Electronic Supplementary Material (ESI) for ChemComm.

Direct Alkylheteroarylation of Alkenes via Photoredox Mediated C-H Functionalization

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Supporting Information

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(A) Materials and equipment

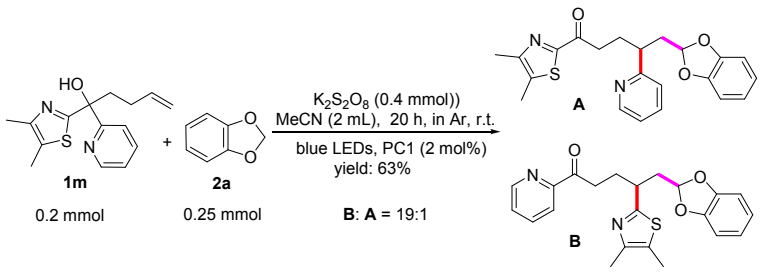
Reagents were obtained commercially and used as received. Solvents were purified and dried by standard methods. Substrates **1** were purchased from Kunming Traditional Chinese Medicine Co. Ltd. All title products were characterized by MS, ^{1}H NMR, ^{13}C NMR and High Resolution mass spectrometer (HRMS). ^{1}H NMR spectra were recorded on 400 MHz in $CDCl_3$, and ^{13}C NMR spectra were recorded on 100 MHz in $CDCl_3$ using tetramethylsilane (TMS) as an internal standard. Chemical shift values (δ) are given in ppm. Coupling constants (*J*) were measured in Hz. Mass spectra were obtained with ionization voltages of 70 eV. HRMS spectra were obtained by ESI on a TOF mass. 200-300 mesh silica gel was used for column chromatography.

(B) Typical experimental procedure for the synthesis of compounds 3:

To a Schlenk tube were added benzothiazole-substituted tertiary alcohol **1** (0.2 mmol), ethers **2** (0.25 mmol), **PC1** (2 mol%), MeCN (2.0 mL), $K_2S_2O_8$ (0.4 mmol). Then the tube was charged with argon, and was stirred at room temperature with the irradiation of a 5 W blue LED for about 16 h. After the reaction was finished, the reaction mixture was diluted in 40 mL ethyl acetate, washed with a saturated solution of $NaHCO_3$ (2 × 8 mL), a saturated solution of brine (10 mL), dried (Na_2SO_4) and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the products **3**.

(C) Experimental for migratory efficiency

To a Schlenk tube were added benzothiazole-substituted tertiary alcohol **1m** (0.2 mmol), ethers **2a** (0.25 mmol), **PC1** (2 mol%), MeCN (2.0 mL), $K_2S_2O_8$ (0.4 mmol). Then the tube was charged with argon, and was stirred at room temperature with the irradiation of a 5 W blue LED for about 20 h. After the reaction was finished, the reaction mixture was diluted in 40 mL ethyl acetate, washed with a saturated solution of $NaHCO_3$ (2 × 8 mL), a saturated solution of brine (10 mL), dried (Na_2SO_4) and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **A** and **B**.

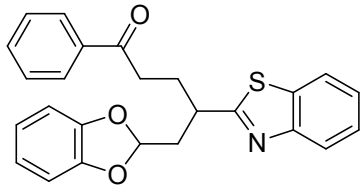


(D) Measurement of quantum yield

A 2 mL MeCN solution containing 29.5 mg **1a**, 12.5 mg **1b**, 54 mg $K_2S_2O_8$ and 2.3 mg **PC1** was irradiated under Ar using 455 nm LEDs of intensity 10 $mW \cdot cm^{-2}$ for 120 s. The light intensity was determined by a radiant power meter (Model 702060 with low noise thermopile probe, Oriel Instruments).

Ø = reactive photons per second/absorbed photons per second = 91%

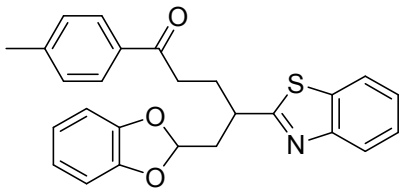
(E) Analytical data



3aa

5-(Benzo[d][1,3]dioxol-2-yl)-4-(benzo[d]thiazol-2-yl)-1-phenylpentan-1-one (3aa):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.99 (d, J = 7.2 Hz, 1H), 7.94-7.90 (m, 3H), 7.57-7.50 (m, 2H), 7.46-7.39 (m, 3H), 6.77-6.64 (m, 4H), 6.01 (t, J = 4.2 Hz, 1H), 3.74-3.63 (m, 1H), 3.01-2.90 (m, 3H), 2.57-2.53 (m, 1H), 2.34-2.23 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.9, 171.7, 153.1, 148.3, 148.2, 136.8, 134.4, 132.6, 128.7, 128.1, 126.2, 125.3, 123.0, 121.4, 120.9, 120.8, 110.1, 109.7, 108.1, 39.8, 38.4, 35.0, 29.2; LRMS (EI 70 ev) *m/z* (%): 415 (M^+, 100); HRMS m/z (ESI) calcd for $C_{25}H_{22}NO_3S$ $(M+H)^+$ 416.1326, found 416.1331.

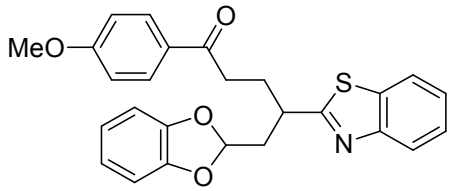


3ab

5-(Benzo[d][1,3]dioxol-2-yl)-4-(benzo[d]thiazol-2-yl)-1-p-tolylpentan-1-one (3ab):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (d, J = 7.2 Hz, 1H), 7.83 (d, J = 7.2 Hz, 1H), 7.71 (d, J = 7.6 Hz, 2H), 7.52-7.49 (m, 1H), 7.36-7.32 (m, 1H), 7.23 (d, J

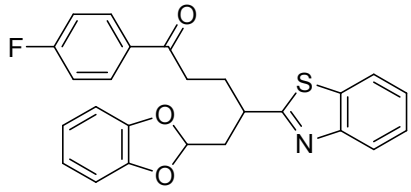
= 7.6 Hz, 2H), 6.80-6.74 (m, 3H), 6.73-6.70 (m, 1H), 6.01-5.98 (m, 1H), 3.76-3.64 (m, 1H), 3.03-2.98 (m, 2H), 2.93-2.89 (m, 1H), 2.55-2.51 (m, 1H), 2.39 (s, 3H), 2.36-2.25 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.7, 170.1, 153.2, 148.1, 148.0, 143.3, 134.3, 134.1, 129.1, 128.4, 126.2, 126.1, 125.1, 121.2, 120.0, 120.6, 110.0, 109.6, 108.1, 40.9, 38.6, 35.4, 29.3, 21.4; LRMS (EI 70 ev) *m/z* (%): 429 (M^+, 81); HRMS m/z (ESI) calcd for $C_{26}H_{24}NO_3S$ $(M+H)^+$ 430.1482, found 430.1476.



3ac

5-(Benzo[d][1,3]dioxol-2-yl)-4-(benzo[d]thiazol-2-yl)-1-(4-methoxyphenyl)pentan-1-one (3ac):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.98 (d, J = 7.6 Hz, 1H), 7.88-7.81 (m, 3H), 7.51-7.48 (m, 1H), 7.41-7.37 (m, 1H), 6.93 (d, J = 8.0 Hz, 1H), 6.75-6.70 (m, 3H), 6.69 (dd, J = 4.4 Hz, J = 0.8 Hz, 1H), 6.01 (dd, J = 4.0 Hz, J = 1.6 Hz, 1H), 3.85 (s, 3H), 3.72-3.60 (m, 1H), 2.97-2.90 (m, 2H), 2.87-2.82 (m, 1H), 2.51-2.47 (m, 1H), 2.31-2.20 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.4, 171.5, 163.2, 153.0, 148.1, 147.9, 136.5, 134.3, 131.1, 128.3, 126.2, 123.1, 122.7, 121.1, 120.2, 119.9, 111.1, 110.6, 108.0, 56.1, 40.1, 38.4, 35.2, 29.3; LRMS (EI 70 ev) *m/z* (%): 445 (M^+, 66); HRMS m/z (ESI) calcd for $C_{26}H_{24}NO_4S$ $(M+H)^+$ 446.1431, found 446.1437.

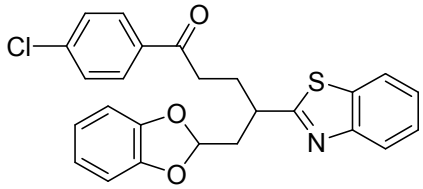


3ad

5-(Benzo[d][1,3]dioxol-2-yl)-4-(benzo[d]thiazol-2-yl)-1-(4-fluorophenyl)pentan-1-one (3ad):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.98 (d, J = 8.0 Hz, 1H), 7.89 (d, J = 7.6 Hz, 1H), 7.85-7.81 (m, 2H), 7.53-7.49 (m, 1H), 7.42 (m, 1H), 7.14 (t, J = 4.4 Hz, 2H), 6.80-6.72 (m, 4H), 6.01 (dd, J = 2.8 Hz, J = 3.2 Hz, 1H), 3.74-3.64 (m, 1H), 3.02-2.98 (m, 2H), 2.96-2.92 (m, 1H), 2.58-2.54 (m, 1H), 2.30-2.21 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.1, 172.0, 163.8, 161.3, 152.8, 148.1, 147.9, 134.3,

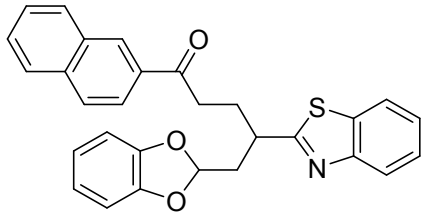
132.7, 132.6, 131.1, 131.0, 125.5, 124.9, 122.8, 121.4, 120.9, 120.6, 120.2, 115.4, 115.2, 111.0, 110.4, 108.1, 39.9, 38.4, 35.1, 29.3; LRMS (EI 70 ev) *m/z* (%): 433 (M^+, 90); HRMS m/z (ESI) calcd for $C_{25}H_{21}FNO_3S$ $(M+H)^+$ 434.1232, found 434.1227.



3ae

5-(Benzo[d][1,3]dioxol-2-yl)-4-(benzo[d]thiazol-2-yl)-1-(4-chlorophenyl)pentan-1-one (3ae):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (d, J = 7.2 Hz, 1H), 7.84 (d, J = 7.2 Hz, 1H), 7.78 (t, J = 7.0 Hz, 2H), 7.51-7.48 (m, 1H), 7.44-7.48 (m, 3H), 6.79-6.70 (m, 4H), 6.01-5.97 (m, 1H), 3.72-3.60 (m, 1H), 3.07-3.01 (m, 2H), 2.94-2.90 (m, 1H), 2.88-2.83 (m, 1H), 2.34-2.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 197.8, 172.0, 152.9, 148.1, 147.9, 138.6, 135.3, 134.4, 129.0, 128.3, 126.0, 125.0, 123.1, 121.5, 120.4, 120.0, 110.2, 109.8, 108.1, 40.2, 38.2, 35.4, 29.2; LRMS (EI 70 ev) *m/z* (%): 449 (M^+, 71); HRMS m/z (ESI) calcd for $C_{25}H_{21}ClNO_3S$ $(M+H)^+$ 450.0937, found 450.0932.

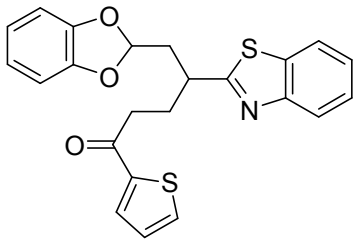


3af

5-(Benzo[d][1,3]dioxol-2-yl)-4-(benzo[d]thiazol-2-yl)-1-(naphthalen-2-yl)pentan-1-one (3af):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.29 (s, 1H), 8.00 (d, J = 8.0 Hz, 1H), 7.92 (dd, J = 0.8 Hz, J = 3.2 Hz, 1H), 7.86-7.80 (m, 4H), 7.57-7.54 (m, 1H), 7.48-7.43 (m, 2H), 7.41-7.38 (m, 1H), 6.76-6.69 (m, 4H), 6.02 (dd, J = 2.4 Hz, J = 5.2 Hz, 1H), 3.74-3.64 (m, 1H), 3.03-2.97 (m, 2H), 2.94-2.90 (m, 1H), 2.60-2.55 (m, 1H), 2.33-2.24 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.4, 171.8, 153.0, 148.2, 148.0, 135.3, 134.7, 134.5, 132.3, 129.5, 128.3, 128.2, 127.6, 126.8, 126.4, 125.7, 123.6, 123.3, 121.5, 120.6, 120.4, 119.8, 110.0, 109.7, 108.2, 40.1, 38.1, 35.1, 29.5; LRMS (EI 70 ev) *m/z* (%): 465 (M^+, 100); HRMS m/z (ESI) calcd for $C_{29}H_{24}NO_3S$ $(M+H)^+$

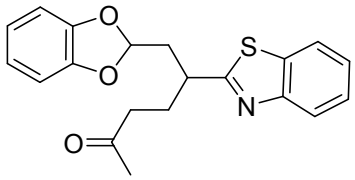
466.1481, found 466.1484.



3ag

5-(Benzo[d][1,3]dioxol-2-yl)-4-(benzo[d]thiazol-2-yl)-1-(thiophen-2-yl)pentan-1-one (3ag):

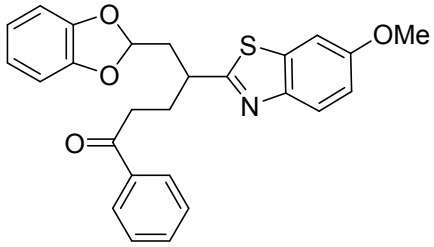
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.00 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 7.6 Hz, 1H), 7.61 (d, J = 4.0 Hz, 2H), 7.51 (t, J = 7.8 Hz, 1H), 7.42 (t, J = 7.4 Hz, 1H), 7.08 (d, J = 4.2 Hz, 1H), 6.78-6.71 (m, 4H), 6.01 (dd, J = 3.2 Hz, J = 3.6 Hz, 1H), 3.44-3.39 (m, 1H), 2.98-2.94 (m, 2H), 2.90-2.85 (m, 1H), 2.56-2.51 (m, 1H), 2.33-2.81 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 191.7, 172.0, 153.2, 148.1, 147.8, 143.4, 134.8, 133.6, 132.0, 128.1, 125.9, 125.1, 122.9, 121.5, 120.3, 120.0, 110.0, 109.7, 108.2, 42.0, 38.2, 35.1, 29.3; LRMS (EI 70 ev) *m/z* (%): 421 (M^+, 100); HRMS m/z (ESI) calcd for $C_{23}H_{20}NO_3S_2$ $(M+H)^+$ 422.0890, found 422.0898.



3ah

6-(Benzo[d][1,3]dioxol-2-yl)-5-(benzo[d]thiazol-2-yl)hexan-2-one (3ah):

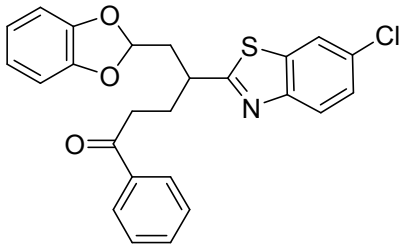
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.98 (d, J = 8.0 Hz, 1H), 7.83 (d, J = 7.6 Hz, 1H), 7.50-7.46 (m, 1H), 7.41-7.38 (m, 1H), 6.77-6.70 (m, 4H), 6.01-5.98 (m, 1H), 3.71-3.63 (m, 1H), 2.99-2.94 (m, 2H), 2.92-2.88 (m, 1H), 2.53-2.49 (m, 1H), 2.39-2.30 (m, 2H), 2.27(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 207.1, 172.0, 153.0, 148.1, 147.7, 134.1, 126.1, 125.0, 123.3, 121.4, 120.4, 120.1, 110.2, 109.9, 108.0, 42.1, 39.9, 38.0, 35.2, 29.7; LRMS (EI 70 ev) *m/z* (%): 353 (M^+, 100); HRMS m/z (ESI) calcd for $C_{20}H_{20}NO_3S$ $(M+H)^+$ 354.1171, found 354.1168.



3ai

5-(Benzo[d][1,3]dioxol-2-yl)-4-(6-methoxybenzo[d]thiazol-2-yl)-1-phenylpentan-1-one (3ai):

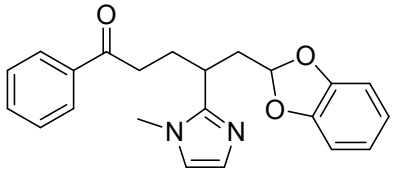
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.91-7.86 (m, 3H), 7.60 (d, J = 7.2 Hz, 1H), 7.46-7.41 (m, 2H), 7.32 (d, J = 3.2 Hz, 1H), 7.10 (dd, J = 0.8 Hz, J = 6.4 Hz, 1H), 6.73-6.67 (m, 4H), 6.02-5.99 (m, 1H), 3.83 (s, 3H), 3.74-3.65 (m, 1H), 2.97-2.92 (m, 2H), 2.90-2.86 (m, 1H), 255-2.51 (m, 1H), 2.38-2.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.2, 171.5, 156.7, 148.2, 148.0, 147.4, 136.2, 135.7, 133.0, 128.4, 127.8, 126.0, 123.1, 120.2, 119.8, 115.1, 110.0, 109.5, 108.1, 56.1, 41.9, 38.3, 35.1, 29.5; LRMS (EI 70 ev) *m/z* (%): 445 (M^+, 79); HRMS m/z (ESI) calcd for $C_{26}H_{24}NO_4S$ $(M+H)^+$ 446.1431, found 446.1435.



3aj

5-(Benzo[d][1,3]dioxol-2-yl)-4-(6-chlorobenzo[d]thiazol-2-yl)-1-phenylpentan-1-one (3aj):

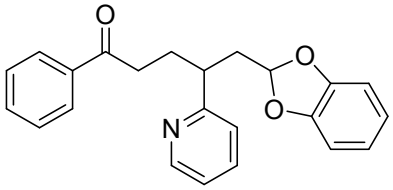
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.01 (d, J = 7.6 Hz, 1H), 7.90-7.86 (m, 2H), 7.81 (s, 1H), 7.56-7.52 (m, 1H), 7.47-7.43 (m, 2H), 7.42 (d, J = 7.2 Hz, 1H), 6.74-6.66 (m, 4H), 6.02 (dd, J = 1.6 Hz, J = 2.8 Hz,1H), 3.75-3.66 (m, 1H), 2.94-2.88 (m, 3H), 2.56-2.52 (m, 1H), 2.37-2.31 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.4, 172.7, 151.9, 148.4, 148.1, 136.3, 133.5, 132.6, 131.1, 128.4, 126.3, 125.0, 123.1, 121.0, 1204, 120.1, 110.4, 109.9, 108.2, 40.1, 38.3, 35.0, 29.6; LRMS (EI 70 ev) *m/z* (%): 449 (M^+, 74); HRMS m/z (ESI) calcd for $C_{25}H_{21}ClNO_3S$ $(M+H)^+$ 450.0937, found 450.0939.



