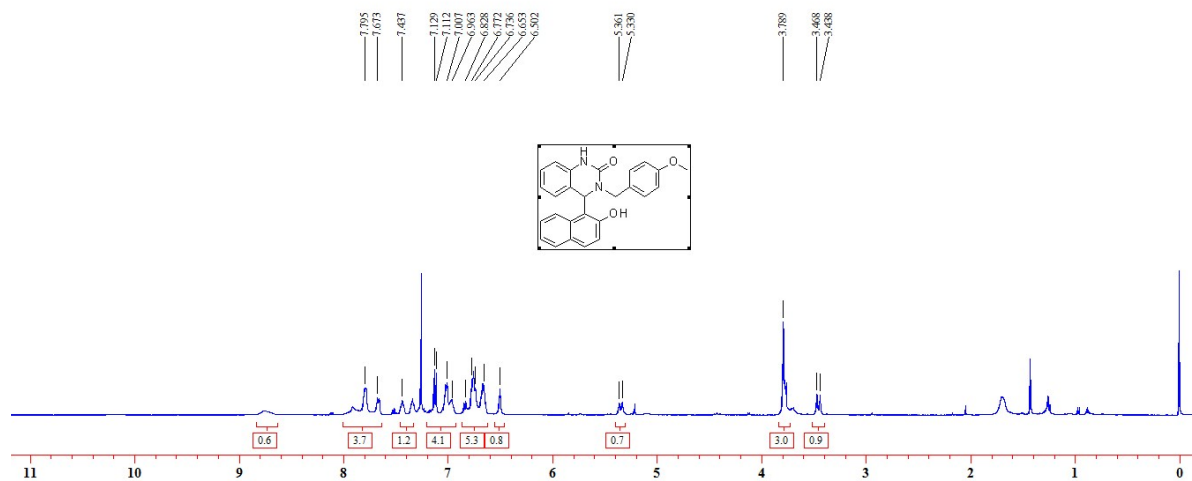
Chemical structure of compound 10 is shown in the center of the spectrum. The structure is a naphthalene derivative with a 2-hydroxy-1-(4-tert-butylphenyl)hydrazono group at position 1 and a 2-hydroxy-1-(4-tert-butylphenyl)hydrazono group at position 2.

The ^1H NMR spectrum (CDCl₃) shows the following chemical shifts (ppm) and integrations:

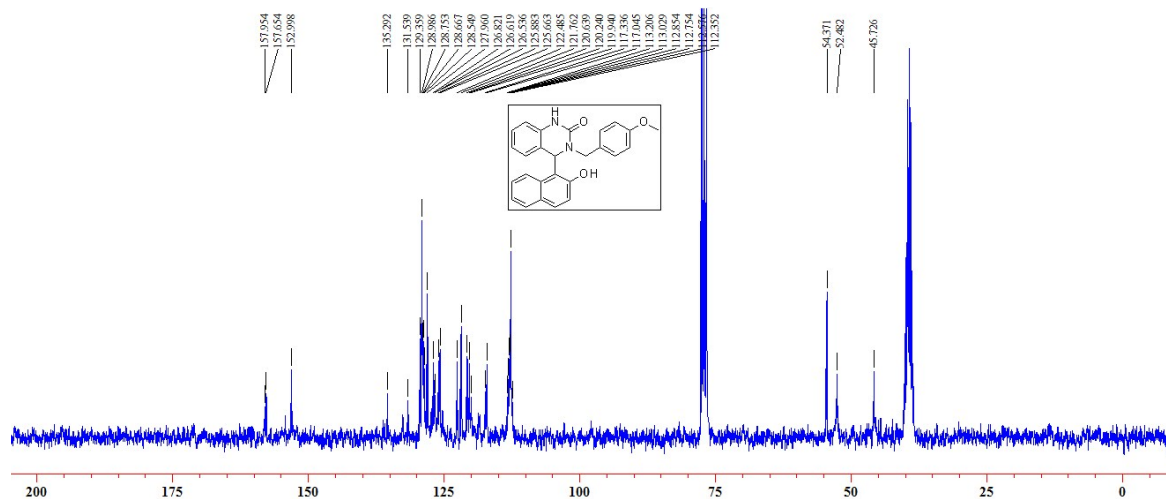
- 9.488 (0.8)
- 8.737 (0.9)
- 8.683 (0.9)
- 7.988 (2.8)
- 7.901 (2.8)
- 7.851 (2.8)
- 7.789 (2.8)
- 7.662 (2.8)
- 7.230 (12.0)
- 7.154 (12.0)
- 7.125 (12.0)
- 7.001 (12.0)
- 6.975 (12.0)
- 6.939 (12.0)
- 6.825 (12.0)
- 6.811 (12.0)
- 6.740 (12.0)
- 6.662 (12.0)
- 6.603 (12.0)
- 6.495 (12.0)
- 5.398 (0.9)
- 5.308 (0.9)
- 4.915 (0.9)
- 4.865 (0.9)
- 3.672 (1.1)
- 3.622 (1.1)
- 3.393 (1.1)
- 1.312 (9.9)
- 1.257 (9.9)

53

¹H & ¹³C NMR spectra of 6d

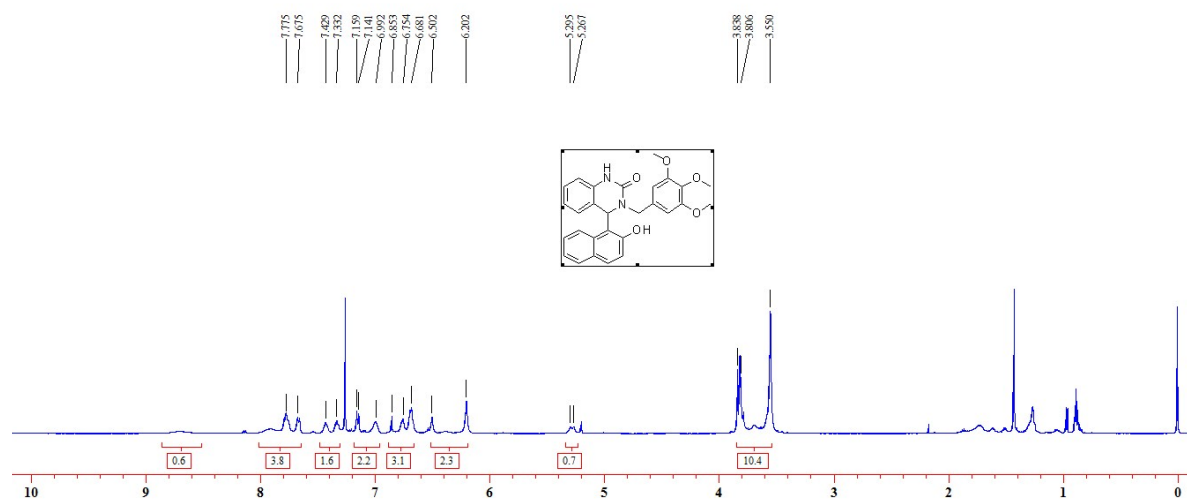


¹H NMR (500 MHz, CDCl₃)

