Electronic Supplementary Material (ESI) for ChemComm.

A formal (5+1) annulation reaction from heterodimerization of two different isocyanides: stereoselective synthesis of *2H*-benzo[b][1,4]oxazin-2-one

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Supporting Information

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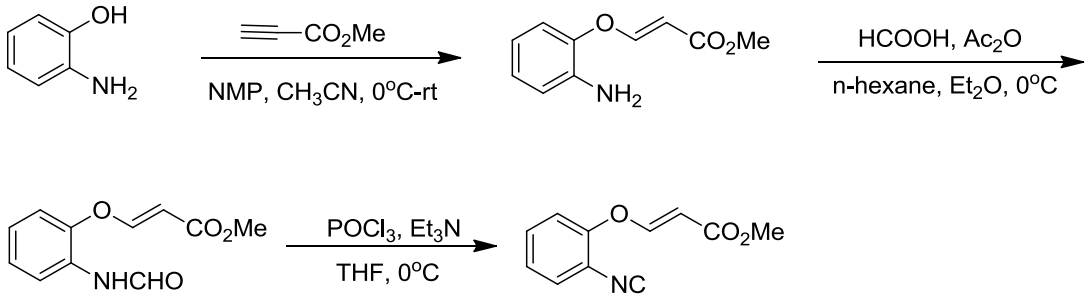
1 General Information

The NMR spectra were recorded on Bruker AC – 500 spectrometer (500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR) with $CDCl_3$ as the solvent and TMS as internal reference. ^{1}H NMR spectral data were reported as follows: chemical shift (δ, ppm), multiplicity, integration, and coupling constant (Hz). ^{13}C NMR spectral data were reported in terms of the chemical shift. The following abbreviations were used to indicate multiplicities: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet. Low-resolution mass spectra were obtained on a Shimadzu LCMS-2010EV spectrometer in ESI mode and reported as m/z. High-resolution mass spectra (HRMS) were recorded on a Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS instrument. Melting points were obtained on a X-4 digital melting point apparatus without correction. Chemical yields referred to pure isolated product. Purification of products was accomplished by column chromatography packed with silica gel. Unless otherwise stated, anhydrous solvents were used in all cases.

2 Synthetic Procedures

2.1 Representative procedure for the preparation of substrates 1



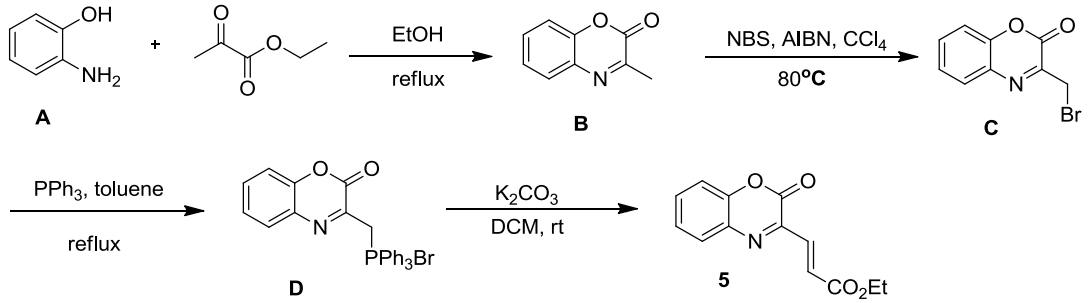
Step 1: In a 100 mL round-bottom flask, a mixture of 2-aminophenol (20 mmol, 1 equiv) propiolate (24 mmol, 1.2 equiv.) was dissolved in acetonitrile (60 mL) and was cooled to 0 ℃. Then N-methylmorpholine (1.2 mmol, 0.06 equiv.) was added into the reaction mixture. The reaction mixture was allowed to warmed to room temperature and stirred for 12 h. After the solvent was removed, the crude product was purified by column chromatography to afforded (*E*)-methyl 3-(2-aminophenoxy)acrylate (3.32 g, 86%) as a yellow liquid.[1]

Step 2: Acetyl formyl anhydride (prepared by stirring 2.0 equiv of acetic anhydride and 2.0 equiv of formic acid for 2 h at 55 ℃) was added dropwise to a solution of (*E*)-methyl 3-(2-aminophenoxy)

acrylate (3.32 g, 17.2 mmol, 1.0 equiv) in Et_2O at 0 ℃ , and the mixture was stirred for 0.5 h at 0 ℃, and then filtered to give (*E*)-methyl 3-(2-formamidophenoxy)acrylate (3.42 g, 90%) as a white solid.

Step 3: A solution of (*E*)-methyl 3-(2-formamidophenoxy)acrylate (3.42 g, 15.48 mmol, 1.0 equiv) and NEt_3 (69.66 mmol, 4.5 equiv) in THF (100 mL) was cooled at 0 ℃, then $POCl_3$ (23.22 mmol, 1.5 equiv) was added dropwise. After the reaction was completed, a saturated Na_2CO_3 aqueous solution was added at 0 ℃ and the mixture was extracted with EA (3 ×100 mL). The combined organic phases were dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The residue was subjected to column chromatography on neutral Al_2O_3 to give (*E*)-methyl 3-(2-isocyanophenoxy)acrylate (**1a**, 2.60 g, 83%) as a white solid.[2,3]

2.2 General procedure for the preparation of substrates 6



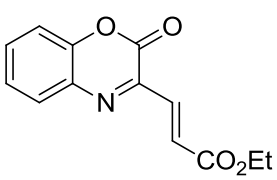
Setp 1: To a 250 mL round-bottomed flask equipped with a magnetic stir bar was added 100 ml absolute ethyl alcohol, active Molecular sieves type 4Å, **A** (2.40 g, 22.0 mmol, 1.1 eq) and ethyl pyruvate (2.32 g, 20.0 mmol, 1.0 eq), the reaction mixture was stirred at 110 ℃ for 12 h. After cooling to room temperature, the mixture was filtered and concentrated under vacuum, purified by flash silica gel column chromatography (petroleum ether : ethyl acetate = 5:1) to afford the desired product **B** as a yellow solid (2.58 g, 80% yield).[4]

Setp 2: To a 250 mL round-bottomed flask equipped with a magnetic stir bar was added **B** (2.58 g, 16.0 mmol, 1.0 eq), CCl_4 (100 mL), bromosuccinimide (2.85 g, 16.0 mmol, 1.0 eq) and AIBN ((0.50 g, 4.8 mmol)). The reaction mixture was stirred at 80 ^oC for 24 h. After cooling to room temperature, H_2O (100 mL) and dichloromethane (50 mL) were added to the mixture, and the layers were separated. The aqueous layer was extracted with dichloromethane (2 x 50 mL). The combined organic layers were

washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate = 5:1) to give 3-(bromomethyl)-2H-benzo[*b*] [1, 4] oxazin-2-one **C** as a yellow solid**.**

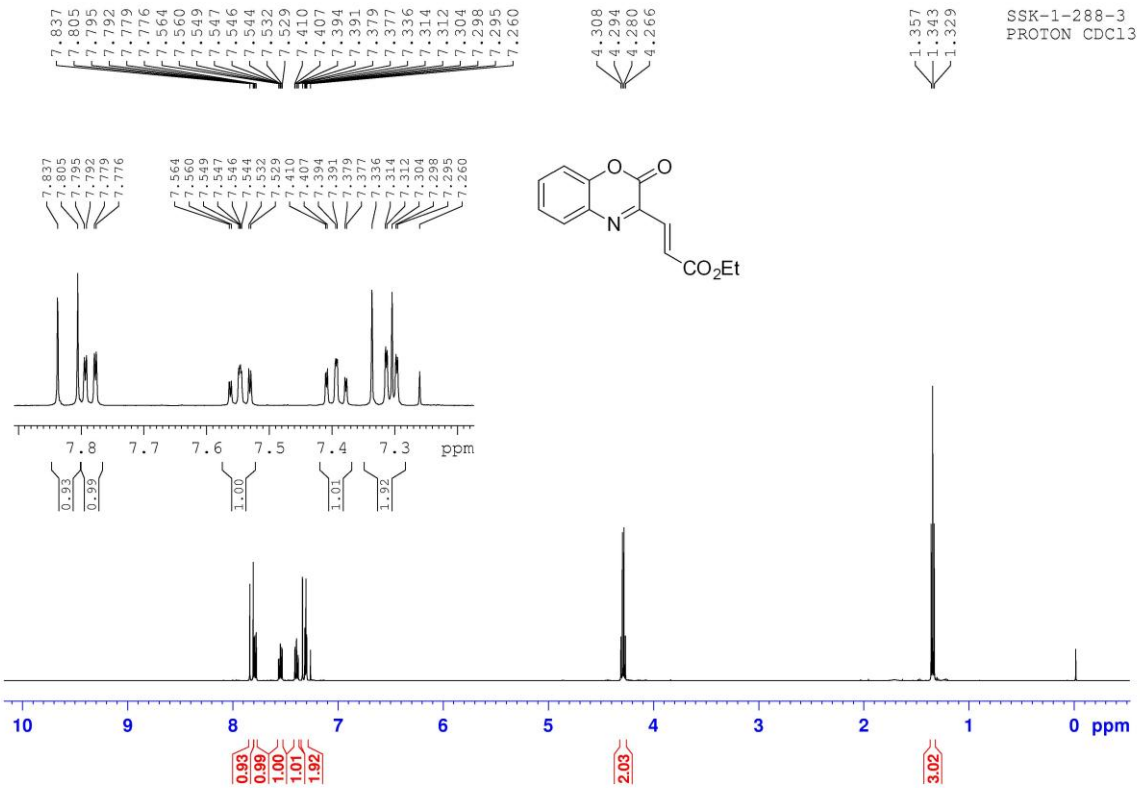
Setp 3: To a solution of above yellow solid was added toluene (60 mL) and triphenylphosphine (4.19 g, 16.0 mmol, 1.0eq). Thereaction mixture was stirred at 110 ^oC for 12h. After cooling to room temperature, the precipiate was isolated by filtration, washed with pentane to afford **D** as a brown solid (4.02 g, 50% yield for two steps).

Setp 4: A mixture of **D** (0.53 g, 1.05 mmol), ethyl glyoxalate (1.0 mmol, 50% in toluene) and potassium carbonate (0.15 g, 1.05 mmol) in 10 mL DCM was stirred at room temperature for 0.5 h. The water (20 mL) was added to the reaction mixture, and extracted with dichloromethane (3 x 20 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, concentrated, and purified by column chromatography (petroleum ether: ethyl acetate = 10:1) to give the desired products **5** as a yellow solid (0.14 g, 57% yield).[5]

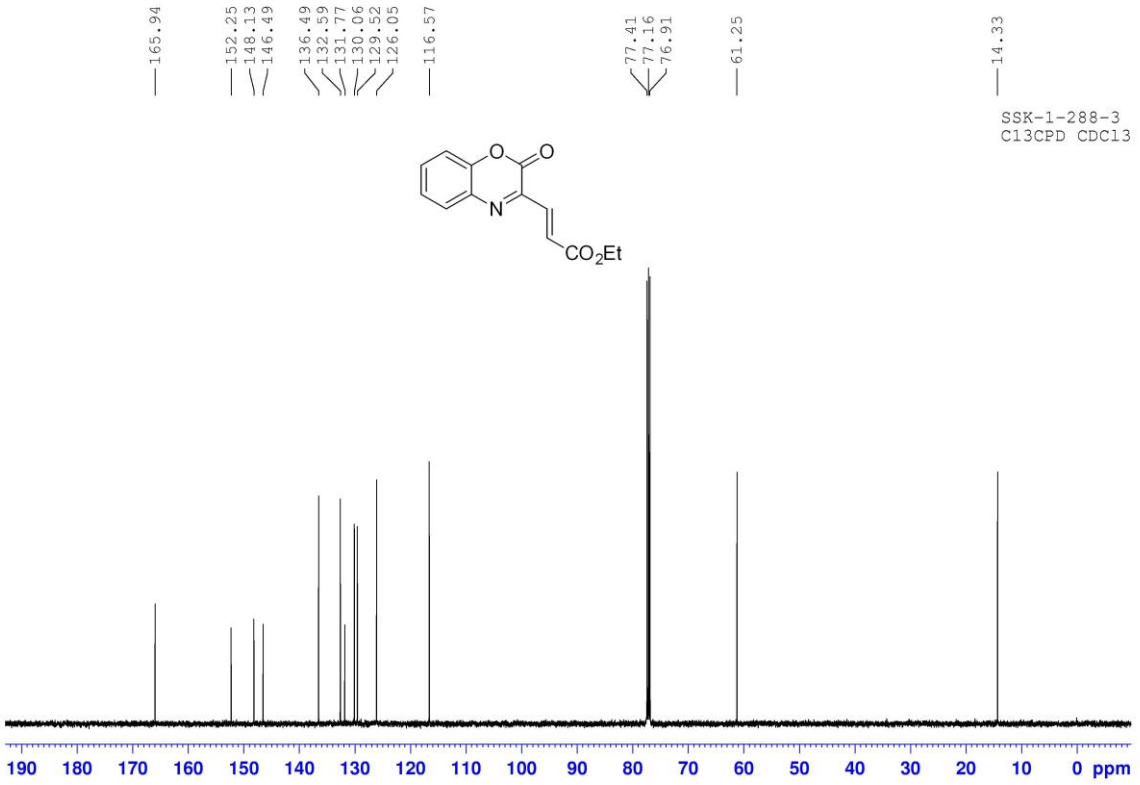


5: 142 mg, 57% yield, yellow solid: m.p. 85-87^oC. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.82 (d, *J* = 16.0 Hz, 1H), 7.79 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.56-7.53 (m, 1H), 7.39 (td, *J* = 8.0, 1.5 Hz, 1H), 7.34-7.29 (m, 2H), 4.29 (q, *J* = 7.0 Hz, 2H), 1.34 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 165.9, 152.3, 148.1, 146.5, 136.5, 132.6, 131.8, 130.1, 129.5, 126.1, 116.6, 61.3, 14.3. HRMS (ESI): calcd. for $C_{13}H_{11}NO_4$ [M+H]+: 246.0761, found: 246.0780.

^{1}H NMR (500 MHz, $CDCl_3$) for **5**



^{13}C NMR (125 MHz, $CDCl_3$) for **5**



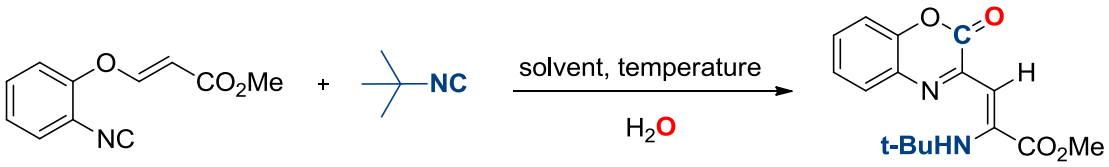
2.3 General Procedure for the Formation of Product 3 or 4.

Under air atmosphere, a flask equipped with a magnetic stir bar and reflux condenser was charged with 2-isocyanophenyloxyacrylate **1** (0.3 mmol, 1.0 eq), isocyanide **2** (0.6 mmol, 2.0 eq) and H_2O (0.6 mmol, 2.0 eq) in DMA (3.0 mL), the resulting solution was heated at 130 ℃ for 12 hours. After the completion of the reaction, H_2O (20 mL) was added, exterted by EA (3×20 mL). The combined organic layer wad dried over anhydrous Na_2SO_4, concentrated under reduced pressure to afford the crude product which was purified by flash silica gel column chromatography using a gradient of ethyl acetate: petroleum ether to afford the corresponding products **3 or 4.**

References:

1. E. Ciganek, *Synthesis*, **1995**, 1311.
2. M. Tobisu, H. Fujihara, K. Koh, N. Chatani, *J. Org. Chem.* **2010**, *75*, 4841.
3. Z. Hu, H. Yuan, Y. Men, Q. Liu, J. Zhang, X. Xu, *Angew. Chem. Int. Ed.* **2016**, *55*, 7077.
4. Le Bris, M. T. *J. Heterocyclic. Chem*. **1985**, *22*, 1275-1280.
5. Y.-Y. Ding, D.-F. Xu, S.-S. Meng, Y. Li, J.-L. Zhao, *Adv. Synth. Catal.* **2018**, *360*, 664.

3. Optimization of Reaction Conditions

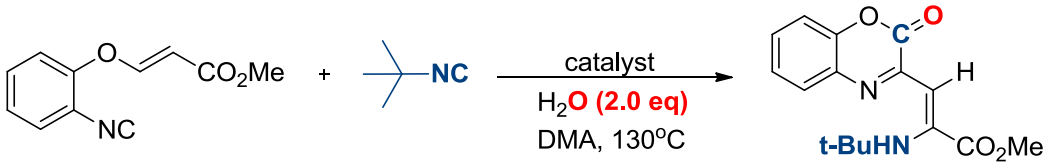


1a **2a** **3a**

(1) Screening the solvent and temperature

Entry	Solvent	Temp (^{o}C)	Yield (%)[b]
1	Toluene	100	8
2	1,4-dioxane	100	15
3	DME	100	13
4	Diglyme	100	6
5	DMSO	100	0
6	DMF	100	31
7	DMA	100	42
8	DMA	120	49
9	DMA	130	71
10	DMA	140	59
11	DMA	80	trace
12[c]	DMA	130	14
13[d]	DMA	130	trace

[a] All reactions were carried out with 0.3 mmol of 2-isocyanophenyloxyacrylate **1a**, 0.6 mmol *tert*-butyl isocyanide **2a**, and 0.6 mmol H_2O in 3 mL solvent. [b] Yields of product after silica gel chromatography. [c] Under N_2 atmosphere. [d] No extra H_2O was added.



1a **2a** **3a**

(2) Screening the catalyst

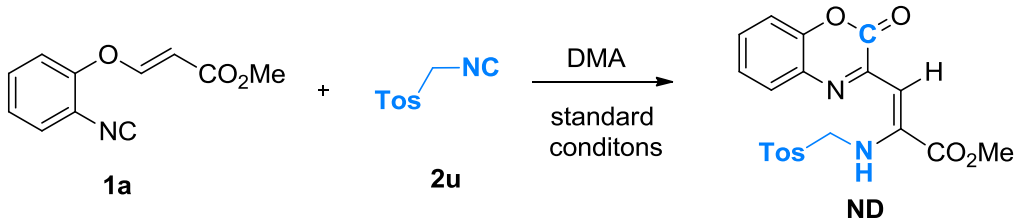
Entry	catalyst	eq	Yield (%)
1	$Sc(OTf)_3$	0.1	-
2	$Cu(OTf)_2$	0.1	-
3	$Y(OTf)_3$	0.1	trace

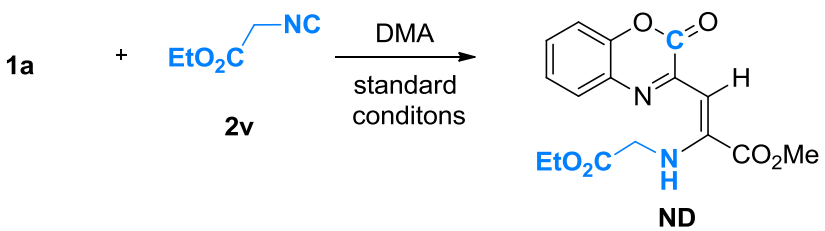
4	$La(OTf)_3$	0.1	-
5	$Yb(OTf_{)3}$	0.1	-
6	$Bi(OTf)_3$	0.1	-
7	$AgNO_3$	0.1	trace
8	AgOAc	0.1	12
9	Ag_2CO_3	0.1	23
10	$Zn(OAc)_2$	0.1	-
11	H_2O_2	1.0	trace
12	DDQ	0.1	-
13	$Pd(TFA)_2$	0.1	18
14	$InCl_3$	0.1	trace
15	K_2PtCl_6	0.1	trace
16	$Mn(acac)_2$	0.1	trace
17	$Ni(acac)_2$	0.1	-
18	HCOOH	0.3	35
19	AcOH	0.3	41
20	$TsOH{\cdot}H_2O$	0.3	-

[a] All reactions were carried out with 0.3 mmol of 2-isocyanophenyloxyacrylate **1a**, 0.6 mmol *tert*-butyl isocyanide **2a**, and 0.6 mmol H_2O in 3 mL DMA. [b] Yields of product after silica gel chromatography.

4 Control Experiments and Mechanistic Studies

4.1 Reactions with activated methylene isocyanides

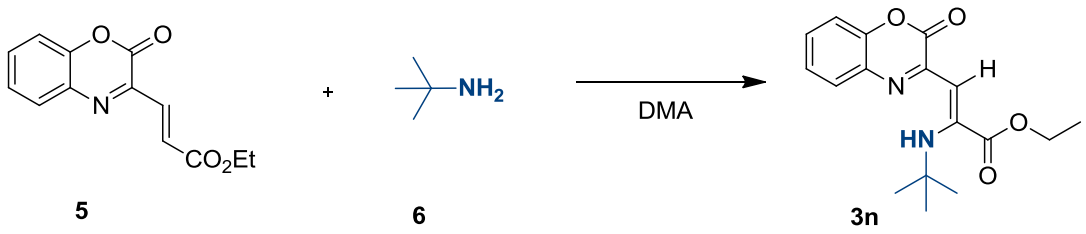




Under air atmosphere, a flask equipped with a magnetic stir bar and reflux condenser was charged with 2-isocyanophenyloxyacrylate **1a** (0.3 mmol, 1.0 eq), isocyanide **2u (2v)** (0.6 mmol, 2.0 eq) and H_2O (0.6 mmol, 2.0 eq) in DMA (3.0 mL), the resulting solution was heated at 130 ℃ for 12 hours. After the

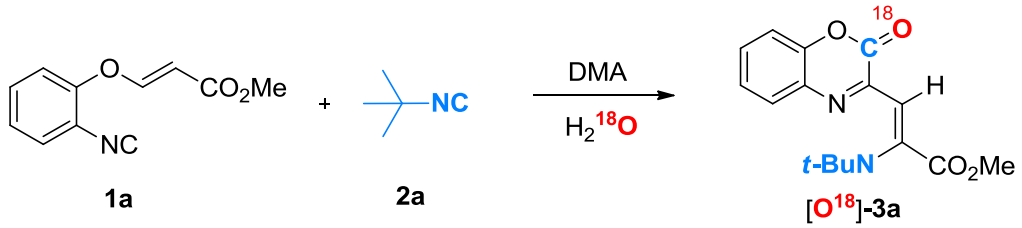
completion of the reaction, H_2O (20 mL) was added, exterted by EA (3×20 mL). In such cases, no desired products **3 or 4** were detected.

4.2 Reactions to verify the possible intermediate



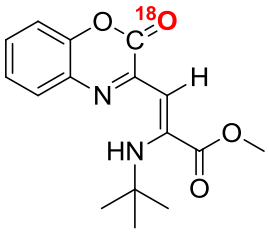
Under air atmosphere, a sealed tube with a magnetic stir bar was charged with (E)-ethyl 3-(2-oxo-2H-benzo[b][1,4]oxazin-3-yl)acrylate **5** (0.3 mmol, 1.0 eq) and *tert*-butylamine **6** (0.6 mmol, 2.0 eq) in DMA (1.5 mL), the resulting solution was heated at 130 ℃ for 12 hours. After the completion of the reaction, H_2O (20 mL) was added, extracted by EA (3×20 mL). The combined organic layer wad dried over anhydrous Na_2SO_4, concentrated under reduced pressure to afford the crude product which was purified by flash silica gel column chromatography using a gradient of ethyl acetate: petroleum ether to afford the product **3n** as a yellow solid (48 mg, 51% yield).

4.3 Isotope reaction to find out the real oxygen source

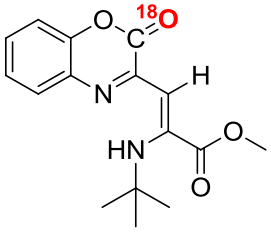


Under air atmosphere, sealed tube with a magnetic stir bar was charged with 2-isocyanophenyloxyacrylate **1a** (0.3 mmol, 1.0 eq), isocyanide **2a** (0.6 mmol, 2.0 eq) and $\mathbf{H_2O^{18}}$ (0.6 mmol, 2.0 eq) in DMA (1.5 mL), the resulting solution was heated at 130 ℃ for 12 hours. After the completion of the reaction, H_2O (20 mL) was added, exterted by EA (3×20 mL). The combined organic layer wad dried over anhydrous Na_2SO_4, concentrated under reduced pressure to afford the crude product

which was purified by flash silica gel column chromatography using a gradient of ethyl acetate: petroleum ether to afford the corresponding products [^{18}O]- **3a** (62 mg, 68% yield).

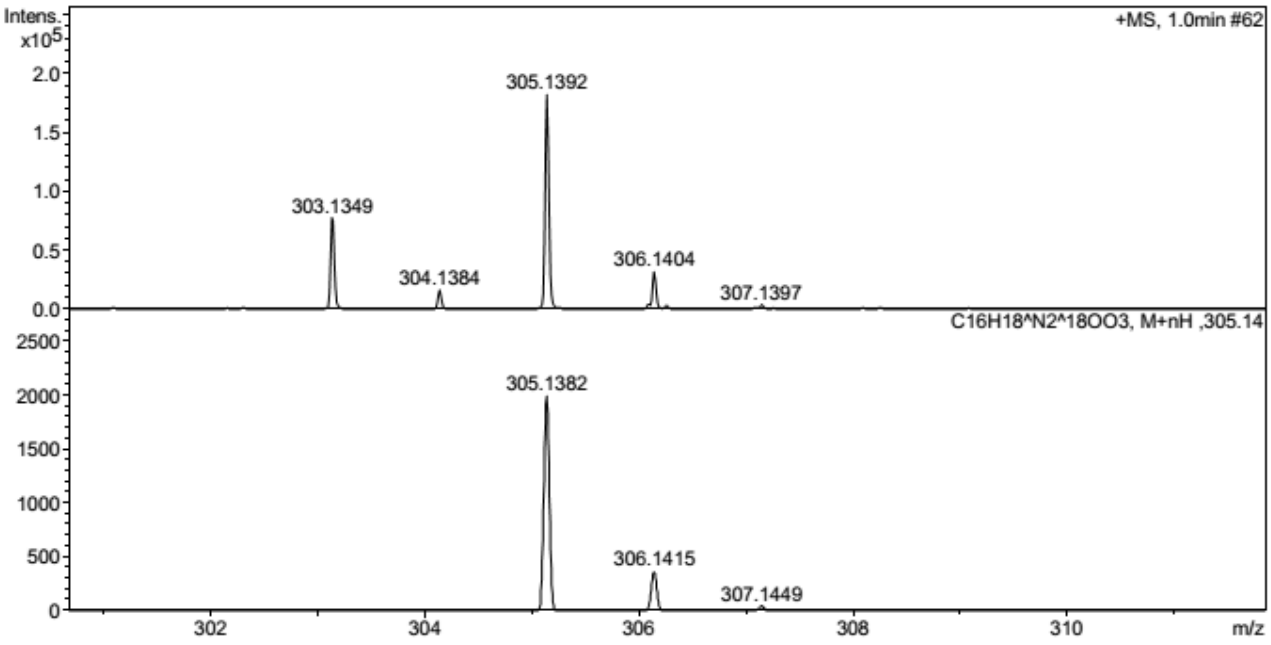


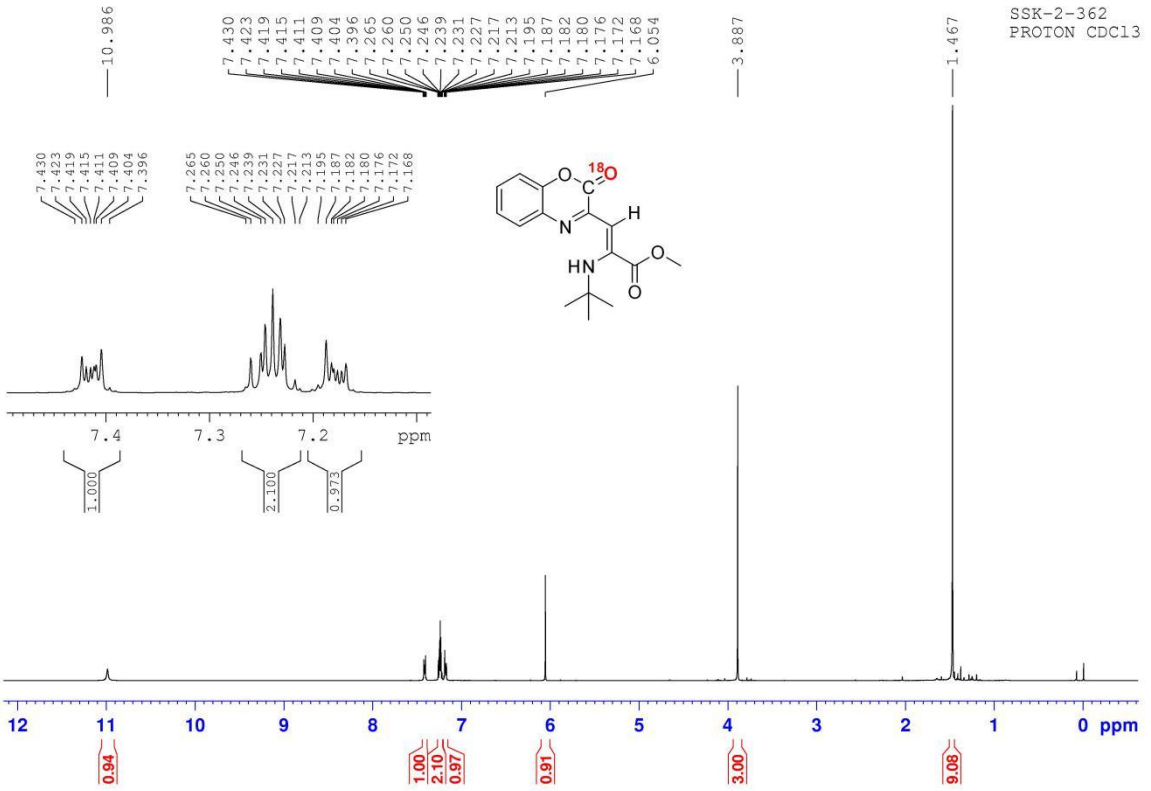
([^{18}O]-**3a**): 62 mg, 68% yield, yellow solid: m.p. 143-145 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.99 (brs, 1H), 7.43-7.40 (m, 1H), 7.27-7.21 (m, 2H), 7.20-7.17 (m, 1H), 6.05 (s, 1H), 3.89 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 165.5, 154.24, 154.21, 150.5, 150.0, 144.9, 131.9, 127.4, 125.9, 125.4, 116.5, 91.2, 54.5, 52.9, 30.7. HRMS (ESI): calcd. for $C_{16}H_{19}N_2O_3{}^{18}O$ $[M+H]^+$ 305.1387, Found: 305.1392.