3ak

5-(Benzo[d][1,3]dioxol-2-yl)-4-(1-methyl-1H-imidazol-2-yl)-1-phenylpentan-1-one (3ak):

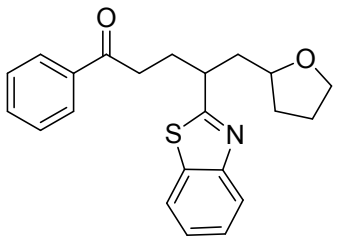
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.90-7.86 (m, 2H), 7.56-7.51 (m, 1H), 7.44-7.40 (m, 2H), 6.97 (d, J = 0.8 Hz, 1H), 6.79-6.71 (m, 5H), 5.99 (dd, J = 1.6 Hz, J = 4.0 Hz, 1H), 3.50 (s, 3H), 3.43-3.35 (m, 1H), 3.04-2.97 (m, 2H), 2.94-2.90 (m, 1H), 2.55-2.50 (m, 1H), 2.32-2.21 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.7, 148.2, 147.8, 147.1, 136.0, 132.5, 128.0, 127.4, 126.9, 120.8, 120.2, 119.7, 110.3, 109.8, 107.8, 41.7, 34.9, 31.2, 29.4, 28.9; LRMS (EI 70 ev) *m/z* (%): 362 (M^+, 100); HRMS m/z (ESI) calcd for $C_{22}H_{23}N_2O_3$ $(M+H)^+$ 363.1714, found 363.1710.



3al

5-(Benzo[d][1,3]dioxol-2-yl)-1-phenyl-4-(pyridin-2-yl)pentan-1-one (3al):

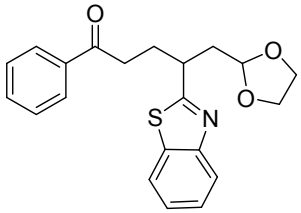
Pale yellow oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.51 (d, J = 4.8 Hz, 1H), 7.85 (d, J = 7.6 Hz, 1H), 7.66-7.58 (m, 1H), 7.34 (dd, J = 7.6 Hz, J = 6.4 Hz, 3H), 7.23-7.14 (m, 3H), 6.86-6.70 (m, 4H), 5.92 (dd, J = 3.6 Hz, J = 2.8 Hz, 1H), 3.34-3.19 (m, 1H), 2.91-2.75 (m, 2H), 2.61-2.54 (m, 1H), 2.35-2.30 (m, 1H), 2.26-2.17 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 199.7, 163.3, 149.6, 147.5, 147.3, 138.6, 137.0, 132.9, 128.4, 128.2, 127.9, 126.8, 121.2, 120.4, 110.1, 109.0, 108.4, 40.3, 36.0, 31.9, 29.6; LRMS (EI 70 ev) *m/z* (%): 359 (M^+, 100); HRMS m/z (ESI) calcd for $C_{23}H_{22}NO_3$ $(M+H)^+$ 360.1605, found 360.1601.



3ba

4-(Benzo[d]thiazol-2-yl)-5-(tetrahydrofuran-2-yl)-1-phenylpentan-1-one (3ba):

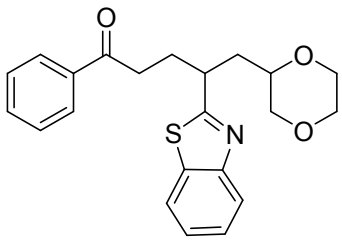
Pale yellow oil, (1:1.4 dr), ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.02 (d, J = 8.0 Hz, 1H), 7.88-7.84 (m, 3H), 7.51-7.46 (m, 2H), 7.41-7.37 (m, 3H), 3.90-3.83 (m, 1H), 3.75-3.66 (m, 3H), 3.58-3.44 (m, 1H), 3.02-2.92 (m, 3H), 2.60-2.56 (m, 0.45H), 2.22-2.17 (m, 0.54H), 2.06-1.79 (m, 4H), 1.54-1.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 199.55, 199.52, 175.7, 175.3, 153.1, 153.0, 136.7, 136.6, 134.7, 134.6, 133.0, 132.9, 128.5, 128.4, 128.0, 127.8, 126.0, 125.9, 124.89, 124.86, 122.8, 122.7, 121.6, 76.6, 76.4, 67.6, 67.5, 42.4, 42.3, 42.0, 41.9, 36.1, 36.0, 31.6, 31.3, 30.9, 30.8, 25.6, 25.5; LRMS (EI 70 ev) *m/z* (%): 365 (M^+, 100); HRMS m/z (ESI) calcd for $C_{22}H_{24}NO_2S$ $(M+H)^+$ 366.1526, found 366.1531.



3ca

4-(Benzo[d]thiazol-2-yl)-5-(1,3-dioxolan-2-yl)-1-phenylpentan-1-one (3ca):

Pale yellow oil, (1:1.4 dr), ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.99 (d, J = 8.4 Hz, 1H), 7.87 (d, J = 7.2 Hz, 1H), 7.82-7.78 (m, 2H), 7.58-7.50 (m, 2H), 7.42-7.36 (m, 3H), 4.92-4.86 (m, 1H), 3.99-3.91 (m, 1H), 3.88-3.73 (m, 3H), 3.70-3.61 (m, 1H), 3.18-3.04 (m, 3H), 2.56-2.46 (m, 1H), 2.30-2.17 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 199.4, 172.9, 153.0, 136.7, 134.5, 133.0, 128.5, 127.9, 126.1, 125.1, 122.8, 121.6, 102.7, 65.8, 65.7, 41.7, 35.1, 30.9, 29.3; LRMS (EI 70 ev) *m/z* (%): 367 (M^+, 100); HRMS m/z (ESI) calcd for $C_{21}H_{22}NO_3S$ $(M+H)^+$ 368.1318, found 368.1325.

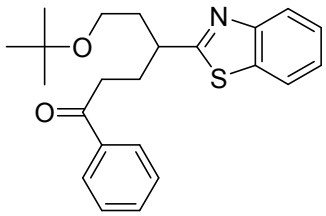


3da

4-(Benzo[d]thiazol-2-yl)-5-(1,4-dioxan-2-yl)-1-phenylpentan-1-one (3da):

Yellow oil, (1:1.5 dr); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.03 (d, J = 8.0 Hz, 1H), 7.90-7.69 (m, 3H), 7.53-7.48 (m, 2H), 7.43-7.35 (m, 3H), 3.73-3.68 (m, 1H), 3.65-3.59 (m, 2H), 3.51-3.44 (m, 1H), 3.35-3.27 (m, 2H), 3.03-2.96 (m, 3H), 2.61-2.56 (m,

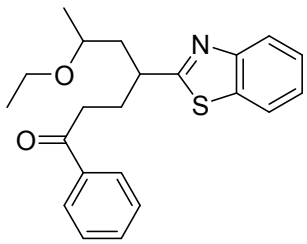
2H), 2.33-2.16 (m, 1H), 1.95-1.86 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 199.3, 199.2, 175.0, 174.4, 153.1, 152.9, 136.6, 135.6, 134.63, 134.60, 133.0, 133.0, 128.49, 128.41, 127.9, 127.6, 126.0, 125.0, 124.9, 123.0, 122.7, 121.68, 121.61, 72.9, 72.6, 71.1, 71.0, 66.67, 66.63, 66.4, 66.3, 40.0, 39.8, 37.8, 37.7, 36.1, 35.9, 30.7, 29.9; LRMS (EI 70 ev) *m/z* (%): 381 (M^+, 100); HRMS m/z (ESI) calcd for $C_{22}H_{24}NO_3S$ $(M+H)^+$ 382.1475, found 382.1478.



3ea

6-*tert*-Butoxy-4-(benzo[d]thiazol-2-yl)-1-phenylhexan-1-one (3ea):

Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.01 (d, J = 8.4 Hz, 1H), 7.87 (t, J = 4.2 Hz, 1H), 7.54-7.46 (m, 2H), 7.42-7.36 (m, 3H), 3.83-3.80 (m, 1H), 3.49-3.41 (m, 2H), 3.04-2.94 (m, 3H), 2.68-2.53 (m, 1H), 2.32-2.14 (m, 2H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.4, 172.1, 152.9, 136.4, 134.6, 133.9, 128.4, 127.4, 126.1, 125.1, 122.9, 121.7, 78.1, 64.3, 39.4, 38.7, 35.2, 29.3, 28.6; LRMS (EI 70 ev) *m/z* (%): 381 (M^+, 100); HRMS m/z (ESI) calcd for $C_{23}H_{28}NO_2S$ $(M+H)^+$ 382.1841, found 382.1837.

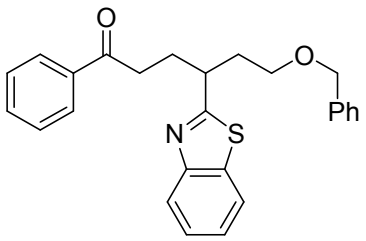


3fa

4-(Benzo[d]thiazol-2-yl)-6-ethoxy-1-phenylheptan-1-one (3fa):

Pale yellow oil, (1:1.3 dr); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.01 (d, J = 8.0 Hz, 1H), 7.88-7.82 (m, 3H), 7.52-7.44 (m, 2H), 3.67-3.57 (m, 1H), 3.49-3.41 (m, 1H), 3.32-3.24 (m, 1H), 3.07-2.97 (m, 2H), 2.61-2.51 (m, 2H), 2.29-2.15 (m, 3H), 1.21 (t, J = 6.0 Hz, 3H), 1.13-1.10 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 199.1, 198.8, 1728, 172.4, 153.8, 153.3, 136.8, 136.4, 135.1, 134.8, 133.3, 133.0, 128.7, 128.4, 127.9, 127.5, 126.5, 126.2, 125.1, 124.8, 123.3, 123.0, 121.8, 121.4, 72.8, 72.4, 64.2, 63.9,

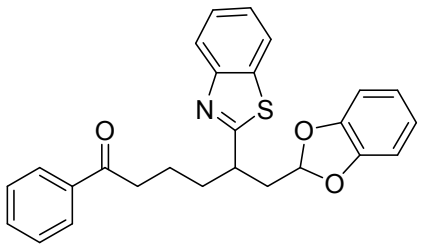
40.1, 39.8, 38.5, 38.1, 35.4, 35.1, 29.7, 29.4, 20.3, 20.1, 15.6, 15.5; LRMS (EI 70 ev) *m/z* (%): 367 (M^+, 100); HRMS m/z (ESI) calcd for $C_{22}H_{26}NO_2S$ $(M+H)^+$ 368.1682, found 368.1685.



3ga

4-(Benzo[d]thiazol-2-yl)-6-(benzyloxy)-1-phenylhexan-1-one (3ga):

Yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ: 8.00 (d, J = 8.0 Hz, 1H), 7.88 (dd, J = 7.2 Hz, J = 1.2 Hz, 3H), 7.53-7.47 (m, 2H), 7.43-7.38 (m, 3H), 7.37-7.30 (m, 5H), 4.49 (s, 2H), 3.74-3.67 (m, 1H), 3.47-3.41 (m, 2H), 3.04-2.97 (m, 3H), 2.45-2.37 (m, 1H), 2.33-2.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.7, 172.5, 153.1, 138.0, 136.5, 134.6, 133.2, 128.6, 128.3, 128.0, 127.7, 127.5, 126.3, 125.3, 122.9, 121.8, 74.8, 65.4, 42.7, 35.8, 31.3, 29.5; LRMS (EI 70 ev) *m/z* (%): 415 (M^+, 100); HRMS m/z (ESI) calcd for $C_{26}H_{26}NO_2S$ $(M+H)^+$ 416.1681, found 416.1678.

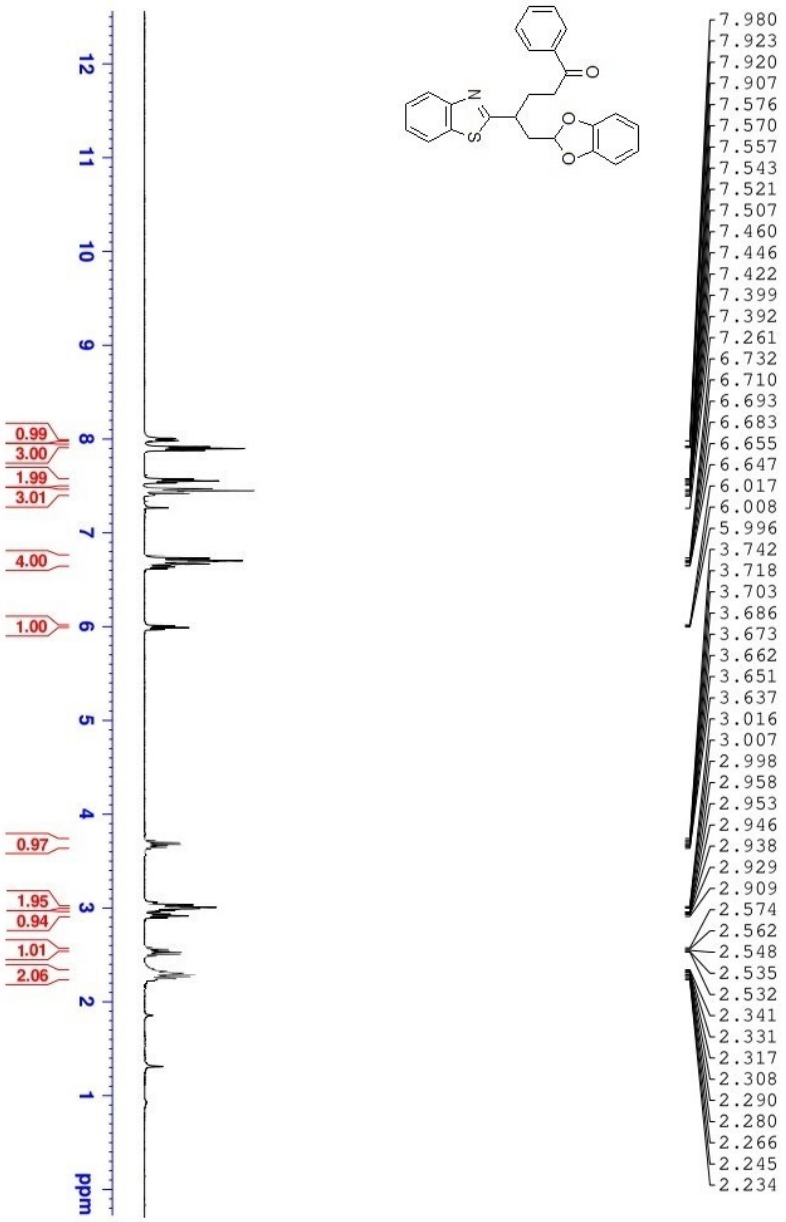


5aa

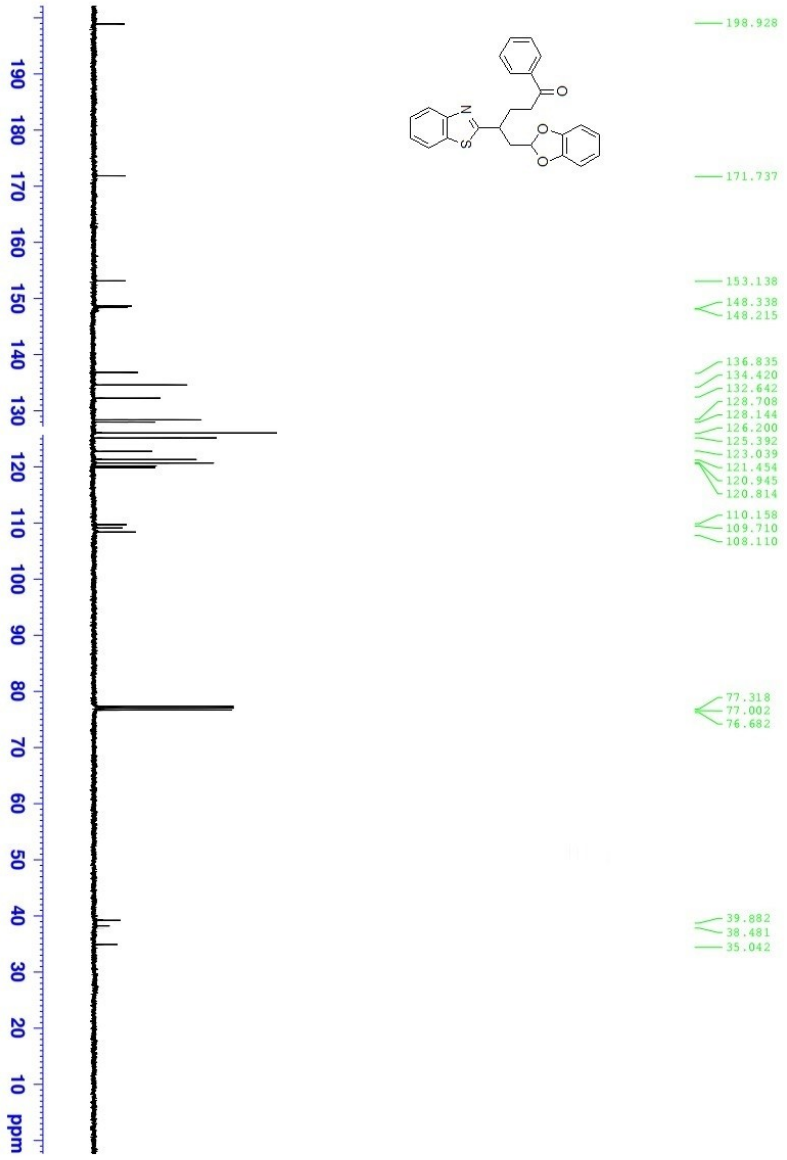
6-(Benzo[d][1,3]dioxol-2-yl)-5-(benzo[d]thiazol-2-yl)-1-phenylhexan-1-one (5aa):

Yellow oil, ^1H NMR (400 MHz, $CDCl_3$) δ: 8.01 (d, J = 8.4 Hz, 1H), 7.91-7.85 (m, 3H), 7.55-7.48 (m, 2H), 7.43-7.39 (m, 3H), 6.75-6.65 (m, 4H), 6.01 (dd, J = 2.0 Hz, J = 4.0 Hz, 1H), 3.65-3.58 (m, 1H), 3.02-2.88 (m, 3H), 2.70-2.58 (m, 1H), 2.08-1.97 (m, 2H), 1.84-1.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 199.2, 173.1, 152.0, 148.1, 147.7, 136.0, 133.8, 132.3, 128.0, 127.7, 125.4, 124.9, 122.5, 121.0, 120.2, 119.8, 110.2, 109.7, 108.2, 41.3, 38.7, 37.8, 34.9, 21.1; LRMS (EI 70 ev) *m/z* (%): 429 (M^+, 62); HRMS m/z (ESI) calcd for $C_{26}H_{24}NO_3S$ $(M+H)^+$ 430.1482, found 430.1480.