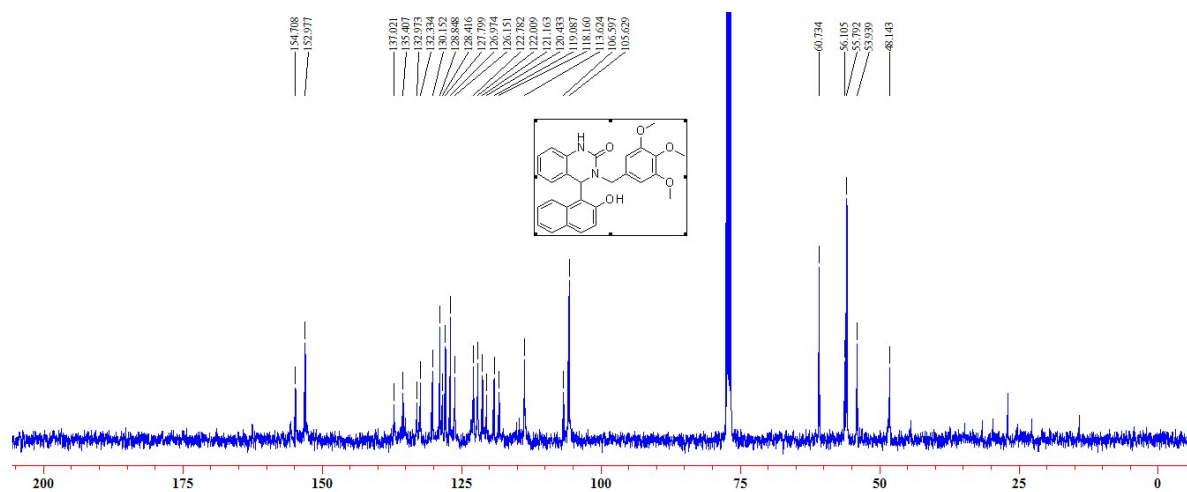


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6e

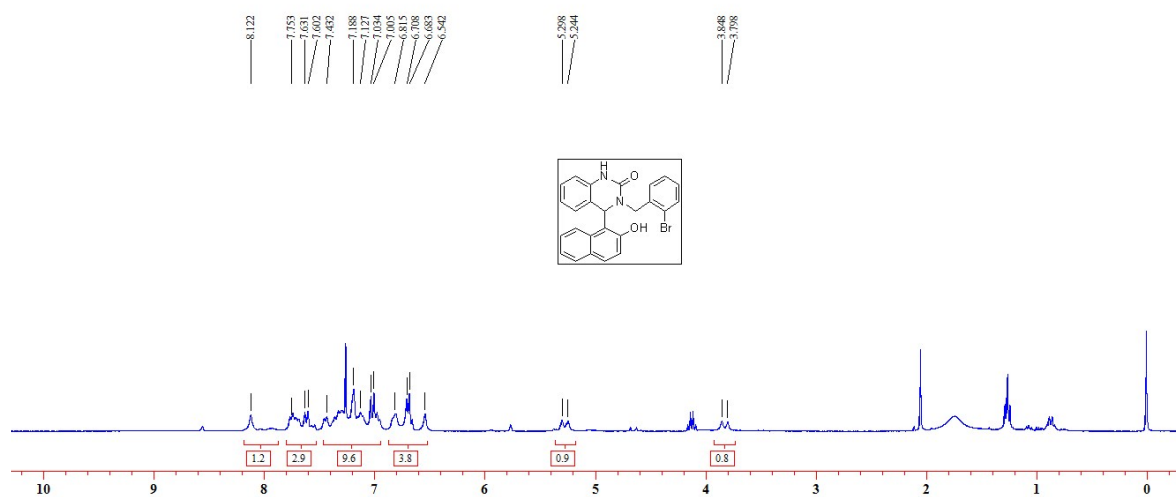


¹H NMR (500 MHz, CDCl₃)

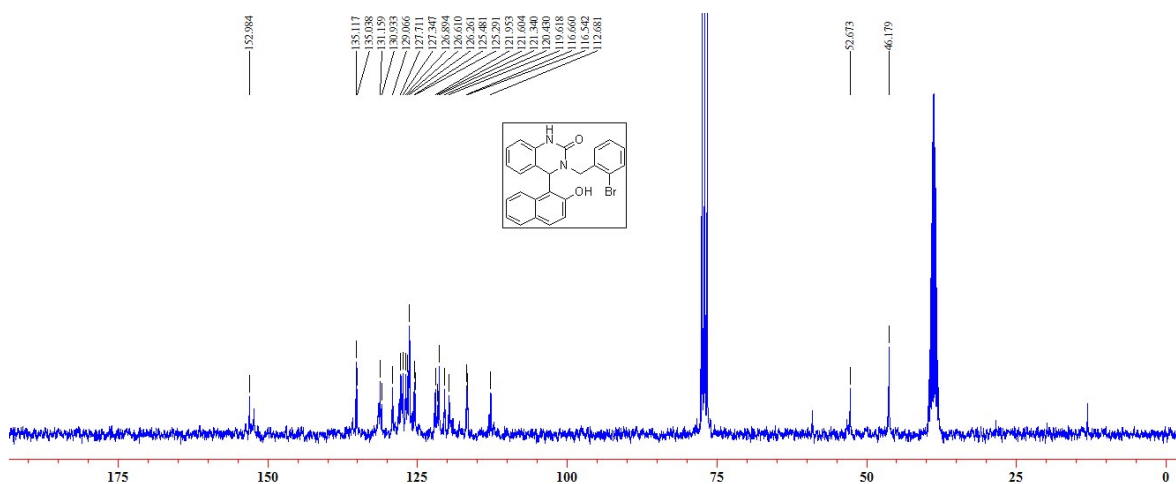


¹³C NMR (100 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6f

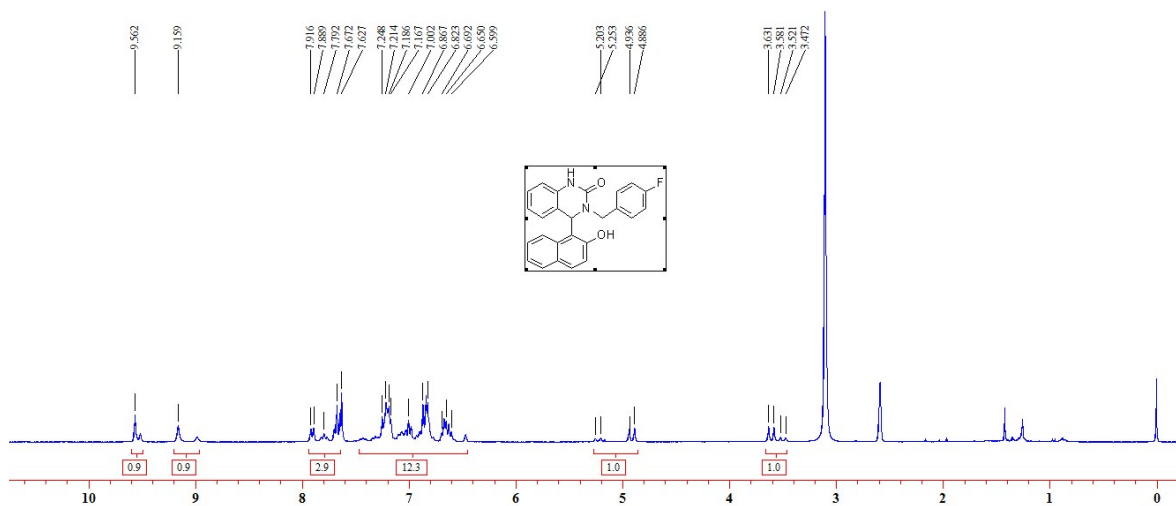


¹H NMR (300 MHz, CDCl₃)