[^{18}O]-**3a**

Chemical Formula: $C_{16}H_{18}N_2O_3{}^{18}O$
[M+H]+
Calcd: 305.1387
Found: 305.1392

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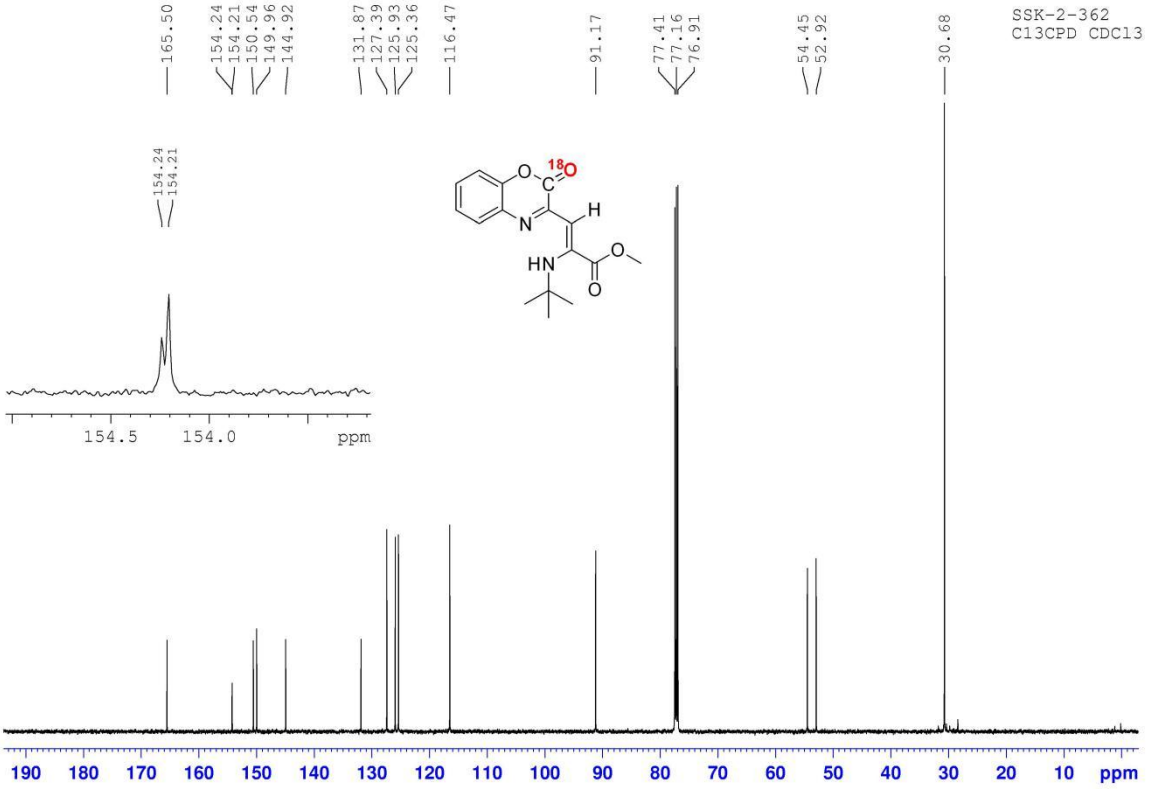
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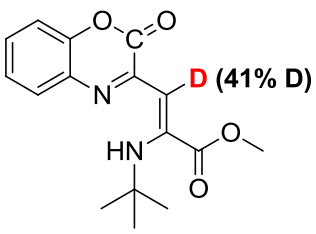
100
90
80
70
60
50
40
30
20
10
ppm

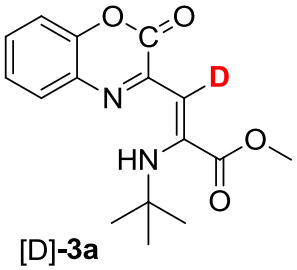
4.4 Isotope reaction to find out the real hydrogen source

1a **2a** **[D]-3a**

Under air atmosphere, sealed tube with a magnetic stir bar was charged with 2-isocyanophenyloxyacrylate **1a** (0.3 mmol, 1.0 eq), isocyanide **2a** (0.6 mmol, 2.0 eq) and **D_2O** (0.6 mmol, 2.0 eq) in DMA (1.5 mL), the resulting solution was heated at 130 ℃ for 12 hours. After the completion of the reaction, H_2O (20 mL) was added, exterted by EA (3×20 mL). The combined organic layer wad dried over anhydrous Na_2SO_4, concentrated under reduced pressure to afford the crude product which was purified by flash silica gel column chromatography using a gradient of ethyl acetate: petroleum ether to afford the corresponding products [**D**]-**3a** (64 mg, 70% yield).

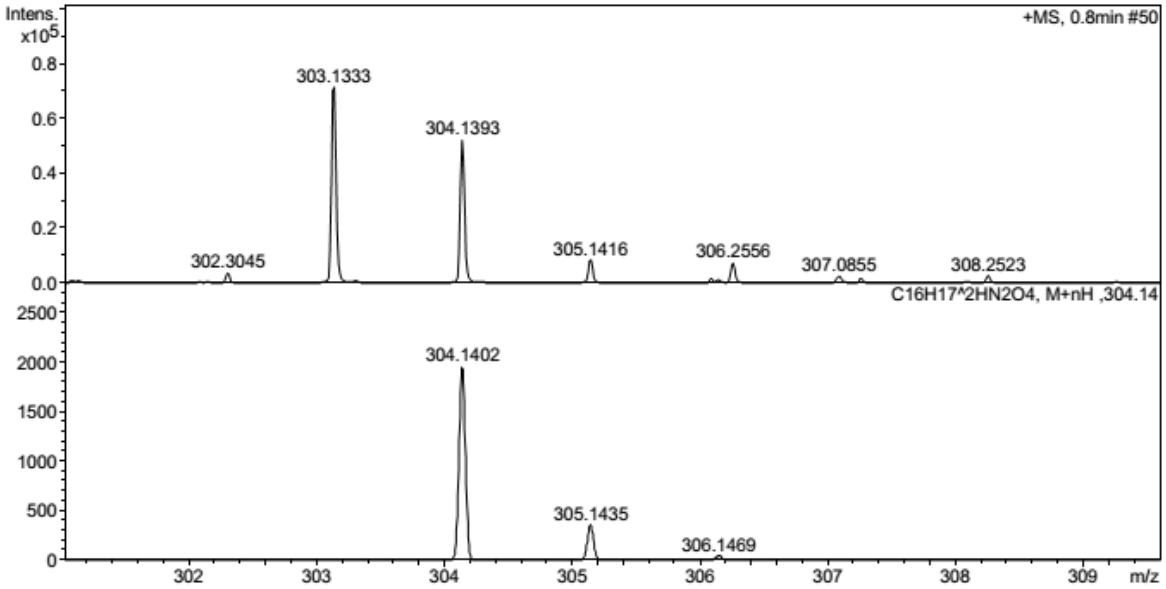


([D]-**3a**): 64 mg, 70% yield, yellow solid: m.p. 144-146°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.00 (brs, 1H), 7.44-7.41 (m, 1H), 7.27-7.23 (m, 2H), 7.21-7.18 (m, 1H), 6.06 (s, 0.59H), 3.89 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 165.5, 154.2, 150.53, 150.48, 149.95, 149.87, 131.9, 127.4, 125.9, 125.4, 116.5, 91.2, 54.4, 52.9, 30.7. HRMS (ESI): calcd. for $C_{16}H_{18}DN_2O_4$ $[M+H]^+$ 304.1408, Found: 304.1393.



[D]-**3a**

Chemical Formula: $C_{16}H_{17}DN_2O_4$
[M+H]+
Calcd: 304.1408
Found: 304.1393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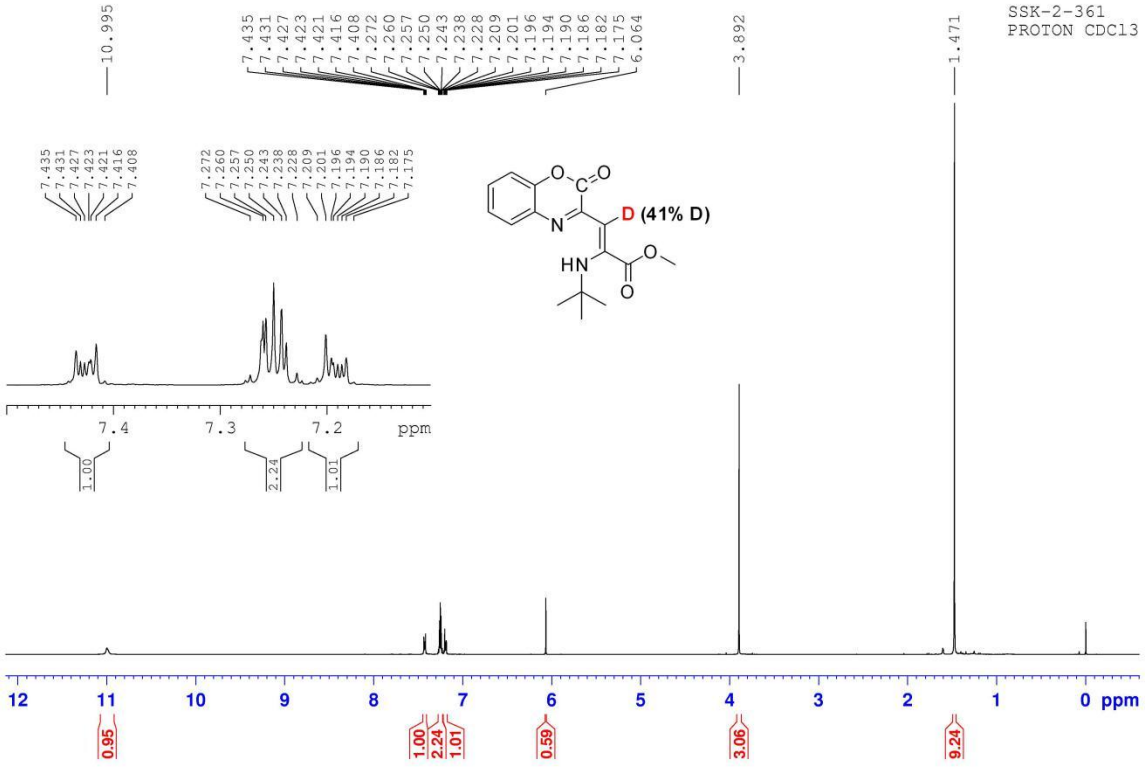
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7.201
7.196
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7.190
7.186
7.182
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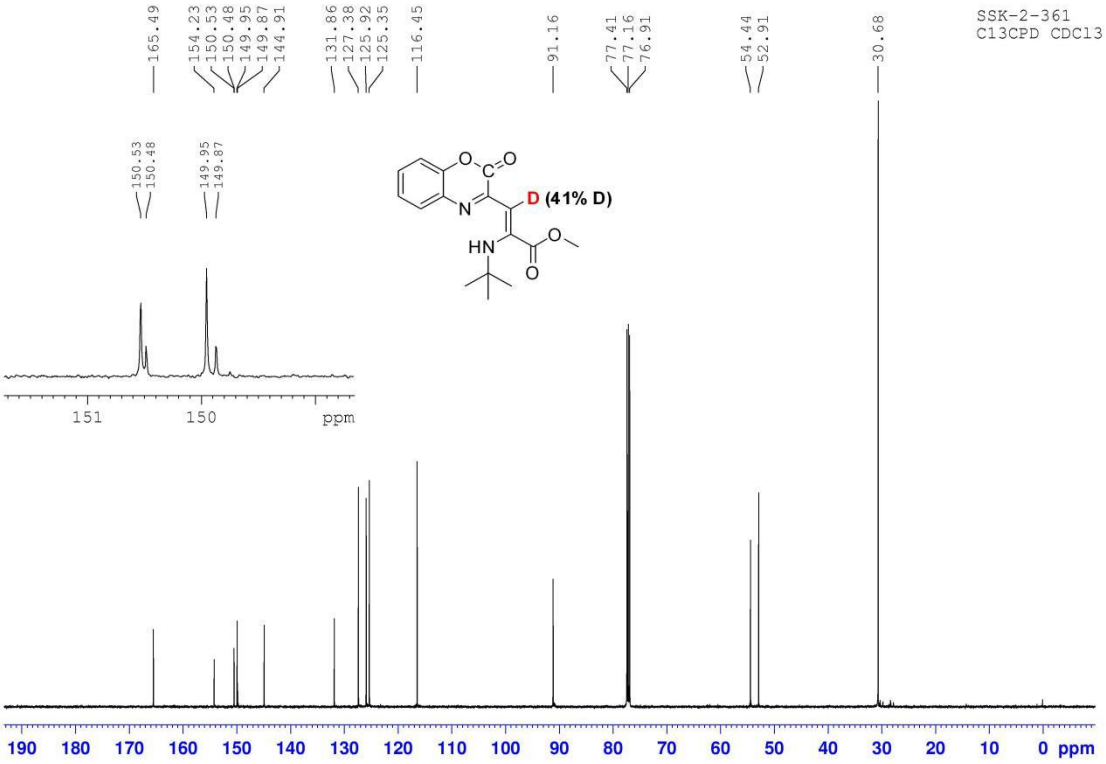
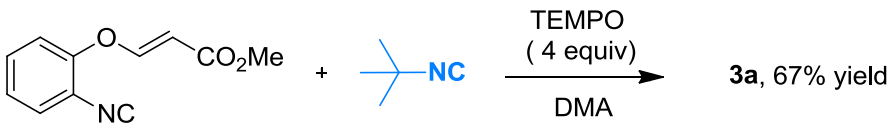
9.24



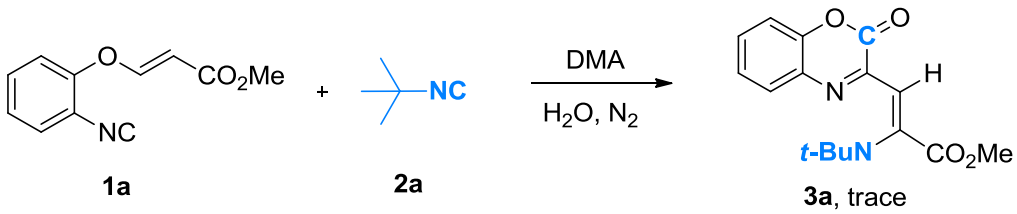
4.5 Reaction with radical radical scavenger TEMPO



1a **2a**

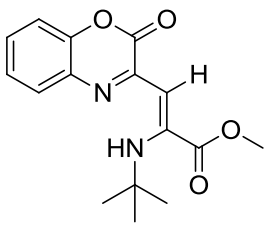
Under air atmosphere, sealed tube with a magnetic stir bar was charged with 2-isocyanophenyloxyacrylate **1a** (0.3 mmol, 1.0 eq), isocyanide **2a** (0.6 mmol, 2.0 eq), TEMPO (4.0 equiv.), and H_2O (0.6 mmol, 2.0 eq) in DMA (1.5 mL), the resulting solution was heated at 130 ℃ for 12 hours. After the completion of the reaction, H_2O (20 mL) was added, exterted by EA (3×20 mL). The combined organic layer wad dried over anhydrous Na_2SO_4, concentrated under reduced pressure to afford the crude product which was purified by flash silica gel column chromatography using a gradient of ethyl acetate: petroleum ether to afford the corresponding product **3a**.

4.6 Reaction under the inert atmosphere

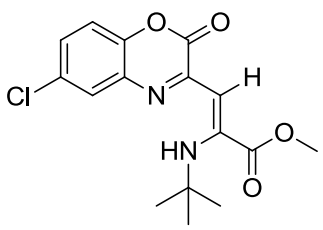


A sealed Schlenk tube was charged with 2-isocyanophenyloxyacrylate **1a** (0.3 mmol, 1.0 eq), isocyanide **2a** (0.6 mmol, 2.0 eq) and H_2O (0.6 mmol, 2.0 eq) in DMA (1.5 mL), the vial was charged with nitrogen and was heated at 130 ℃ for 12 hours. The progress of the reaction was monitored by TLC. After the completion of the reaction, H_2O (20 mL) was added, exterted by EA (3×20 mL). The combined organic layer wad dried over anhydrous Na_2SO_4, concentrated under reduced pressure to afford the crude product which was purified by flash silica gel column chromatography using a gradient of ethyl acetate: petroleum ether to afford the corresponding products.

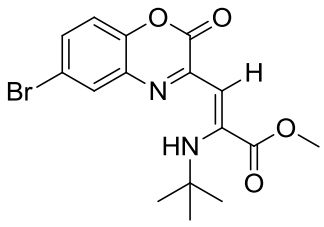
5 Characterization Data



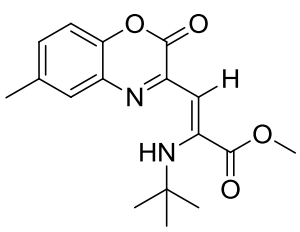
(**3a**): 66 mg, 73% yield, yellow solid: m.p. 137-139 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.99 (brs, 1H), 7.42-7.40 (m, 1H), 7.25-7.22 (m, 2H), 7.19-7.17 (m, 1H), 6.05 (s, 1H), 3.89 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 165.5, 154.2, 150.5, 150.0, 144.9, 131.9, 127.4, 125.9, 125.4, 116.5, 91.2, 54.5, 52.9, 30.7. HRMS (ESI): calcd. for $C_{16}H_{19}N_2O_4$ $[M+H]^+$ 303.1345, Found: 303.1341.



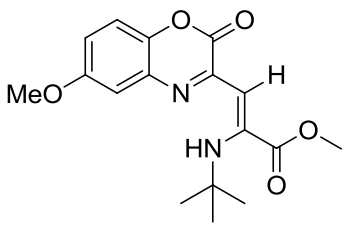
(**3b**): 63 mg, 62% yield, yellow solid: m.p. 140-141 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.03 (brs, 1H), 7.35 (d, *J* = 2.5 Hz, 1H), 7.18 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.11 (d, *J* = 9.0 Hz, 1H), 6.02 (s, 1H), 3.90 (s, 3H), 1.48 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.2, 153.8, 151.0, 151.0, 143.5, 132.7, 130.3, 126.8, 125.2, 117.5, 90.9, 54.8, 53.1, 30.6. HRMS (ESI): calcd. for $C_{16}H_{18}ClN_2O_4$ $[M+H]^+$ 337.0955, Found: 337.0951.



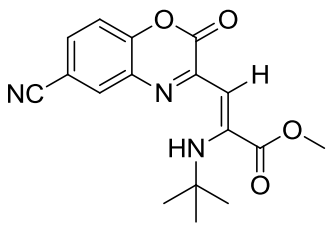
(**3c**): 73 mg, 64% yield, yellow solid: m.p. 139-140 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.02 (brs, 1H), 7.50 (d, *J* = 2.5 Hz, 1H), 7.32 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.05 (d, *J* = 8.5 Hz, 1H), 6.02 (s, 1H), 3.90 (s, 3H), 1.48 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.2, 153.8, 151.0, 151.0, 144.0, 133.1, 129.7, 128.2, 117.9, 117.7, 90.9, 54.8, 53.1, 30.7. HRMS (ESI): calcd. for $C_{16}H_{18}BrN_2O_4$ $[M+H]^+$ 381.0450, Found: 381.0439.



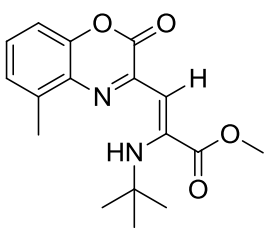
(**3d**): 68 mg, 72% yield, yellow solid: m.p. 150-151 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.93 (brs, 1H), 7.20 (s, 1H), 7.08-7.04 (m, 2H), 6.06 (s, 1H), 3.89 (s, 3H), 2.39 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.6, 154.5, 150.5, 149.8, 142.9, 135.2, 131.6, 128.4, 125.9, 116.1, 91.4, 54.4, 52.9, 30.8, 21.0. HRMS (ESI): calcd. for $C_{17}H_{21}N_2O_4$ $[M+H]^+$ 317.1501, Found: 317.1502.



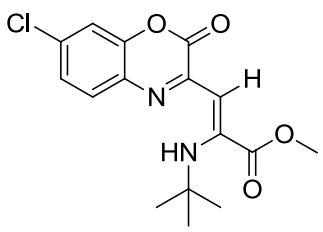
(**3e**): 66 mg, 66% yield, yellow solid: m.p. 161-162 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.98 (brs, 1H), 7.12 (d, *J* = 8.5 Hz, 1H), 6.89 (d, *J* = 2.5 Hz, 2H), 6.84 (dd, *J* = 9.0, 3.0 Hz, 1H), 6.07 (s, 3H), 3.89 (s, 3H), 3.85 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.6, 154.5, 150.5, 149.8, 142.9, 135.2, 131.6, 128.4, 125.9, 116.1, 91.4, 54.4, 52.9, 30.8, 21.0. HRMS (ESI): calcd. for $C_{17}H_{21}N_2O_5$ $[M+H]^+$ 333.1450, Found: 333.1444.



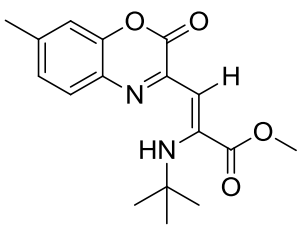
(**3f**): 52 mg, 53% yield, yellow solid: m.p. 181-183 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.18 (brs, 1H), 7.68 (d, *J* = 1.5 Hz, 1H), 7.49 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.27 (d, *J* = 3.0 Hz, 1H), 6.03 (s, 1H), 3.93 (s, 3H), 1.50 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.9, 153.1, 151.9, 151.3, 147.7, 132.5, 129.8, 129.7, 118.2, 117.8, 109.3, 90.6, 55.2, 53.2, 30.6. HRMS (ESI): calcd. for $C_{17}H_{18}N_3O_4$ $[M+H]^+$ 328.1297, Found: 328.1294.



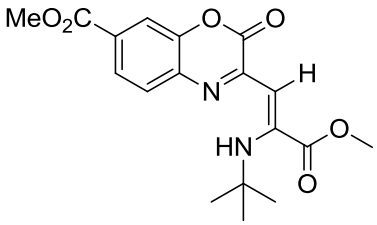
(**3g**): 57 mg, 60% yield, yellow solid: m.p. 161-162 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.10 (brs, 1H), 7.16 (t, *J* = 8.5 Hz, 1H), 7.12 (d, *J* = 7.0 Hz, 1H), 7.04 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.07 (s, 1H), 3.90 (s, 3H), 2.52 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.9, 154.4, 149.7, 149.6, 145.1, 134.6, 130.7, 127.1, 126.5, 114.4, 91.6, 54.3, 53.0, 31.2, 18.7. HRMS (ESI): calcd. for $C_{17}H_{21}N_2O_4$ $[M+H]^+$ 317.1501, Found: 317.1498.



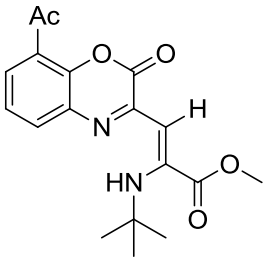
(**3h**): 72 mg, 71% yield, yellow solid: m.p. 157-158 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.94 (brs, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.20-7.17 (m, 2H), 6.01 (s, 1H), 3.89 (s, 3H), 1.46 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.3, 153.6, 150.4, 150.2, 145.1, 132.3, 130.6, 126.5, 125.7, 116.7, 91.0, 54.6, 53.0, 30.6. HRMS (ESI): calcd. for $C_{16}H_{18}ClN_2O_4$ $[M+H]^+$ 337.0955, Found: 337.0948.



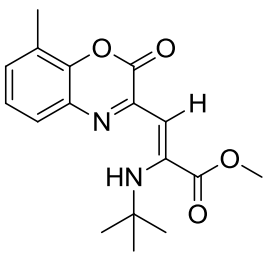
(**3i**): 71 mg, 75% yield, yellow solid: m.p. 120-121 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.81 (brs, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.03 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.97 (s, 1H), 6.04 (s, 1H), 3.88 (s, 3H), 1.45 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.6, 154.4, 149.7, 149.3, 144.8, 138.4, 129.7, 126.4, 125.6, 116.6, 91.4, 54.3, 52.9, 30.7, 21.5. HRMS (ESI): calcd. for $C_{17}H_{21}N_2O_4$ $[M+H]^+$ 317.1501, Found: 317.1507.



(**3j**): 53 mg, 43% yield, yellow solid: m.p. 160-161 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.30 (brs, 1H), 7.86 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.78 (d, *J* = 1.5 Hz, 1H), 7.37 (d, *J* = 8.5 Hz, 1H), 6.02 (s, 1H), 3.91 (s, 3H), 3.89 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.9, 165.0, 153.9, 151.6, 151.5, 144.3, 135.4, 128.1, 126.5, 125.3, 117.8, 91.1, 54.9, 53.1, 52.5, 30.5. HRMS (ESI): calcd. for $C_{18}H_{21}N_2O_6$ $[M+H]^+$ 361.1400, Found: 361.1398.

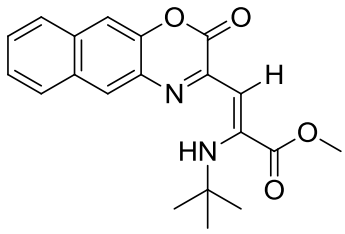


(**3k**): 39 mg, 38% yield, yellow solid: m.p. 145-147 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.04 (brs, 1H), 7.71 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.56 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 6.04 (s, 1H), 3.91 (s, 3H), 2.79 (s, 3H), 1.48 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 197.0, 165.3, 152.9, 150.7, 150.3, 143.8, 132.2, 130.0, 128.0, 127.3, 125.0, 90.8, 54.7, 53.1, 32.2, 30.7. HRMS (ESI): calcd. for $C_{18}H_{21}N_2O_5$ $[M+H]^+$ 345.1450, Found: 345.1451.

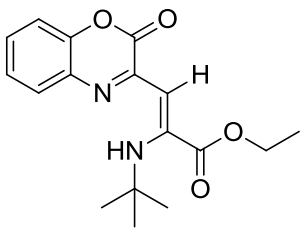


(**3l**): 62 mg, 65% yield, yellow solid: m.p. 180-182 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.04 (brs, 1H), 7.26 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.13 (t, *J* = 7.5 Hz, 1H), 7.10-7.09 (m, 1H), 6.07 (s, 1H), 3.89 (s, 3H), 2.38 (s, 3H), 1.46 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.6, 154.4, 150.24, 149.7, 143.3, 131.6, 129.0, 125.9, 124.8, 123.7, 91.3, 54.4, 52.9, 30.7, 14.9. HRMS (ESI):

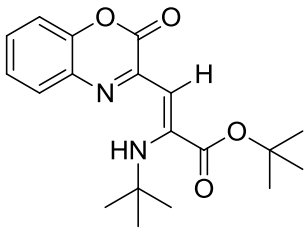
calcd. for $C_{17}H_{21}N_2O_4$ $[M+H]^+$ 317.1501, Found: 317.1498.