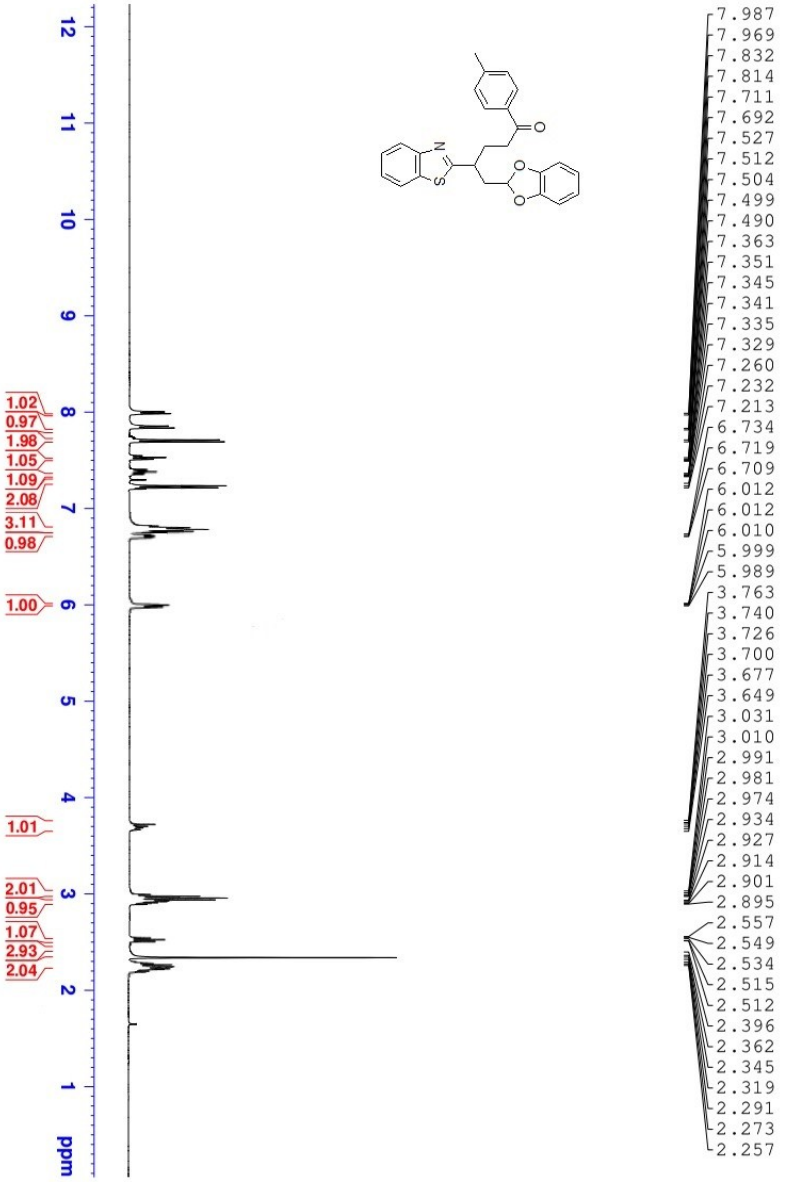
(F) Spectra



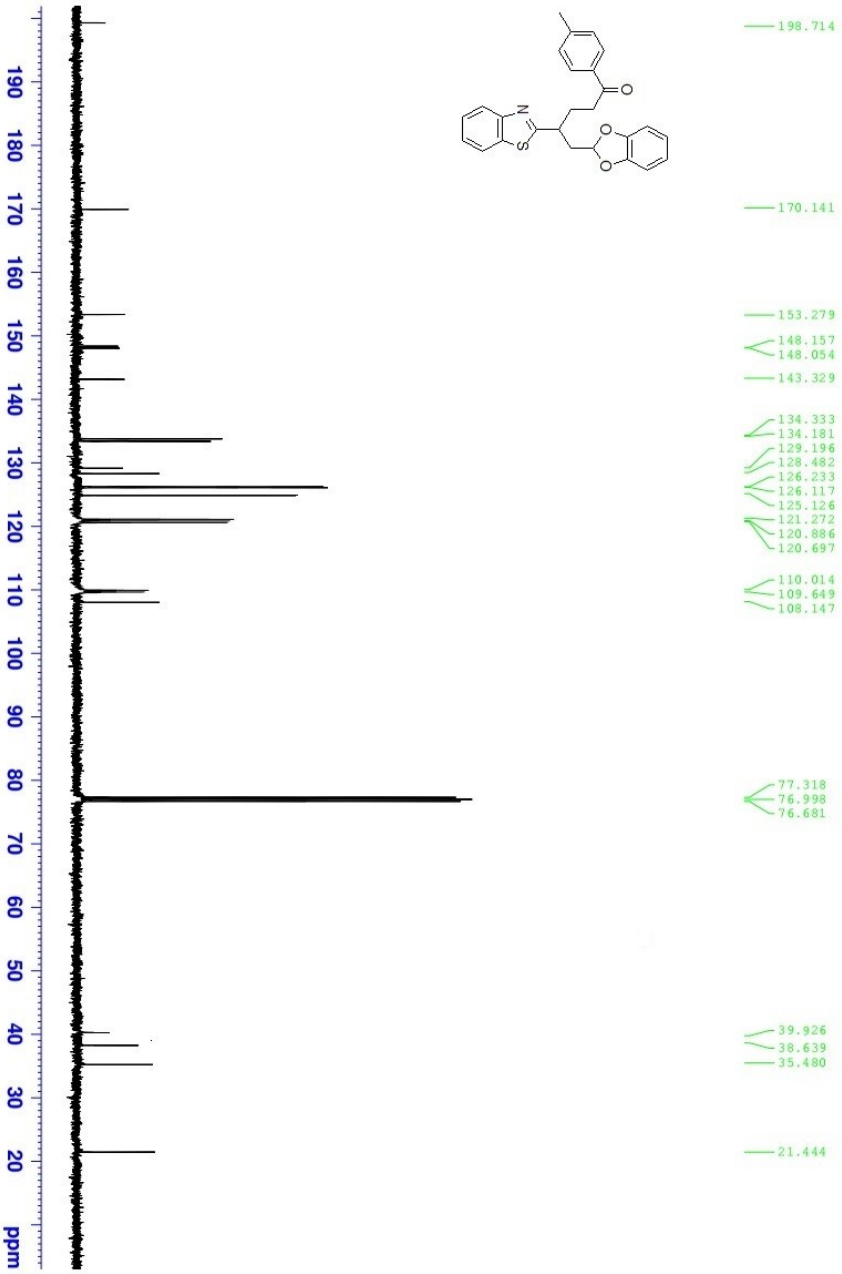
^{1}H NMR of Compound 3aa



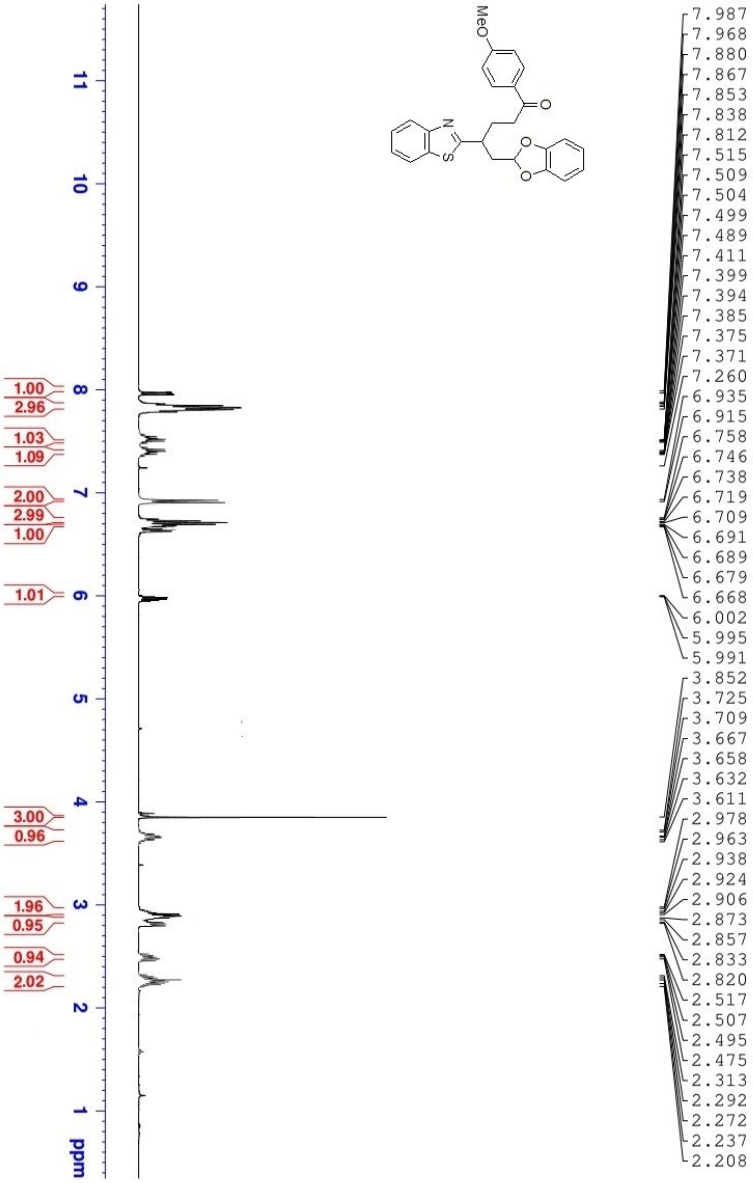
^{13}C NMR of Compound 3aa



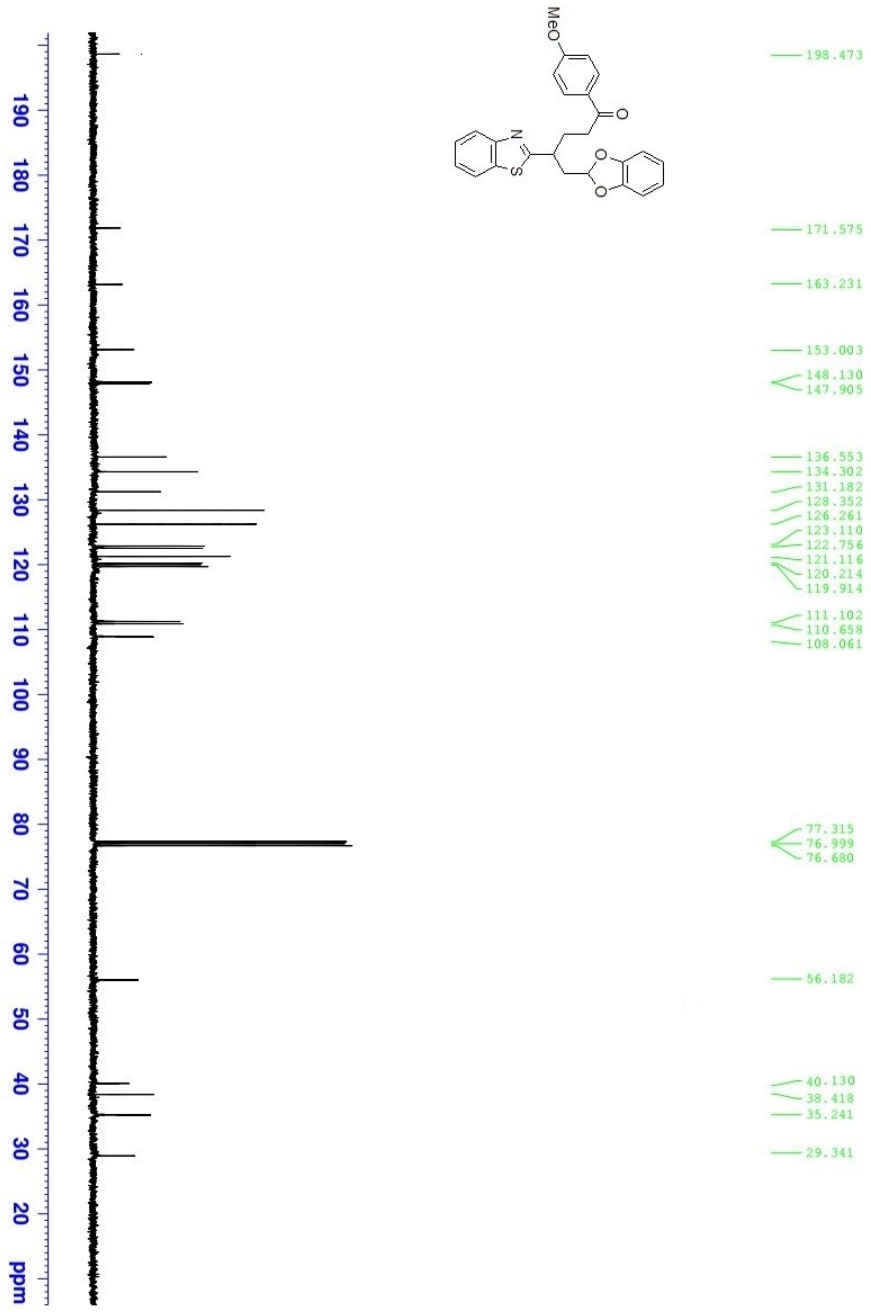
^{1}H NMR of Compound 3ab



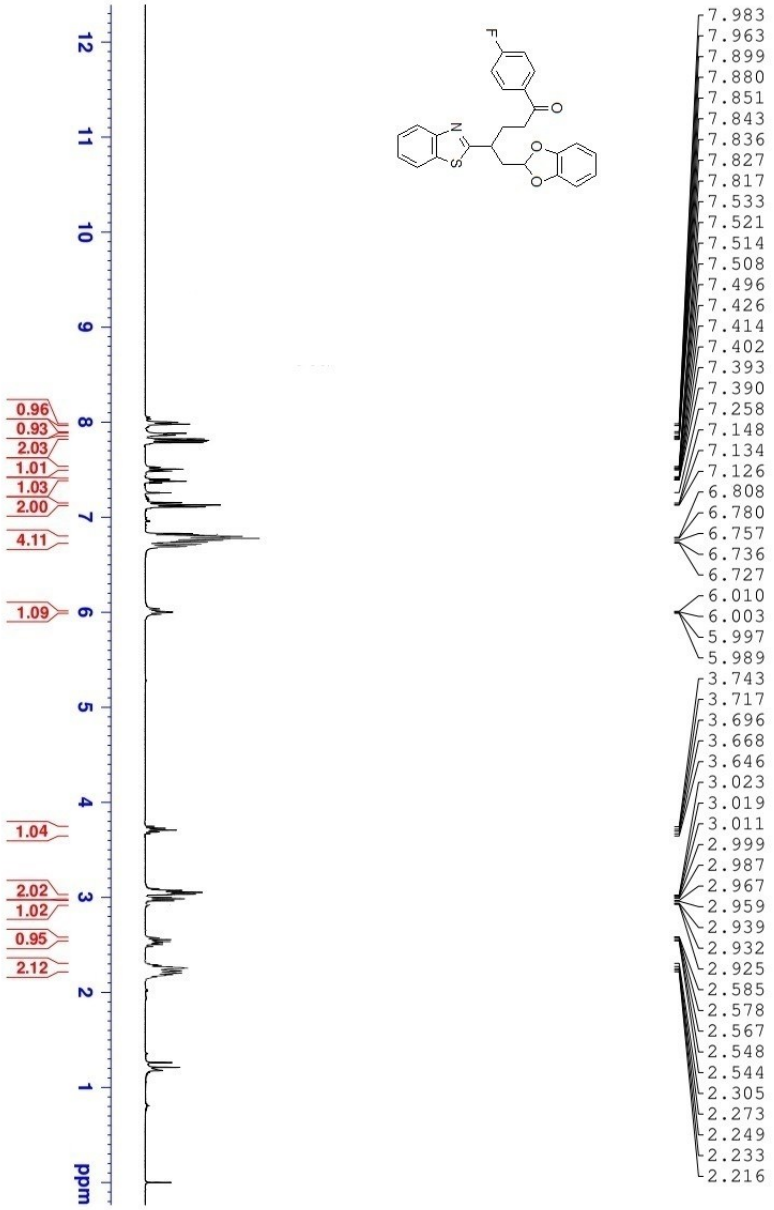
^{13}C NMR of Compound 3ab



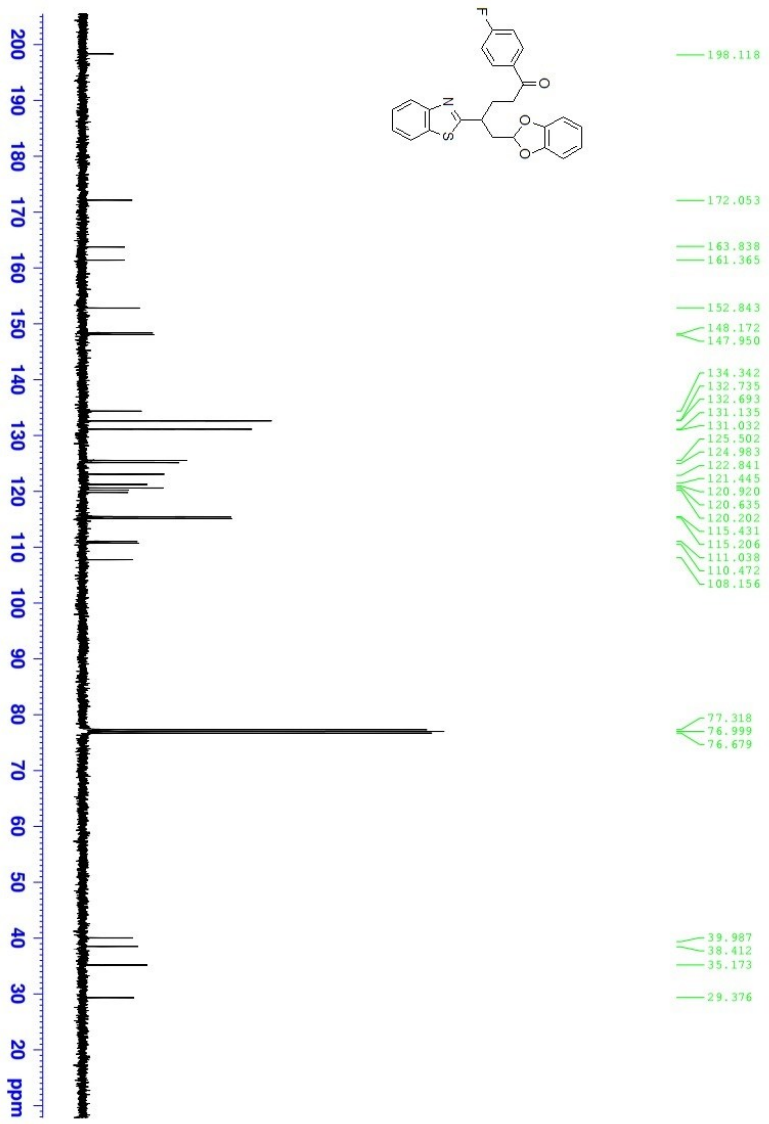
^{1}H NMR of Compound 3ac



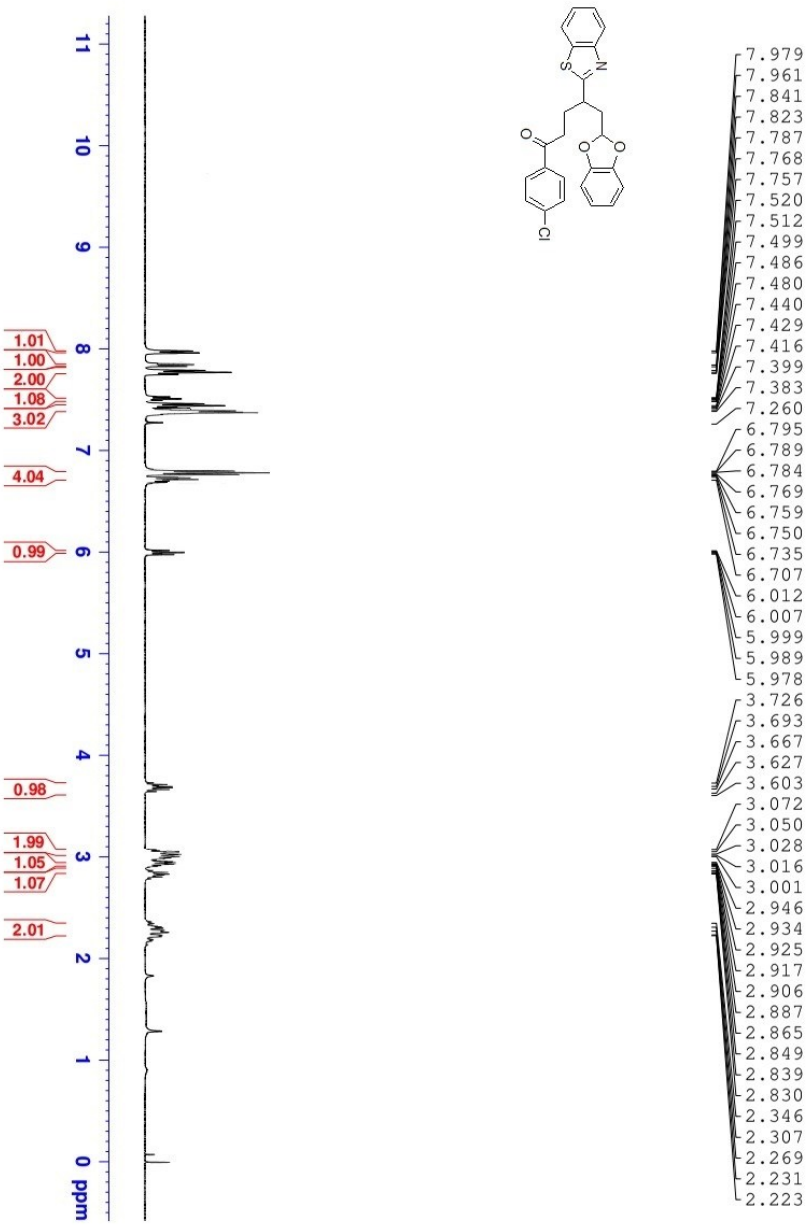