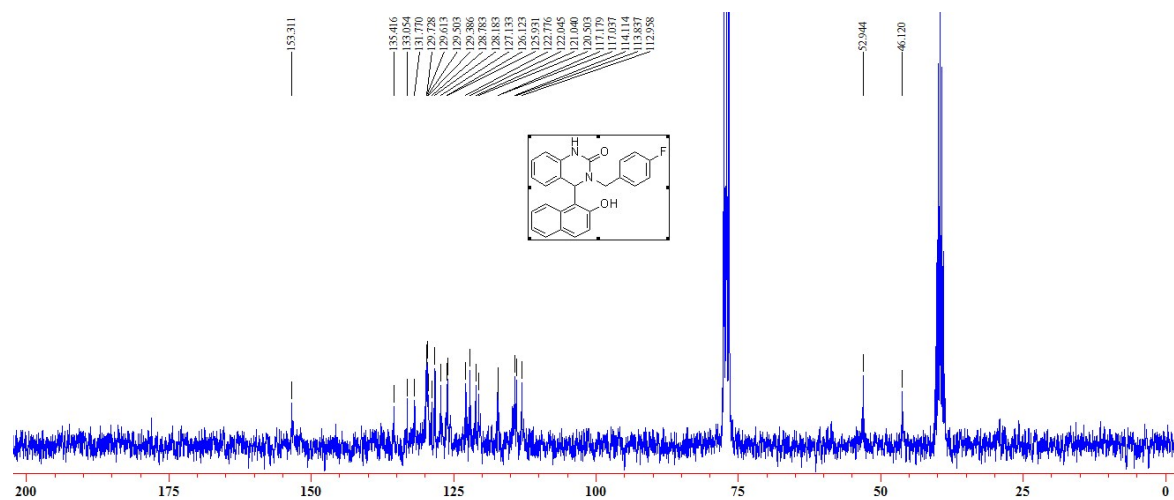


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6g

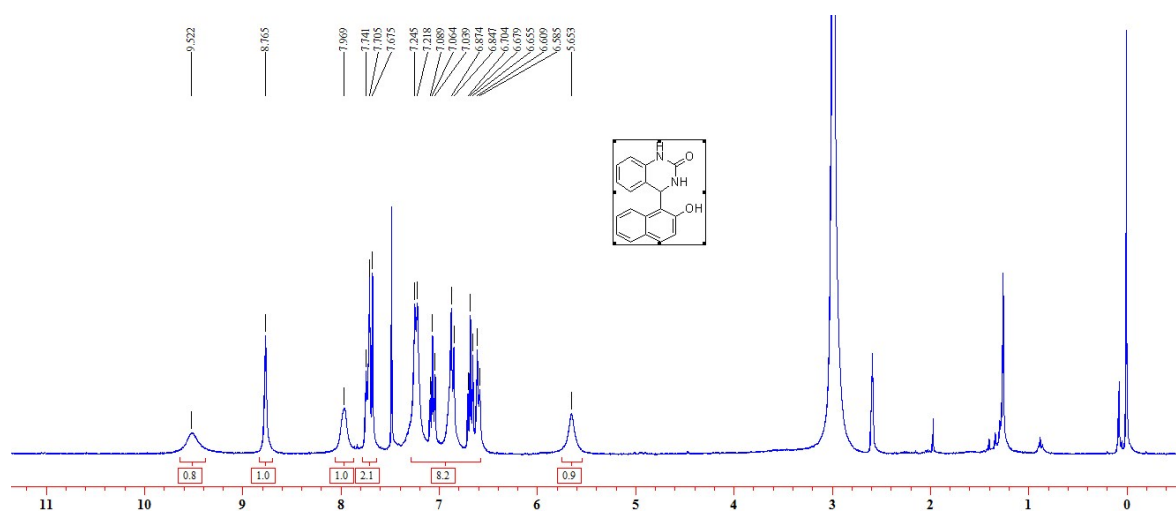


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

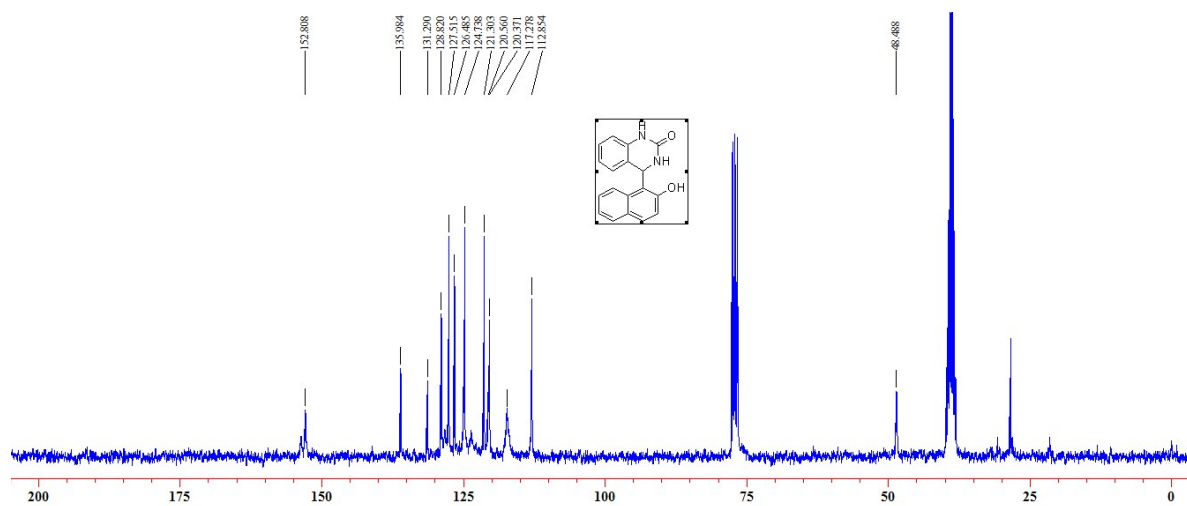


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6h

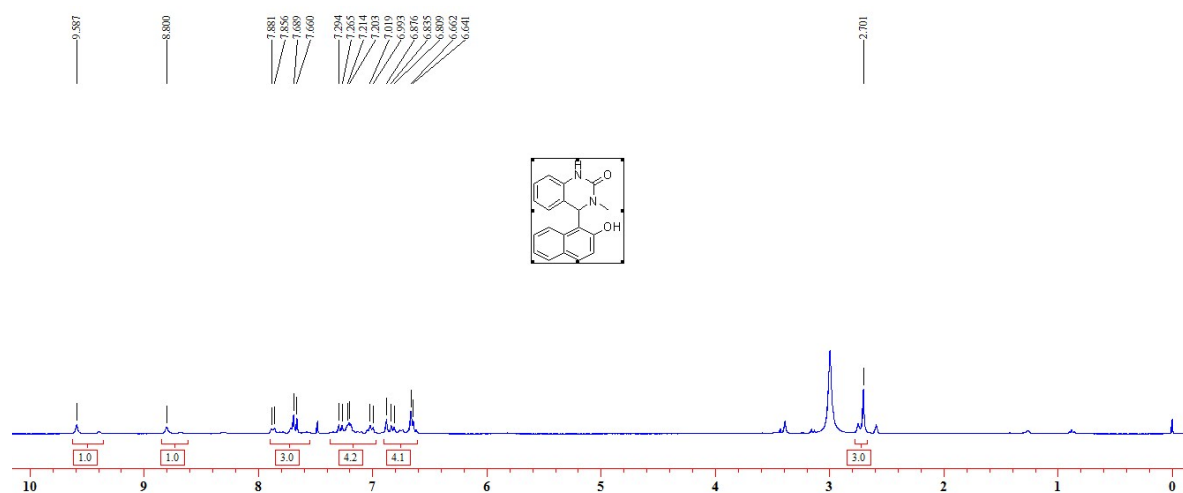


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