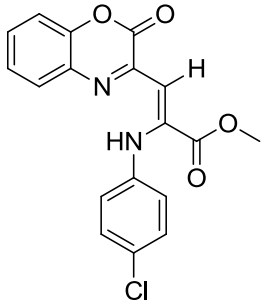
(**3m**): 71 mg, 67% yield, yellow solid: m.p. 189-191 ^oC. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.14 (brs, 1H), 7.85 (dd, *J* = 7.0, 2.0 Hz, 1H), 7.80 (s, 1H), 7.79 (d, *J* = 7.0 Hz, 1H), 7.53 (s, 1H), 7.48-7.42 (m, 2H), 6.09 (s, 1H), 3.91 (s, 3H), 1.53 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.5, 154.2, 150.4, 150.1, 143.7, 132.1, 131.3, 128.0, 127.5, 126.8, 125.9, 123.7, 112.6, 91.5, 54.6, 53.0, 30.7. HRMS (ESI): calcd. for $C_{20}H_{21}N_2O_4$ $[M+H]^+$ 353.1501, Found: 353.1498.



(**3n**): 73 mg, 77% yield, yellow solid: m.p. 97-99 ^oC. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.04 (brs, 1H), 7.43-7.42 (m, 1H), 7.27-7.23 (m, 2H), 7.21-7.18 (m, 1H), 6.05 (s, 1H), 4.35 (q, *J* = 7.0 Hz, 2H), 1.48 (s, 9H), 1.40 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.1, 154.3, 150.6, 144.9, 131.9, 127.3, 125.9, 125.3, 116.5, 90.9, 62.3, 54.5, 30.7, 14.1. HRMS (ESI): calcd. for $C_{17}H_{21}N_2O_4$ $[M+H]^+$ 317.1501, Found: 317.1499.

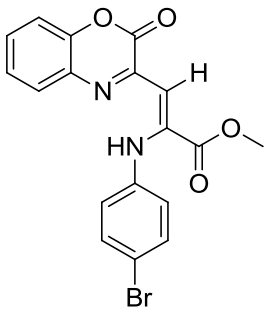


(**3o**): 66 mg, 64% yield, yellow solid: m.p. 165-166 ^oC. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.15 (brs, 1H), 7.42-7.38 (m, 1H), 7.24-7.21 (m, 2H), 7.19-7.16 (m, 1H), 5.94 (s, 1H), 1.59 (s, 9H), 1.50 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.3, 154.4, 152.2, 150.6, 144.8, 132.0, 127.0, 125.7, 125.3, 116.4, 90.2, 83.9, 54.5, 30.8, 28.0. HRMS (ESI): calcd. for $C_{19}H_{25}N_2O_4$ $[M+H]^+$ 345.1814, Found: 345.1804.

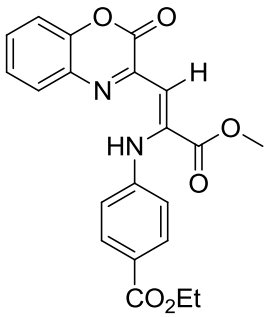


(**4a**): 69 mg, 65% yield, yellow solid: m.p. 152-154 ^oC. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.79 (brs, 1H), 7.56 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.37 (td, *J* = 7.5, 1.5 Hz, 1H), 7.32-7.28 (m, 3H), 7.25 (dd, *J* = 8.5, 1.5 Hz, 1H), 6.95-6.92 (m, 2H), 6.68 (s, 1H), 3.80 (s, 3H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.3, 153.7,

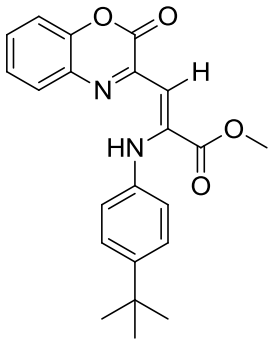
150.4, 145.4, 144.2, 138.9, 131.2, 130.3, 129.5, 129.4, 127.0, 125.7, 122.5, 116.8, 97.8, 53.06. HRMS (ESI): calcd. for $C_{18}H_{14}ClN_2O_4$ $[M+H]^+$ 357.0642, Found: 357.0640.



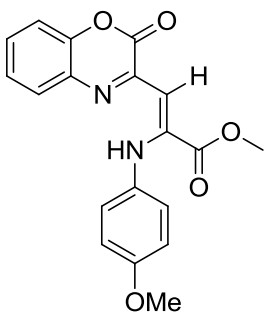
(**4b**): 82 mg, 68% yield, yellow solid: m.p. 159-160 ^oC. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.76 (brs, 1H), 7.56 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.46-7.43 (m, 2H), 7.38 (td, *J* = 7.5, 1.5 Hz, 1H), 7.30 (td, *J* = 8.0, 1.5 Hz, 1H), 7.25 (d, *J* = 3.0, 1.0 Hz, 1H), 6.89-6.86 (m, 2H), 6.68 (s, 1H), 3.80 (s, 3H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.2, 153.7, 150.4, 145.4, 144.0, 139.4, 132.4, 131.2, 129.4, 127.0, 125.7, 122.7, 117.8, 116.8, 98.0, 53.1. HRMS (ESI): calcd. for $C_{18}H_{14}BrN_2O_4$ $[M+H]^+$ 401.0137, Found: 401.0125.



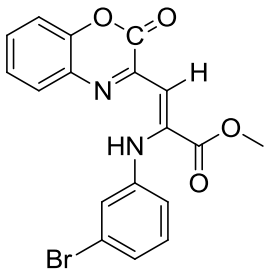
(**4c**): 63 mg, 53% yield, yellow solid: m.p. 195-197 ^oC. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.80 (brs, 1H), 8.02 (d, *J* = 9.0 Hz, 2H), 7.59 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.42-7.38 (m, 1H), 7.34-7.31 (m, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 6.98 (d, *J* = 8.5 Hz, 2H), 6.75 (s, 1H), 4.37 (q, *J* = 7.0 Hz, 2H), 3.82 (s, 1H), 1.39 (t, *J* = 7.0 Hz, 1H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 166.1, 164.3, 153.5, 150.4, 145.5, 144.2, 143.2, 131.1, 131.0, 129.8, 127.2, 126.1, 125.8, 119.8, 116.8, 99.4, 61.1, 53.1, 14.5. HRMS (ESI): calcd. for $C_{21}H_{19}N_2O_6$ $[M+H]^+$ 395.1243, Found: 395.1256



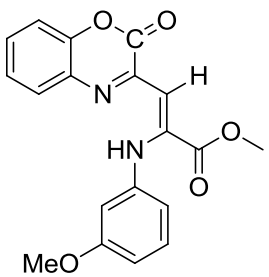
(**4d**): 58mg, 51% yield, yellow solid: m.p. 58-59 ^oC. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.93 (brs, 1H), 7.54 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.38-7.32 (m, 3H), 7.28 (td, *J* = 7.5, 1.5 Hz, 1H), 7.24 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.98-6.95 (m, 2H), 6.60 (s, 1H), 3.80 (s, 3H), 1.33 (m, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.6, 153.9, 150.5, 148.1, 145.3, 145.0, 137.5, 131.5, 128.9, 126.8, 126.3, 125.6, 120.9, 116.7, 96.4, 53.0, 34.6, 31.5. HRMS (ESI): calcd. for $C_{22}H_{23}N_2O_4$ $[M+H]^+$ 379.1658, Found: 379.1664.



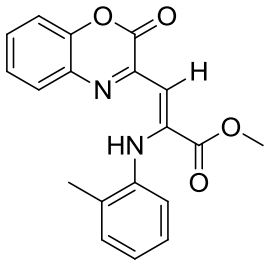
(**4e**): 80 mg, 76% yield, yellow solid: m.p. 145-146 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.89 (brs, 1H), 7.54 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.34 (td, *J* = 7.5, 1.5 Hz, 1H), 7.29 (td, *J* = 7.5, 1.5 Hz, 1H), 7.24 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.01-6.98 (m, 2H), 6.90-6.87 (m, 2H), 6.56 (s, 1H), 3.82 (s, 1H), 3.77 (s, 1H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.5, 157.4, 154.0, 150.5, 145.6, 145.3, 133.4, 131.5, 128.7, 126.74, 125.6, 123.2, 116.7, 114.7, 95.8, 55.7, 52.9. HRMS (ESI): calcd. for $C_{19}H_{17}N_2O_5$ $[M+H]^+$ 353.1137, Found: 353.1128.



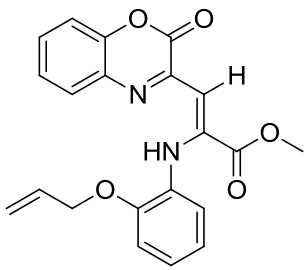
(**4f**): 76 mg, 63% yield, yellow solid: m.p. 168-170 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.75 (brs, 1H), 7.60 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.39 (td, *J* = 8.0, 1.5 Hz, 1H), 7.32 (td, *J* = 8.0, 1.5 Hz, 1H), 7.28-7.26 (m, 2H), 7.22-7.18 (m, 2H), 6.91 (dd, J = 7.5, 1.5 Hz, 1H), 6.71 (s, 1H), 3.81 (s, 1H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.2, 153.7, 150.4, 145.4, 143.9, 141.7, 131.2, 130.6, 129.6, 127.7, 127.2, 125.8, 124.2, 123.0, 119.7, 116.8, 98.4, 53.1. HRMS (ESI): calcd. for $C_{18}H_{14}BrN_2O_4$ $[M+H]^+$ 401.0137, Found: 401.0125.



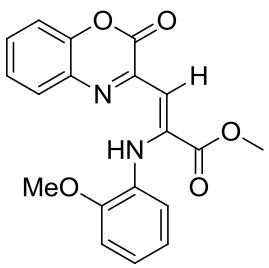
(**4g**): 75 mg, 71% yield, yellow solid: m.p. 129-131 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.83 (brs, 1H), 7.57 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.36 (td, *J* = 7.5, 1.5 Hz, 1H), 7.30 (td, *J* = 8.0, 1.5 Hz, 1H), 7.26-7.23 (m, 2H), 6.71 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.61-6.57 (m, 3H), 3.82 (s, 1H), 3.80 (s, 1H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.7, 160.6, 153.8, 150.5, 145.4, 144.8, 141.4, 131.4, 130.2, 129.2, 127.0, 125.7, 116.7, 113.7, 110.4, 107.2, 97.1, 55.5, 53.0. HRMS (ESI): calcd. for $C_{19}H_{17}N_2O_5$ $[M+H]^+$ 353.1137, Found: 353.1138.



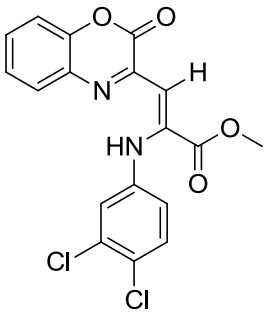
(**4h**): 47 mg, 46% yield, yellow solid: m.p. 146-148 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.86 (brs, 1H), 7.50 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.35 (td, *J* = 7.5, 1.5 Hz, 1H), 7.30 (td, *J* = 8.0, 1.5 Hz, 1H), 7.28-7.25 (m, 2H), 7.16 (td, *J* = 7.5, 1.0 Hz, 1H), 7.09 (td, *J* = 7.5, 1.0 Hz, 1H), 6.84 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.65 (s, 1H), 3.77 (s, 1H), 2.49 (s, 1H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.6, 153.9, 150.5, 145.5, 145.4, 139.0, 131.5, 130.9, 129.7, 128.8, 126.9, 126.8, 125.7, 125.2, 121.5, 116.7, 96.8, 52.9, 18.4. HRMS (ESI): calcd. for $C_{19}H_{17}N_2O_4$ $[M+H]^+$ 337.1188, Found: 337.1176.



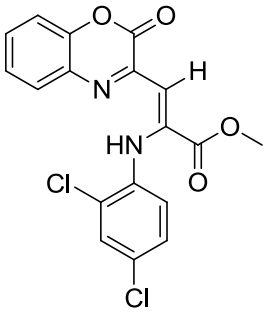
(**4i**): 79 mg, 70% yield, yellow solid: m.p. 162-164 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.99 (brs, 1H), 7.58 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.33 (td, *J* = 7.5, 1.5 Hz, 1H), 7.28-7.22 (m, 2H), 7.09-7.06 (m, 1H), 6.95-6.88 (m, 3H), 6.64 (s, 1H), 6.16-6.08 (m, 1H), 5.49 (dq, *J* = 17.5, 1.5 Hz, 1H), 5.31 (dq, *J* = 10.5, 1.5 Hz, 1H), 4.66 (dt, *J* = 5.0, 1.5 Hz, 2H), 3.81 (s, 1H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.7, 153.9, 150.3, 149.6, 145.4, 144.2, 133.0, 131.6, 129.6, 128.8, 127.3, 125.5, 125.0, 121.1, 120.6, 118.0, 116.5, 112.6, 96.8, 69.6, 52.8. HRMS (ESI): calcd. for $C_{21}H_{19}N_2O_5$ $[M+H]^+$ 379.1294, Found: 379.1286.



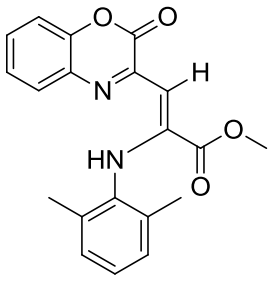
(**4j**): 72 mg, 68% yield, yellow solid: m.p. 133-135 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 12.05 (brs, 1H), 7.54 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.34 (td, *J* = 7.5, 1.5 Hz, 1H), 7.29 (td, *J* = 7.5, 1.5 Hz, 1H), 7.24 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.12-7.08 (m, 1H), 6.94 (qd, *J* = 8.5, 1.0 Hz, 2H), 6.89 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.61 (s, 1H), 3.96 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.7, 153.9, 150.6, 150.3, 145.4, 144.4, 131.6, 129.3, 128.8, 127.0, 125.6, 125.1, 121.0, 120.5, 116.6, 111.3, 96.4, 55.8, 52.8. HRMS (ESI): calcd. for $C_{19}H_{17}N_2O_5$ $[M+H]^+$ 353.1137, Found: 353.1150.



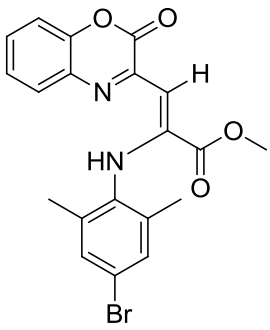
(**4k**): 77 mg, 66% yield, yellow solid: m.p. 182-184 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.69 (brs, 1H), 7.59 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.42-7.37 (m, 3H), 7.32 (td, *J* = 7.5, 1.5 Hz, 1H), 7.27 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.11 (d, *J* = 2.5 Hz, 1H), 6.82 (dd, J = 8.5, 2.5 Hz, 1H), 6.74 (s, 1H), 3.83 (s, 3H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.0, 153.6, 150.3, 145.4, 143.5, 140.0, 133.2, 131.0, 130.8, 129.8, 128.3, 127.2, 125.8, 122.9, 120.5, 116.8, 99.0, 53.2. HRMS (ESI): calcd. for $C_{18}H_{13}Cl_2N_2O_4$ $[M+H]^+$ 391.0252, Found: 391.0251.



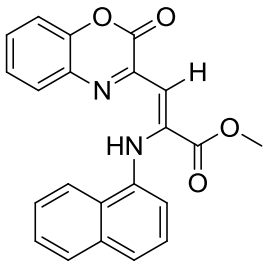
(**4l**): 72 mg, 61% yield, yellow solid: m.p. 239-241 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.98 (brs, 1H), 7.63 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.47 (d, *J* = 2.5 Hz, 1H), 7.41 (td, *J* = 8.0, 1.5 Hz, 1H), 7.34 (td, *J* = 8.0, 1.5 Hz, 1H), 7.28 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.18 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.83 (s, 1H), 6.78 (d, *J* = 8.5 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.1, 153.6, 150.0, 145.7, 142.6, 136.4, 131.2, 129.8, 129.8, 129.5, 127.7, 127.6, 125.9, 125.8, 121.8, 116.8, 100.2, 53.2. HRMS (ESI): calcd. for $C_{18}H_{13}Cl_2N_2O_4$ $[M+H]^+$ 391.0252, Found: 391.0246.



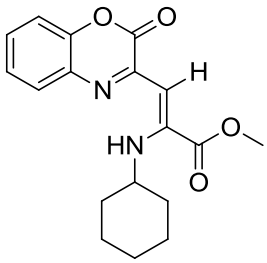
(**4m**): 61 mg, 58% yield, yellow solid: m.p. 128-129 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.64 (brs, 1H), 7.50 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.33 (td, *J* = 8.0, 1.5 Hz, 1H), 7.28 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.27-7.25 (m, 1H), 7.12-7.11 (m, 3H), 6.68 (s, 1H), 3.68 (s, 3H), 2.28 (s, 6H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 163.6, 154.1, 150.9, 148.1, 145.2, 138.3, 134.8, 131.6, 128.4, 128.3, 127.0, 126.7, 125.6, 116.7, 93.6, 52.8, 18.7. HRMS (ESI): calcd. for $C_{20}H_{19}N_2O_4$ $[M+H]^+$ 351.1345, Found: 351.1344.



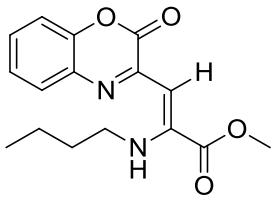
(**4n**): 58 mg, 45% yield, yellow solid: m.p. 157-158 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.75 (brs, 1H), 7.50 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.36-7.33 (m, 1H), 7.30-7.25 (m, 2H), 7.25 (s, 2H), 6.71 (s, 1H), 3.71 (s, 3H), 2.24 (s, 6H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 163.4, 154.0, 150.7, 147.5, 145.2, 137.6, 136.8, 131.4, 131.1, 128.7, 126.7, 125.7, 120.1, 116.7, 94.3, 52.9, 18.5. HRMS (ESI): calcd. for $C_{20}H_{18}BrN_2O_4$ $[M+H]^+$ 429.0450, Found: 429.0477.



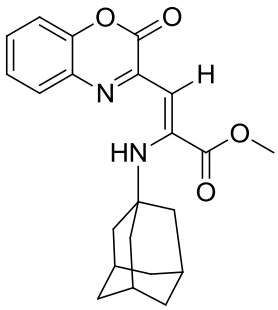
(**4o**): 76 mg, 68% yield, yellow solid: m.p. 180-182 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 12.53 (brs, 1H), 8.26 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.5 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H) , 7.36 (t, *J* = 7.5 Hz, 1H), 7.29-7.26 (m, 2H), 7.30 (d, *J* = 7.0 Hz, 1H), 6.77 (s, 1H), 3.72 (s, 3H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.6, 153.9, 150.5, 146.0, 145.4, 136.6, 134.4, 131.35, 129.0, 128.7, 127.6, 127.0, 126.9, 126.7, 125.7, 125.7, 125.6, 121.8, 118.2, 116.7, 97.6, 52.90. HRMS (ESI): calcd. for $C_{22}H_{17}N_2O_4$ $[M+H]^+$ 373.1188, Found: 373.1188.



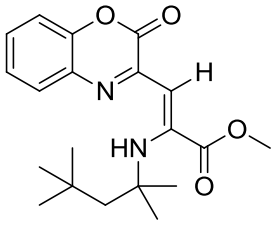
(**4p**): 51 mg, 52% yield, yellow solid: m.p. 122-123 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.83 (brs, 1H), 7.48-7.45 (m, 1H), 7.29-7.24 (m, 2H), 7.22-7.19 (m, 1H), 6.37 (s, 1H), 4.00 (s, 1H), 3.89 (s, 1H), 1.99-1.97 (m, 2H), 1.80-1.76 (m, 2H), 1.62-1.59 (m, 1H), 1.46-1.37 (m, 5H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 164.0, 154.4, 150.6, 147.9, 145.0, 132.1, 127.5, 126.1, 125.4, 116.5, 92.0, 53.3, 52.8, 34.5, 25.6, 24.2.HRMS (ESI): calcd. for $C_{18}H_{21}N_2O_4$ $[M+H]^+$ 329.1501, Found: 329.1490.



(**4q**): 70 mg, 77% yield, yellow solid: m.p. 101-103 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.69 (brs, 1H), 7.46-7.43 (m, 1H), 7.29-7.25 (m, 2H), 7.22-7.19 (m, 1H), 6.41 (s, 1H), 3.89 (s, 1H), 3.64 (t, *J* = 7.0 Hz, 2H), 1.72-1.66 (m, 1H), 1.55-1.49 (m, 1H), 1.00 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 163.9, 154.4, 150.6, 148.6, 145.1, 132.0, 127.6, 126.2, 125.5, 116.6, 92.0, 52.8, 45.2, 32.8, 20.1, 13.9. HRMS (ESI): calcd. for $C_{16}H_{19}N_2O_4$ $[M+H]^+$ 303.1345, Found: 303.1349.



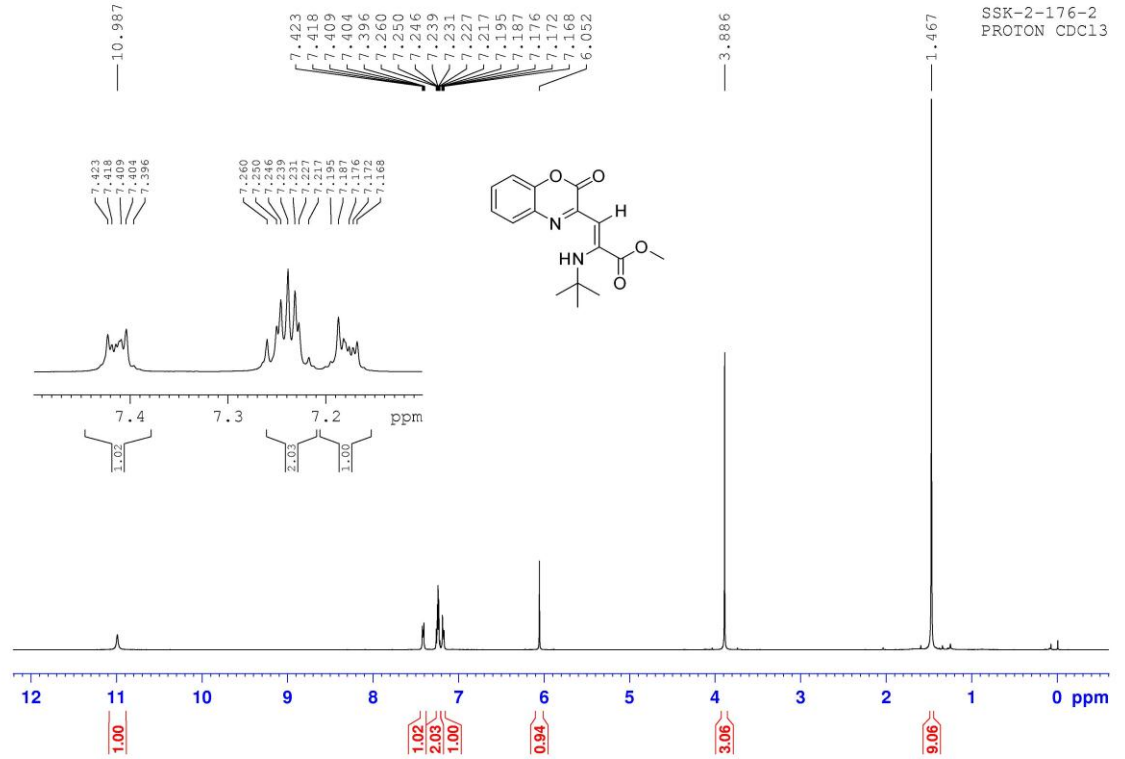
(**4r**): 63 mg, 55% yield, yellow solid: m.p. 178-179 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.92 (brs, 1H), 7.45-7.43 (m, 1H), 7.27-7.23 (m, 2H), 7.21-7.17 (m, 1H), 6.04 (s, 1H), 3.89 (s, 3H), 2.15 (s, 2H), 2.03 (t, *J* = 3.0 Hz, 6H), 1.70 (t, *J* = 15.0 Hz, 6H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.8, 154.3, 150.5, 149.8, 144.9, 132.0, 127.3, 126.0, 125.4, 116.5, 91.2, 55.3, 52.9, 43.4, 36.1, 29.8. HRMS (ESI): calcd. for $C_{22}H_{25}N_2O_4$$[M+H]^+$ 381.1814, Found: 381.1836.

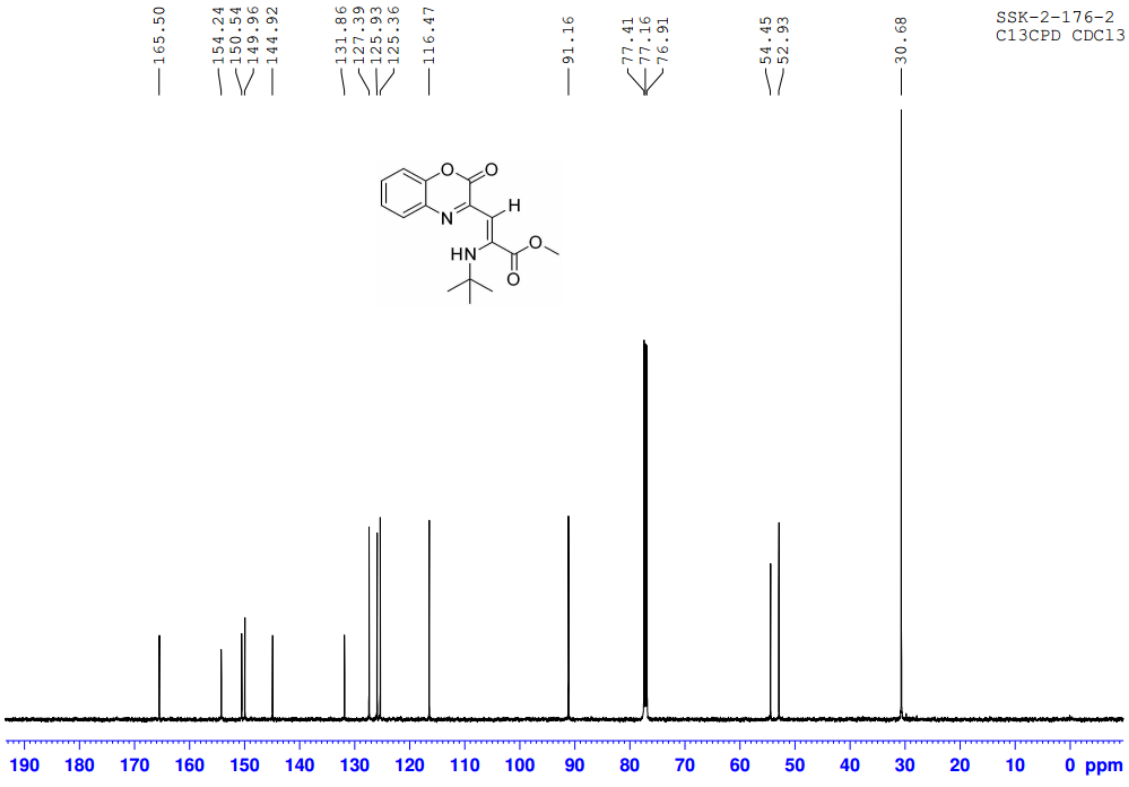


(**4s**): 68 mg, 63% yield, yellow solid: m.p. 100-102 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 11.15 (brs, 1H), 7.43-7.40 (m, 1H), 7.27-7.23 (m, 2H), 7.21-7.18 (m, 1H), 6.00 (s, 1H), 3.89 (s, 3H), 1.81 (s, 2H), 1.48 (s, 6H), 1.04 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ (ppm) = 165.6, 154.4, 150.5, 150.2, 145.0, 132.0, 127.1, 125.7, 125.4, 116.6, 90.5, 58.1, 54.6, 52.9, 31.9, 31.6, 30.9. HRMS (ESI): calcd. for $C_{20}H_{27}N_2O_4$ $[M+H]^+$ 359.1971, Found: 359.1977.