^{13}C NMR of Compound 3ac



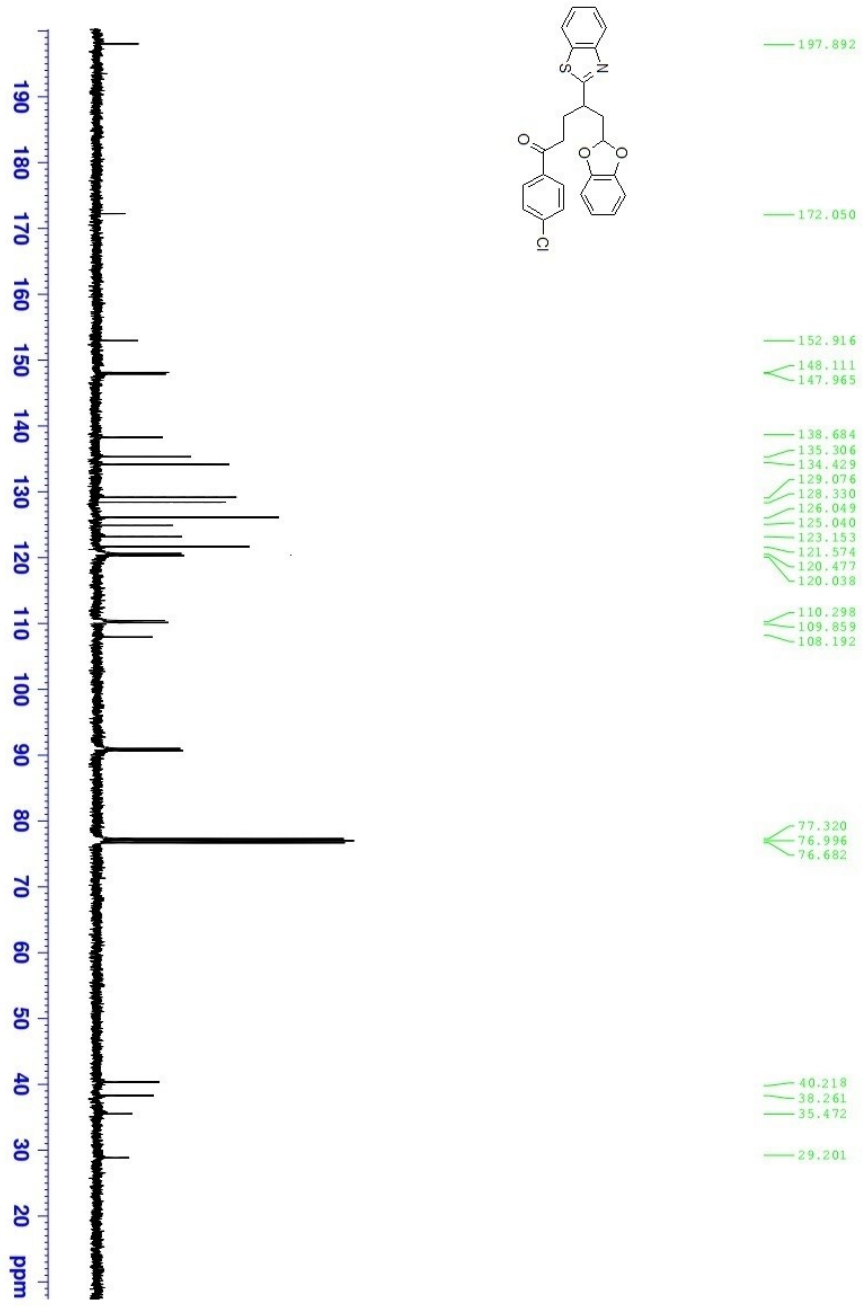
^{1}H NMR of Compound 3ad



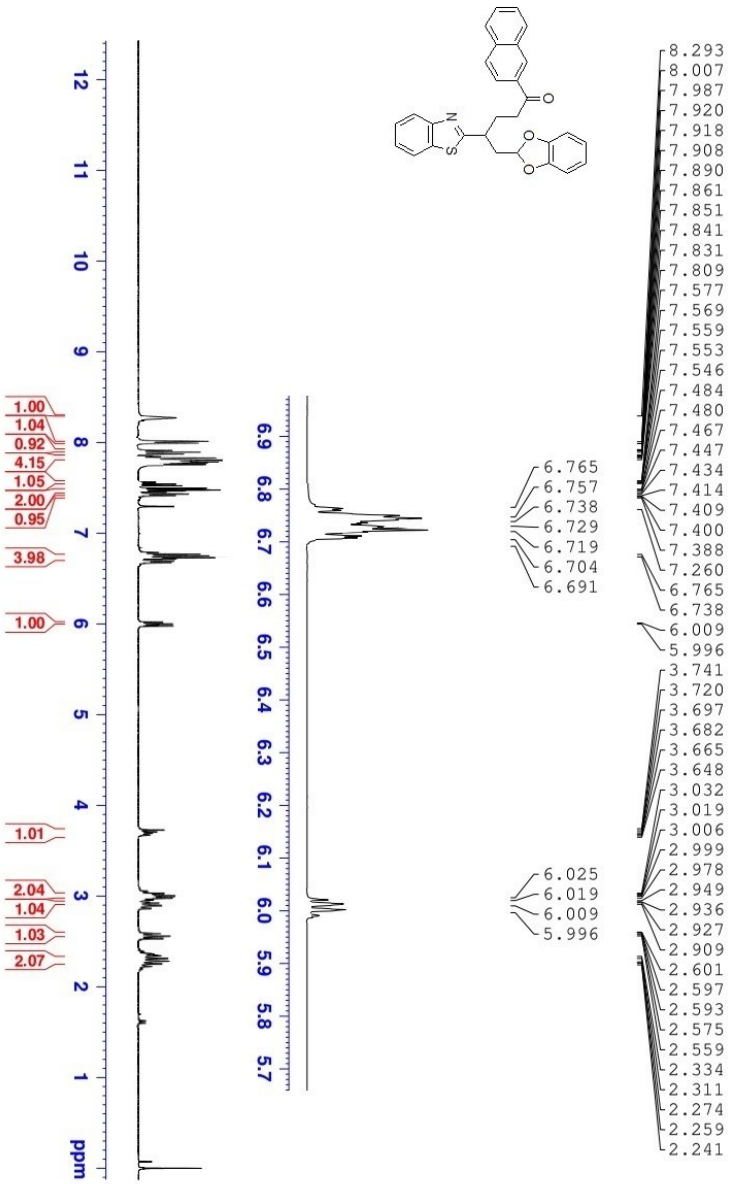
^{13}C NMR of Compound 3ad



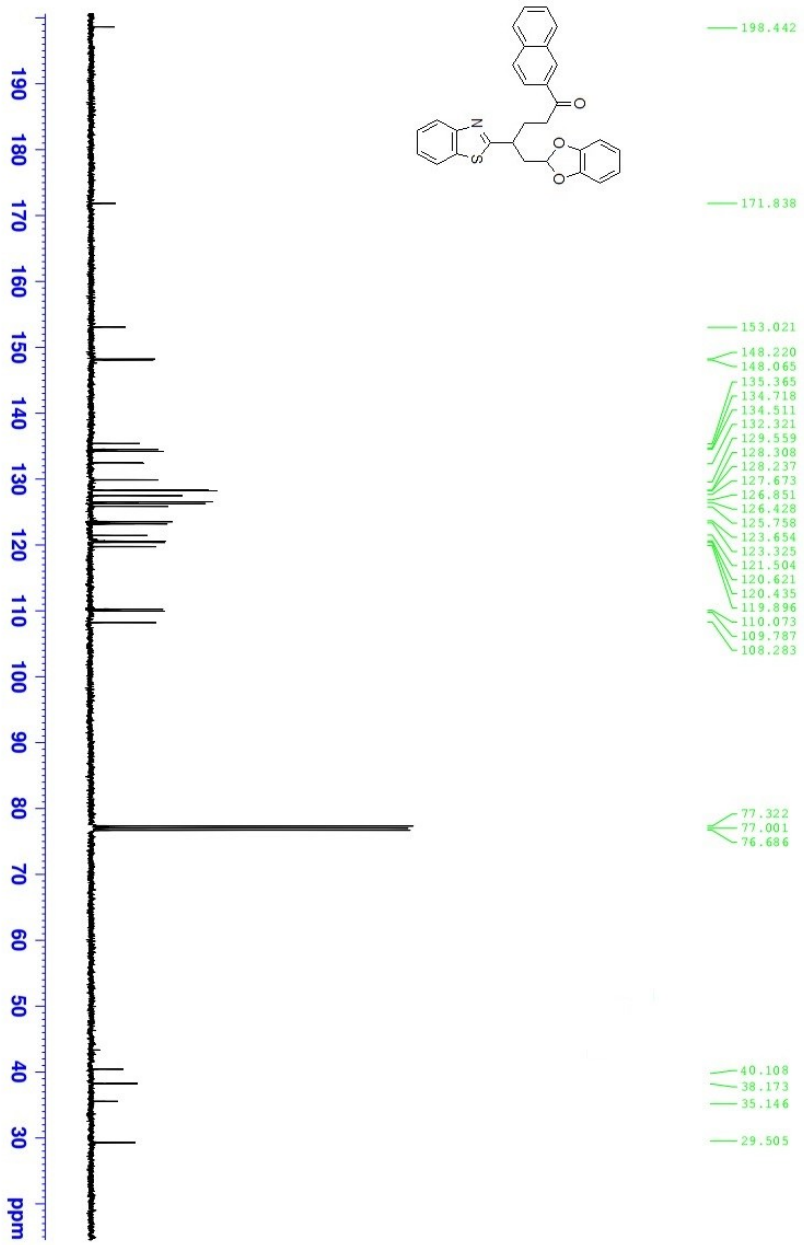
^{1}H NMR of Compound 3ae



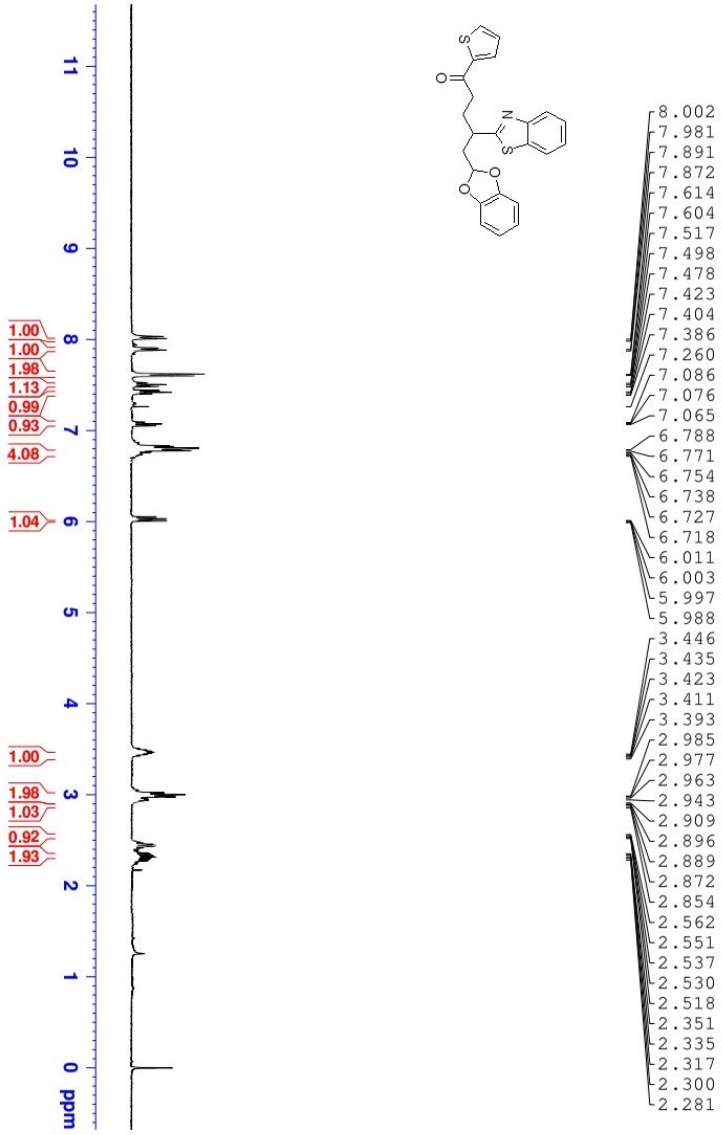
^{13}C NMR of Compound 3ae



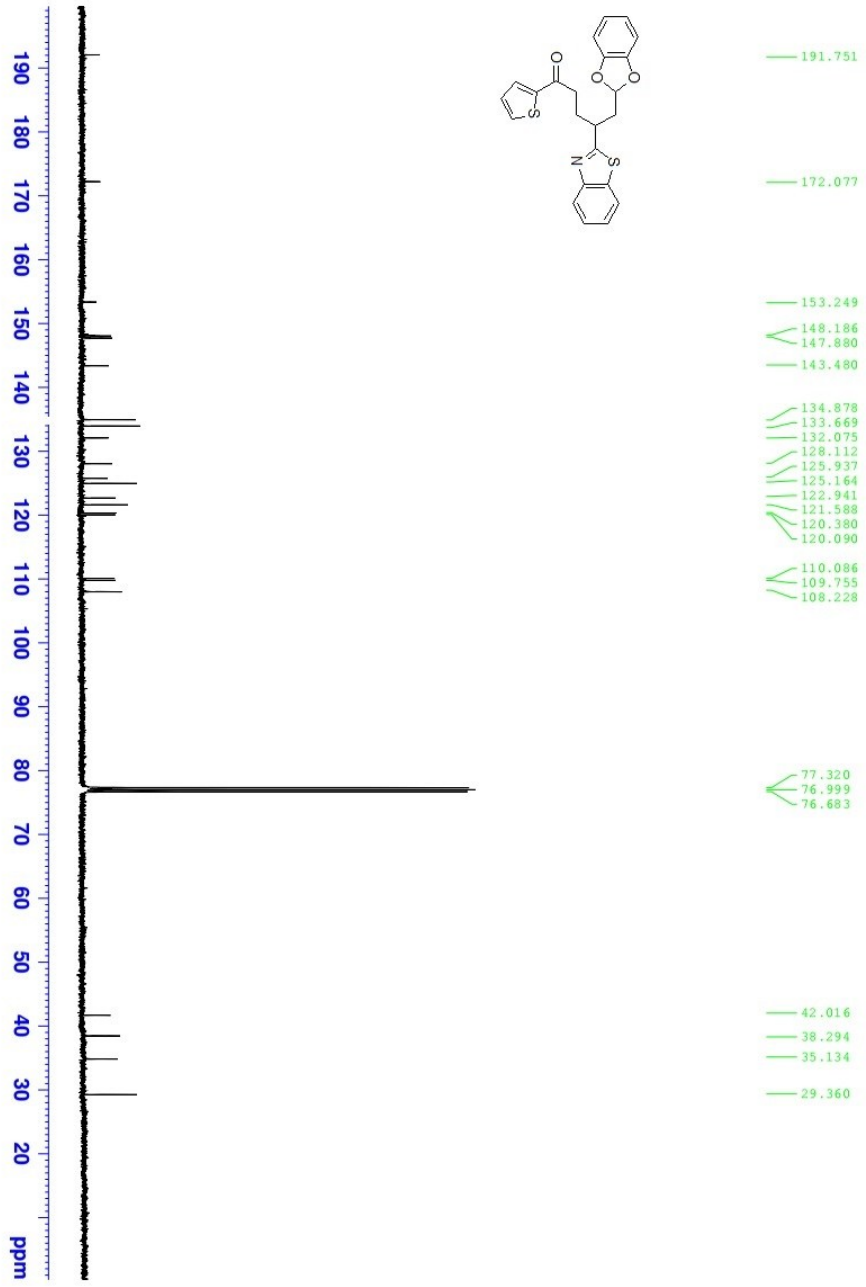
[1]H NMR of Compound 3af



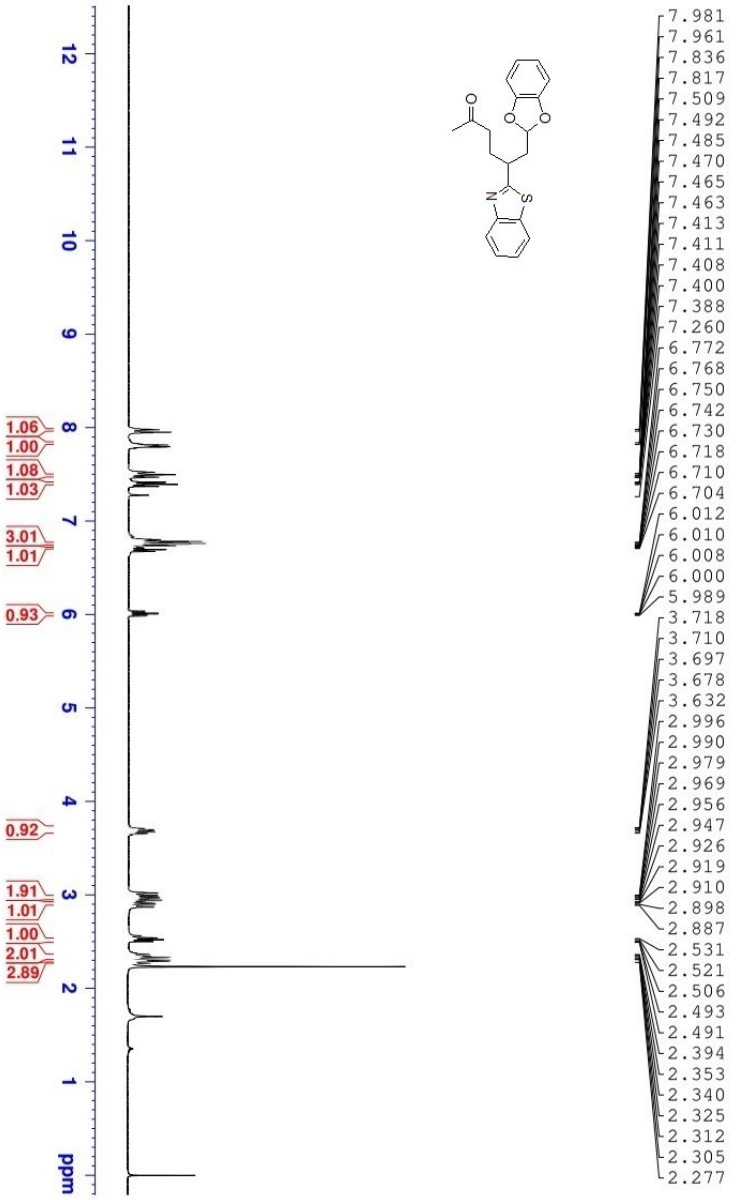
^{13}C NMR of Compound 3af