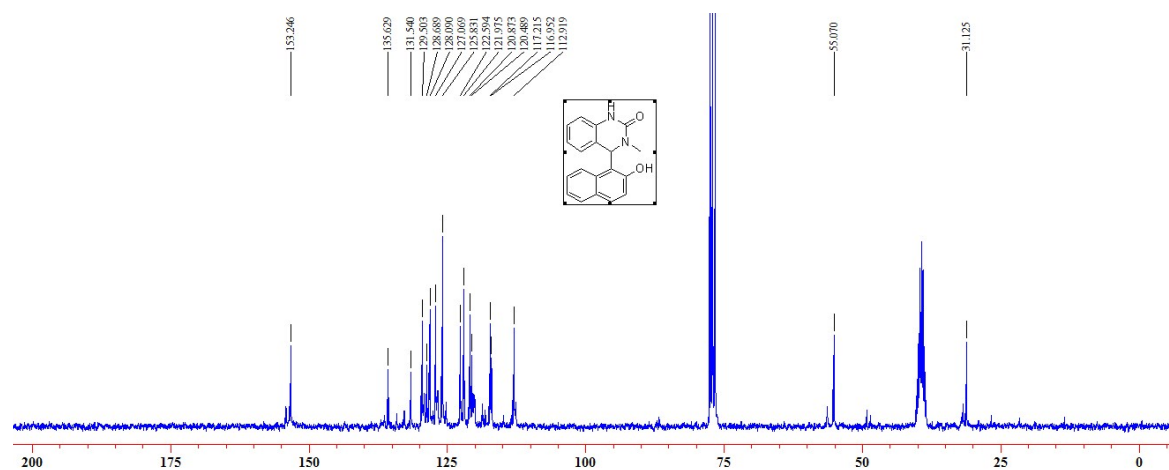


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6i

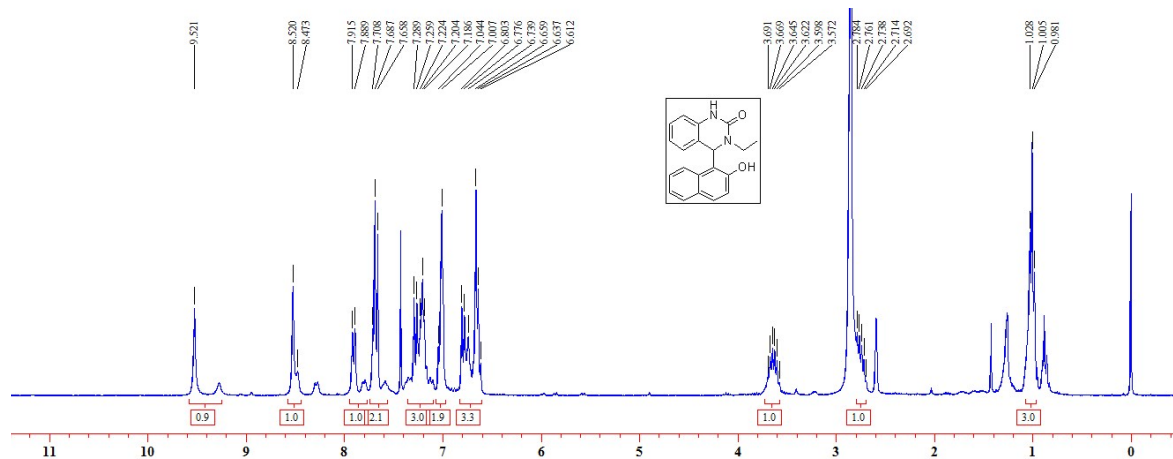


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

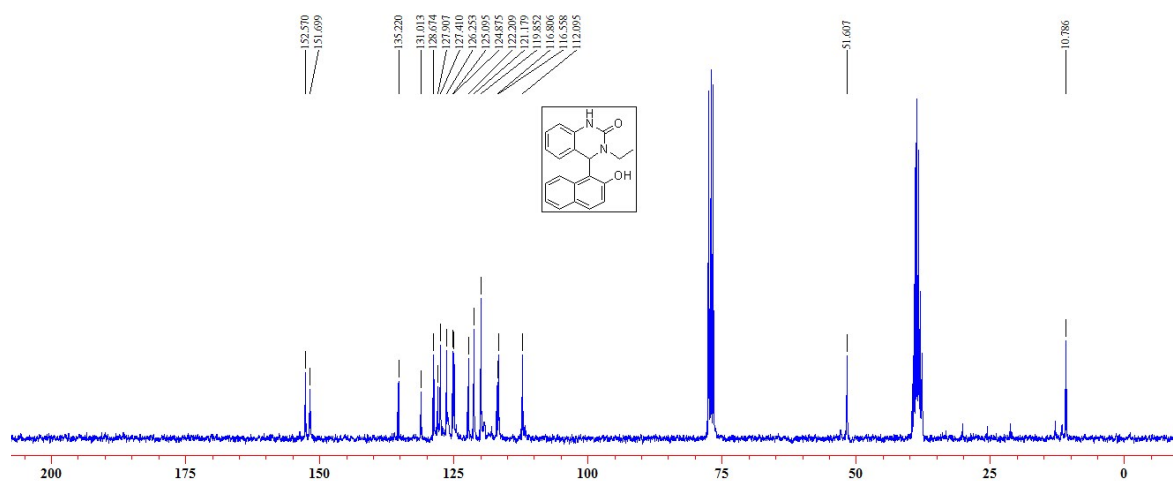


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6j

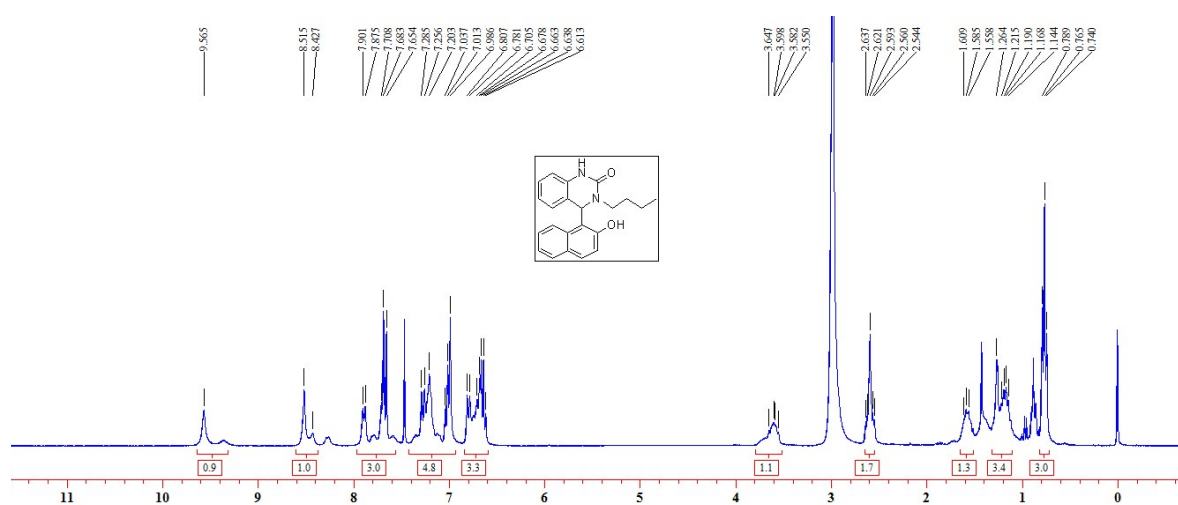


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

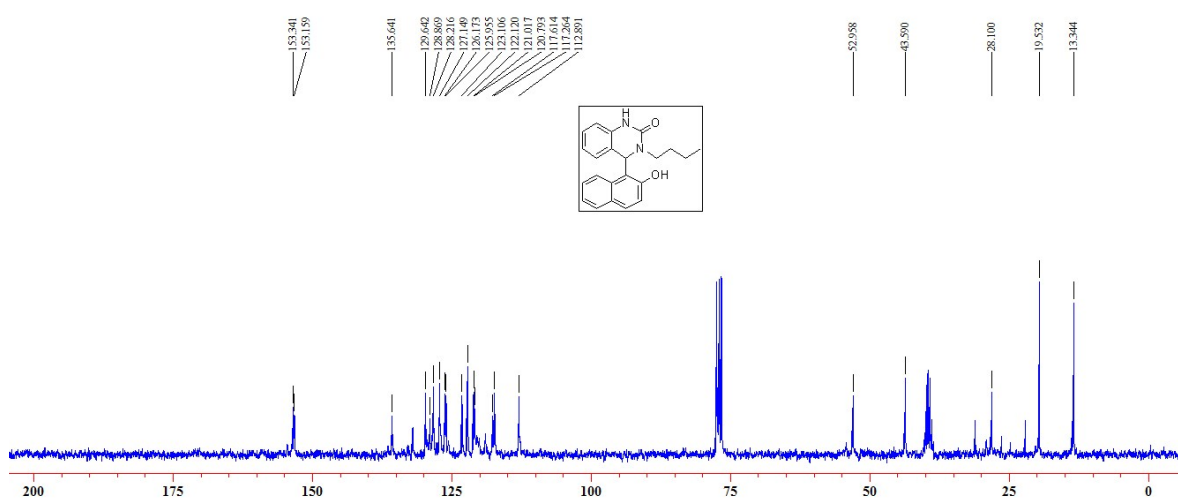