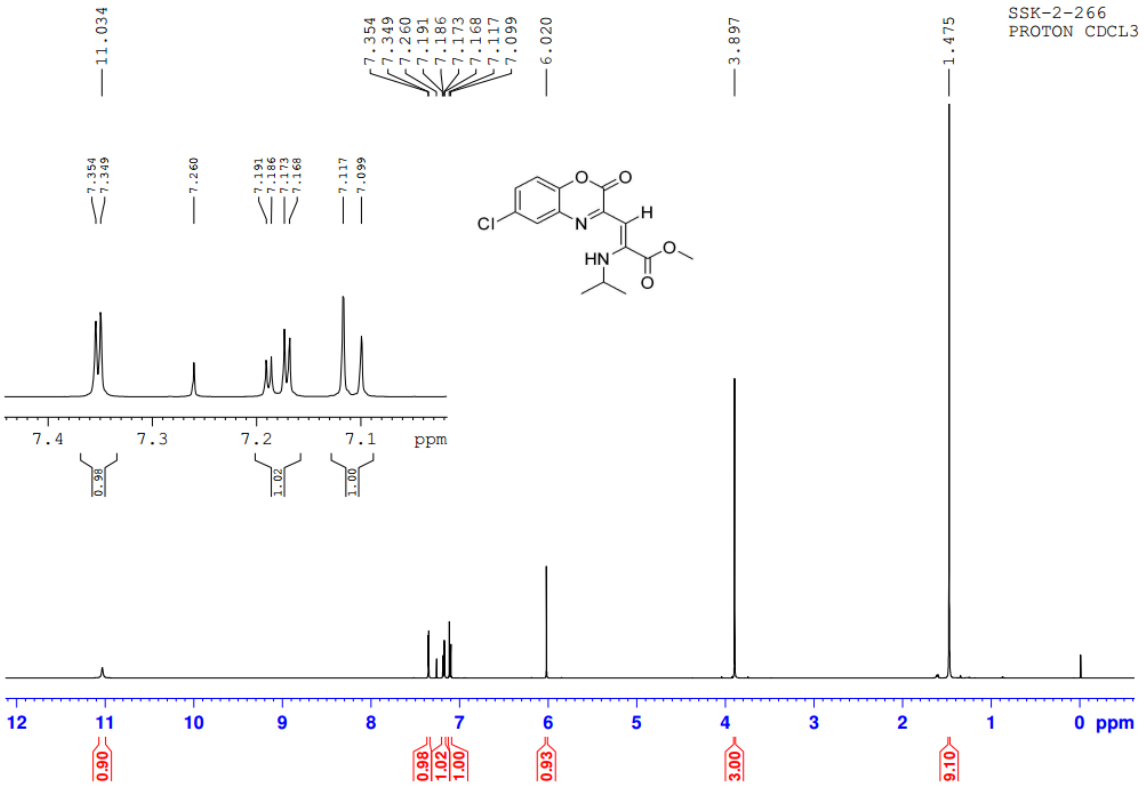
6 ^{1}H NMR and ^{13}C NMR Spectra of All Compounds

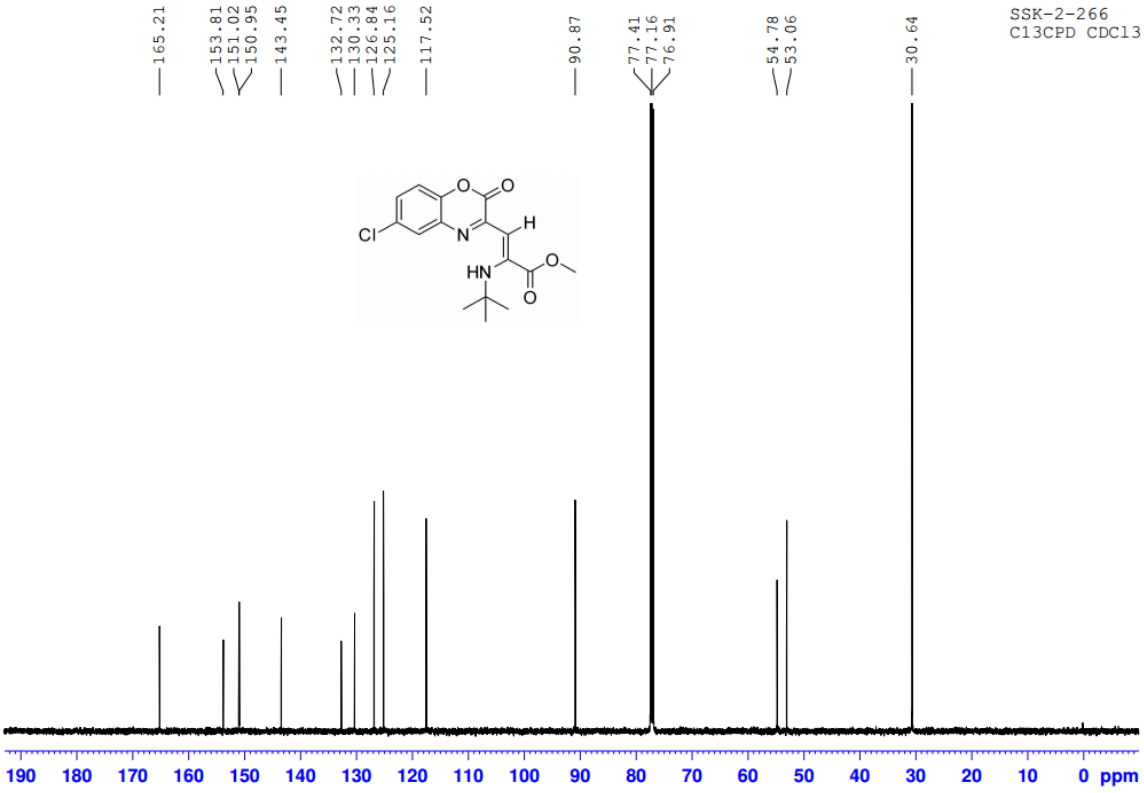
Compound **3a**



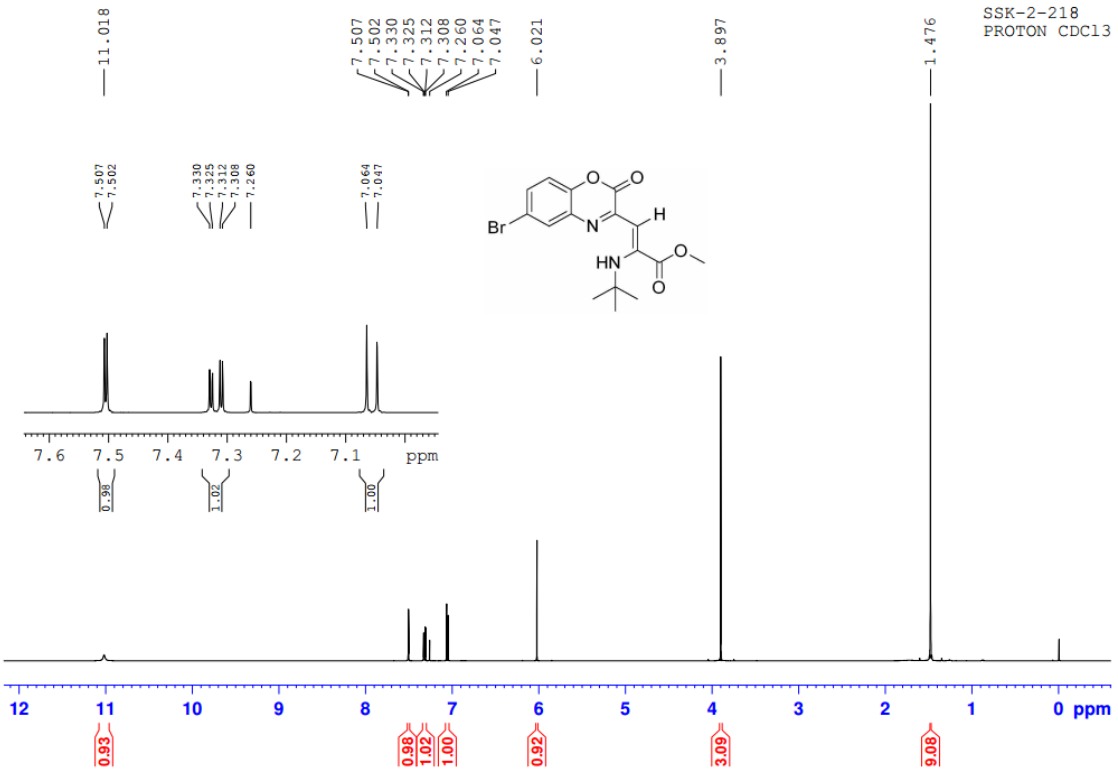


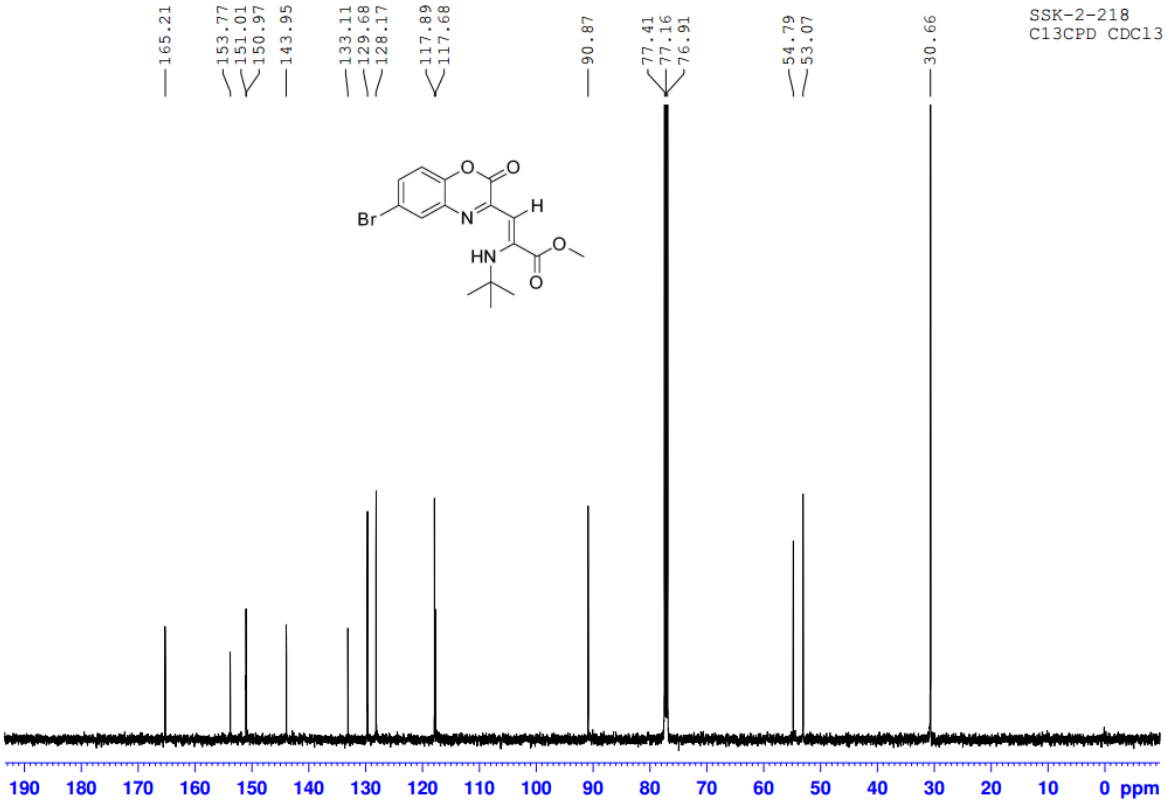
Compound **3b**


SSK-2-266
PROTON CDCL3
11.034
7.354
7.349
7.260
7.191
7.186
7.173
7.168
7.117
7.099
6.020
3.897
1.475
Cl
O
N
H
HN
O
O
7.4
7.3
7.2
7.1
ppm
0.98
1.02
1.00
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.90
0.98
1.02
1.00
0.93
3.00
9.10

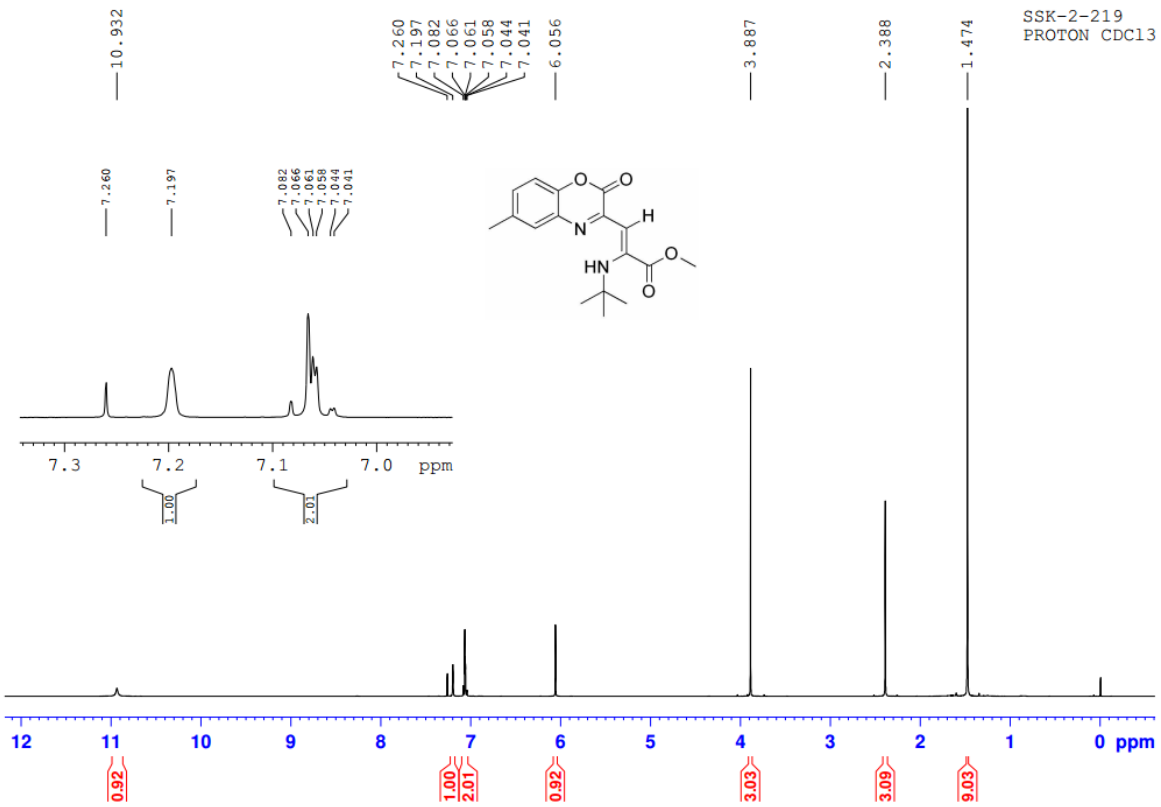

SSK-2-266
C13CPD CDCl3
165.21
153.81
151.02
150.95
143.45
132.72
130.33
126.84
125.16
117.52
90.87
77.41
77.16
76.91
54.78
53.06
30.64
Cl
O
N
H
HN
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

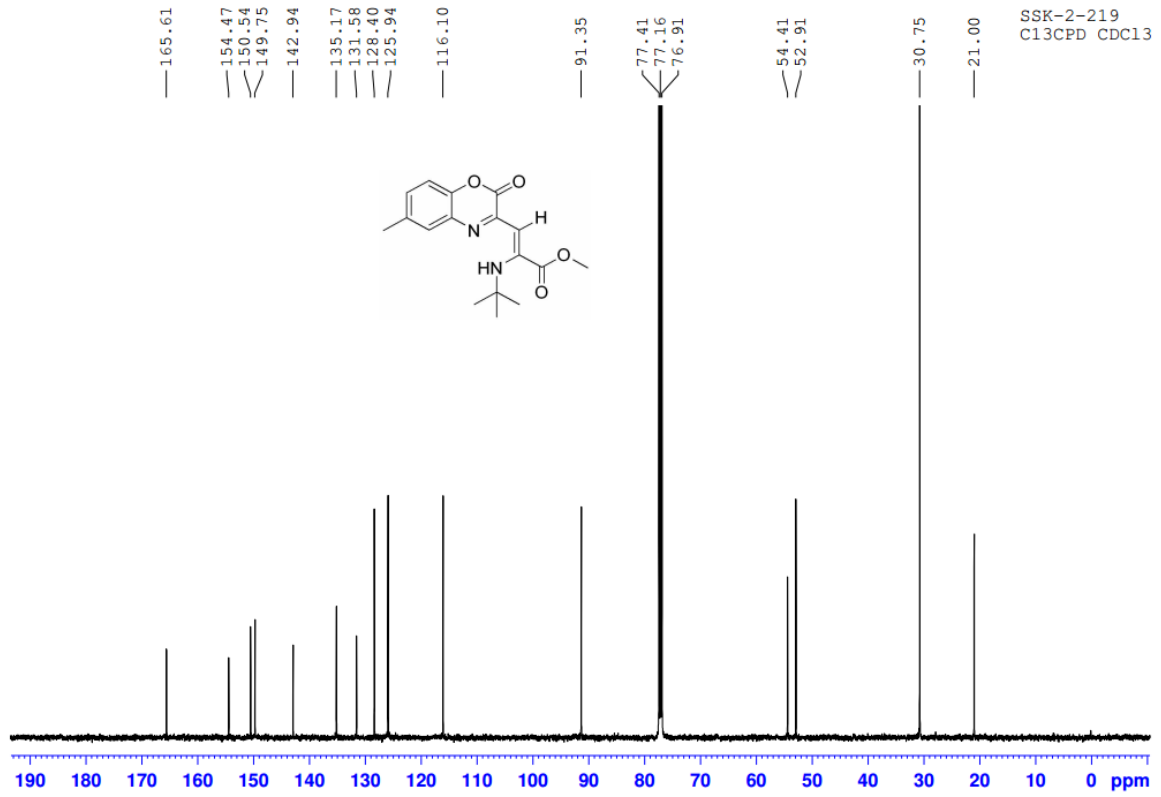
Compound **3c**


SSK-2-218
PROTON CDCl3
11.018
7.507
7.502
7.330
7.325
7.312
7.308
7.260
7.064
7.047
6.021
3.897
1.476
Br
O
N
H
HN
O
O
7.6
7.5
7.4
7.3
7.2
7.1
ppm
0.98
1.02
1.00
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.93
0.98
1.02
1.00
0.92
3.09
9.08

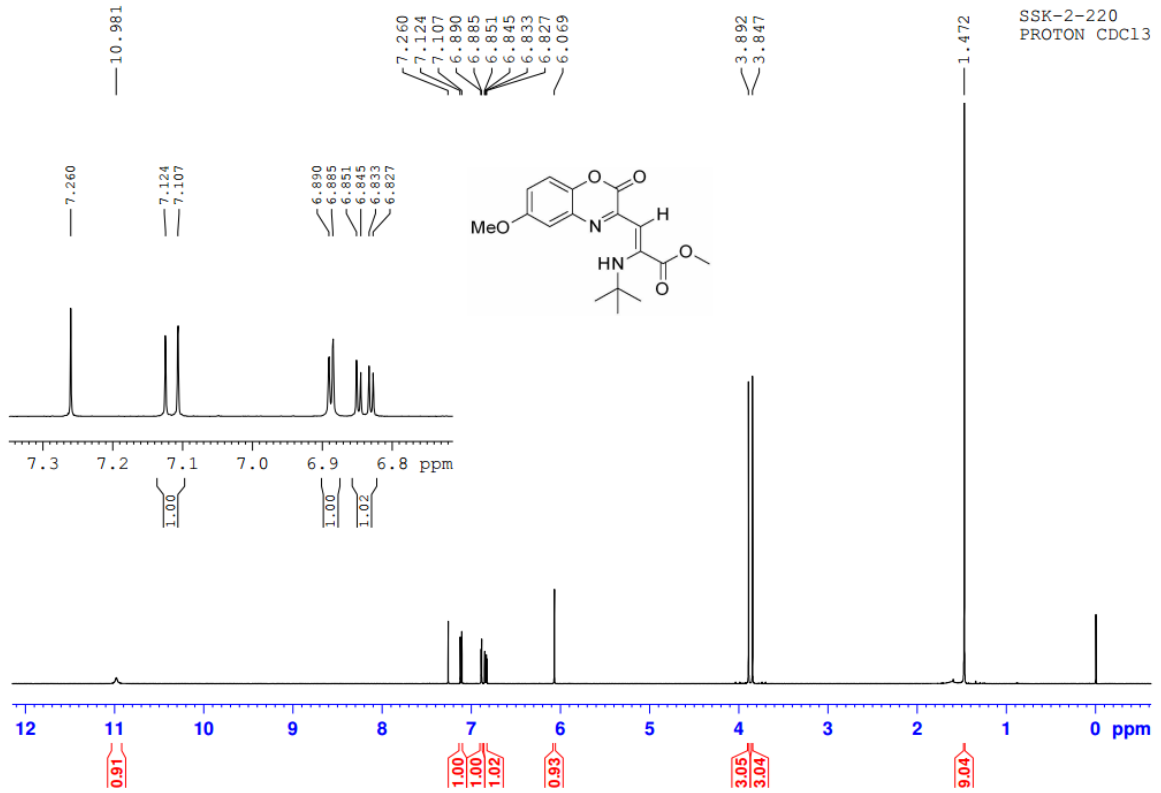

SSK-2-218
C13CPD CDCl3
165.21
153.77
151.01
150.97
143.95
133.11
129.68
128.17
117.89
117.68
90.87
77.41
77.16
76.91
54.79
53.07
30.66
Br
O
N
H
HN
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

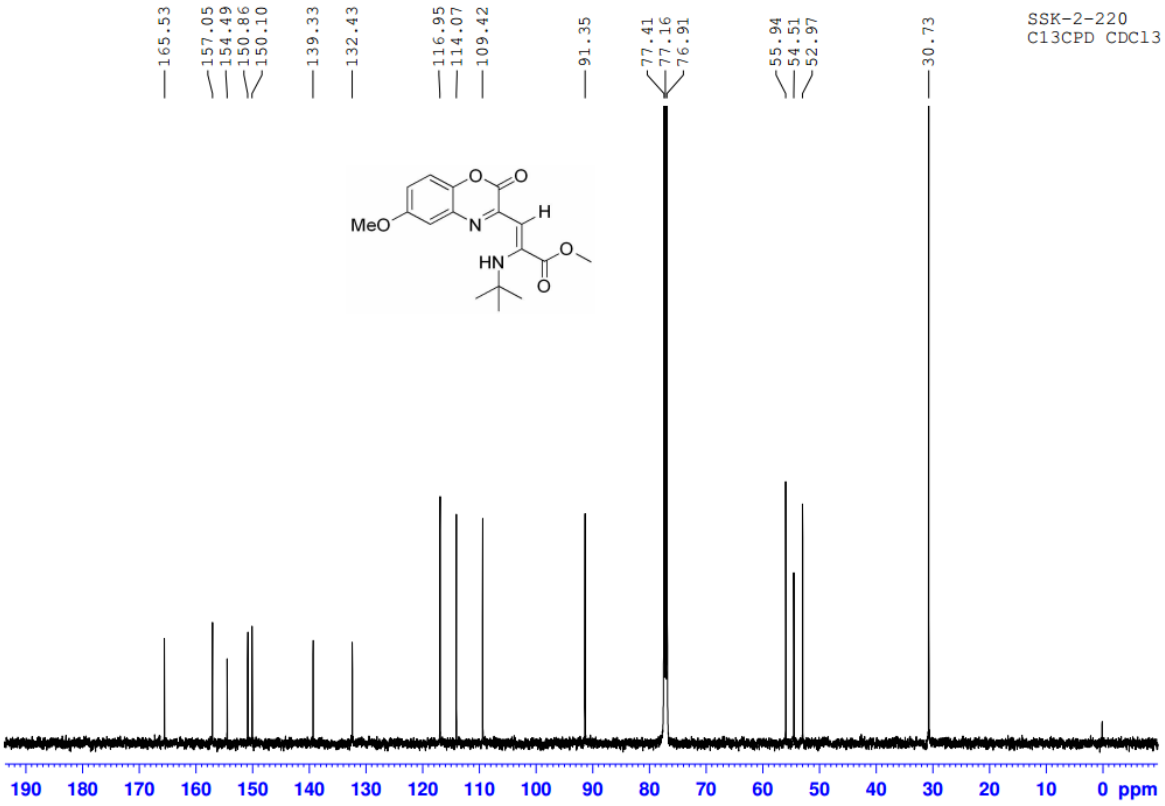
Compound **3d**


SSK-2-219
PROTON CDCl3
10.932
7.260
7.197
7.082
7.066
7.061
7.058
7.044
7.041
6.056
3.887
2.388
1.474
7.3
7.2
7.1
7.0
ppm
1.00
2.01
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.92
1.00
2.01
0.92
3.03
3.09
9.03

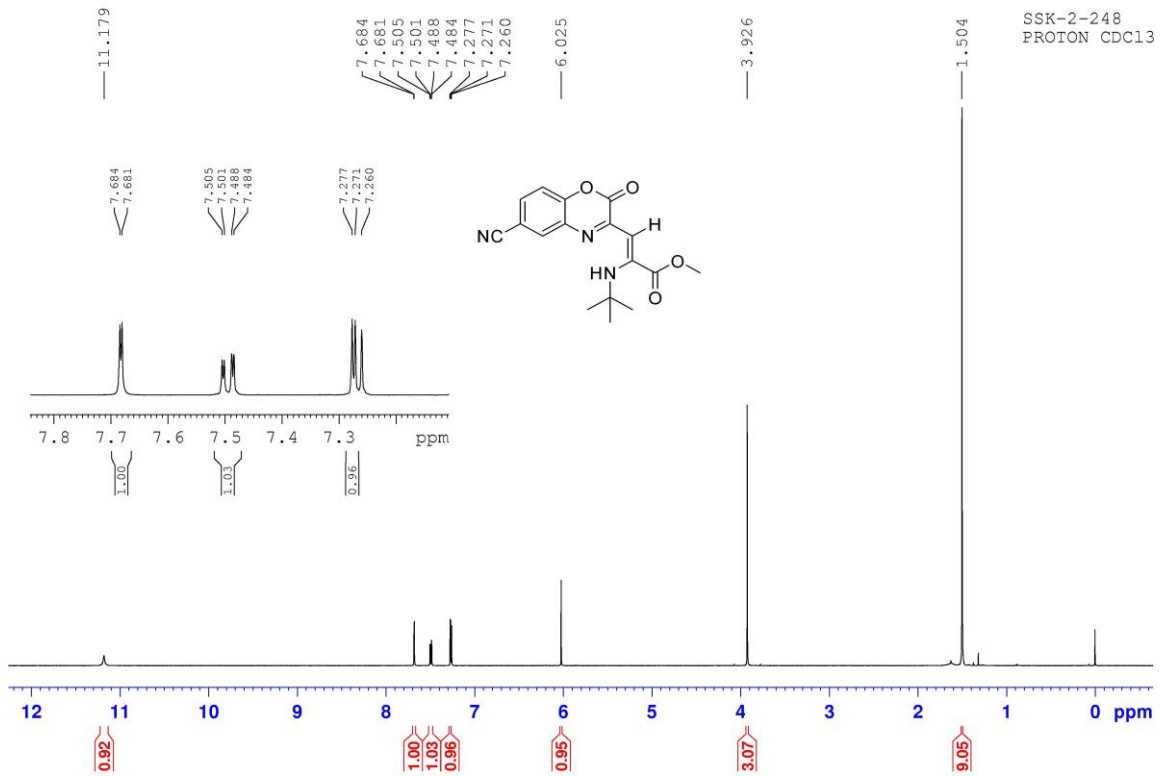

SSK-2-219
C13CPD CDCl3
165.61
154.47
150.54
149.75
142.94
135.17
131.58
128.40
125.94
116.10
91.35
77.41
77.16
76.91
54.41
52.91
30.75
21.00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

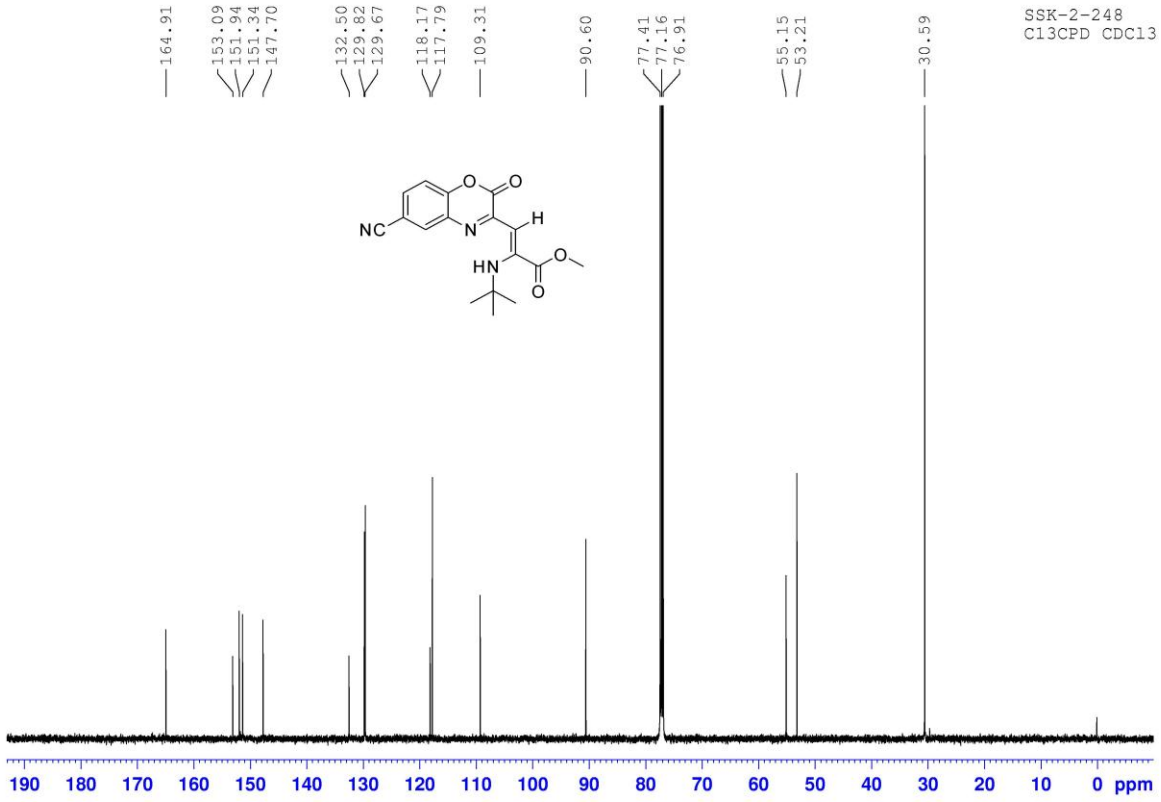
Compound **3e**


SSK-2-220
PROTON CDCl3
10.981
7.260
7.124
7.107
6.890
6.885
6.851
6.845
6.833
6.827
6.069
3.892
3.847
1.472
MeO
HN
7.3
7.2
7.1
7.0
6.9
6.8 ppm
1.00
1.00
1.02
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.91
1.00
1.00
1.02
0.93
3.05
3.04
9.04