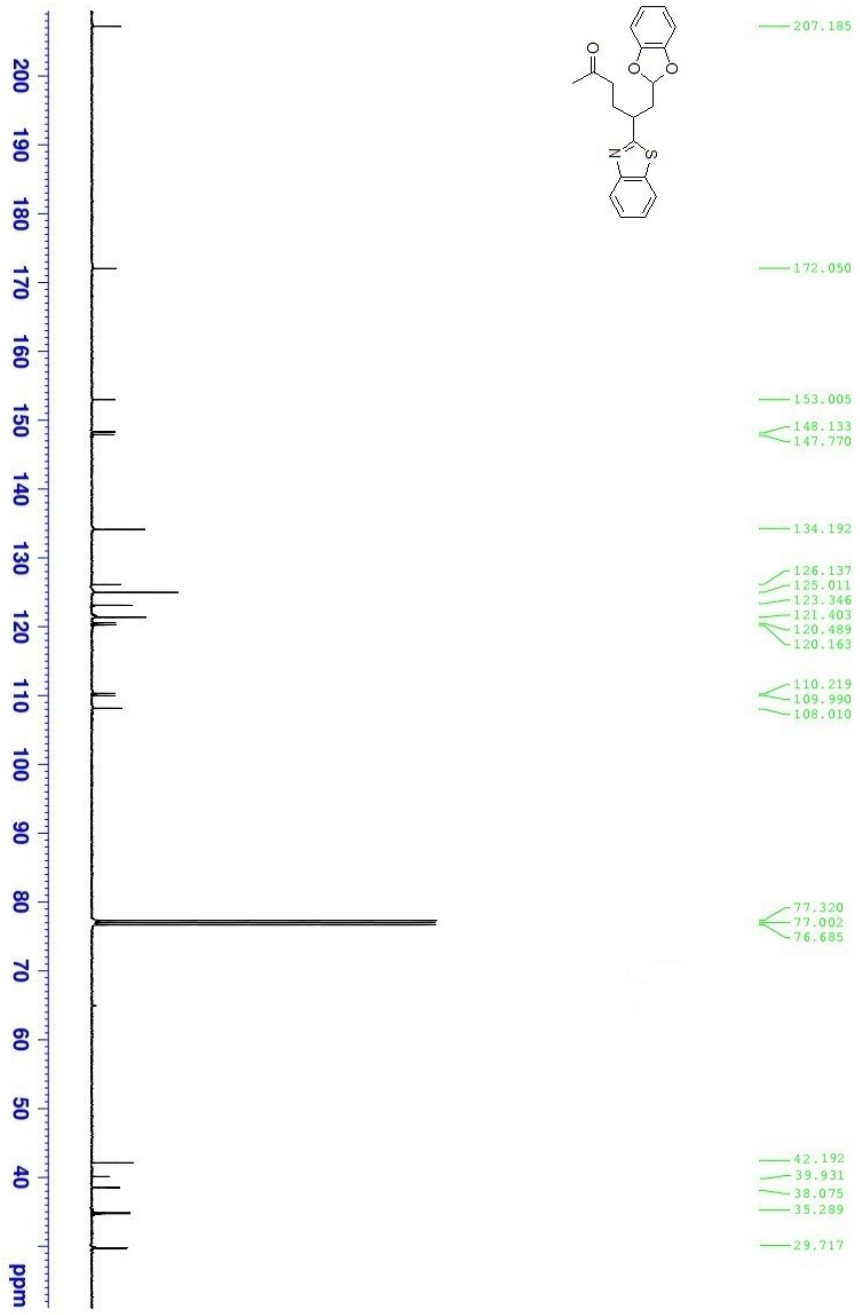
[1]H NMR of Compound 3ag



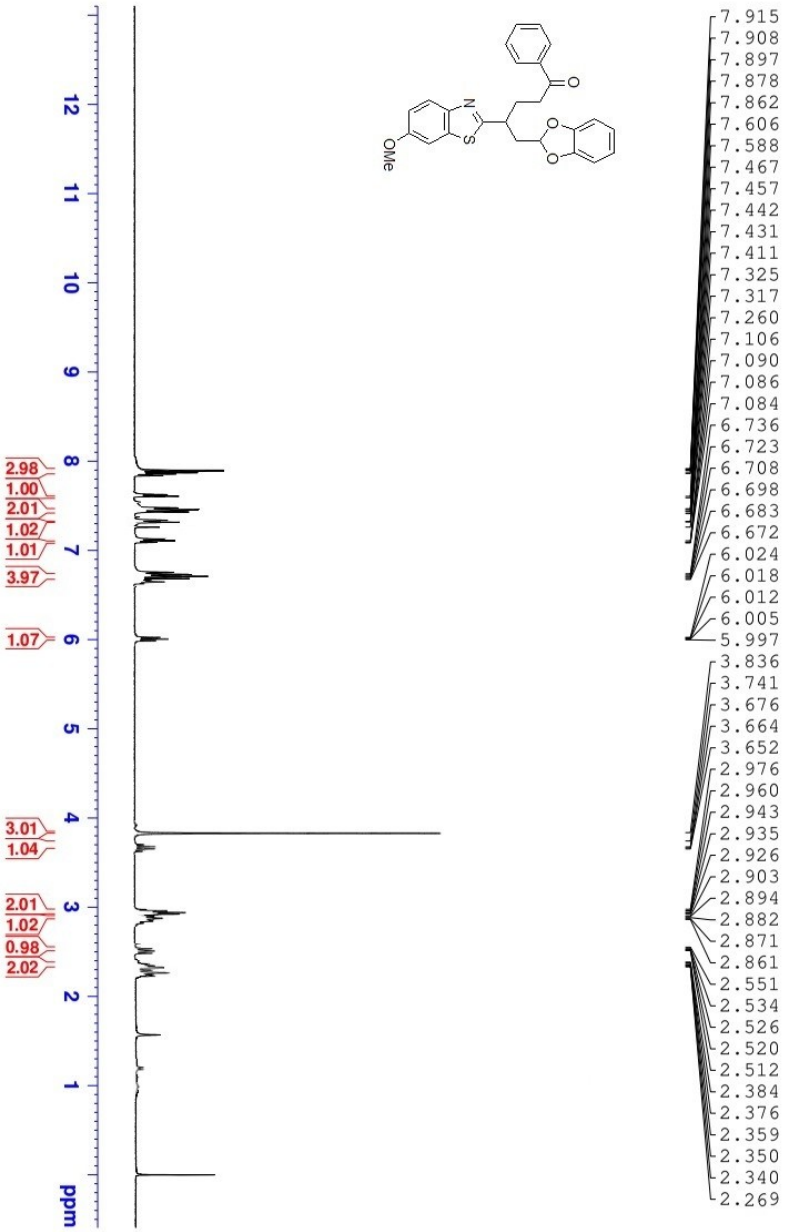
^{13}C NMR of Compound 3ag



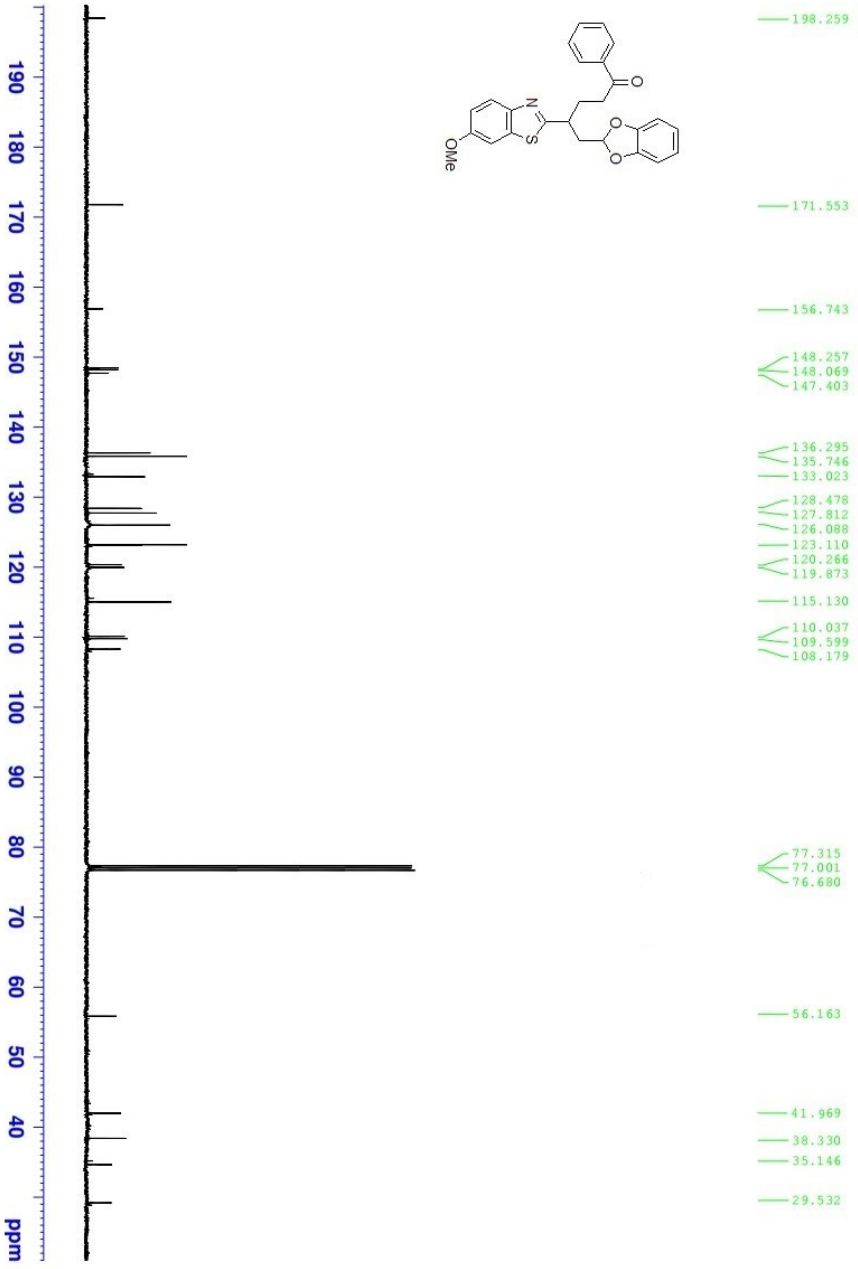
^{1}H NMR of Compound 3ah



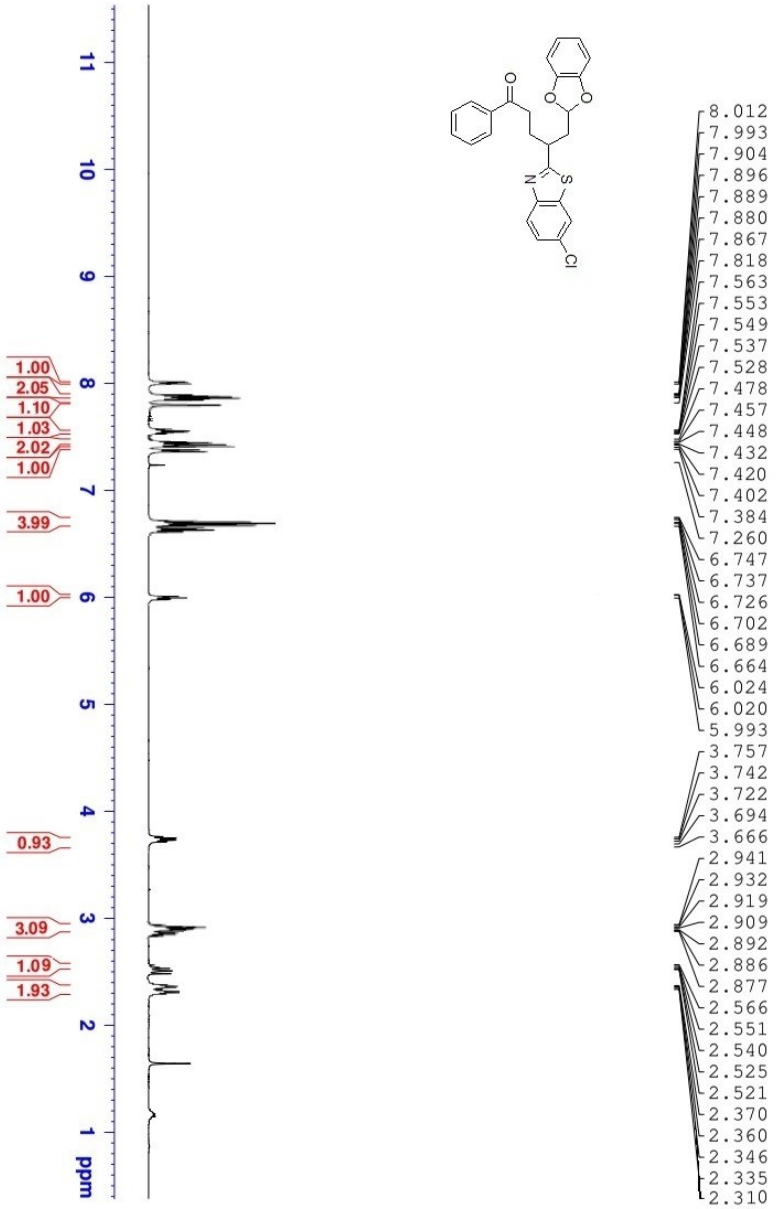
^{13}C NMR of Compound 3ah



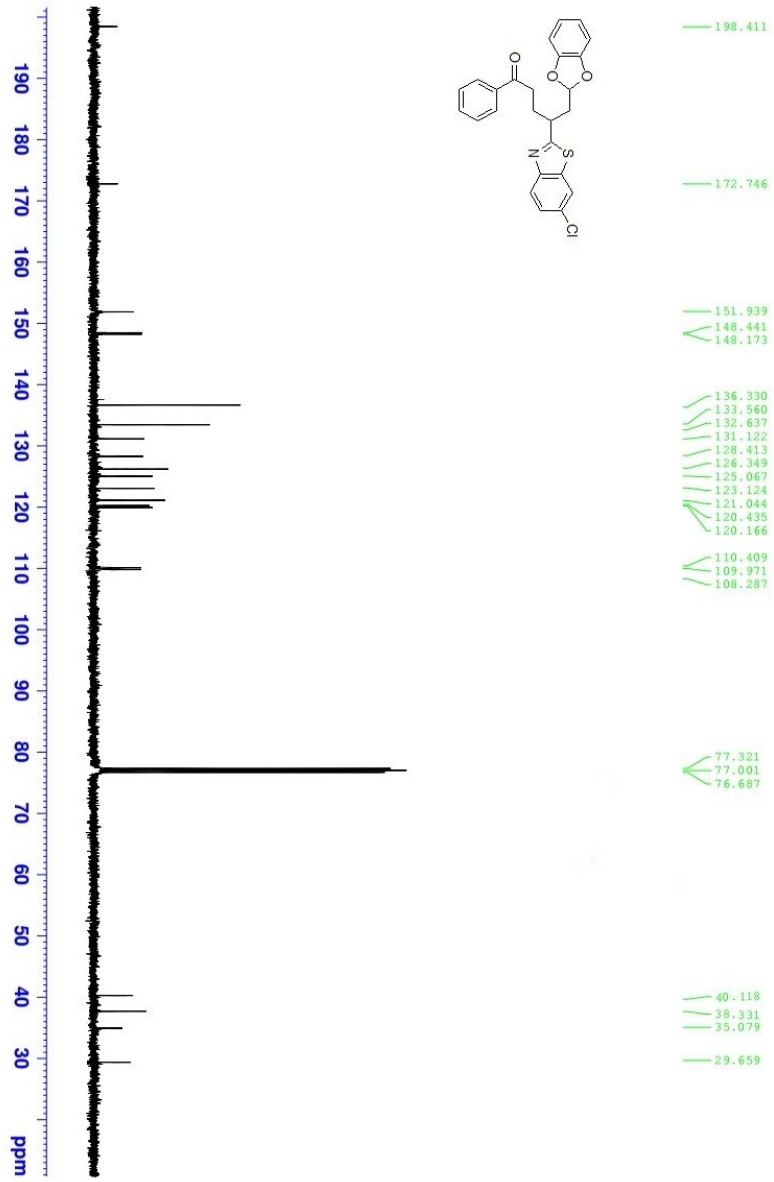
^{1}H NMR of Compound 3ai



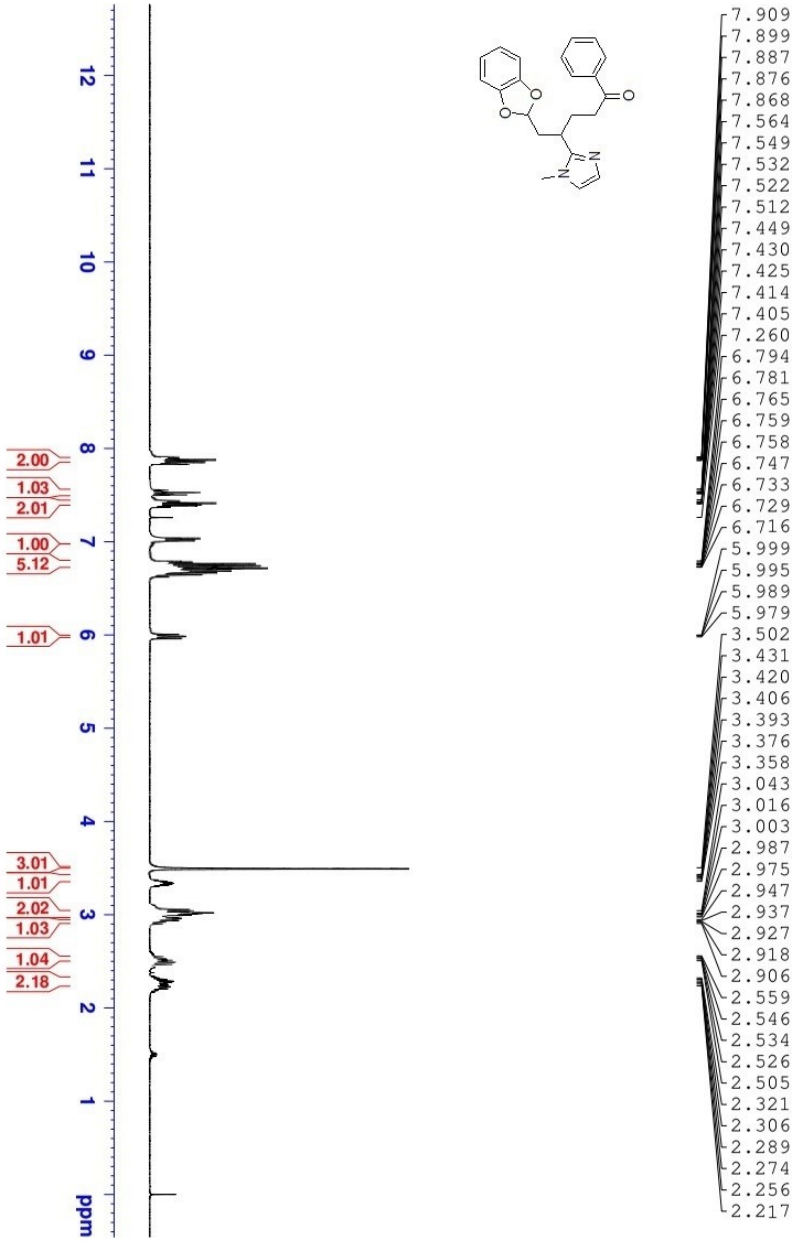
^{13}C NMR of Compound 3ai



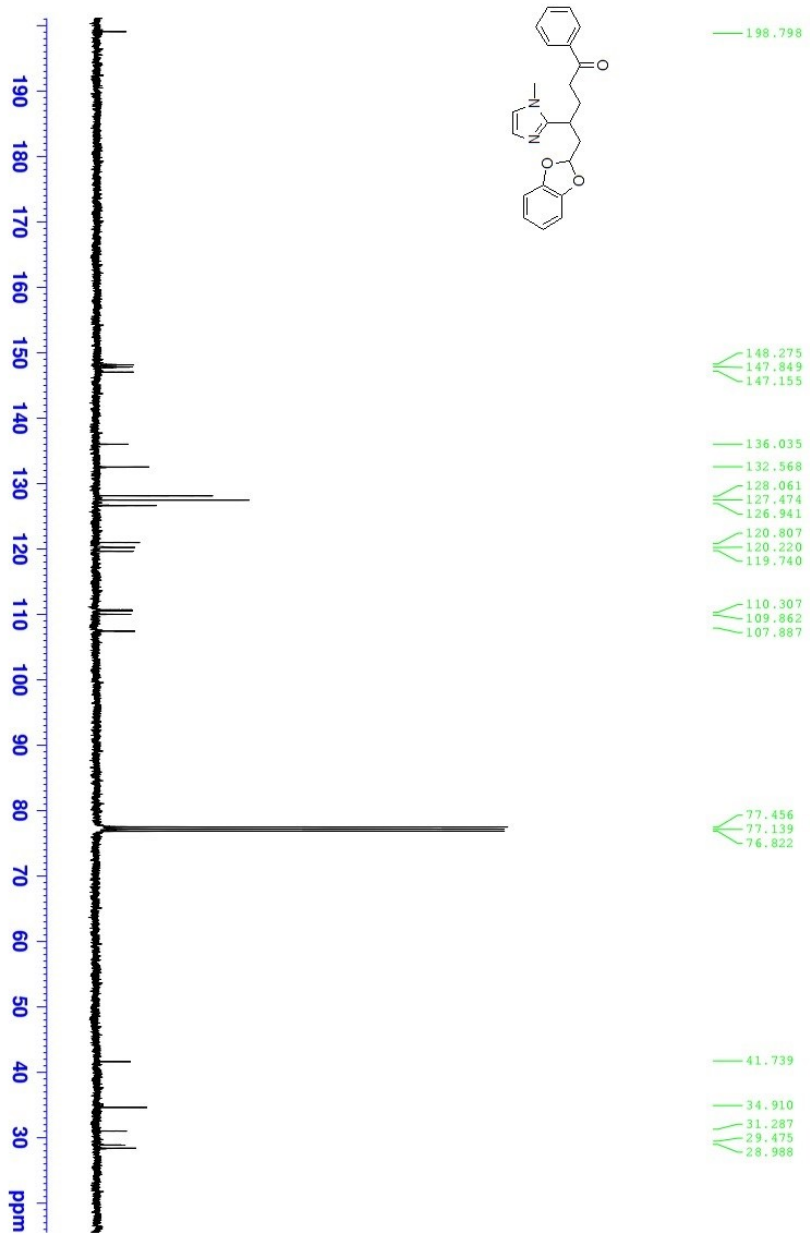