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6k

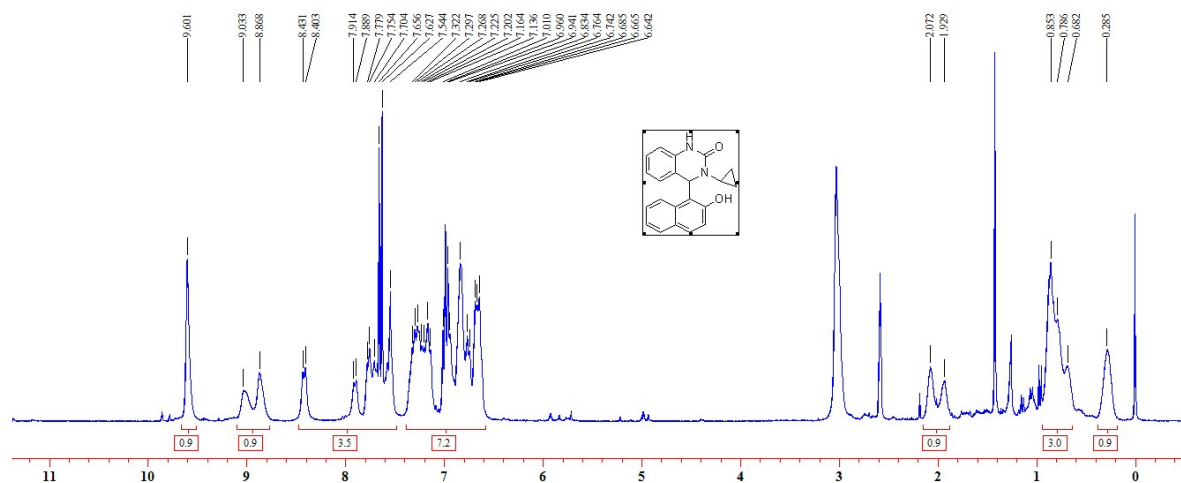


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

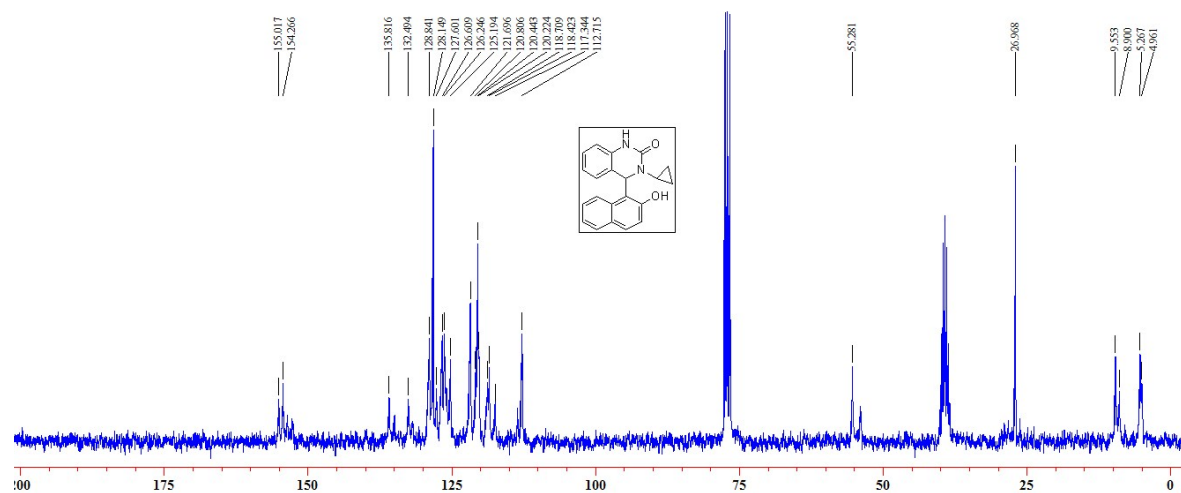


^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$)

^1H & ^{13}C NMR spectra of 6l

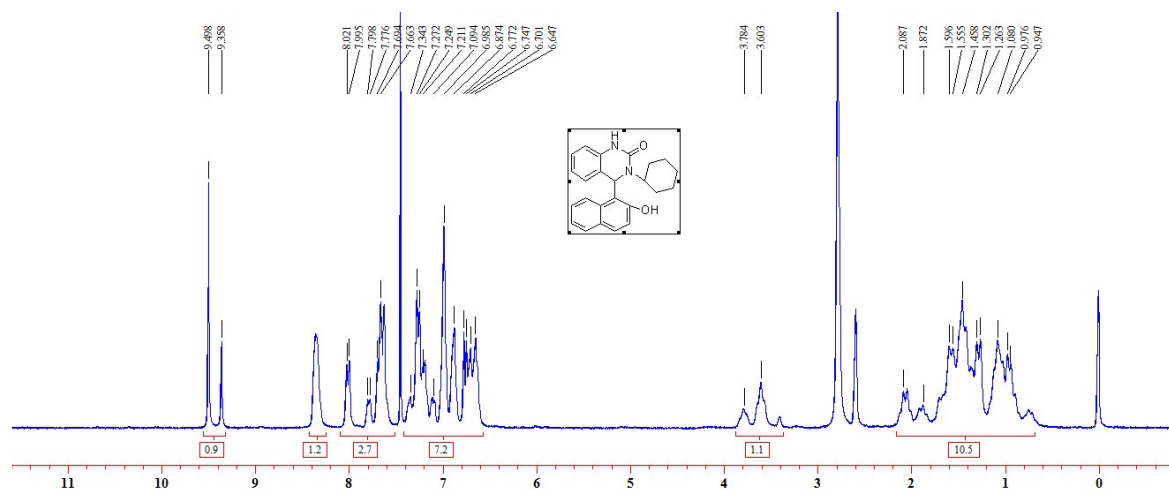


^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$)