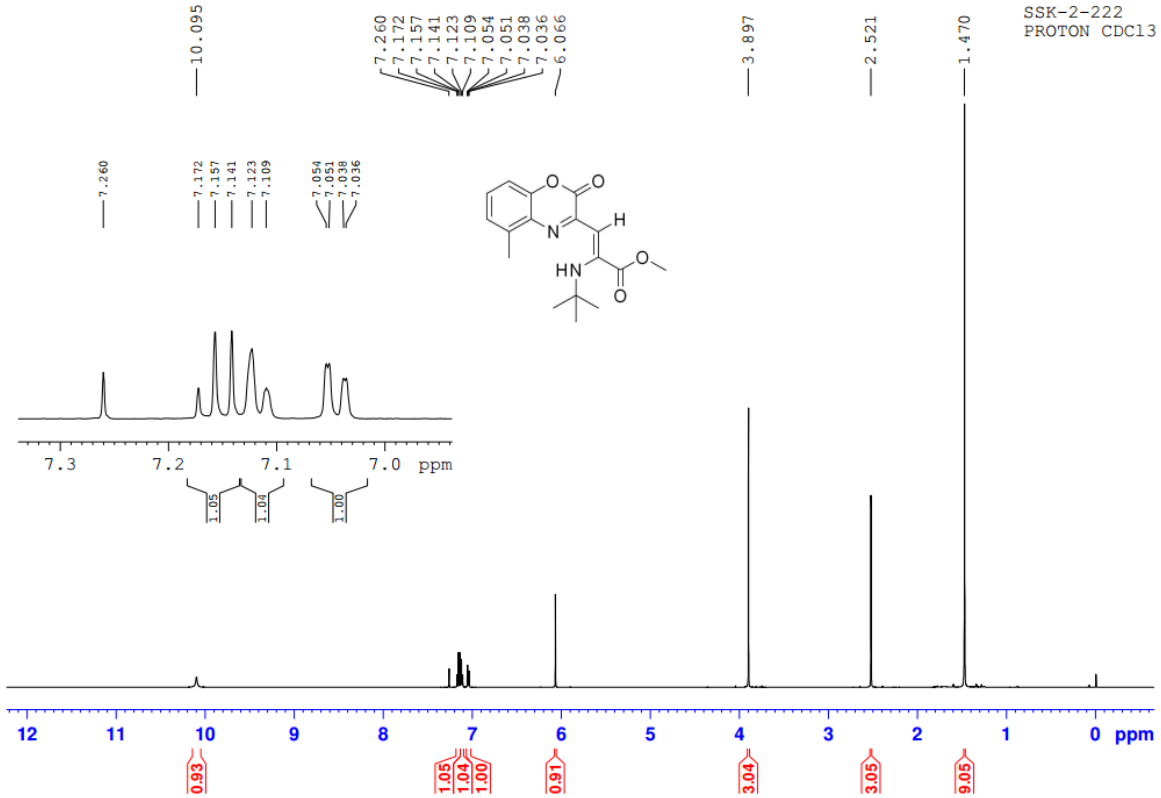

SSK-2-220
C13CPD CDCl3
165.53
157.05
154.49
150.86
150.10
139.33
132.43
116.95
114.07
109.42
91.35
77.41
77.16
76.91
55.94
54.51
52.97
30.73
MeO
HN
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

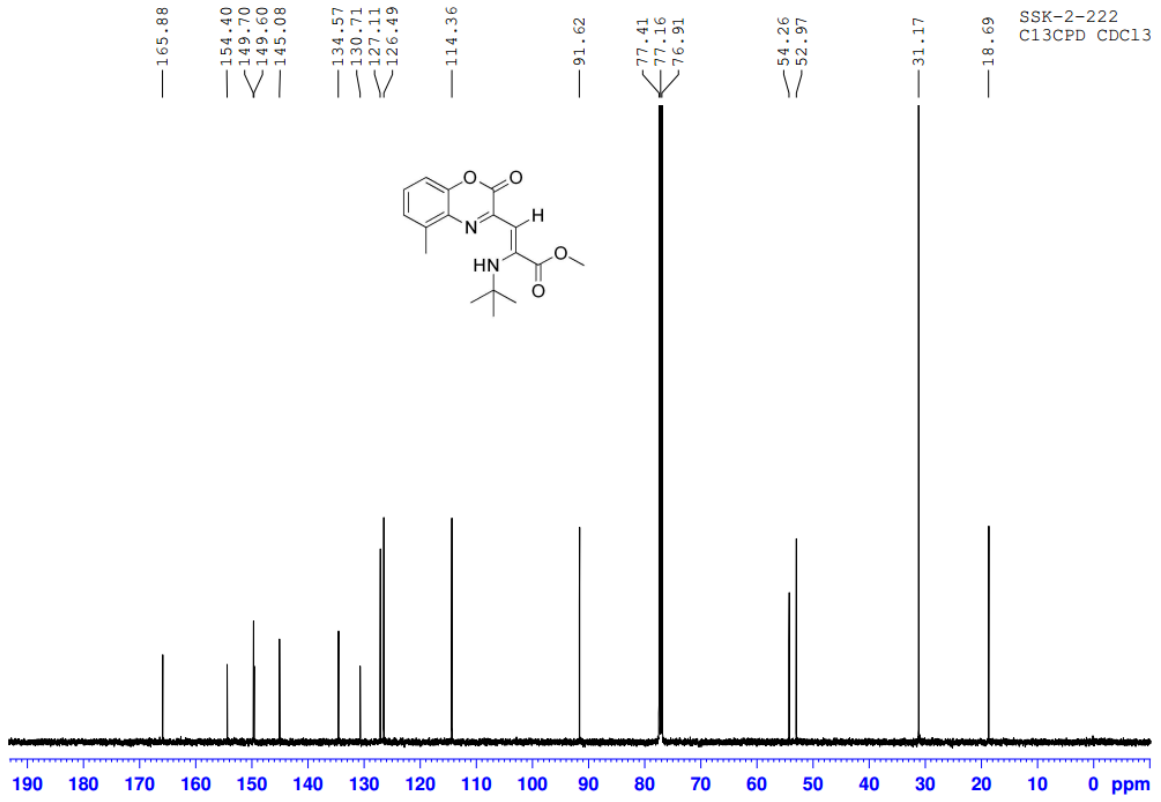
Compound **3f**


SSK-2-248
PROTON CDCl3
11.179
7.684
7.681
7.505
7.501
7.488
7.484
7.277
7.271
7.260
6.025
3.926
1.504
NC
O
N
H
HN
O
O
ppm
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.92
1.00
1.03
0.96
0.95
3.07
9.05

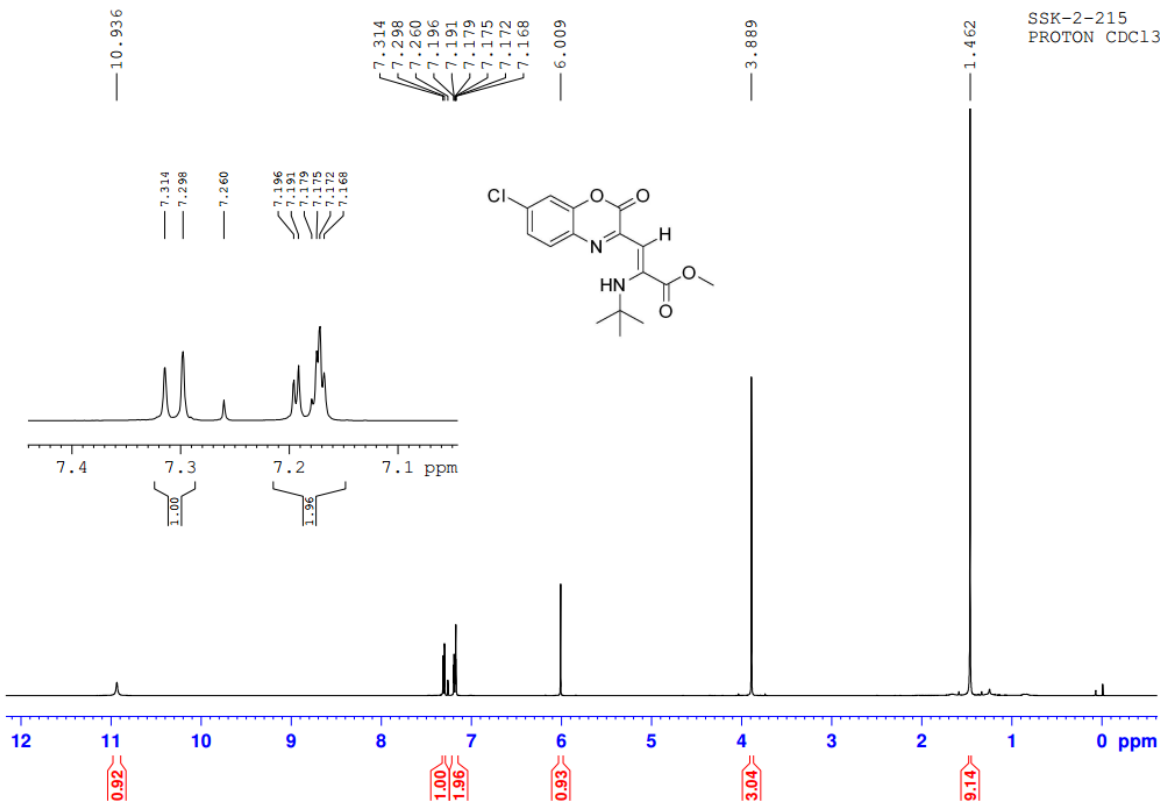

SSK-2-248
C13CPD CDCl3
164.91
153.09
151.94
151.34
147.70
132.50
129.82
129.67
118.17
117.79
109.31
90.60
77.41
77.16
76.91
55.15
53.21
30.59
NC
O
N
H
HN
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

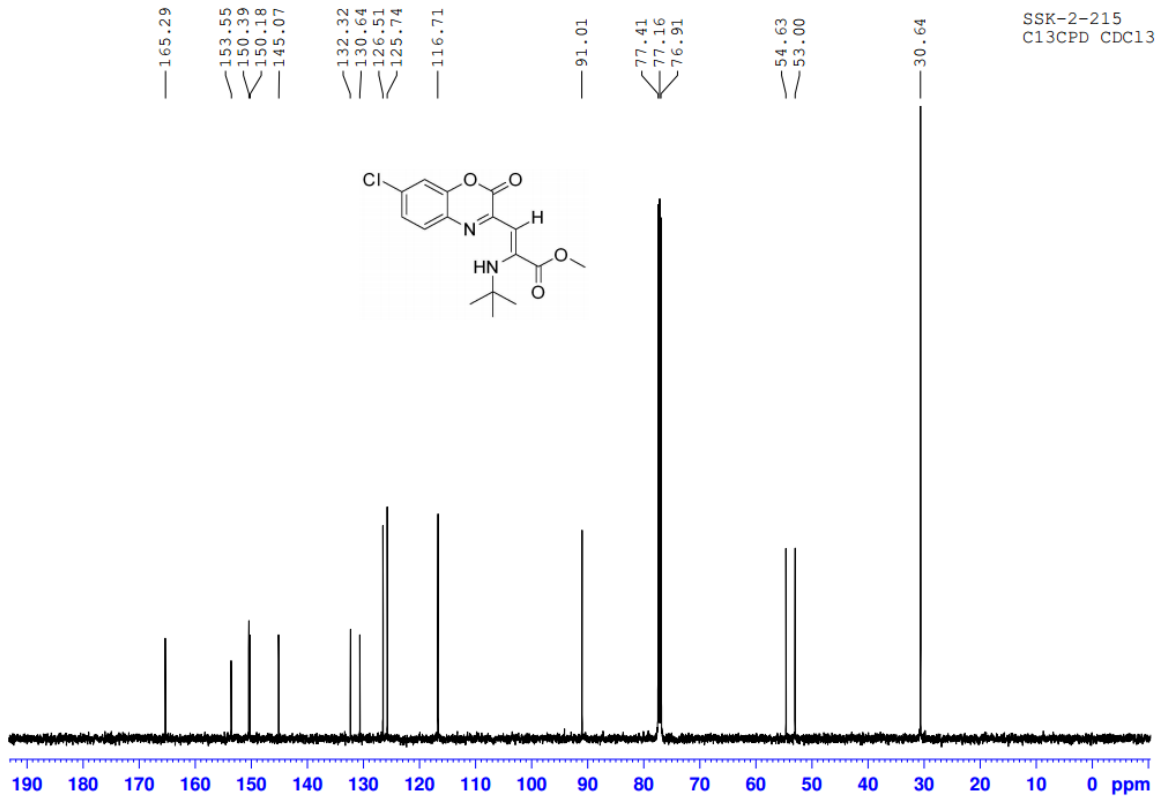
Compound **3g**


SSK-2-222
PROTON CDCl3
10.095
7.260
7.172
7.157
7.141
7.123
7.109
7.054
7.051
7.038
7.036
6.066
3.897
2.521
1.470
7.3
7.2
7.1
7.0 ppm
1.05
1.04
1.00
0.93
0.91
3.04
3.05
9.05
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

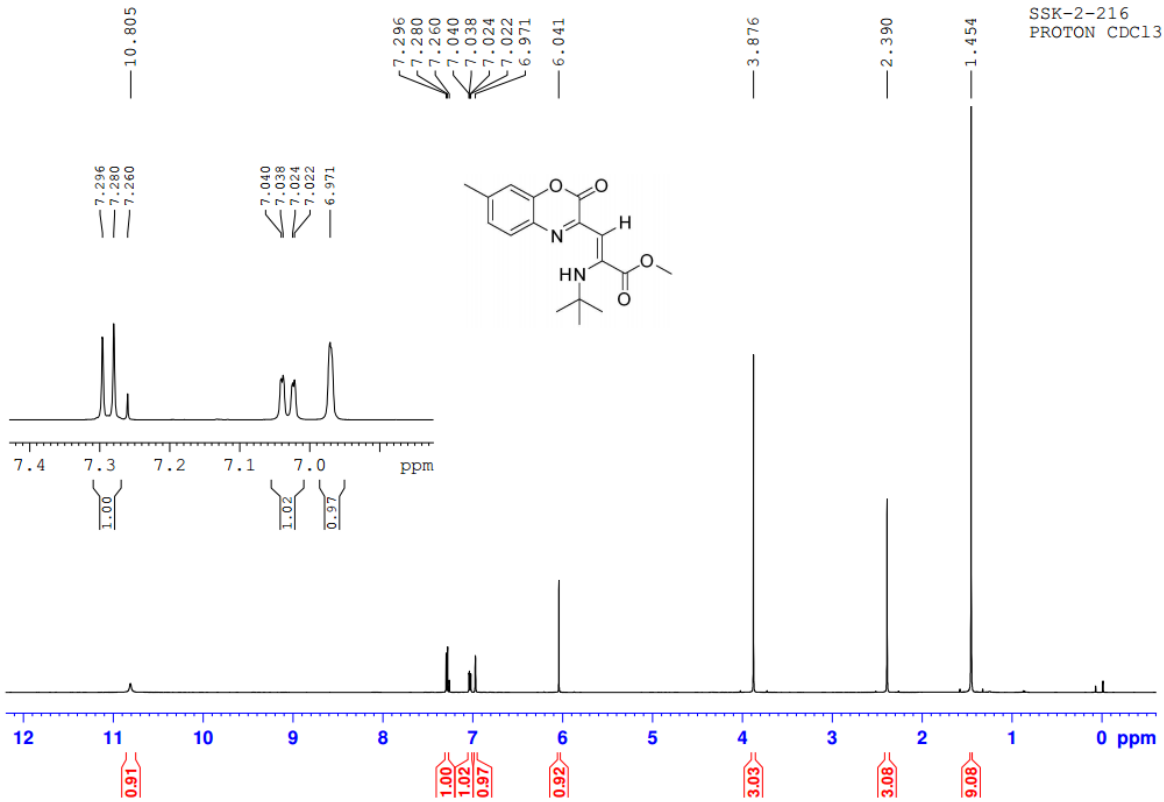

SSK-2-222
C13CPD CDCl3
165.88
154.40
149.70
149.60
145.08
134.57
130.71
127.11
126.49
114.36
91.62
77.41
77.16
76.91
54.26
52.97
31.17
18.69
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

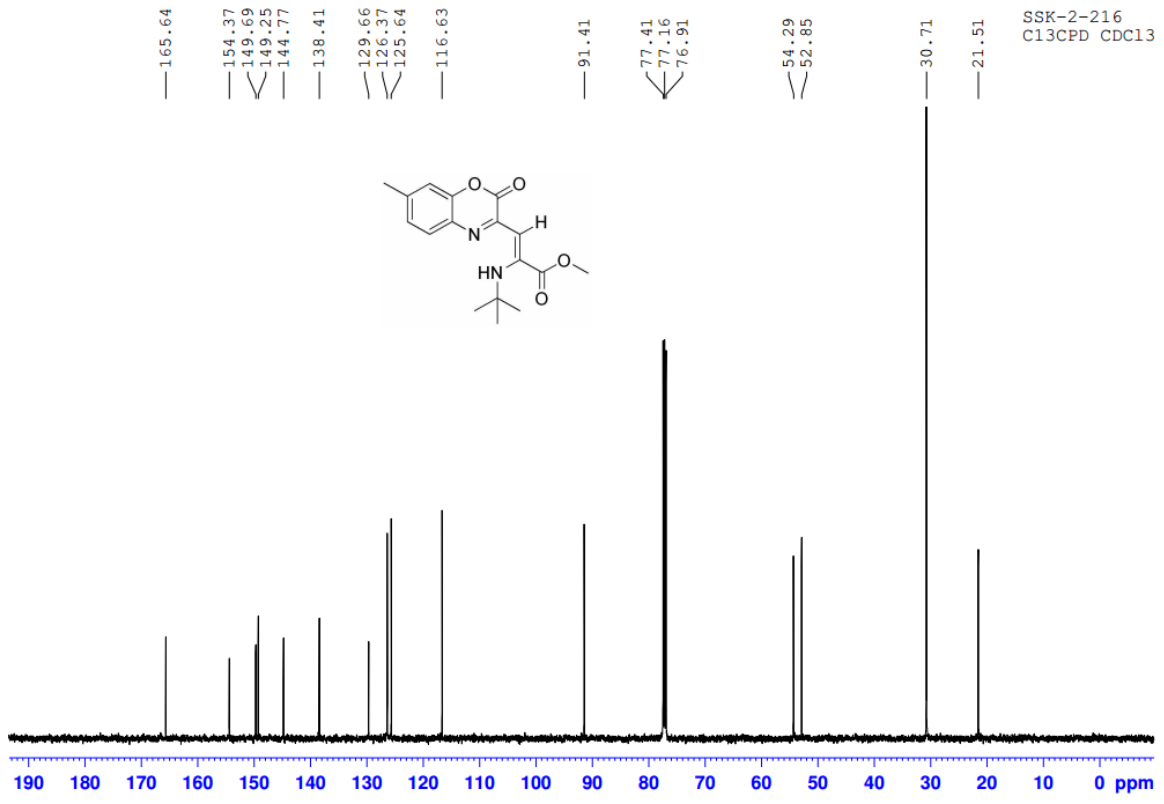
Compound **3h**


SSK-2-215
PROTON CDC13
10.936
7.314
7.298
7.260
7.196
7.191
7.179
7.175
7.172
7.168
6.009
3.889
1.462
Cl
O
N
H
HN
O
O
7.4
7.3
7.2
7.1 ppm
1.00
1.96
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.92
1.00
1.96
0.93
3.04
9.14

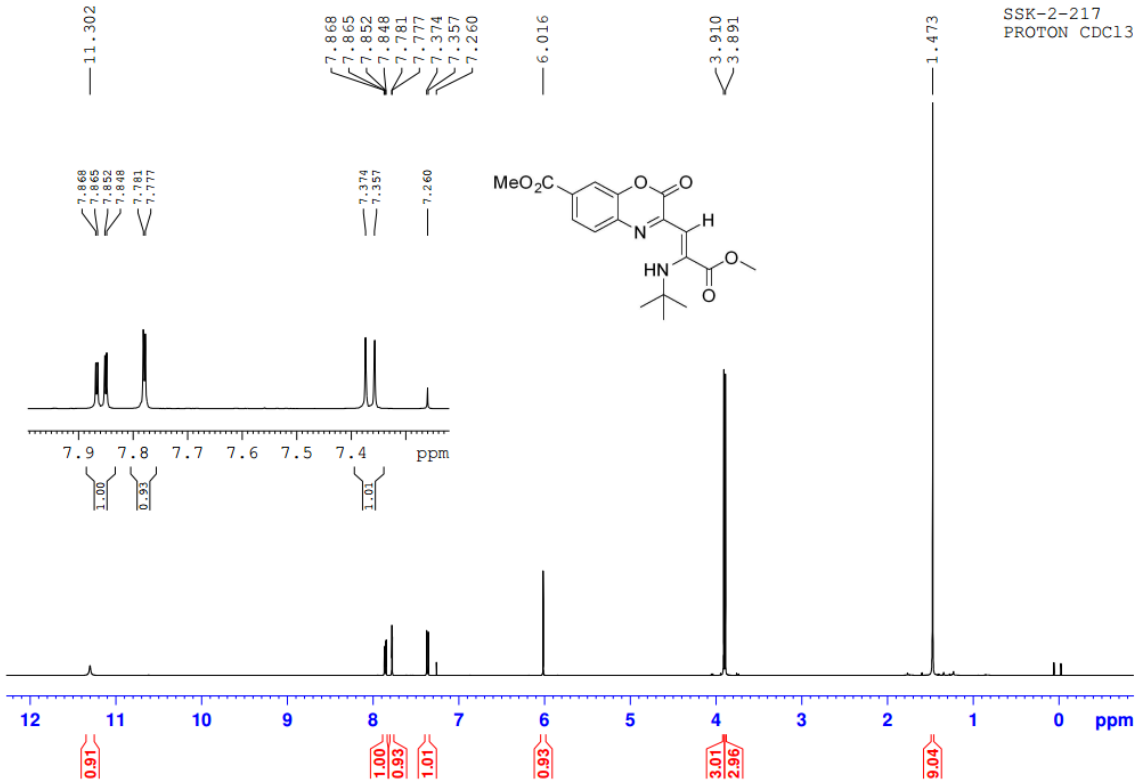

SSK-2-215
C13CPD CDC13
165.29
153.55
150.39
150.18
145.07
132.32
130.64
126.51
125.74
116.71
91.01
77.41
77.16
76.91
54.63
53.00
30.64
Cl
O
N
H
HN
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

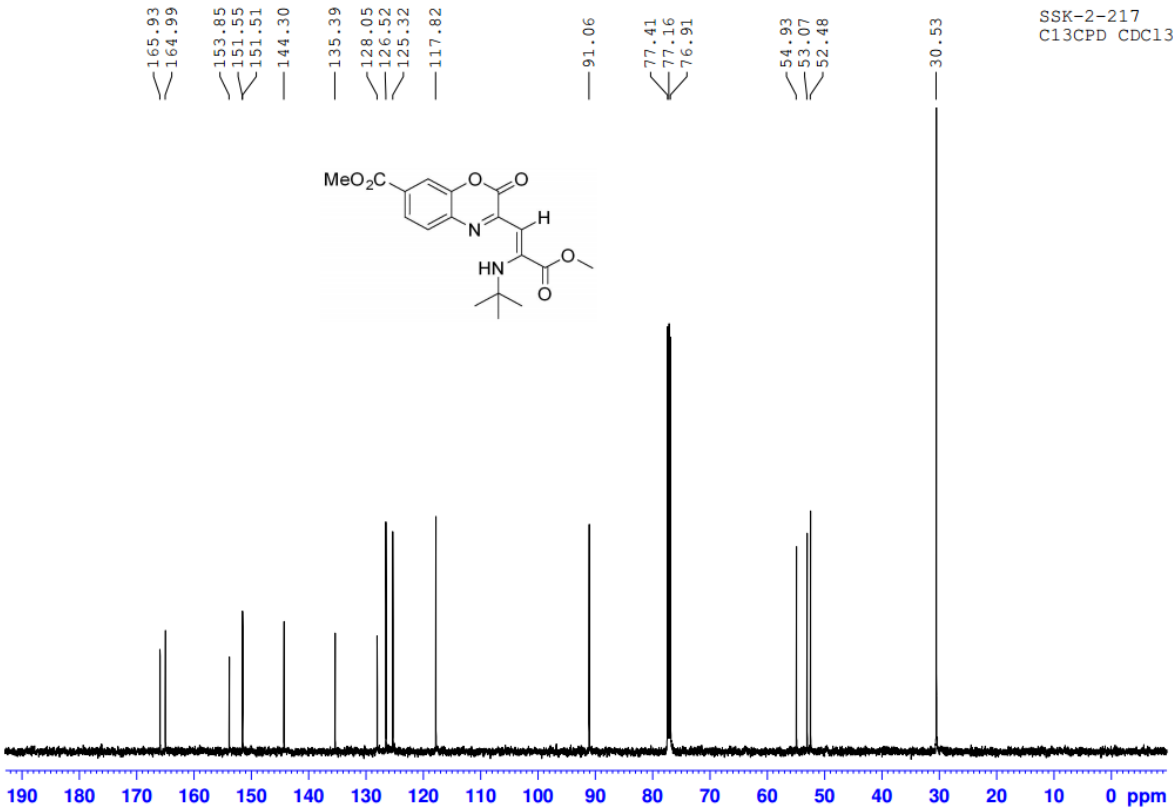
Compound **3i**


SSK-2-216
PROTON CDC13
10.805
7.296
7.280
7.260
7.040
7.038
7.024
7.022
6.971
6.041
3.876
2.390
1.454
ppm
0.91
1.00
1.02
0.97
0.92
3.03
3.08
9.08

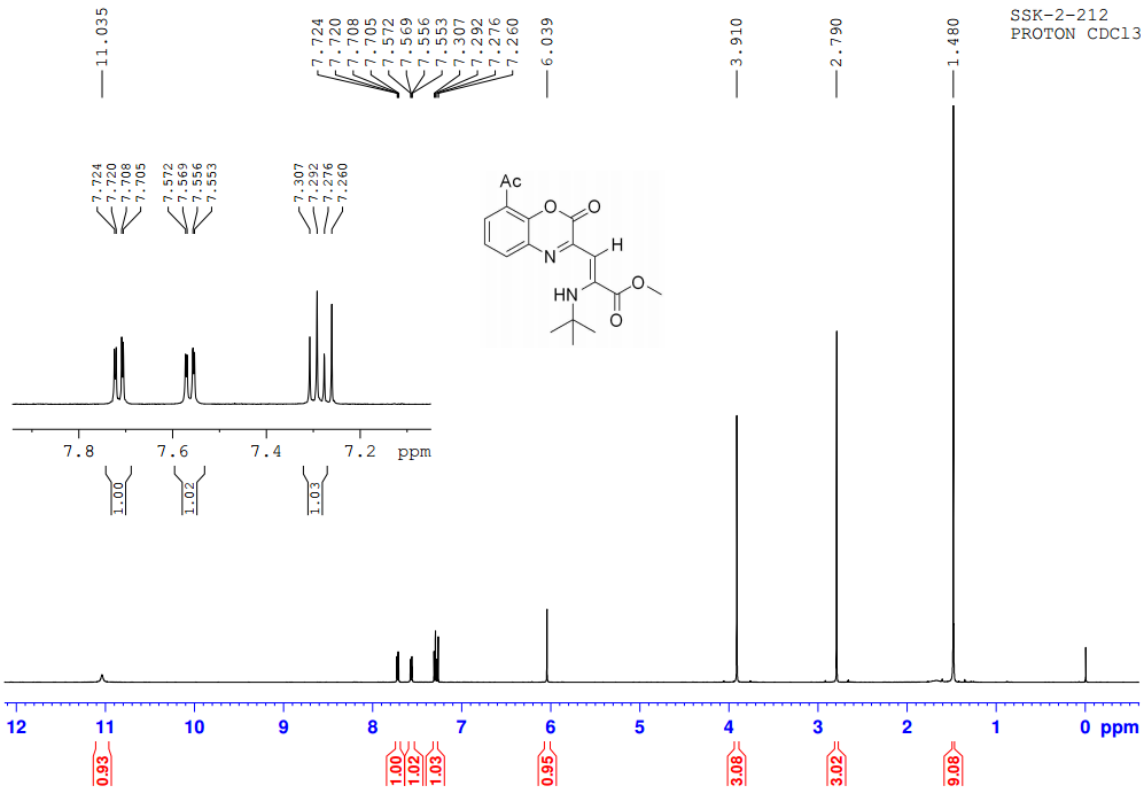

SSK-2-216
C13CPD CDC13
165.64
154.37
149.69
149.25
144.77
138.41
129.66
126.37
125.64
116.63
91.41
77.41
77.16
76.91
54.29
52.85
30.71
21.51
ppm