^{1}H NMR of Compound 3aj



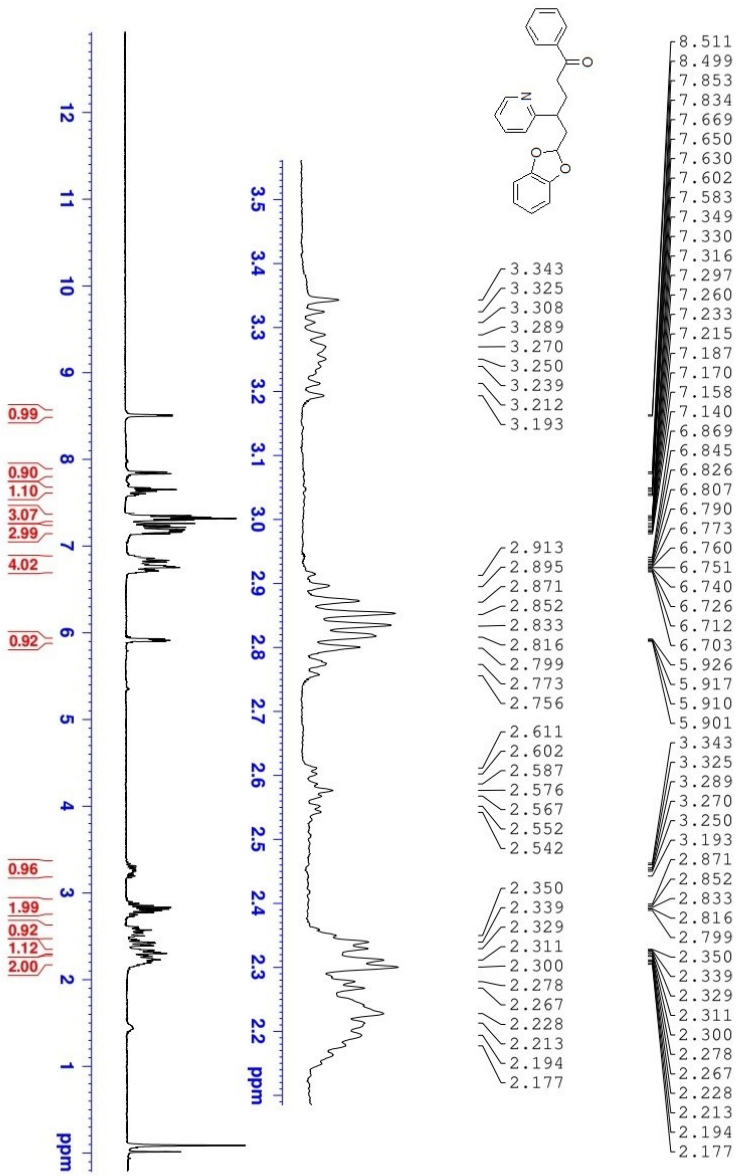
^{13}C NMR of Compound 3aj



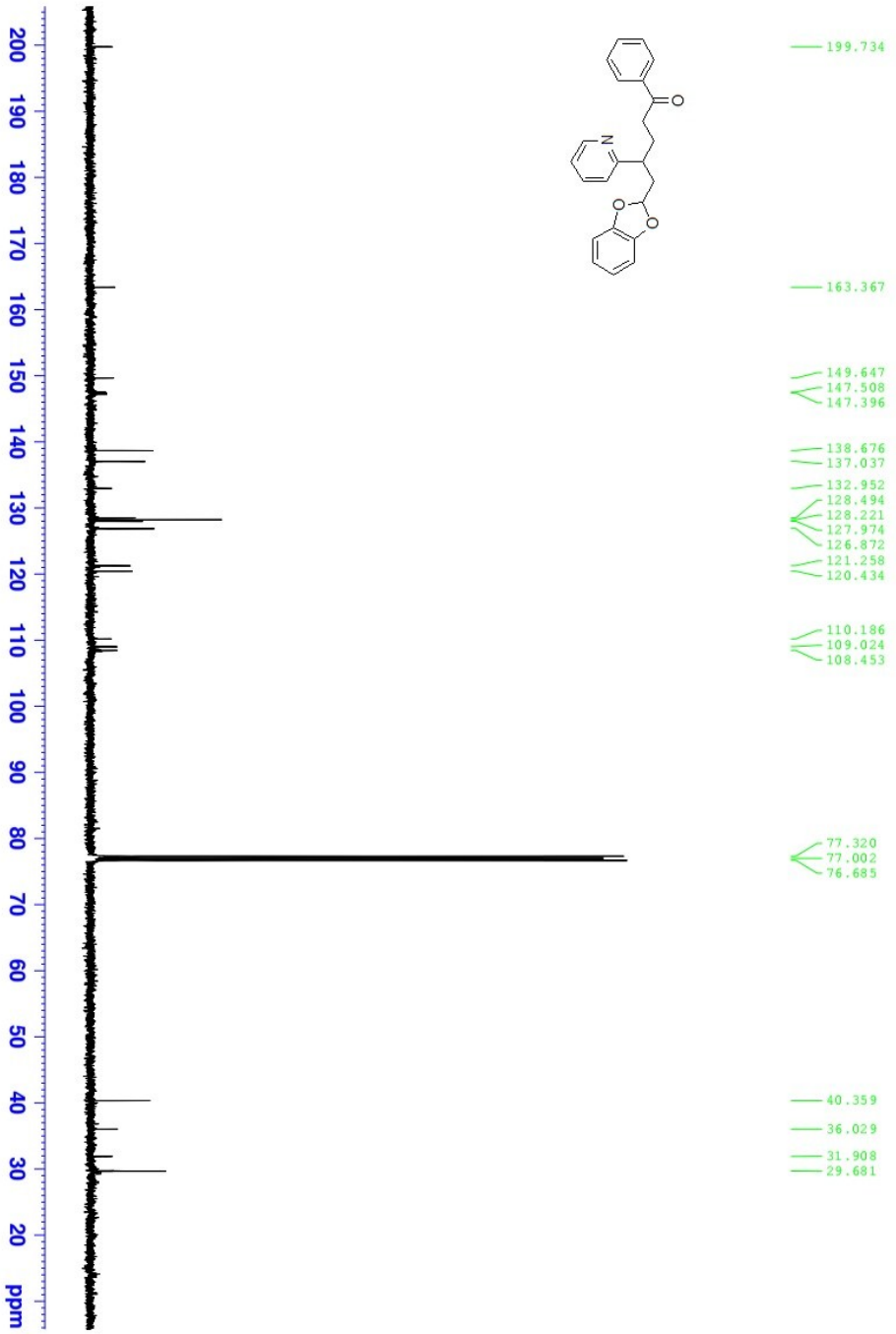
^{1}H NMR of Compound 3ak



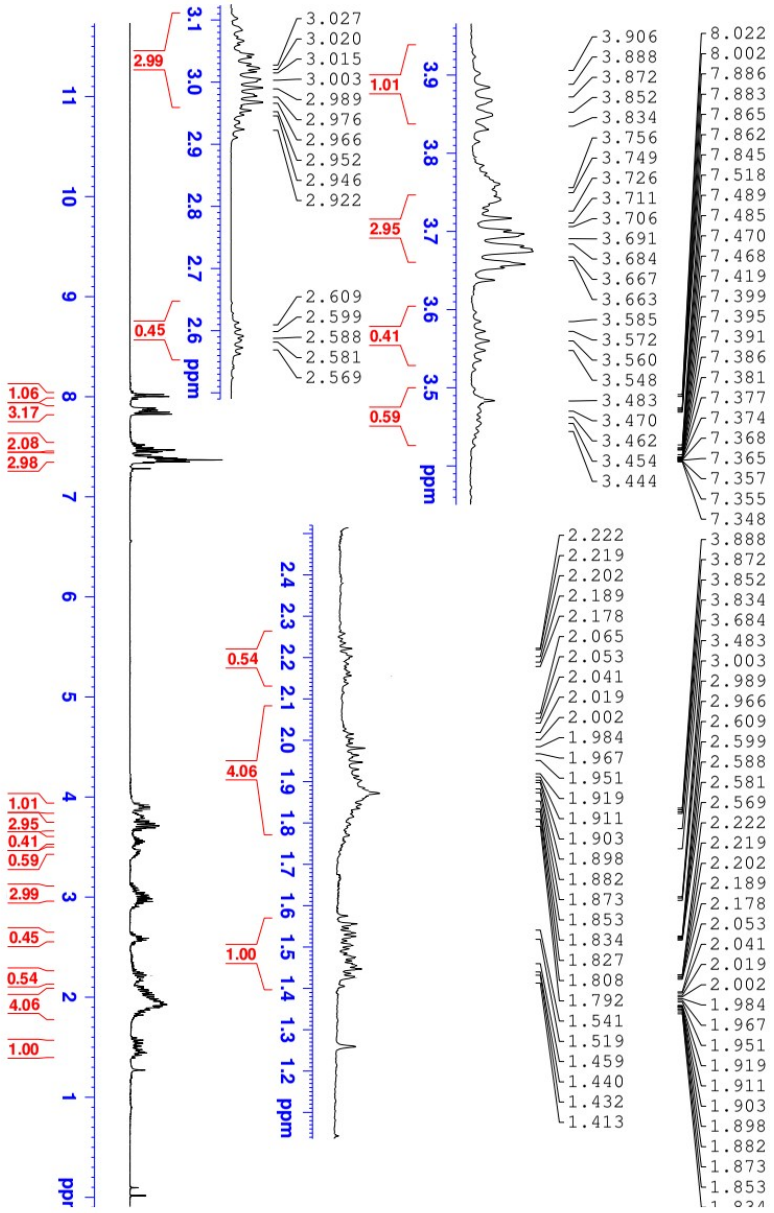
^{13}C NMR of Compound 3ak



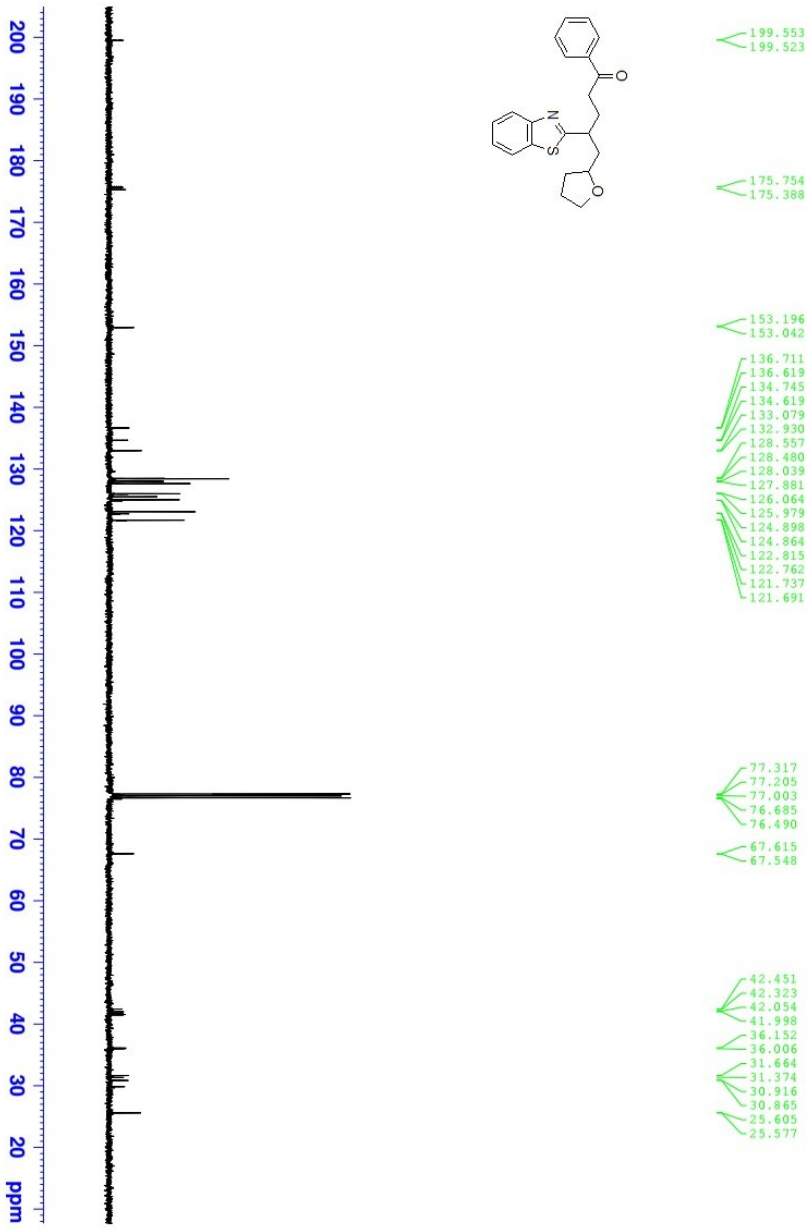
^{1}H NMR of Compound 3al



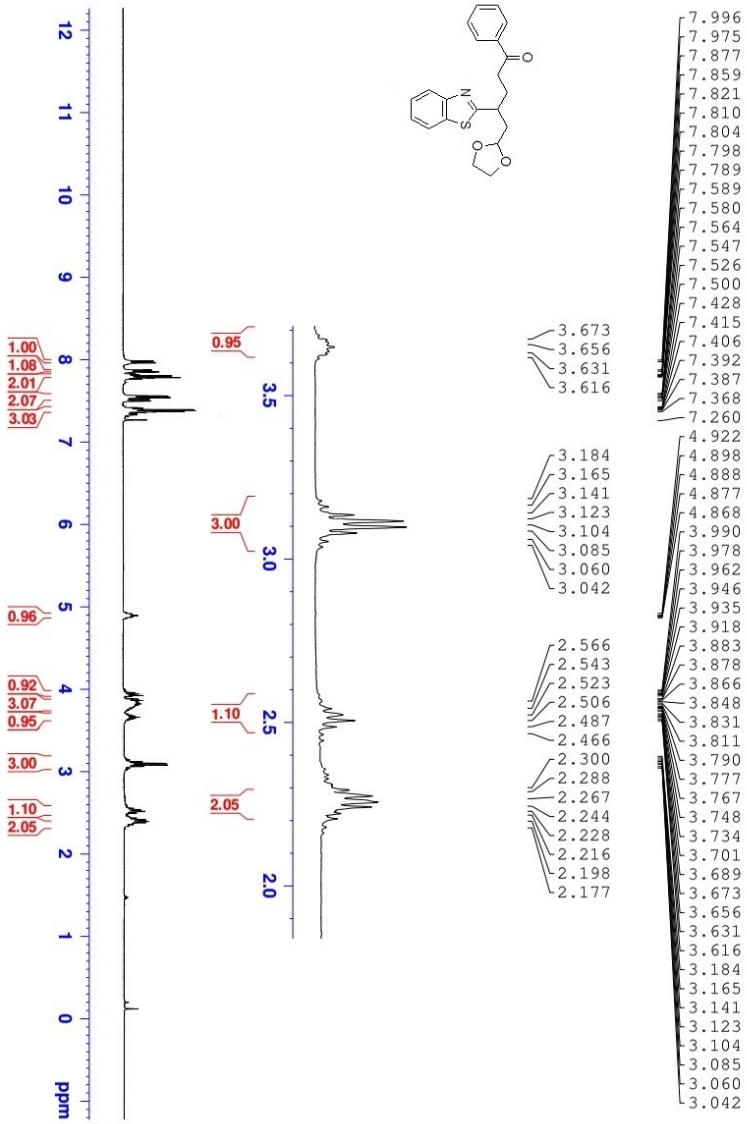
^{13}C NMR of Compound 3al



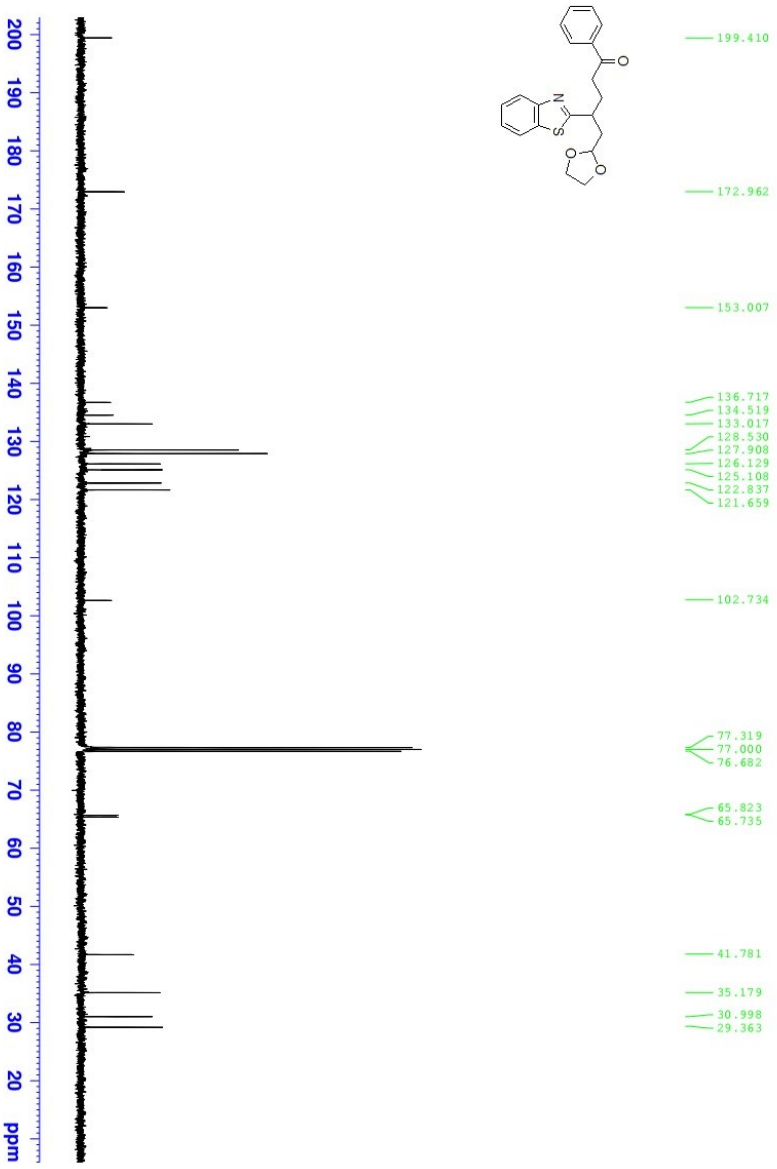
^{1}H NMR of Compound 3ba