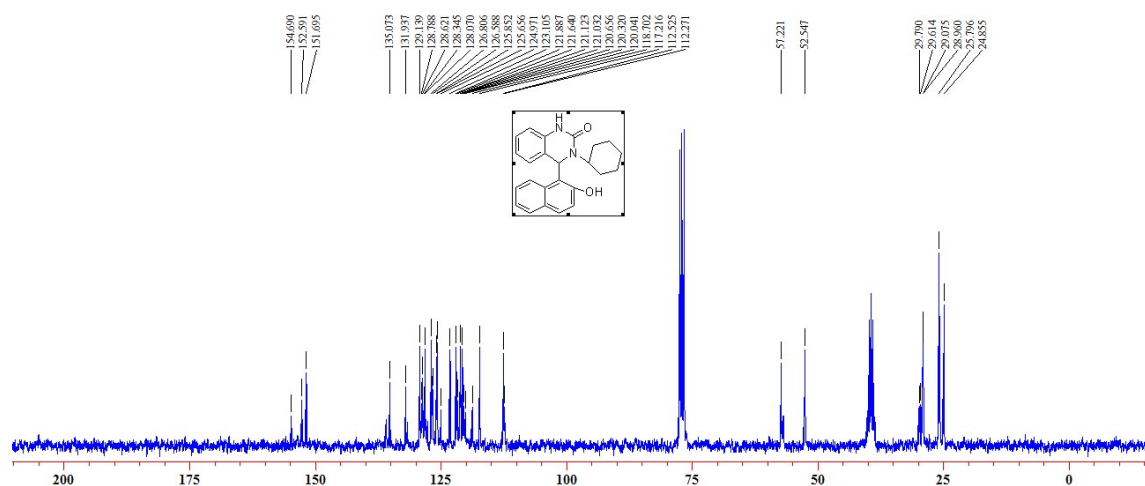


^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}-d_6$)

¹H & ¹³C NMR spectra of 6m

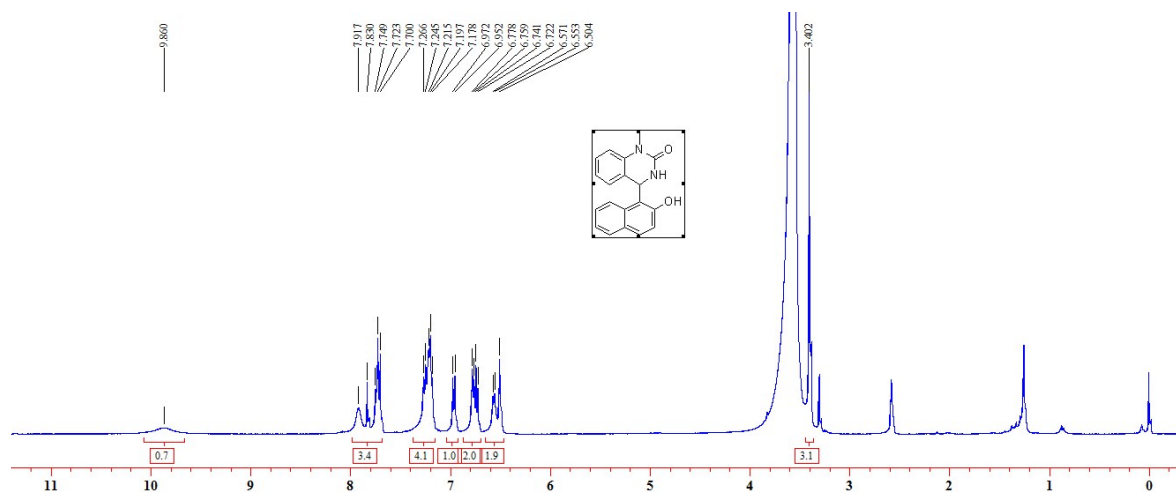


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

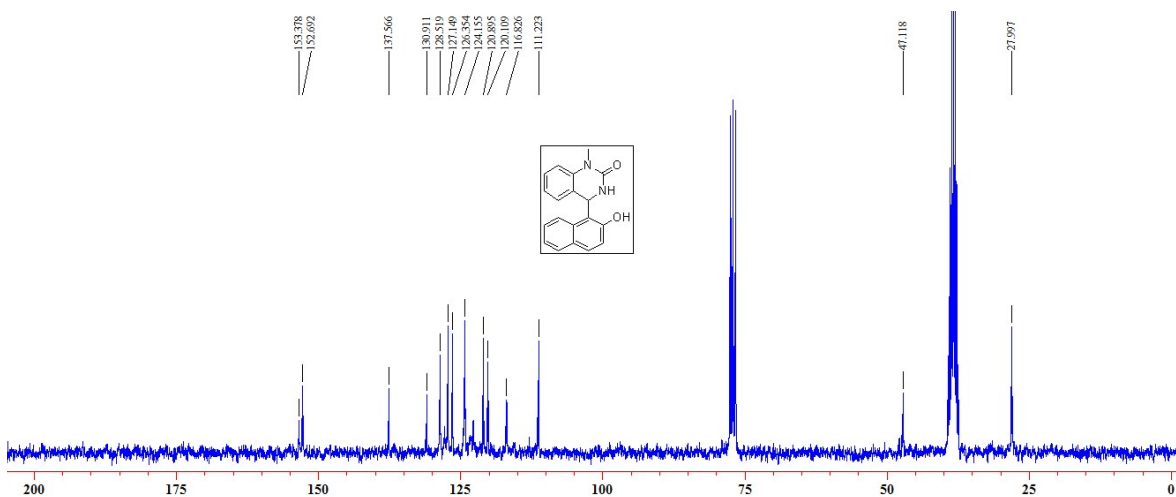


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6n

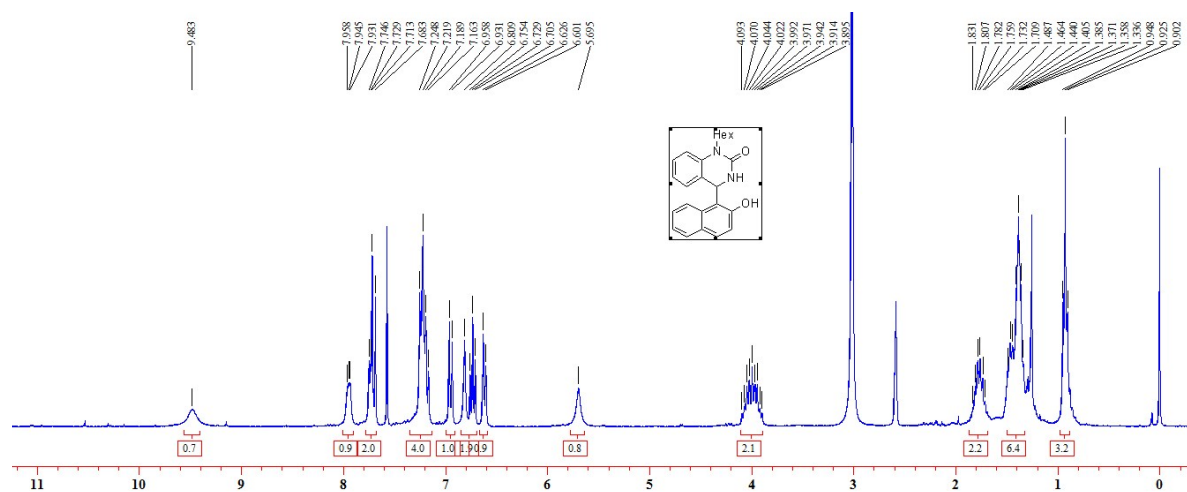


¹H NMR (400 MHz, CDCl₃+DMSO-d₆)