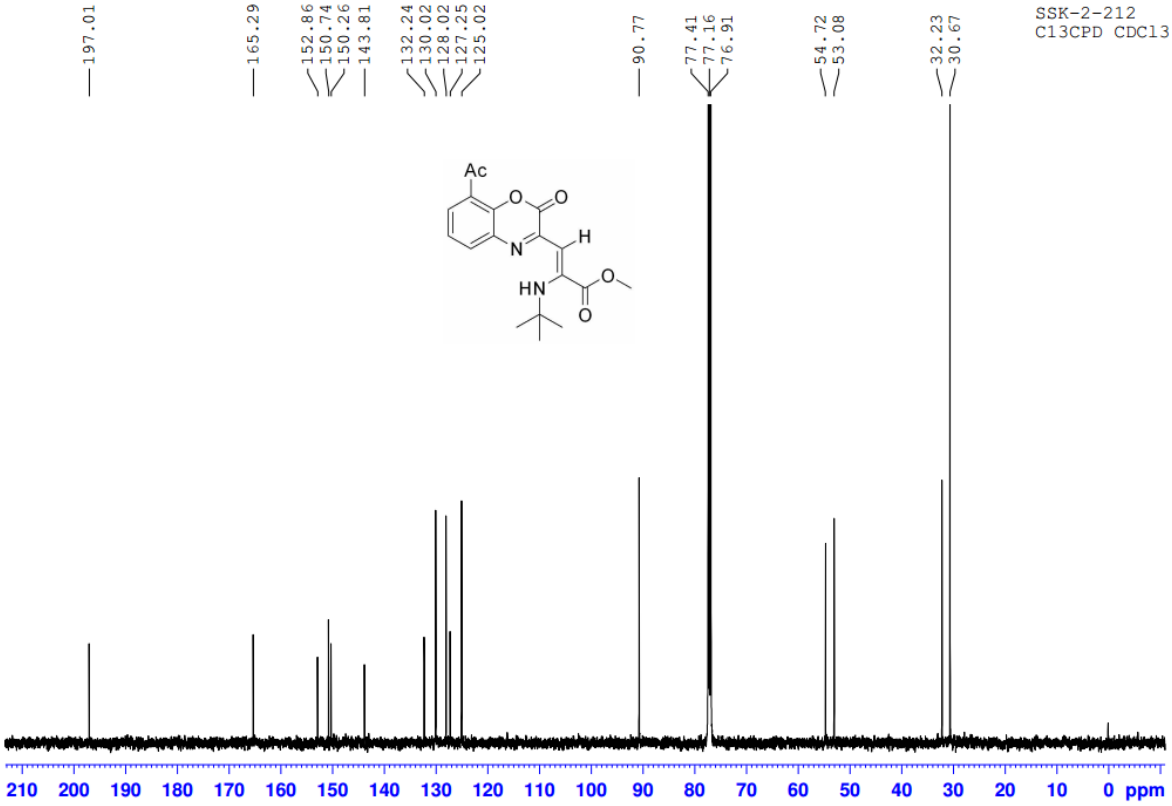
Compound **3j**


SSK-2-217
PROTON CDCl3
11.302
7.868
7.865
7.852
7.848
7.781
7.777
7.374
7.357
7.260
6.016
3.910
3.891
1.473
MeO2C
O
O
H
N
HN
O
O
7.9
7.8
7.7
7.6
7.5
7.4
ppm
1.00
0.93
1.01
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.91
1.00
0.93
1.01
0.93
3.01
2.96
9.04

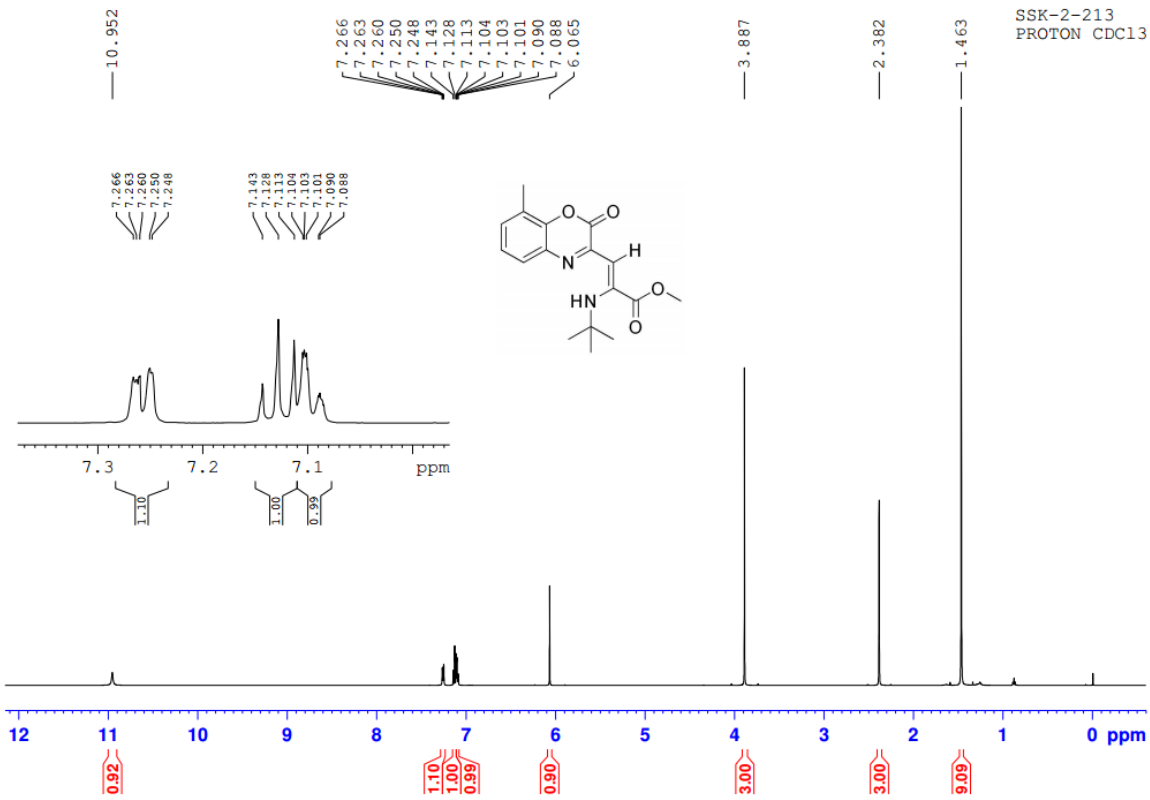

SSK-2-217
C13CPD CDCl3
165.93
164.99
153.85
151.55
151.51
144.30
135.39
128.05
126.52
125.32
117.82
91.06
77.41
77.16
76.91
54.93
53.07
52.48
30.53
MeO2C
O
O
H
N
HN
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

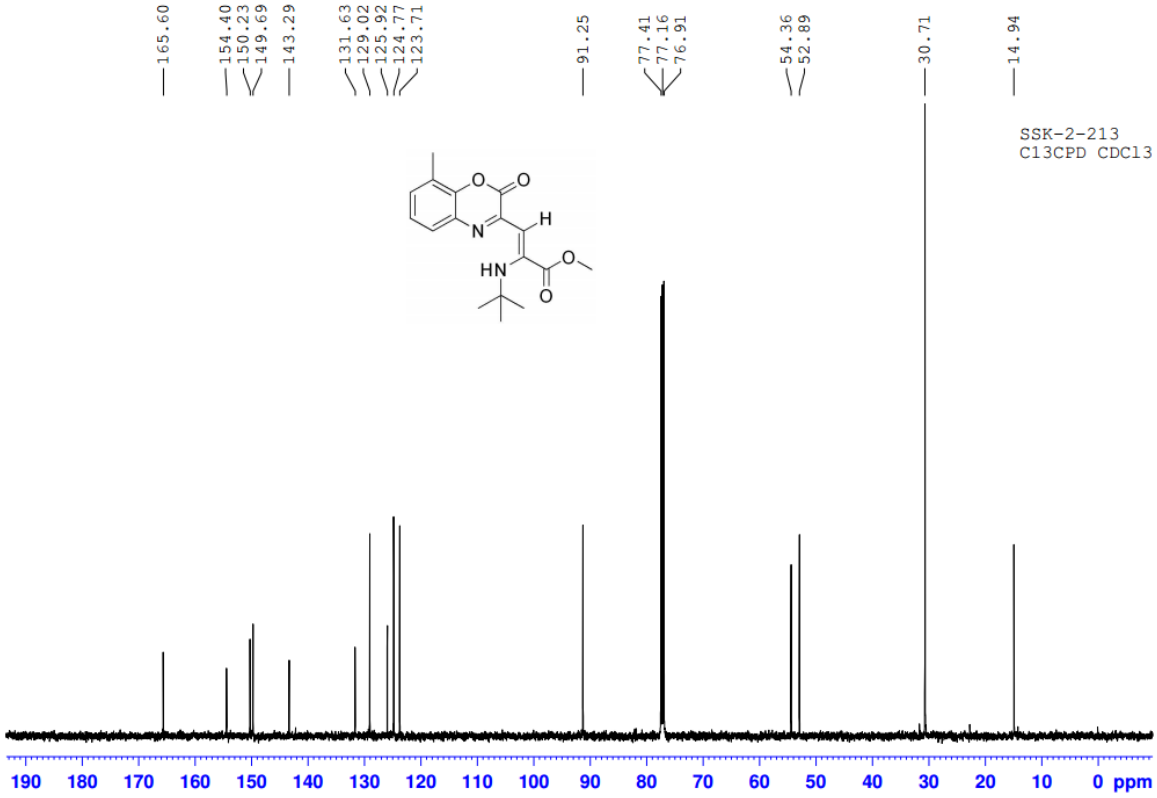
Compound **3k**


SSK-2-212
PROTON CDCl3
11.035
7.724
7.720
7.708
7.705
7.572
7.569
7.556
7.553
7.307
7.292
7.276
7.260
6.039
3.910
2.790
1.480
Ac
O
O
N
H
HN
O
O
7.8
7.6
7.4
7.2
ppm
1.00
1.02
1.03
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.93
1.00
1.02
1.03
0.95
3.08
3.02
9.08

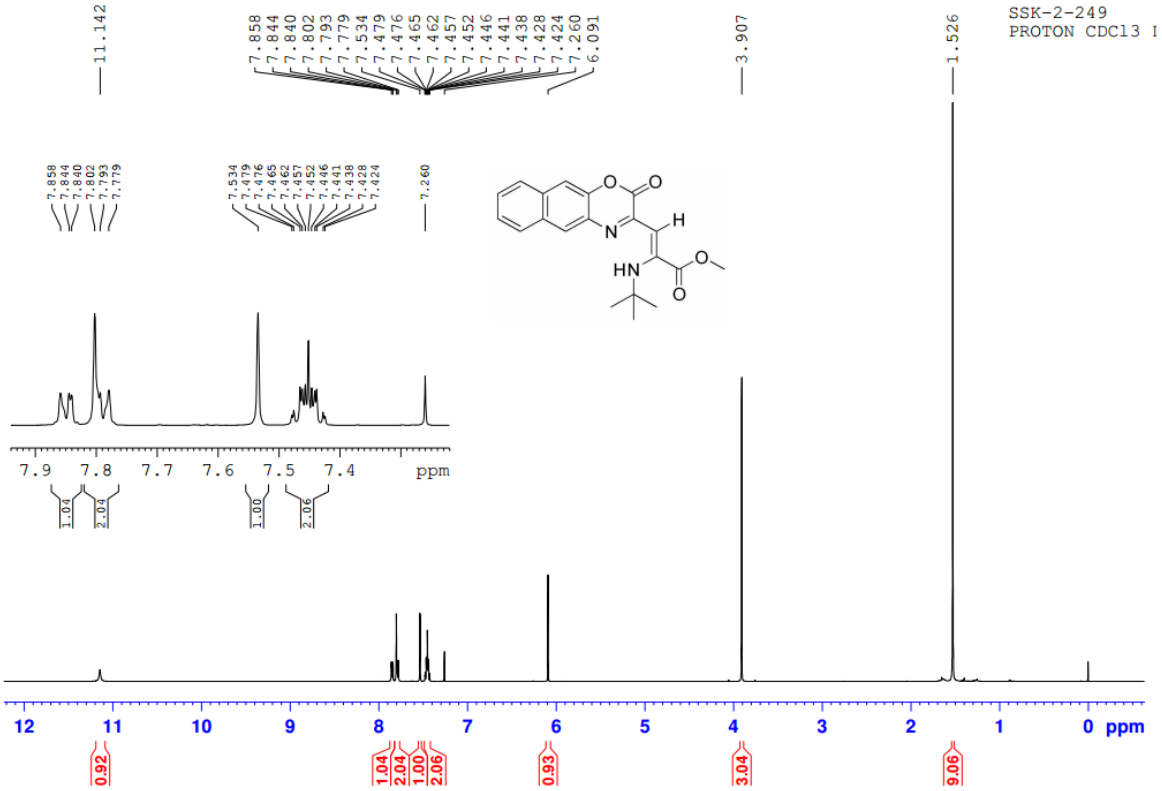

SSK-2-212
C13CPD CDCl3
197.01
165.29
152.86
150.74
150.26
143.81
132.24
130.02
128.02
127.25
125.02
90.77
77.41
77.16
76.91
54.72
53.08
32.23
30.67
Ac
O
O
N
H
HN
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

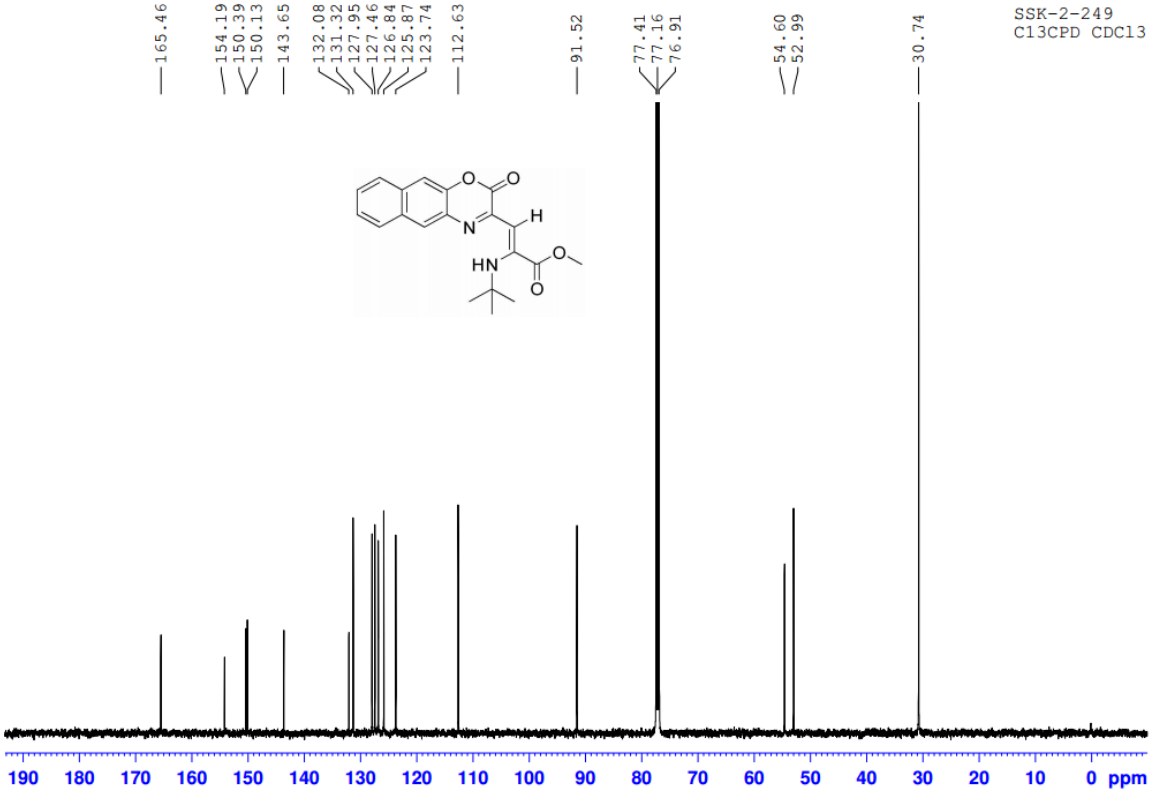
Compound **3l**


SSK-2-213
PROTON CDCl3
10.952
7.266
7.263
7.260
7.250
7.248
7.143
7.128
7.113
7.104
7.103
7.101
7.090
7.088
6.065
3.887
2.382
1.463
ppm
0.92
1.10
1.00
0.99
0.90
3.00
3.00
9.09

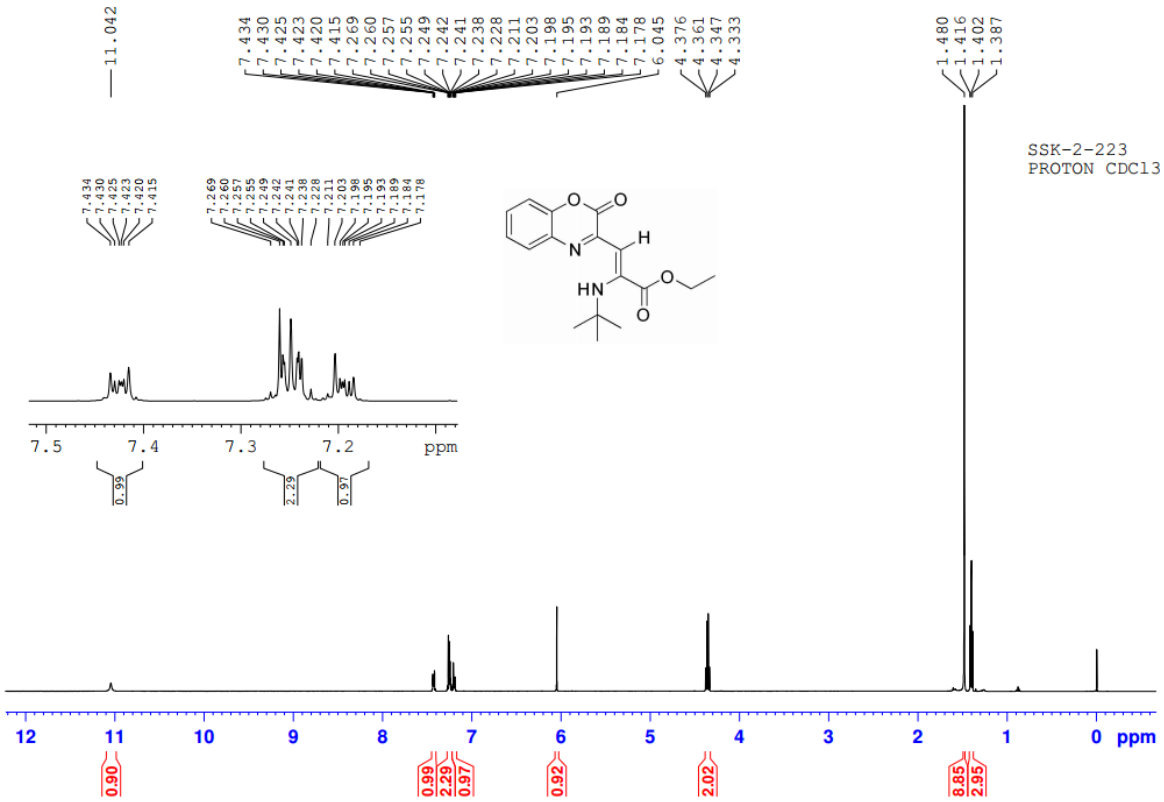

SSK-2-213
C13CPD CDCl3
165.60
154.40
150.23
149.69
143.29
131.63
129.02
125.92
124.77
123.71
91.25
77.41
77.16
76.91
54.36
52.89
30.71
14.94
ppm

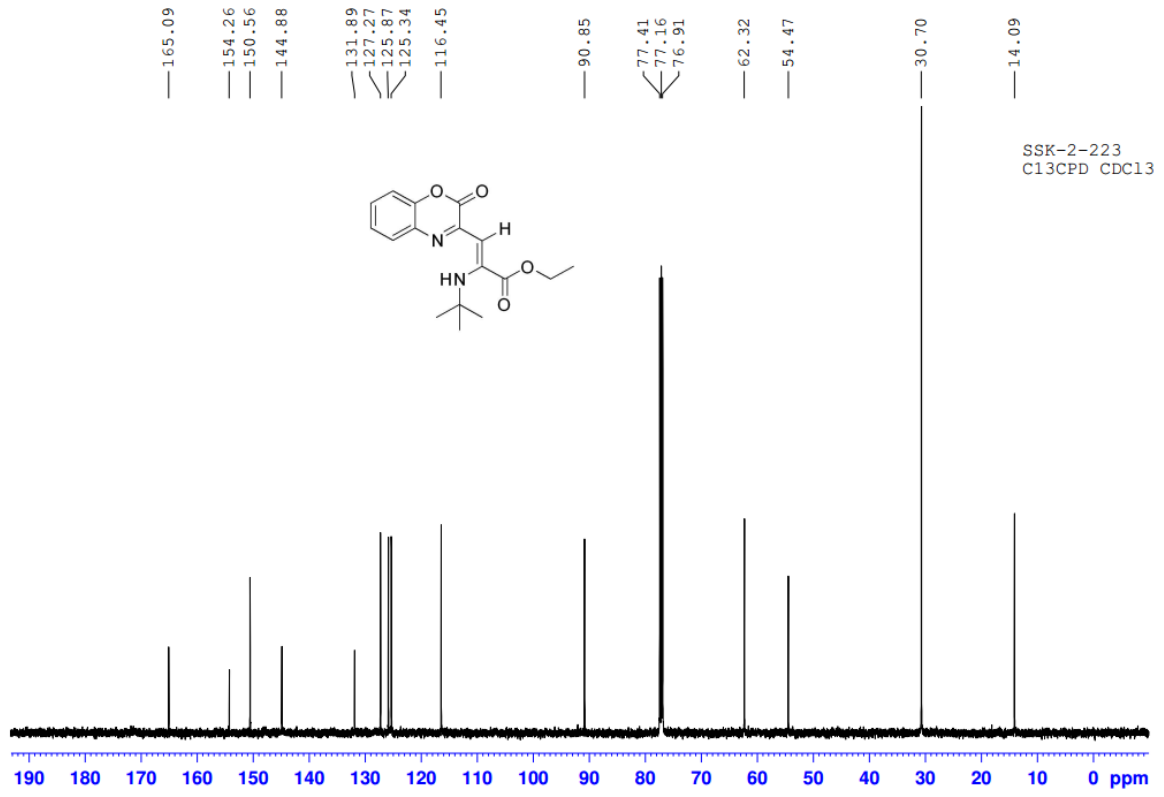
Compound **3m**


SSK-2-249
PROTON CDCl3 I
11.142
7.858
7.844
7.840
7.802
7.793
7.779
7.534
7.479
7.476
7.465
7.462
7.457
7.452
7.446
7.441
7.438
7.428
7.424
7.260
6.091
3.907
1.526
ppm

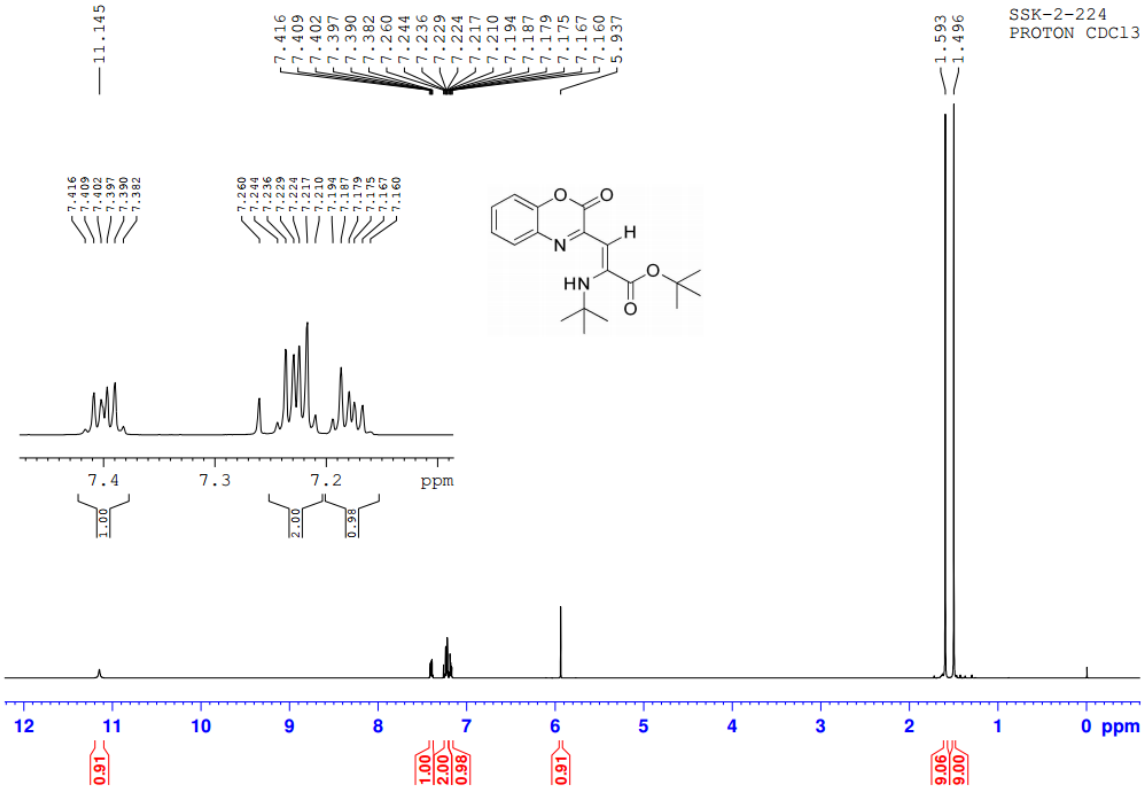

SSK-2-249
C13CPD CDCl3
165.46
154.19
150.39
150.13
143.65
132.08
131.32
127.95
127.46
126.84
125.87
123.74
112.63
91.52
77.41
77.16
76.91
54.60
52.99
30.74
ppm