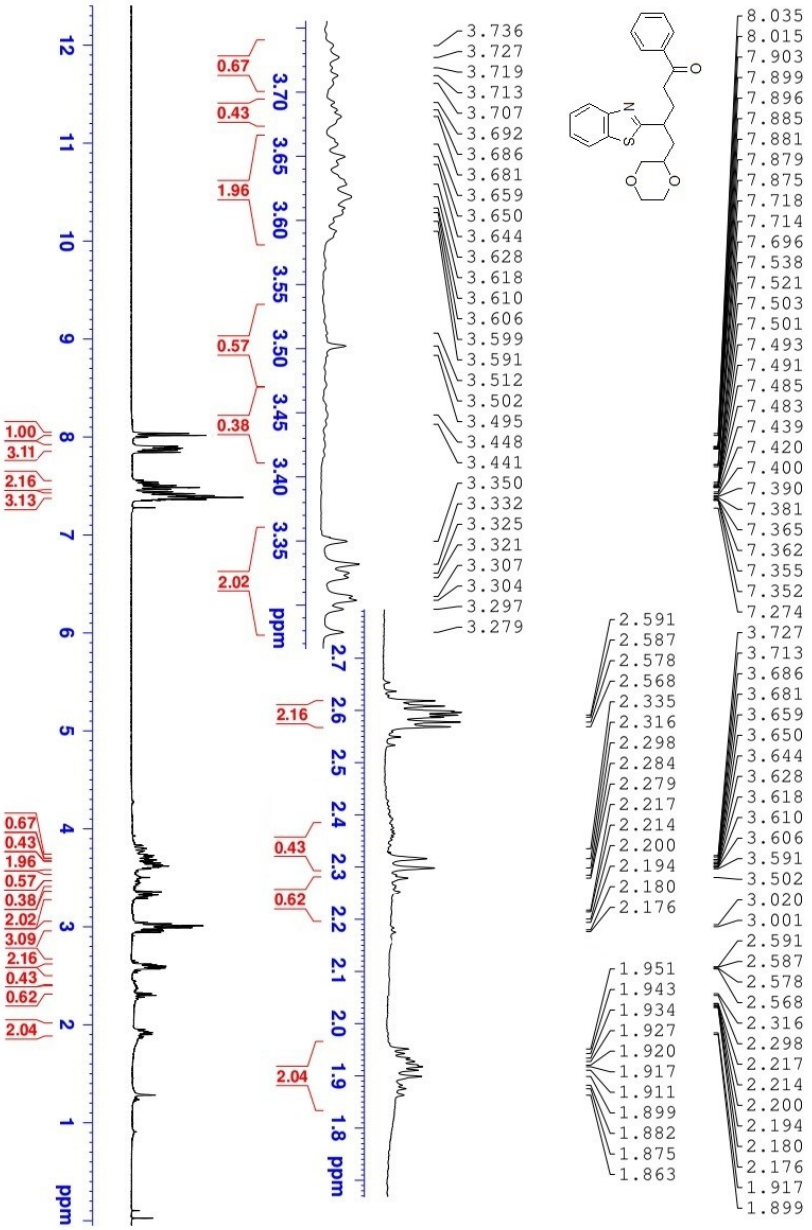
^{13}C NMR of Compound 3ba



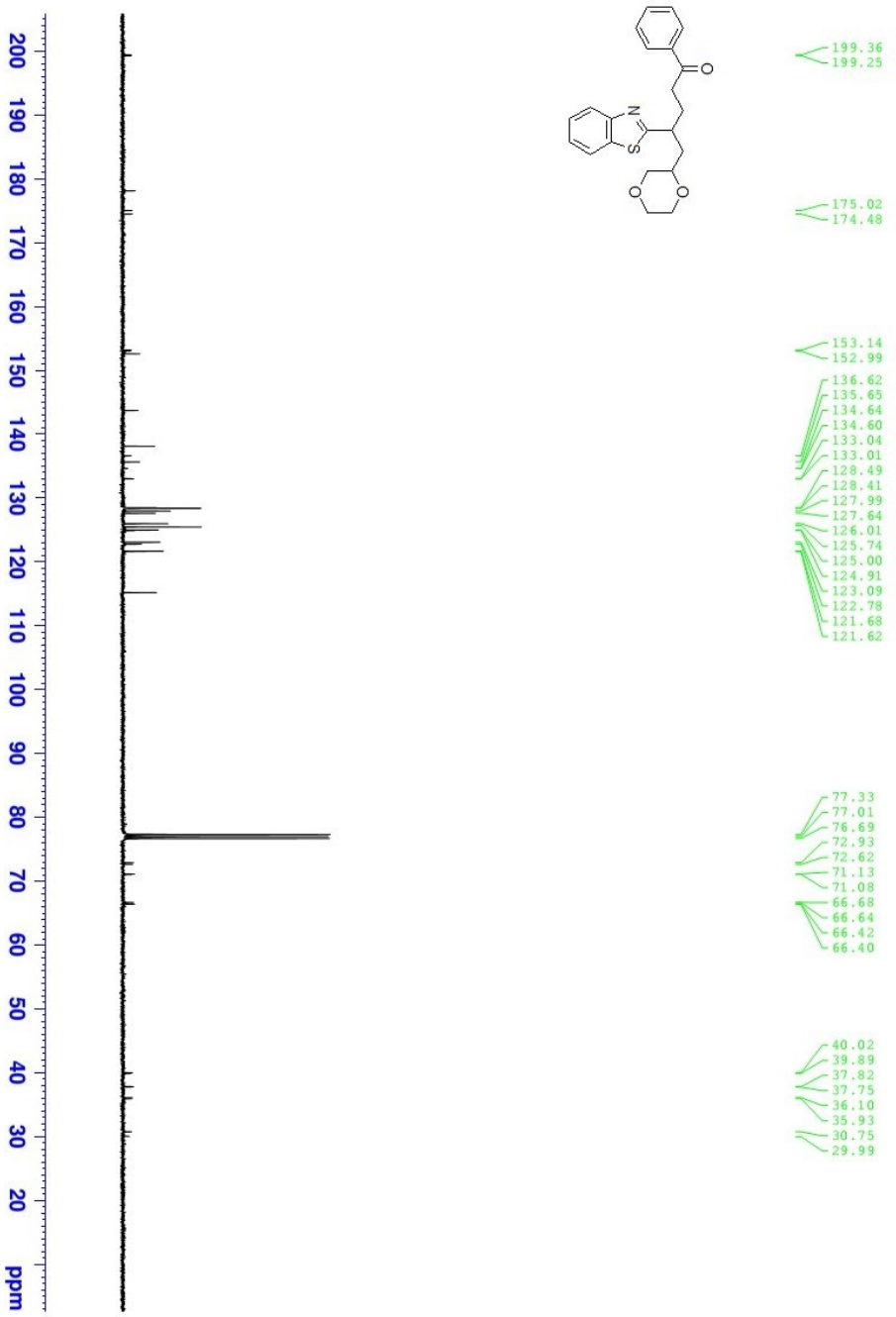
^{1}H NMR of Compound 3ca



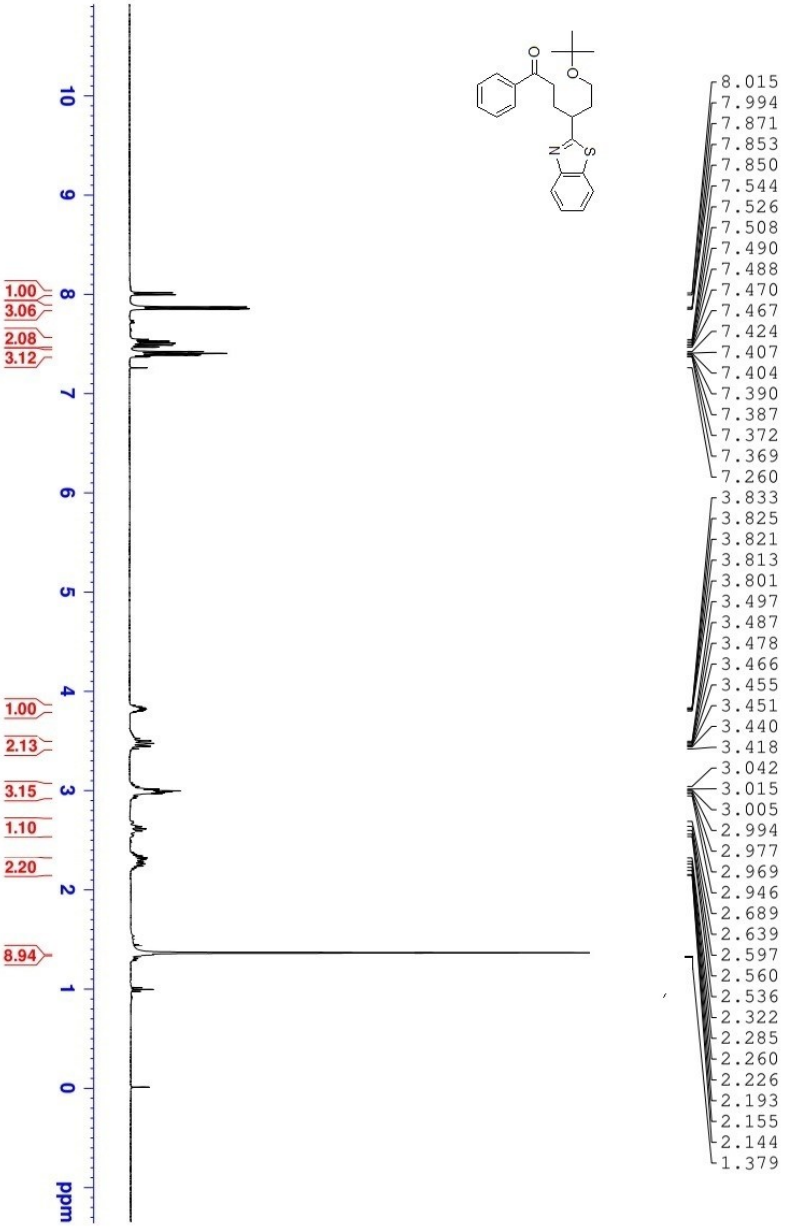
^{13}C NMR of Compound 3ca



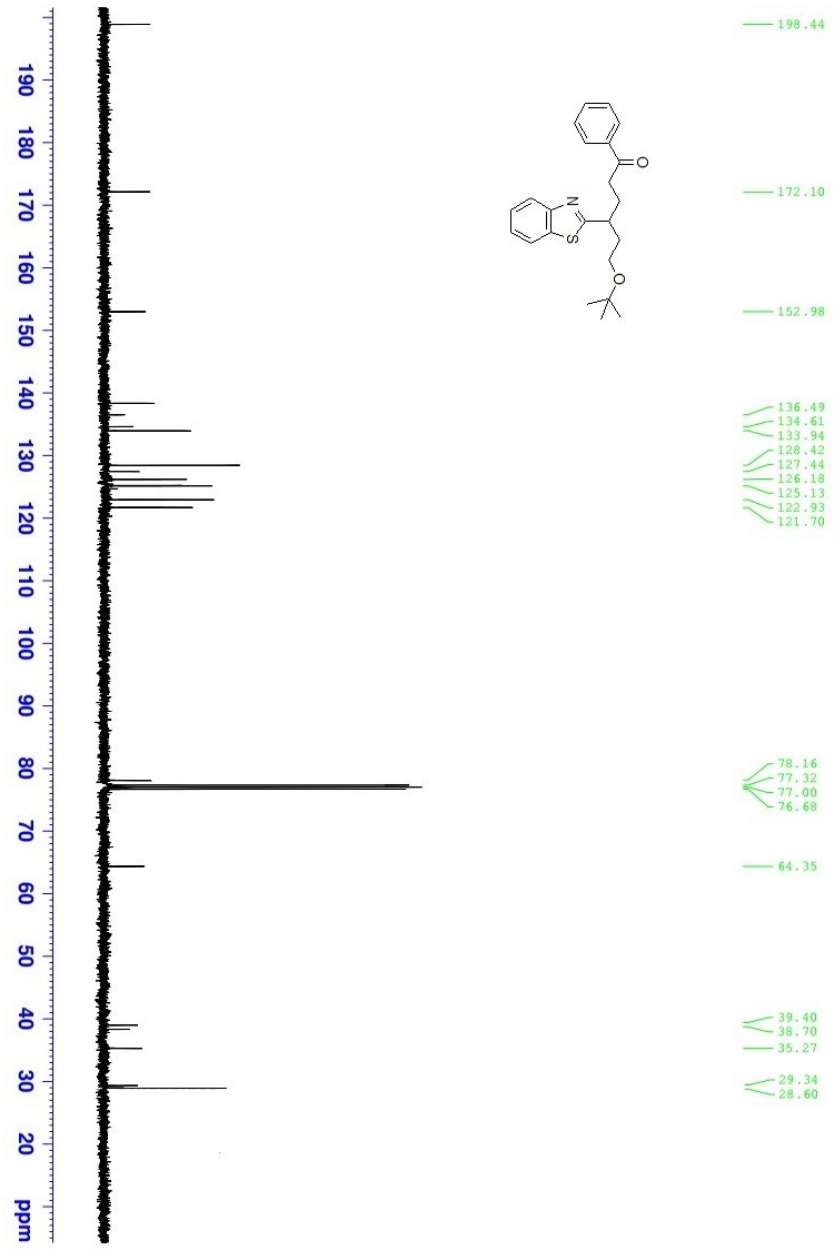
^{1}H NMR of Compound 3da



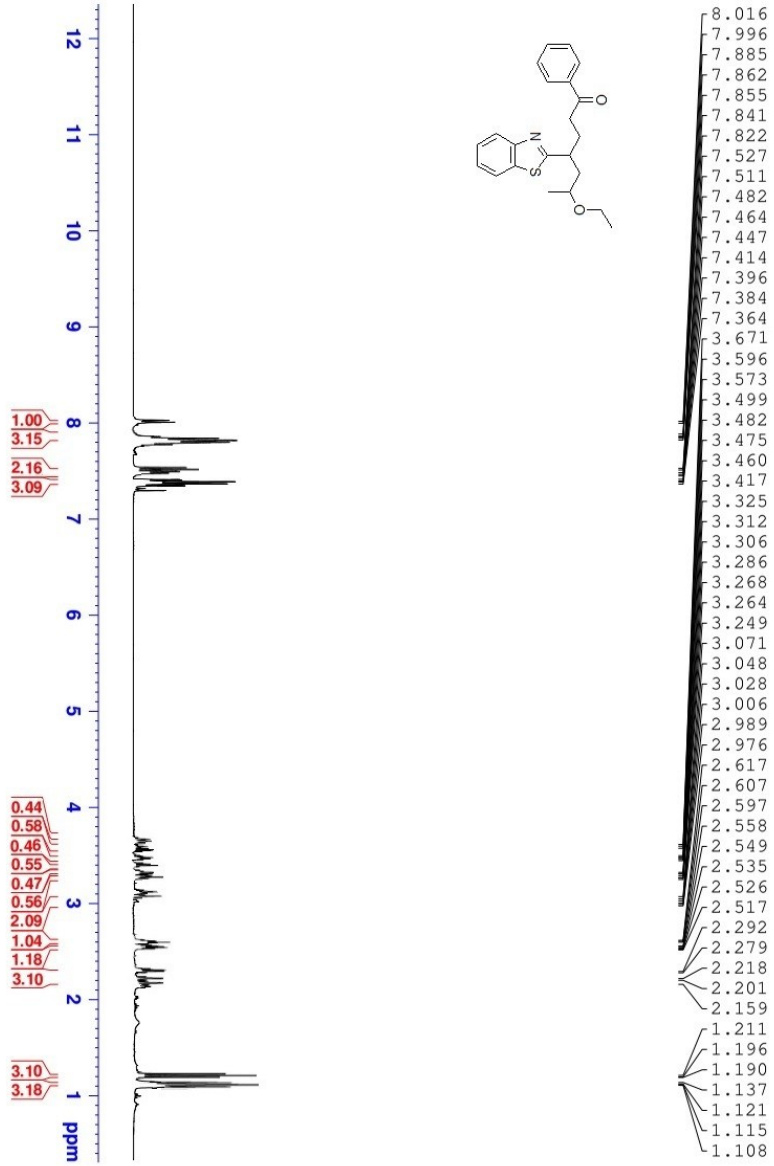
^{13}C NMR of Compound 3da



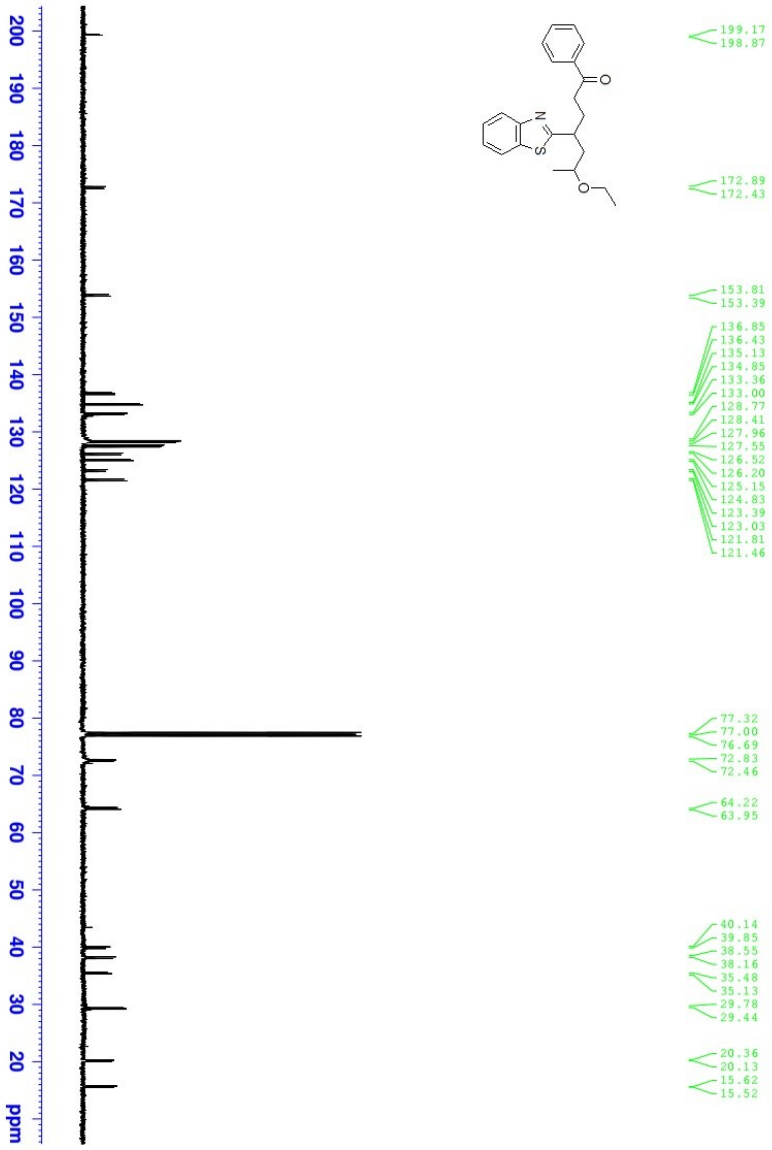
^{1}H NMR of Compound 3ea



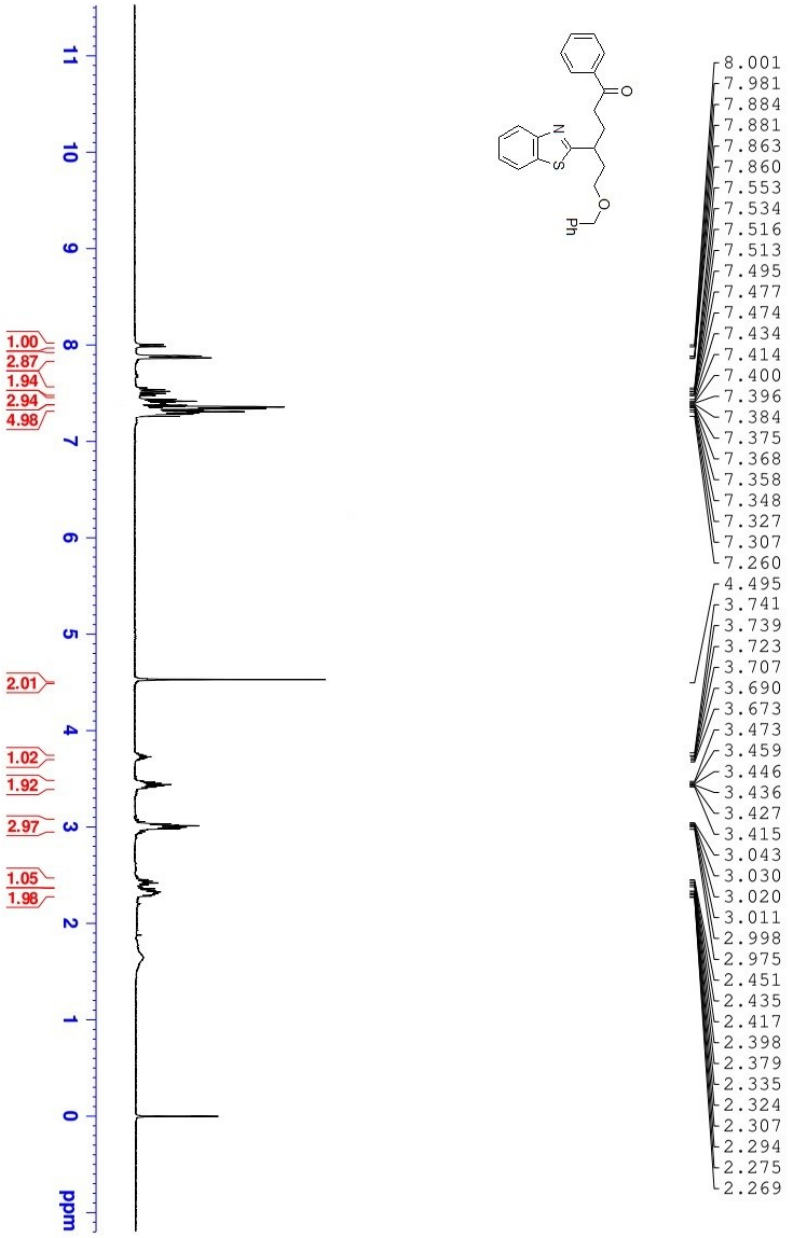