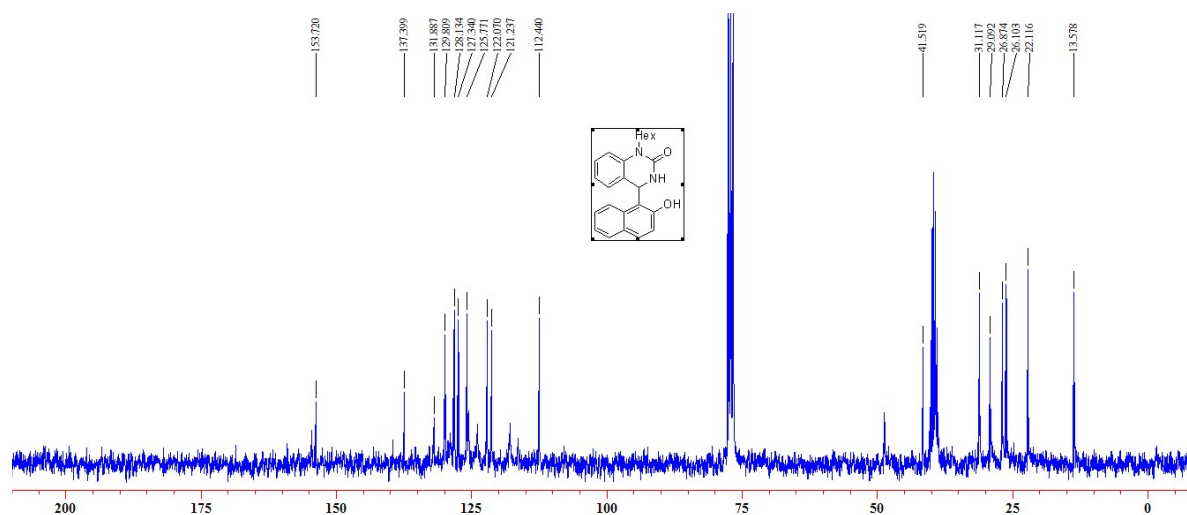


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6o

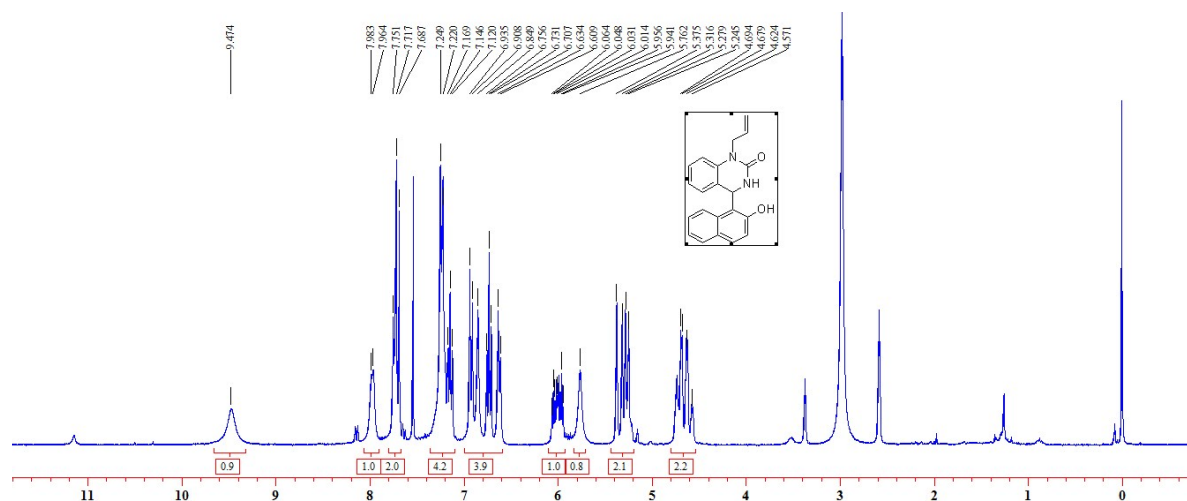


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

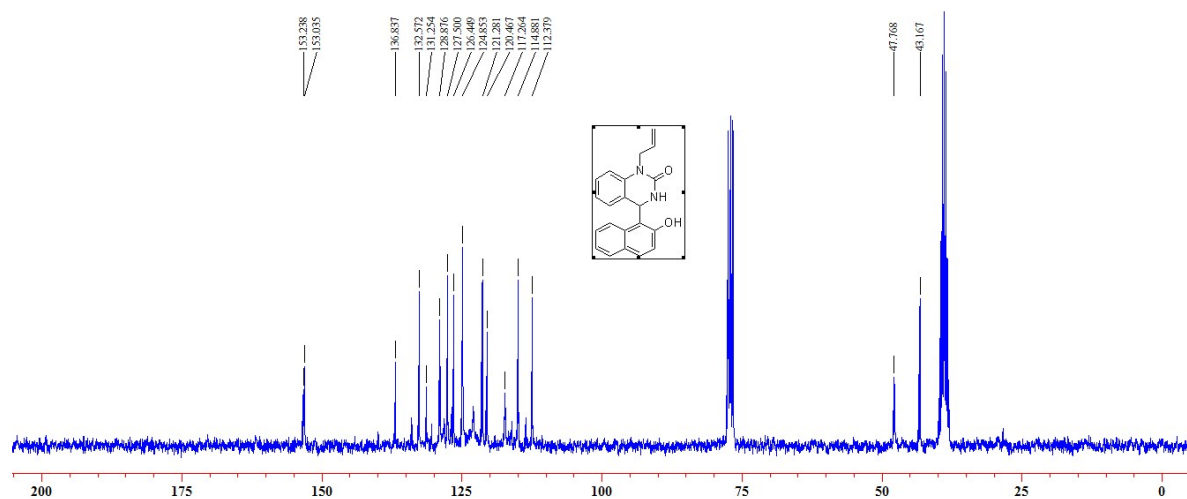


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6p

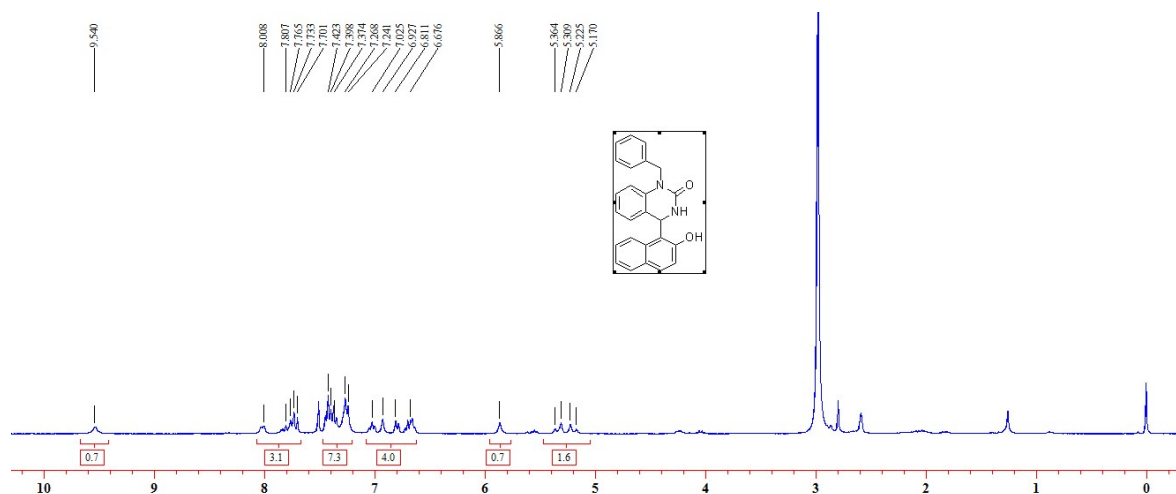


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