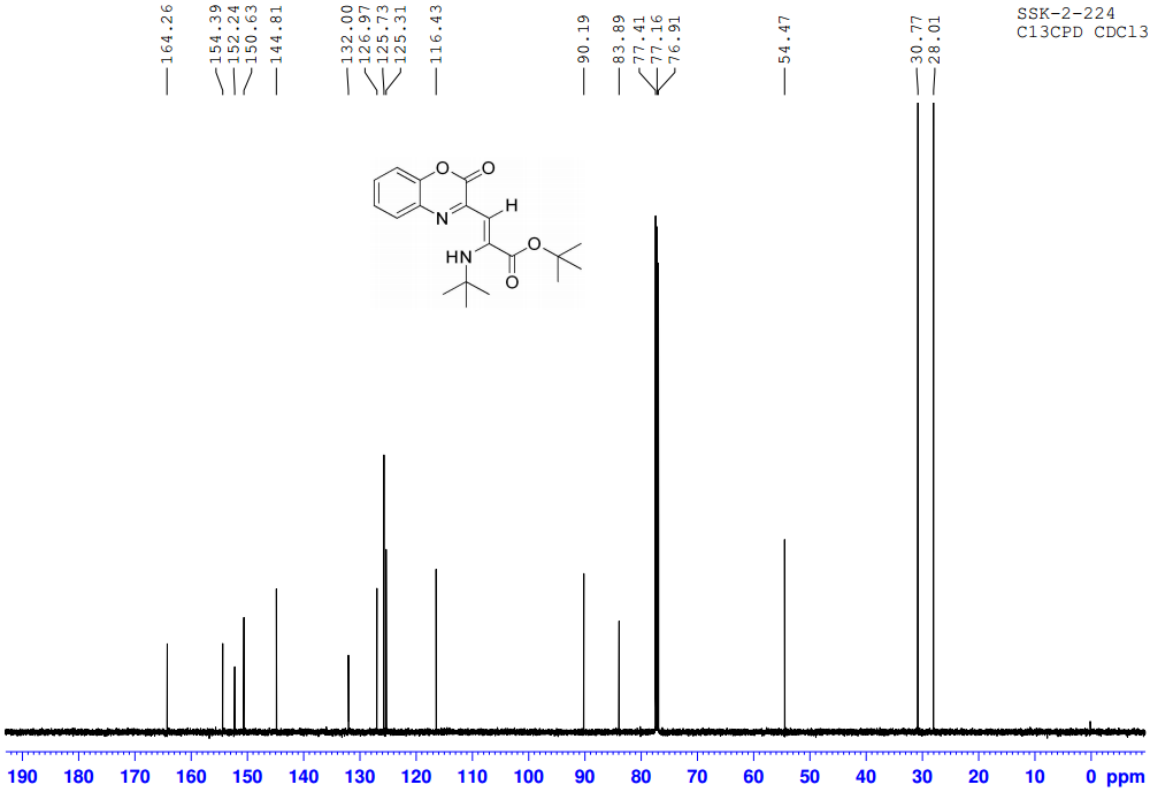
Compound **3n**


11.042
7.434
7.430
7.425
7.423
7.420
7.415
7.269
7.260
7.257
7.255
7.249
7.242
7.241
7.238
7.228
7.211
7.203
7.198
7.195
7.193
7.189
7.184
7.178
6.045
4.376
4.361
4.347
4.333
1.480
1.416
1.402
1.387
SSK-2-223
PROTON CDCl3
ppm
0.99
2.29
0.97
0.90
0.92
2.02
8.85
2.95

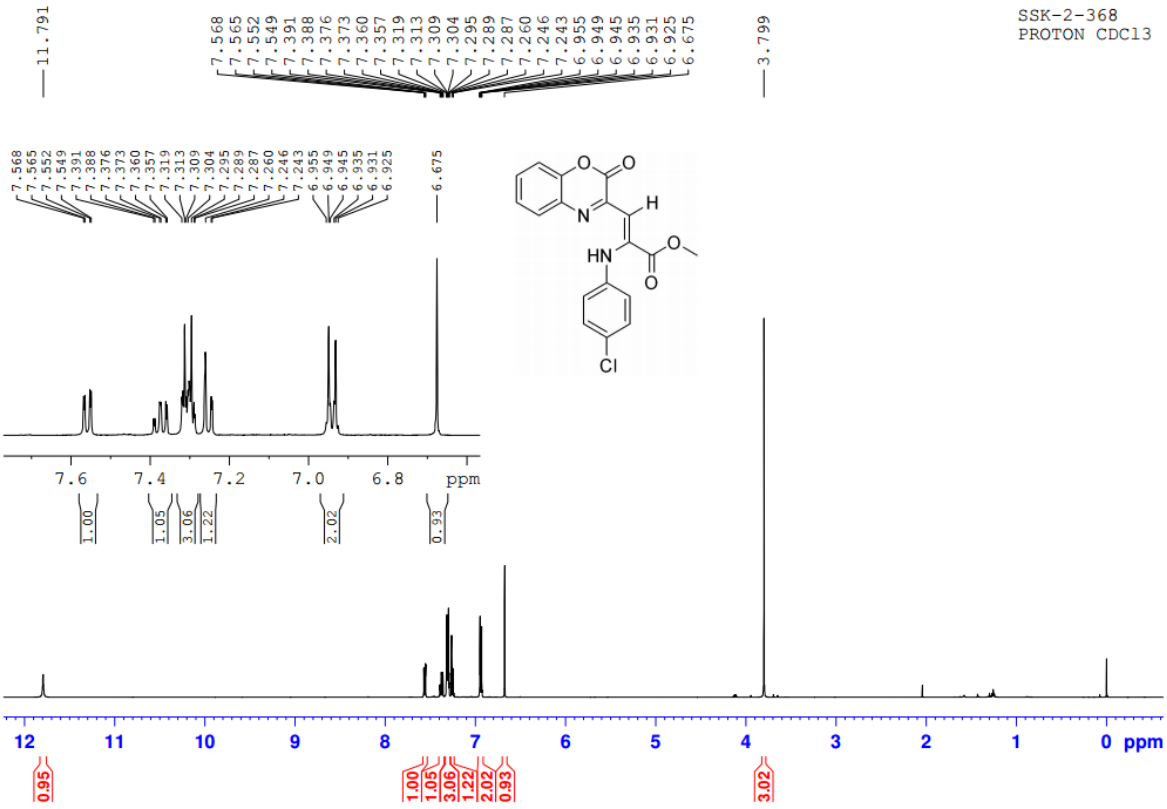

165.09
154.26
150.56
144.88
131.89
127.27
125.87
125.34
116.45
90.85
77.41
77.16
76.91
62.32
54.47
30.70
14.09
SSK-2-223
C13CPD CDCl3
ppm

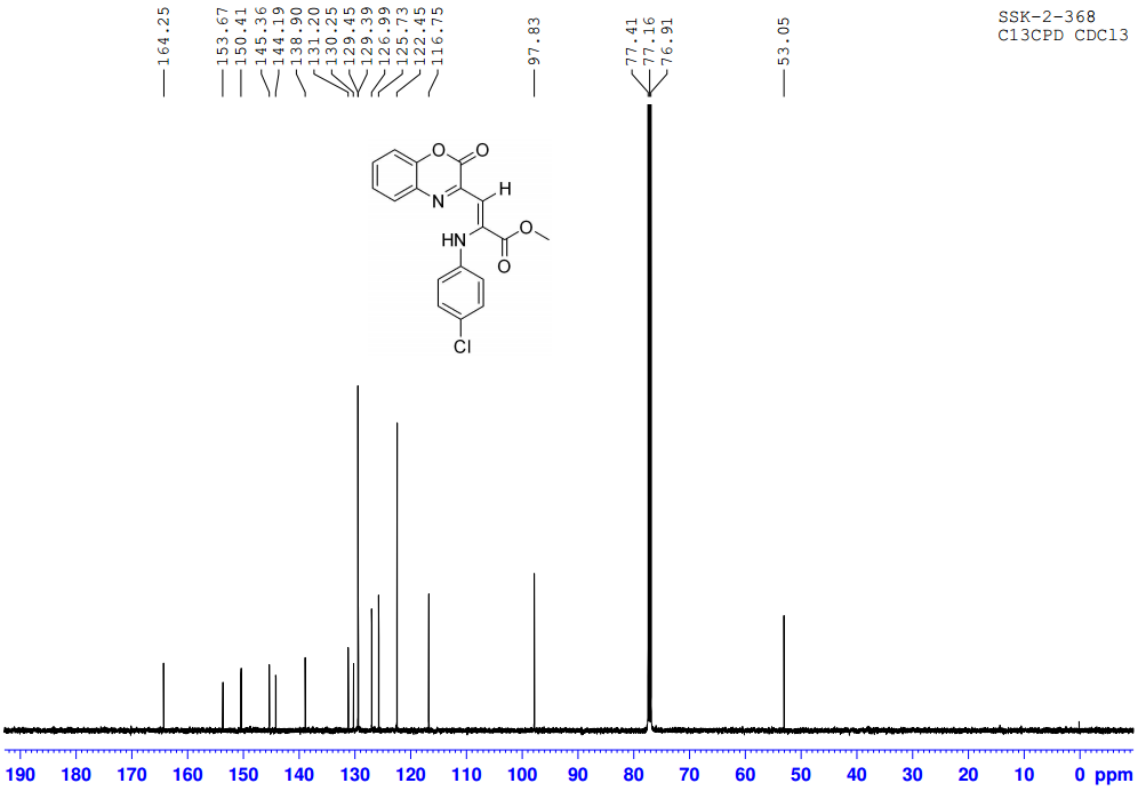
Compound **3o**


SSK-2-224
PROTON CDCl3
11.145
7.416
7.409
7.402
7.397
7.390
7.382
7.260
7.244
7.236
7.229
7.224
7.217
7.210
7.194
7.187
7.179
7.175
7.167
7.160
5.937
1.593
1.496
7.4
7.3
7.2
ppm
1.00
2.00
0.98
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.91
1.00
2.00
0.98
0.91
9.06
9.00

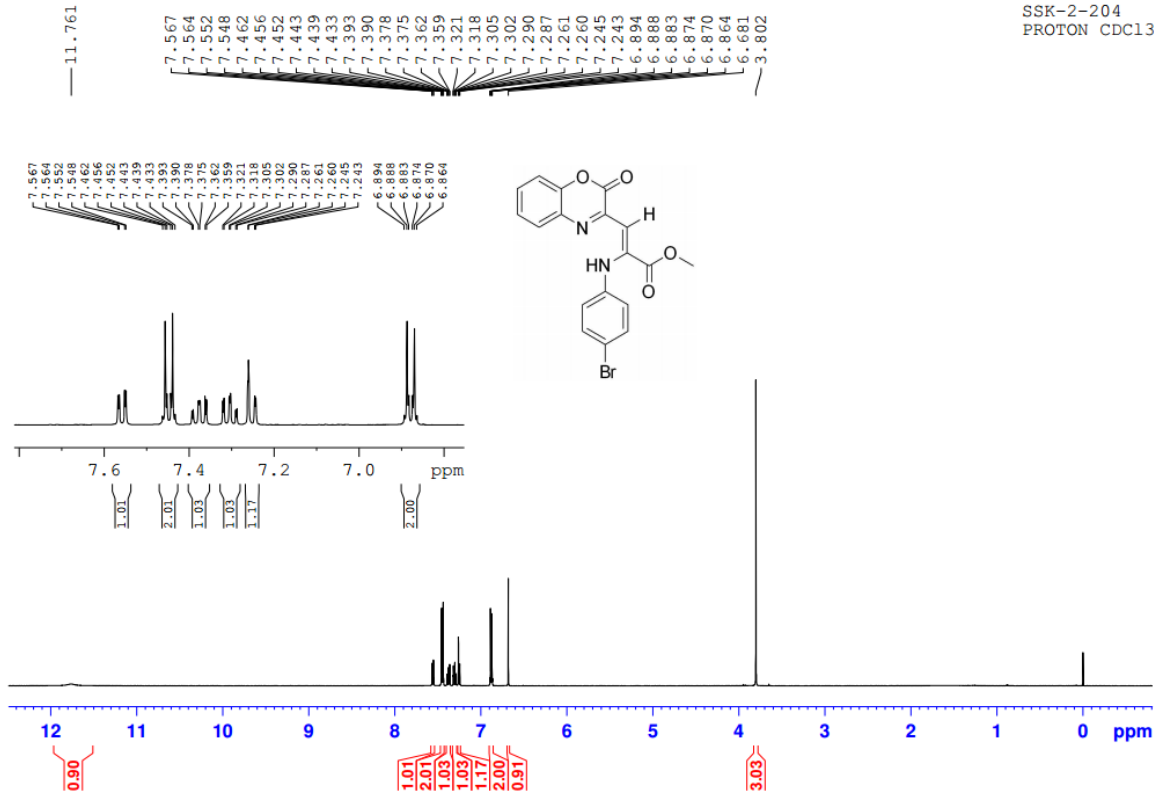

SSK-2-224
C13CPD CDCl3
164.26
154.39
152.24
150.63
144.81
132.00
126.97
125.73
125.31
116.43
90.19
83.89
77.41
77.16
76.91
54.47
30.77
28.01
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

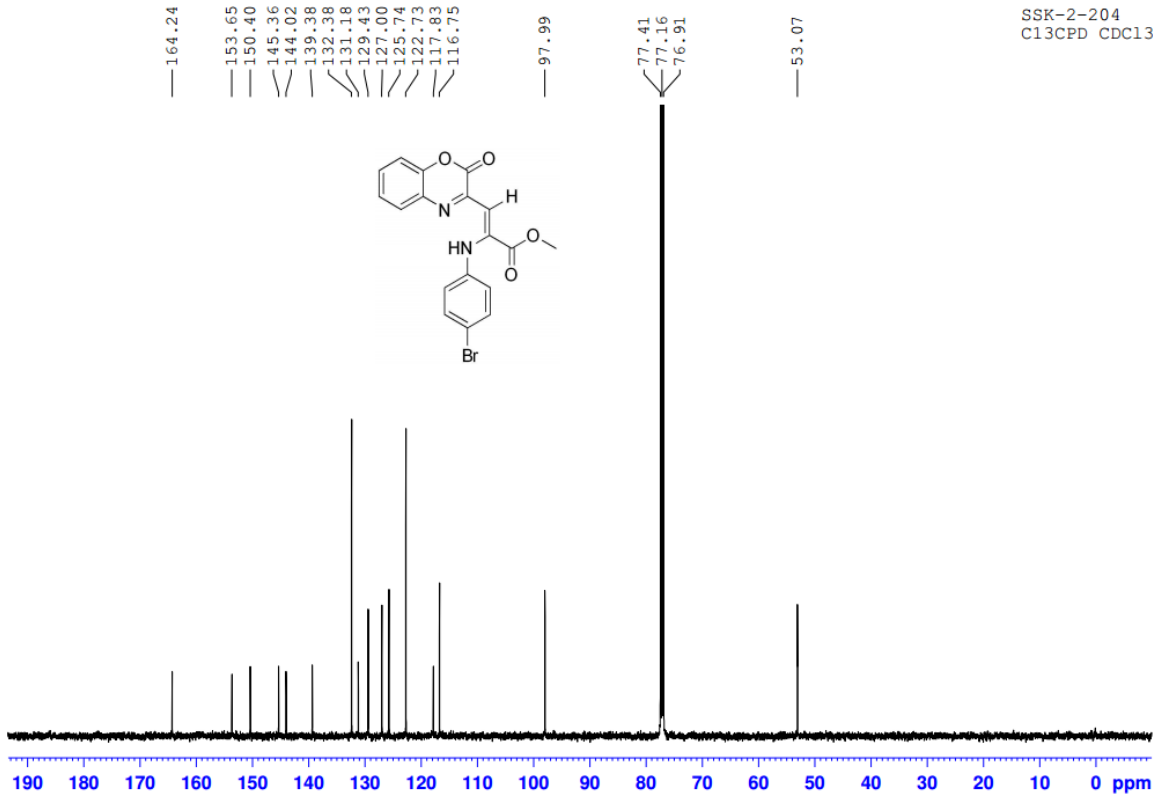
Compound **4a**


SSK-2-368
PROTON CDC13
11.791
7.568
7.565
7.552
7.549
7.391
7.388
7.376
7.373
7.360
7.357
7.319
7.313
7.309
7.304
7.295
7.289
7.287
7.260
7.246
7.243
6.955
6.949
6.945
6.935
6.931
6.925
6.675
3.799
O
O
H
N
HN
O
O
Cl
7.6
7.4
7.2
7.0
6.8
ppm
1.00
1.05
3.06
1.22
2.02
0.93
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.95
1.00
1.05
3.06
1.22
2.02
0.93
3.02

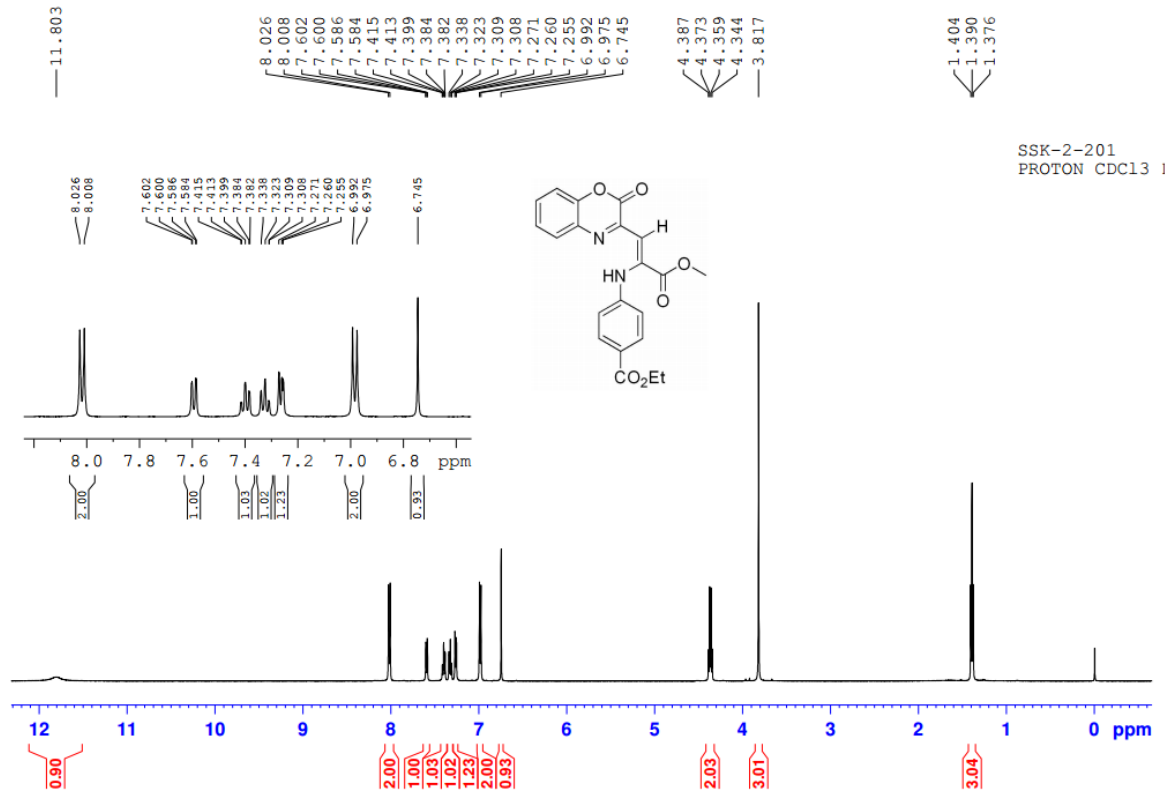

SSK-2-368
C13CPD CDC13
164.25
153.67
150.41
145.36
144.19
138.90
131.20
130.25
129.45
129.39
126.99
125.73
122.45
116.75
97.83
77.41
77.16
76.91
53.05
O
O
H
N
HN
O
O
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

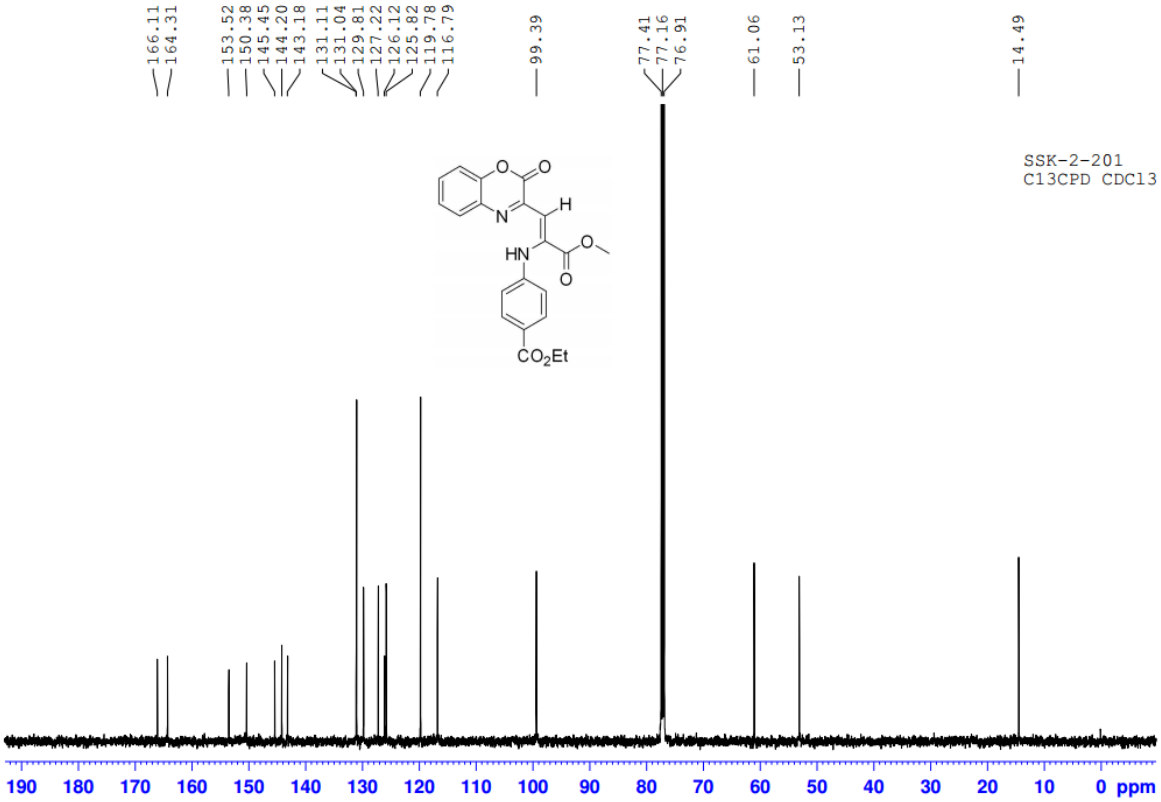
Compound **4b**


SSK-2-204
PROTON CDCl3
11.761
7.567
7.564
7.552
7.548
7.462
7.456
7.452
7.443
7.439
7.433
7.393
7.390
7.378
7.375
7.362
7.359
7.321
7.318
7.305
7.302
7.290
7.287
7.261
7.260
7.245
7.243
6.894
6.888
6.883
6.874
6.870
6.864
6.681
3.802
O
O
N
H
HN
O
O
Br
7.6
7.4
7.2
7.0
ppm
1.01
2.01
1.03
1.03
1.17
2.00
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.90
1.01
2.01
1.03
1.03
1.17
2.00
0.91
3.03

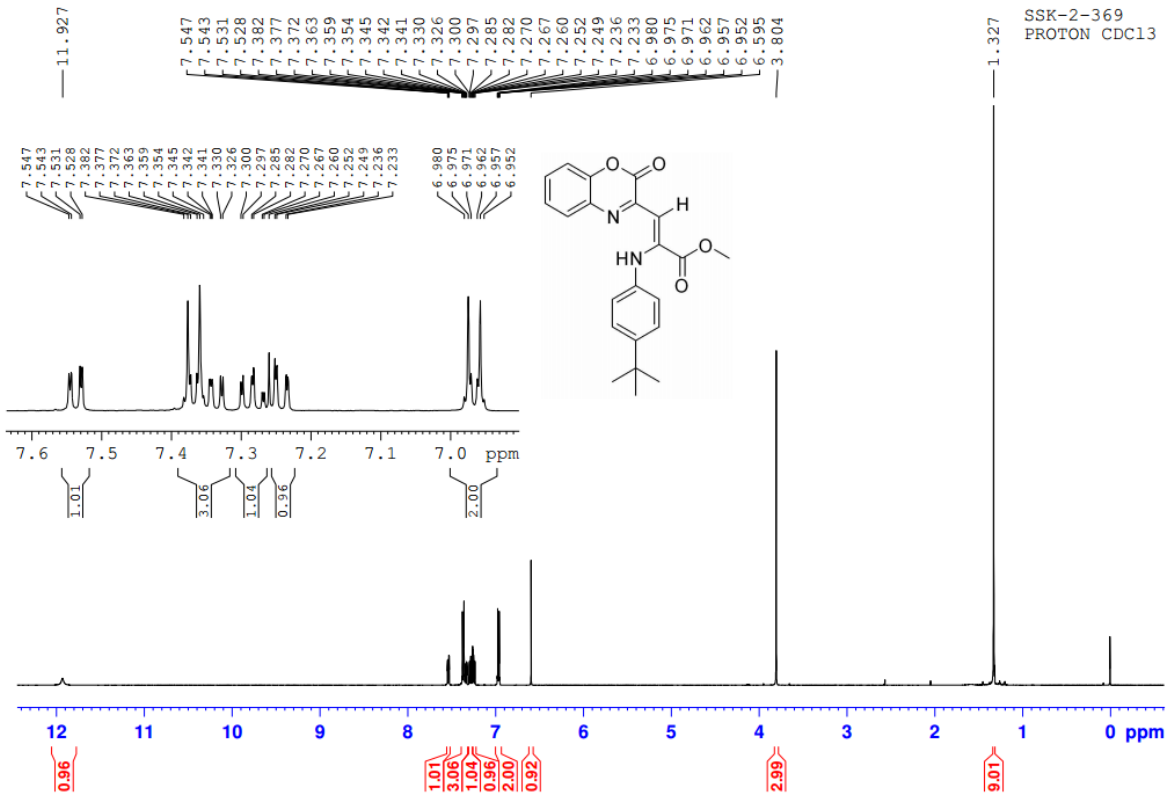

SSK-2-204
C13CPD CDCl3
164.24
153.65
150.40
145.36
144.02
139.38
132.38
131.18
129.43
127.00
125.74
122.73
117.83
116.75
97.99
77.41
77.16
76.91
53.07
O
O
N
H
HN
O
O
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