^{13}C NMR of Compound 3ea



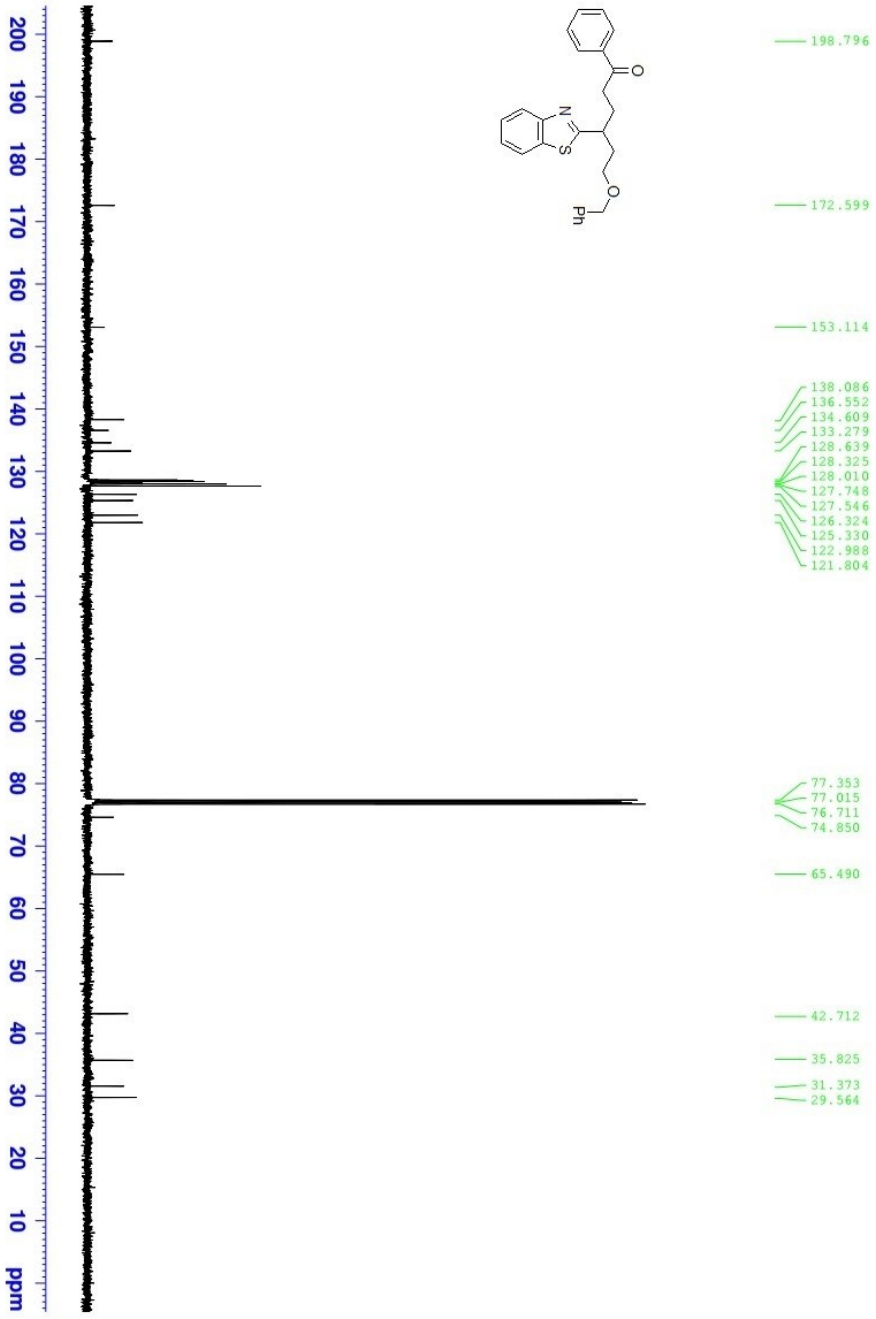
[1]H NMR of Compound 3fa



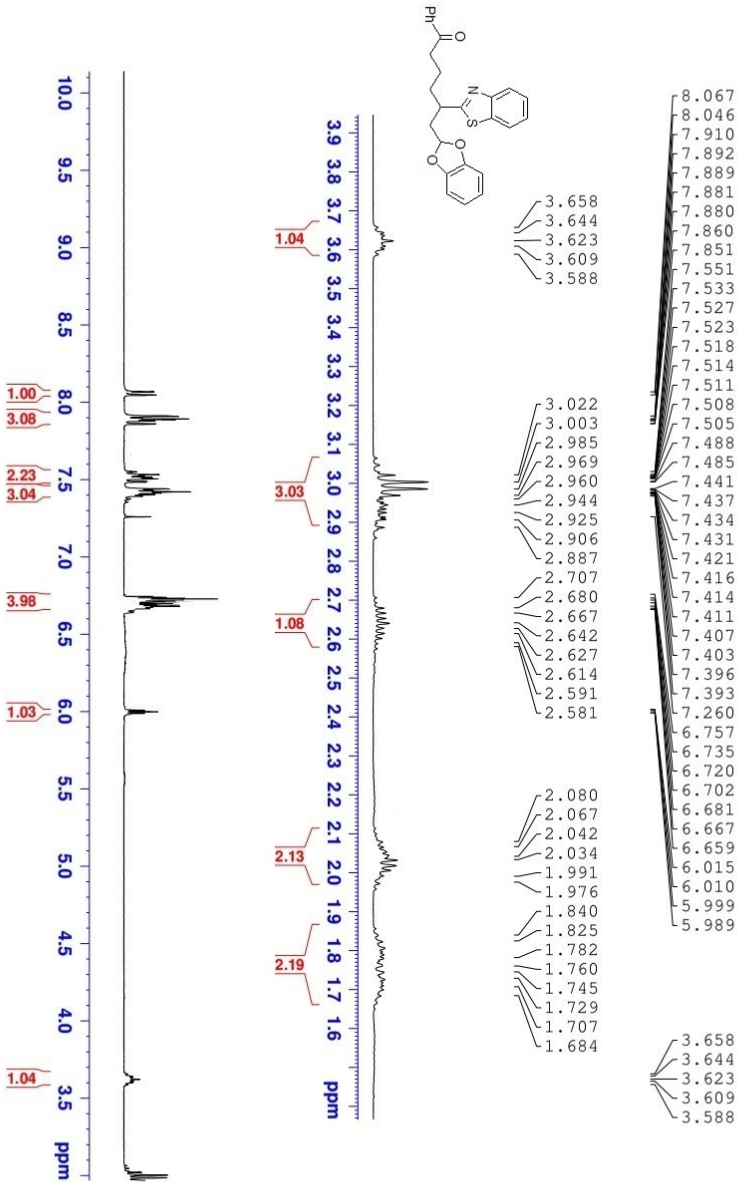
^{13}C NMR of Compound 3fa



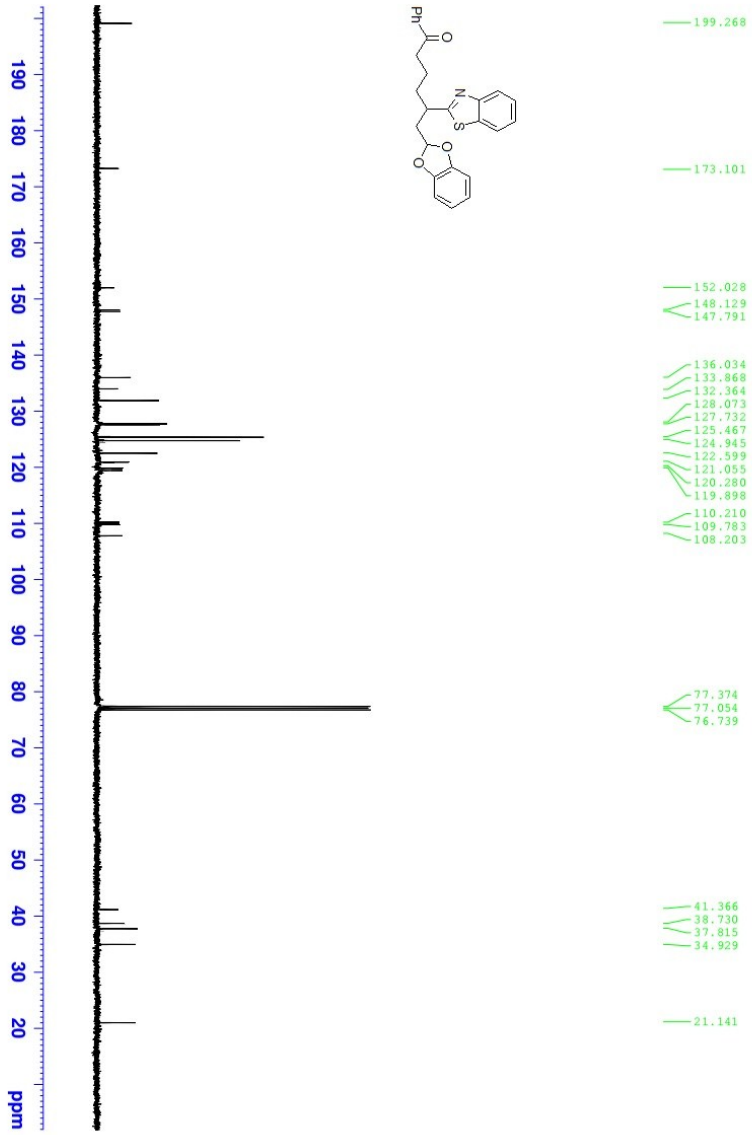
^{1}H NMR of Compound 3ga



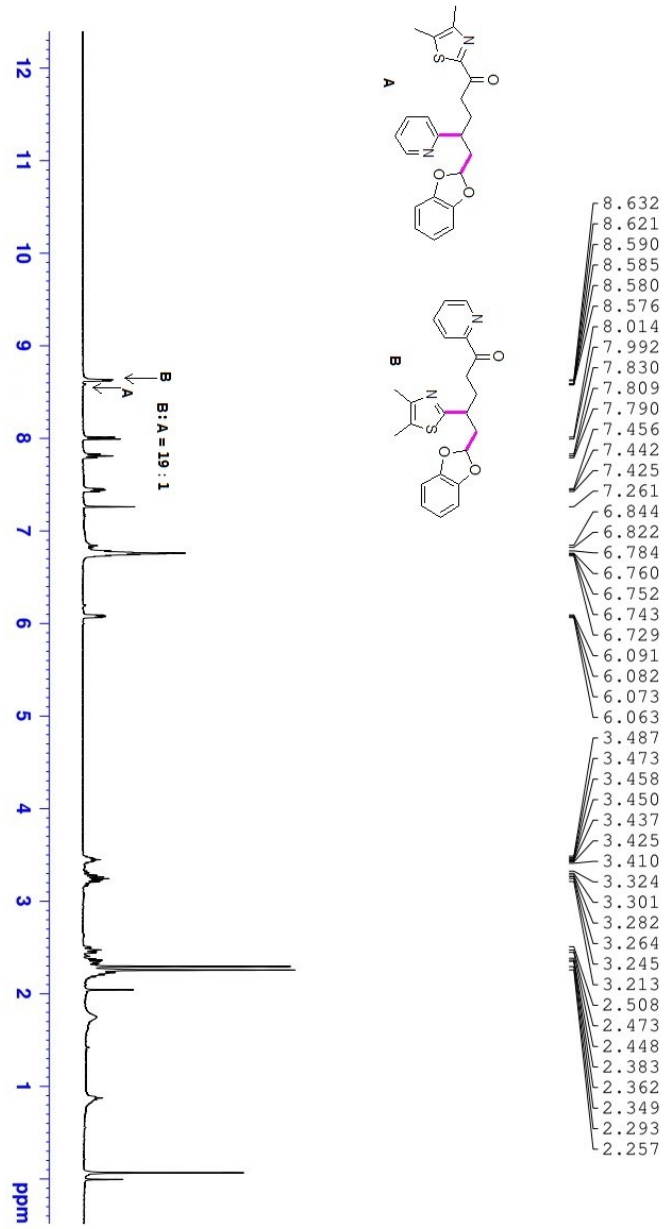
^{13}C NMR of Compound 3ga



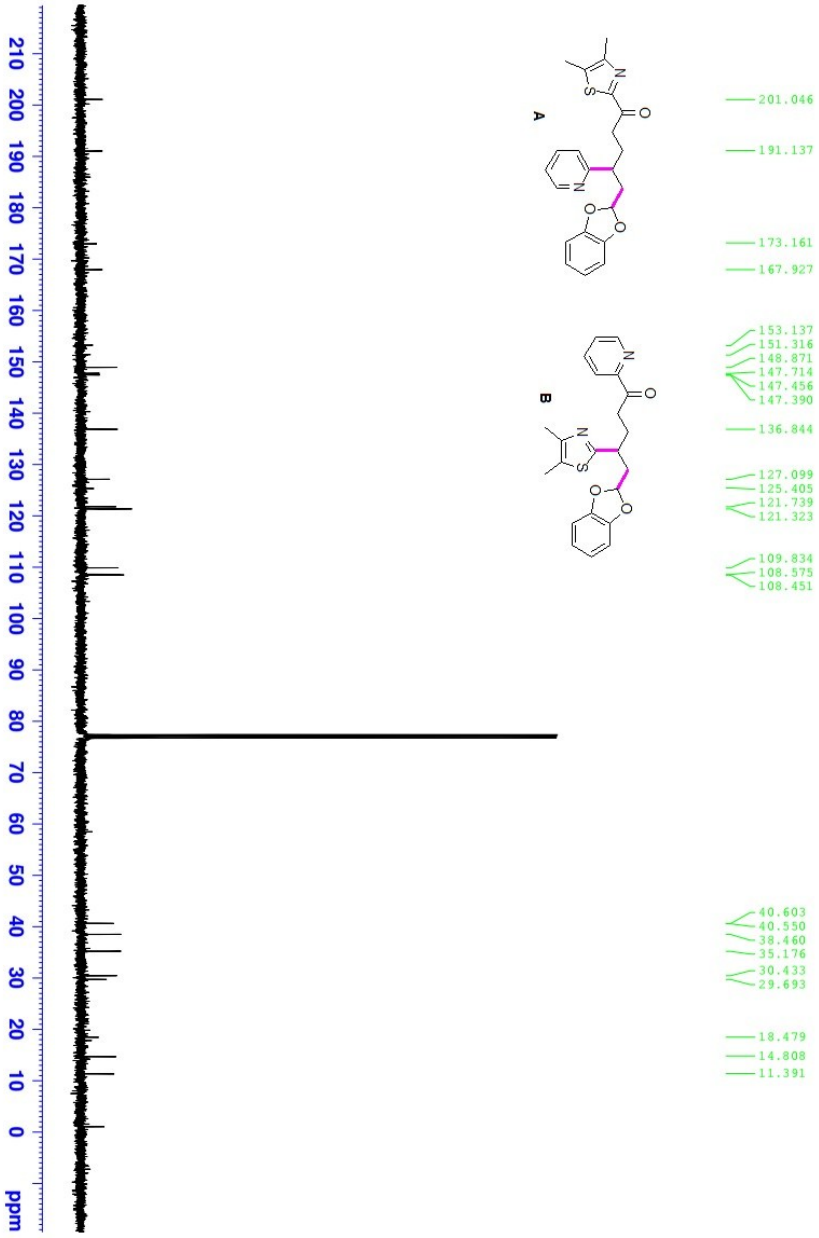
^{1}H NMR of Compound 5aa



^{13}C NMR of Compound 5aa



^{1}H NMR of Compound 6



^{13}C NMR of Compound 6