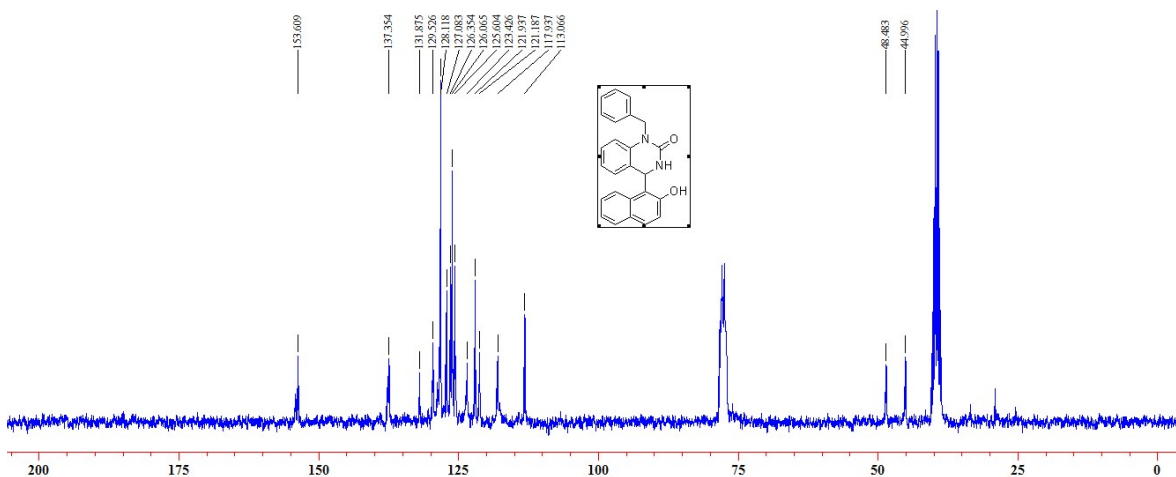


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 6q

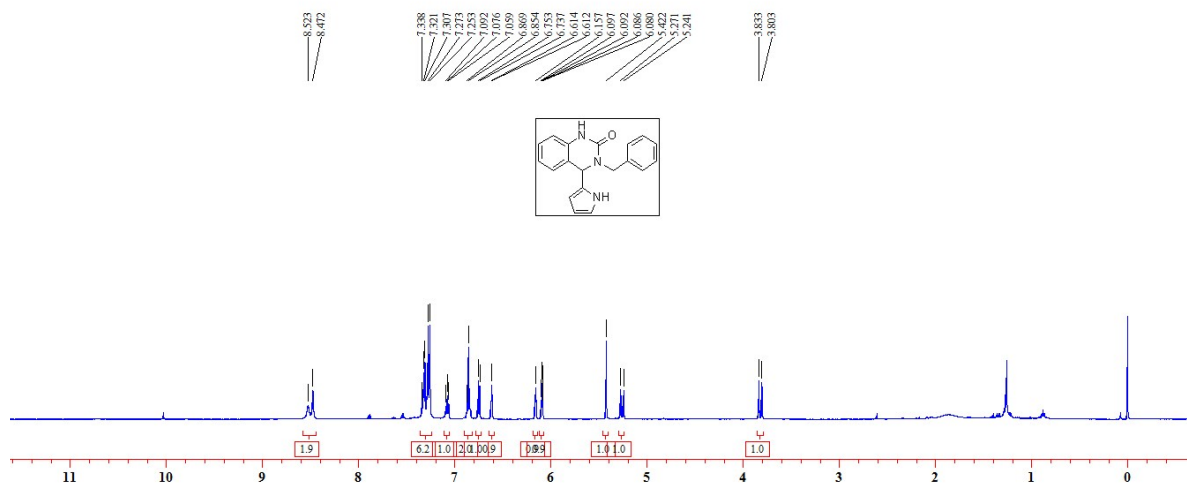


¹H NMR (300 MHz, CDCl₃+DMSO-d₆)

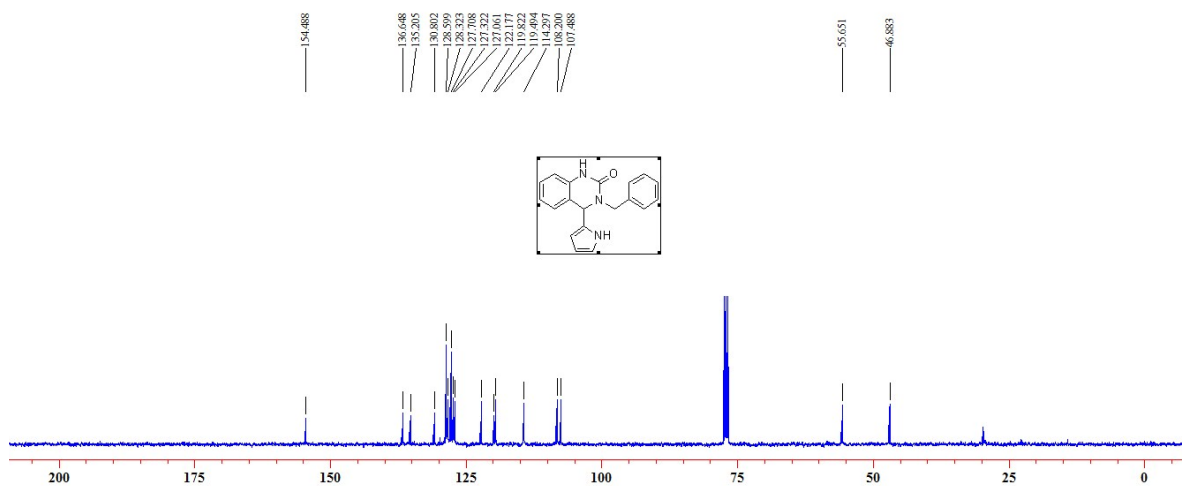


¹³C NMR (75 MHz, CDCl₃+DMSO-d₆)

¹H & ¹³C NMR spectra of 8



¹H NMR (500 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)