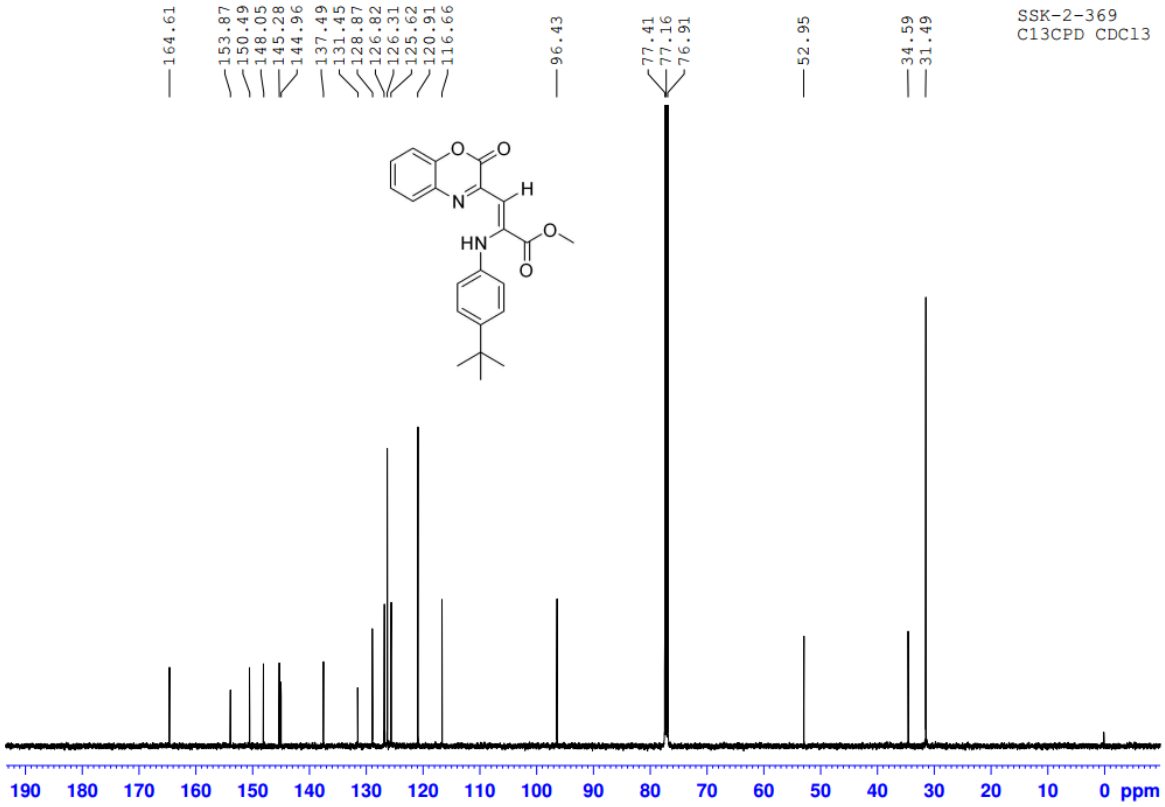
Compound **4c**



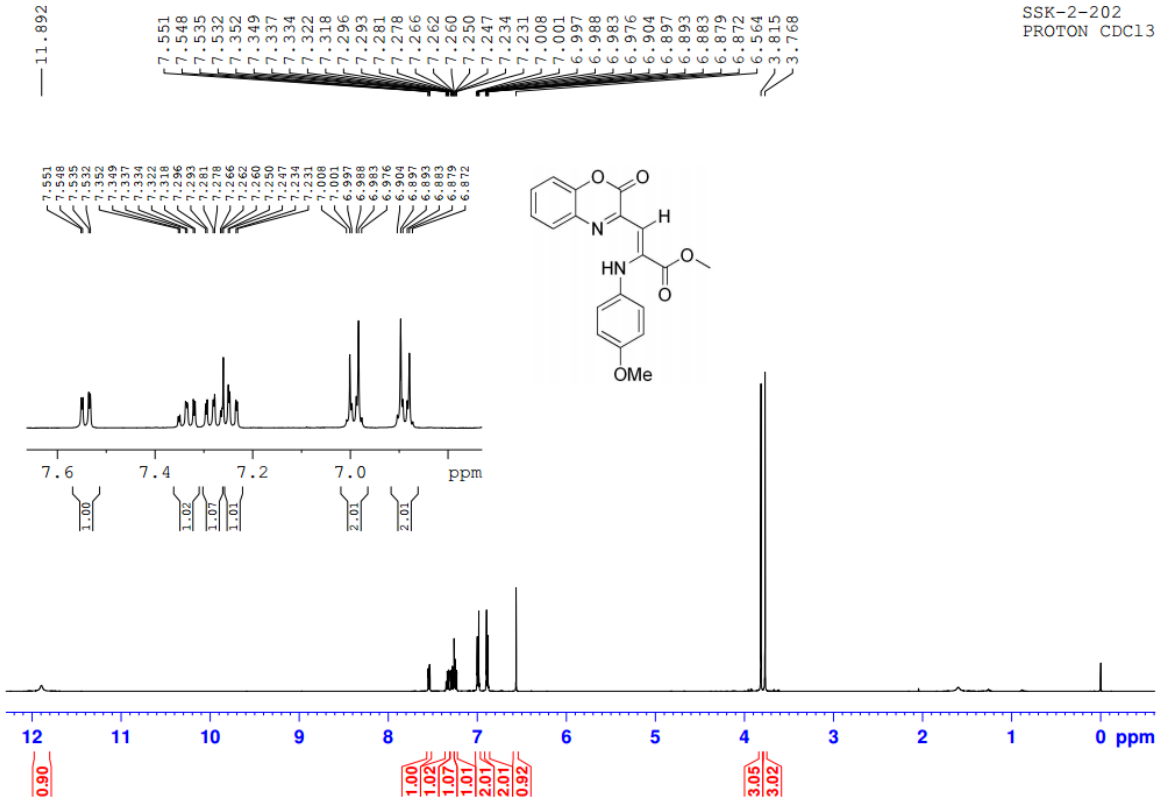


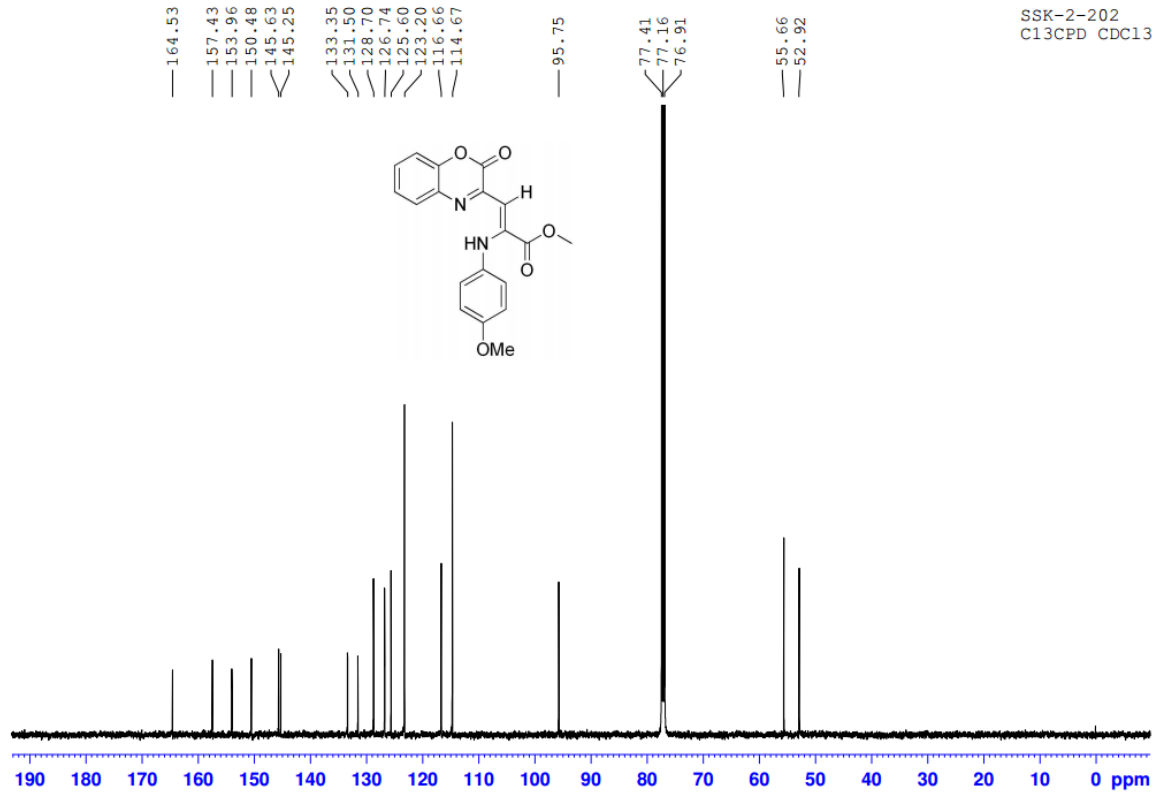
Compound **4d**


SSK-2-369
PROTON CDCl3
11.927
7.547
7.543
7.531
7.528
7.382
7.377
7.372
7.363
7.359
7.354
7.345
7.342
7.341
7.330
7.326
7.300
7.297
7.285
7.282
7.270
7.267
7.260
7.252
7.249
7.236
7.233
6.980
6.975
6.971
6.962
6.957
6.952
6.595
3.804
1.327
7.6
7.5
7.4
7.3
7.2
7.1
7.0 ppm
1.01
3.06
1.04
0.96
2.00
0.92
2.99
9.01
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm

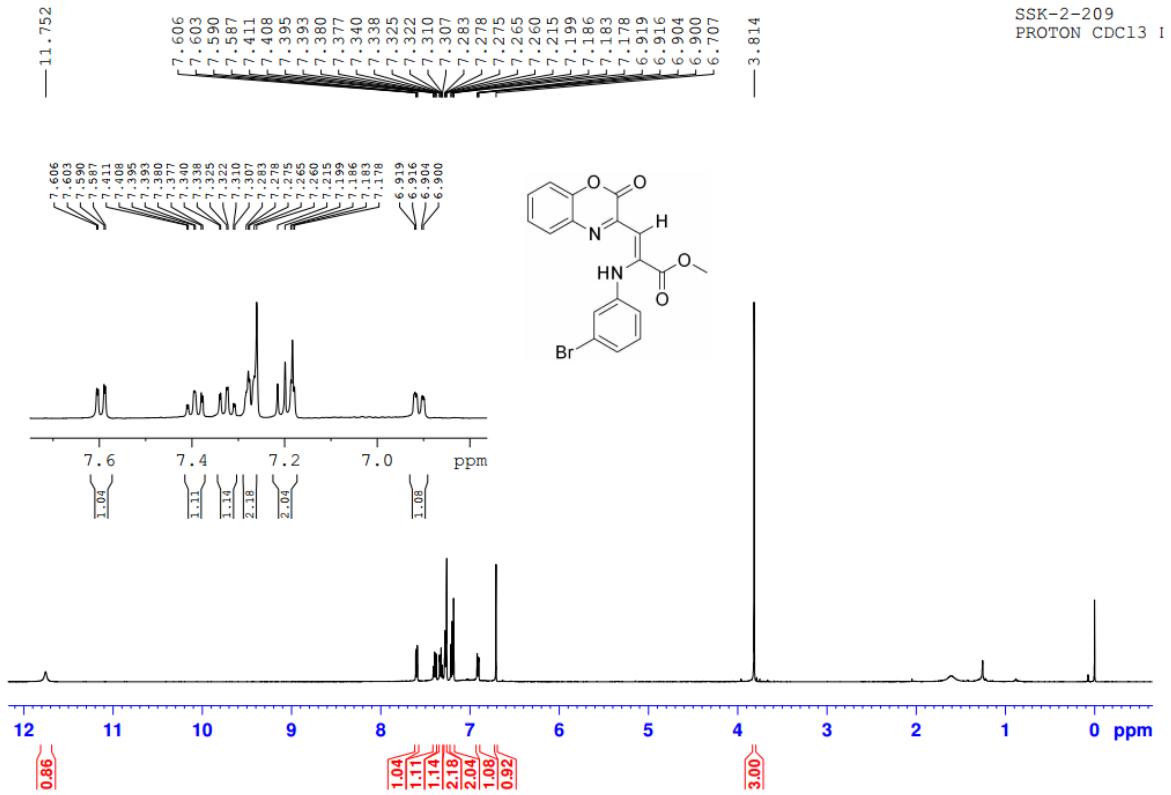

SSK-2-369
C13CPD CDCl3
164.61
153.87
150.49
148.05
145.28
144.96
137.49
131.45
128.87
126.82
126.31
125.62
120.91
116.66
96.43
77.41
77.16
76.91
52.95
34.59
31.49
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

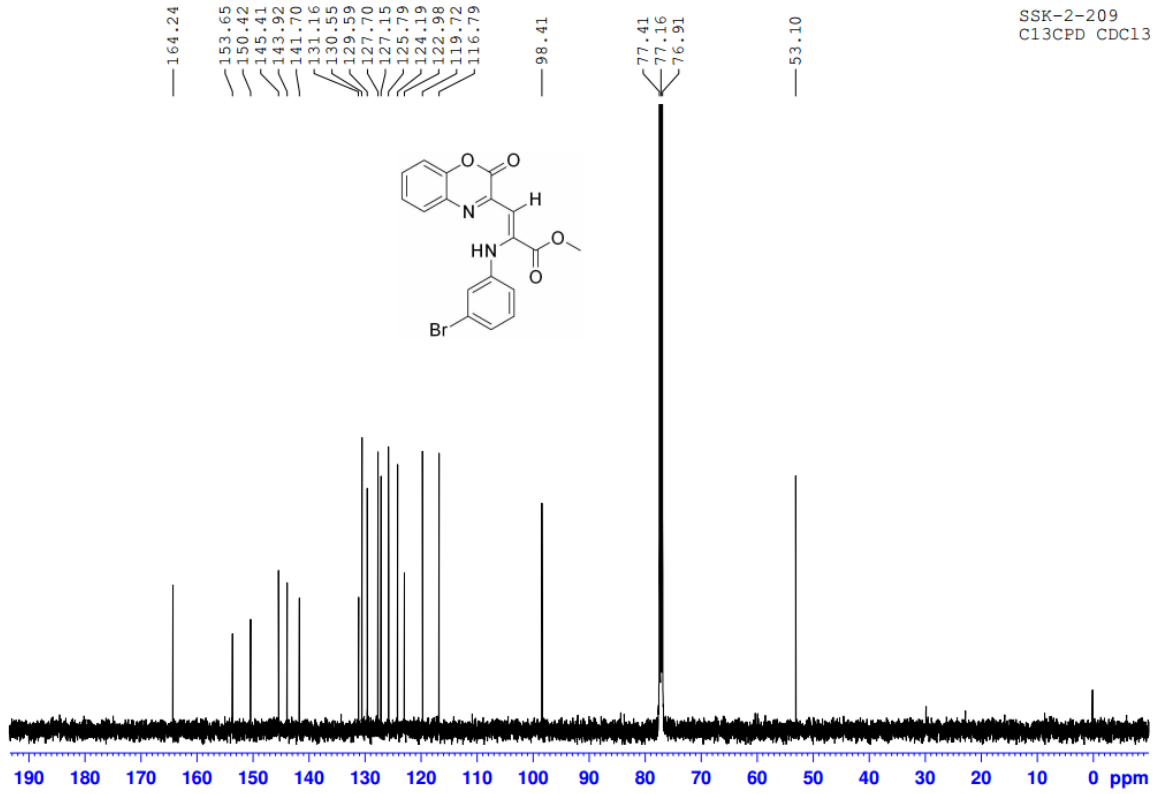
Compound **4e**


SSK-2-202
PROTON CDCl3
11.892
7.551
7.548
7.535
7.532
7.352
7.349
7.337
7.334
7.322
7.318
7.296
7.293
7.281
7.278
7.266
7.262
7.260
7.250
7.247
7.234
7.231
7.008
7.001
6.997
6.988
6.983
6.976
6.904
6.897
6.893
6.883
6.879
6.872
6.564
3.815
3.768
O
O
N
H
HN
O
O
OMe
7.6
7.4
7.2
7.0
ppm
1.00
1.02
1.07
1.01
2.01
2.01
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.90
1.00
1.02
1.07
1.01
2.01
2.01
0.92
3.05
3.02

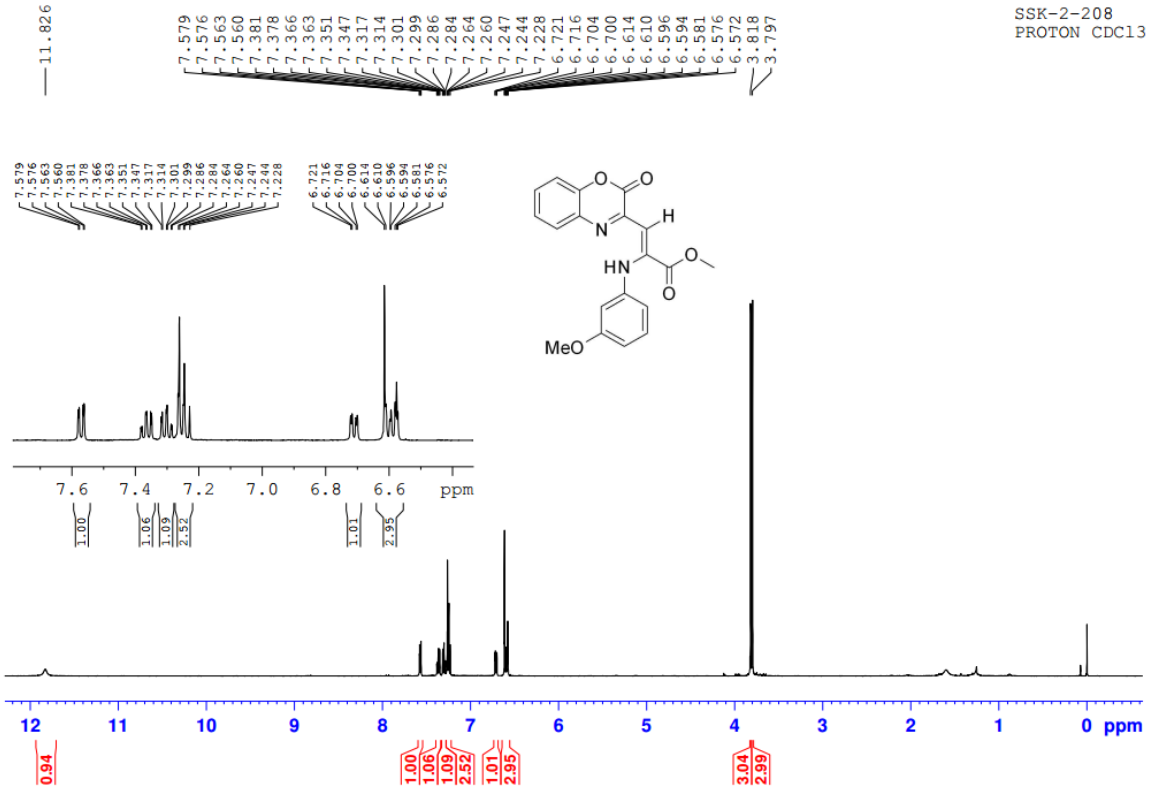

SSK-2-202
C13CPD CDCl3
164.53
157.43
153.96
150.48
145.63
145.25
133.35
131.50
128.70
126.74
125.60
123.20
116.66
114.67
95.75
77.41
77.16
76.91
55.66
52.92
O
O
N
H
HN
O
O
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

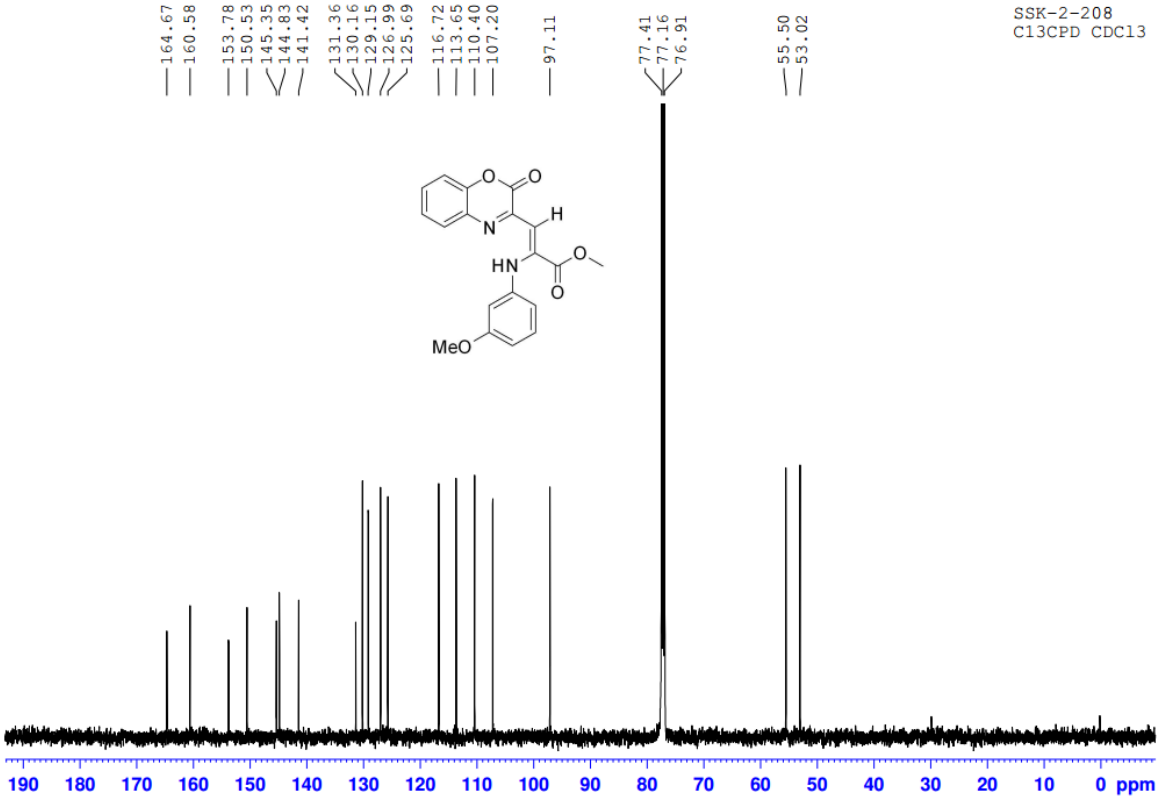
Compound **4f**


SSK-2-209
PROTON CDC13 I
11.752
7.606
7.603
7.590
7.587
7.411
7.408
7.395
7.393
7.380
7.377
7.340
7.338
7.325
7.322
7.310
7.307
7.283
7.278
7.275
7.265
7.260
7.215
7.199
7.186
7.183
7.178
6.919
6.916
6.904
6.900
6.707
3.814
HN
Br
ppm
0.86
1.04
1.11
1.14
2.18
2.04
1.08
0.92
3.00

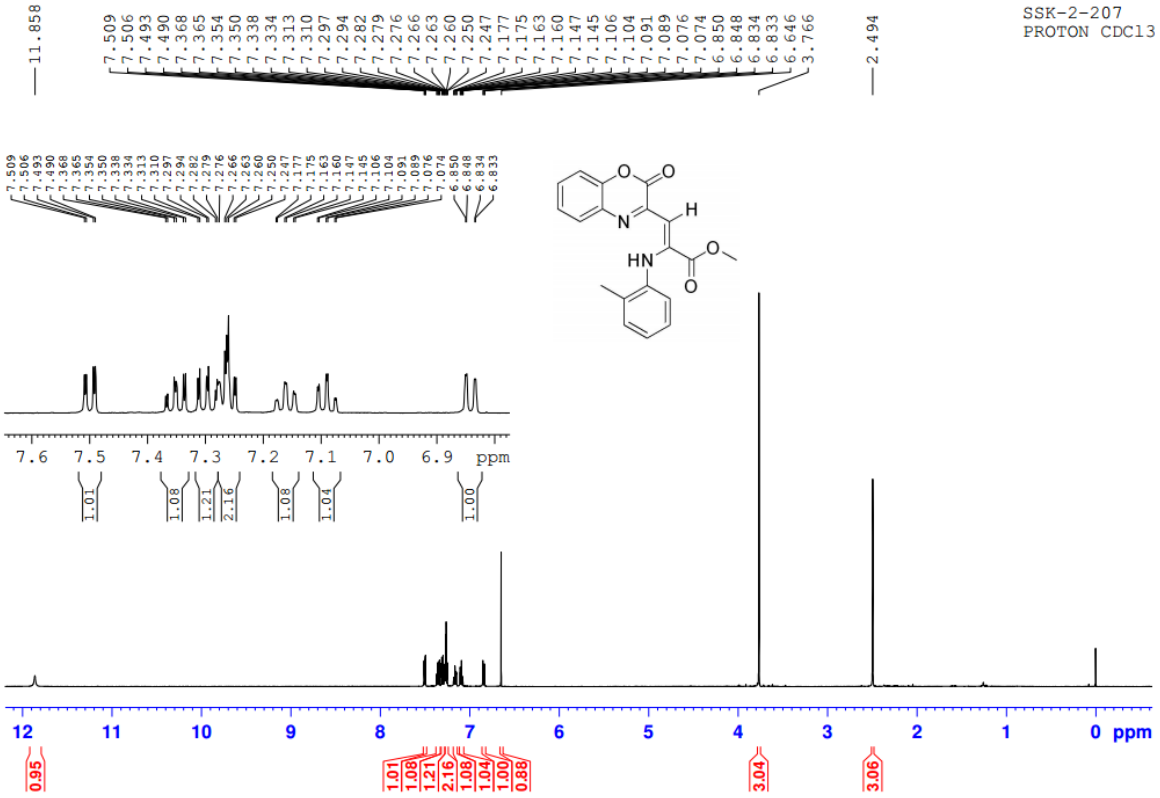

SSK-2-209
C13CPD CDC13
164.24
153.65
150.42
145.41
143.92
141.70
131.16
130.55
129.59
127.70
127.15
125.79
124.19
122.98
119.72
116.79
98.41
77.41
77.16
76.91
53.10
HN
Br
ppm

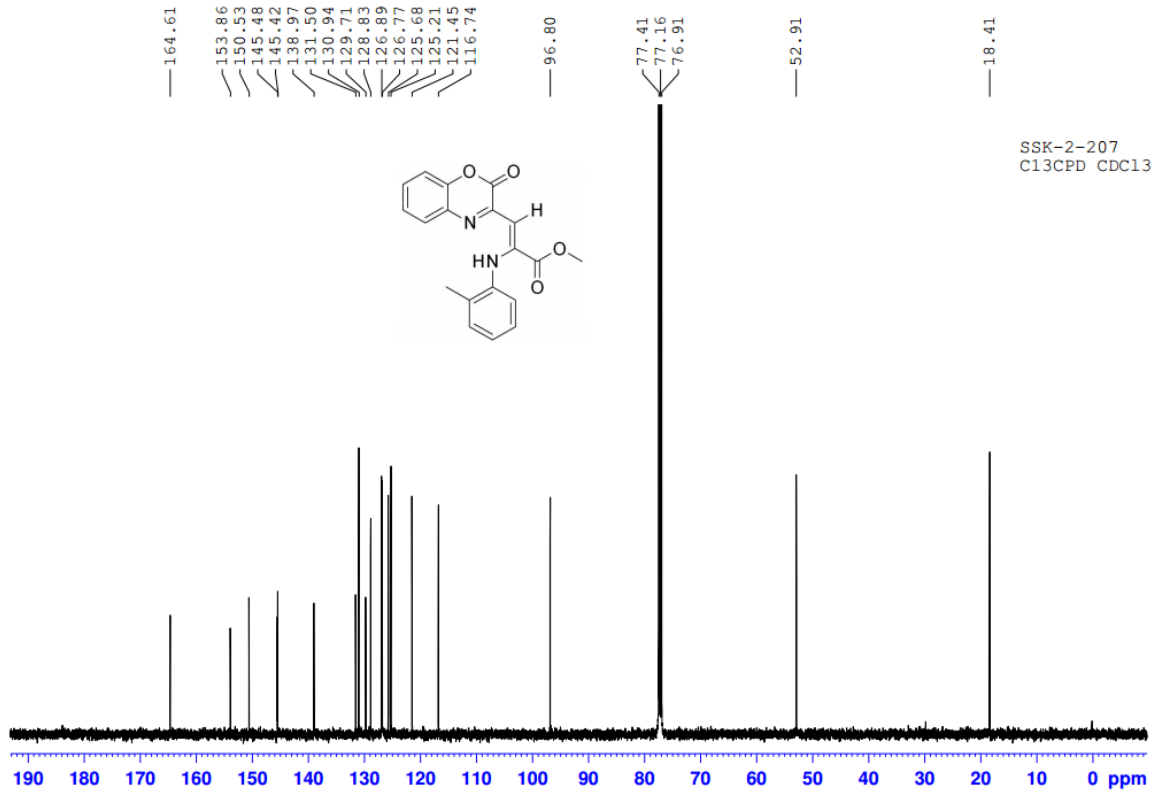
Compound **4g**


SSK-2-208
PROTON CDCl3
11.826
7.579
7.576
7.563
7.560
7.381
7.378
7.366
7.363
7.351
7.347
7.317
7.314
7.301
7.299
7.286
7.284
7.264
7.260
7.247
7.244
7.228
6.721
6.716
6.704
6.700
6.614
6.610
6.596
6.594
6.581
6.576
6.572
3.818
3.797
MeO
ppm
0.94
1.00
1.06
1.09
2.52
1.01
2.95
3.04
2.99

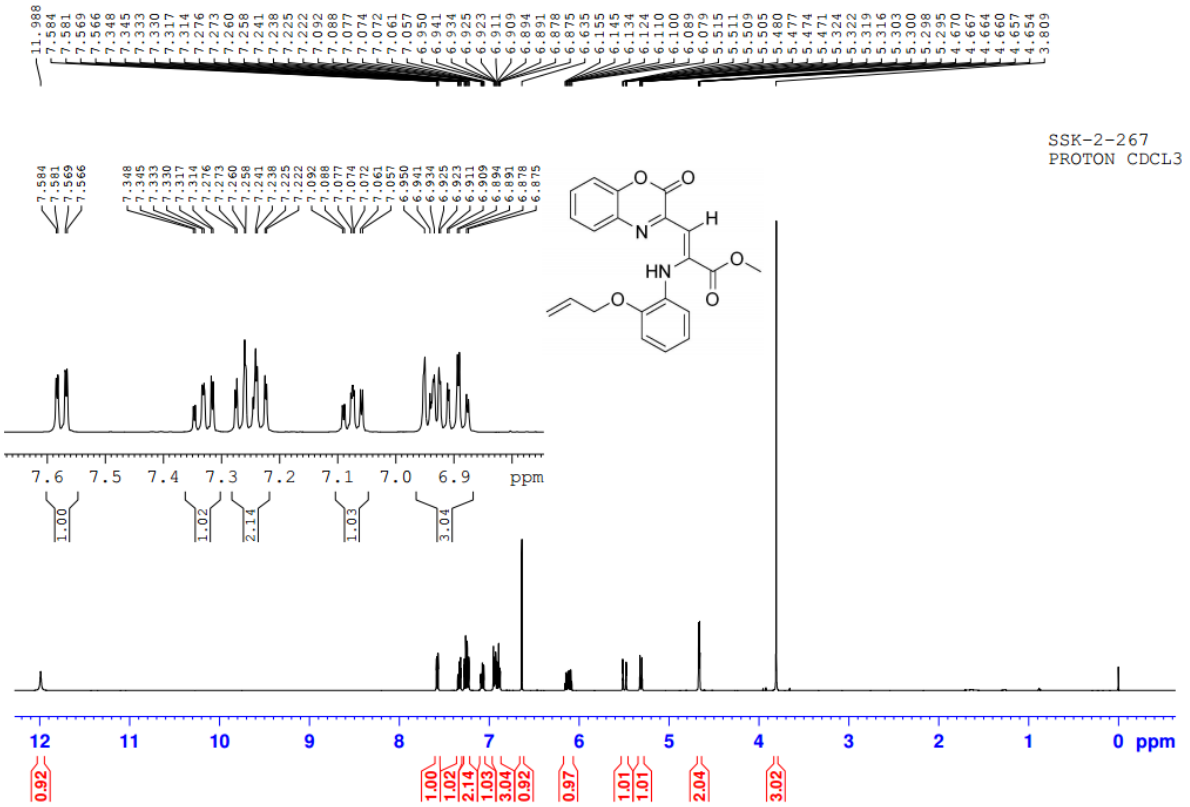

SSK-2-208
C13CPD CDCl3
164.67
160.58
153.78
150.53
145.35
144.83
141.42
131.36
130.16
129.15
126.99
125.69
116.72
113.65
110.40
107.20
97.11
77.41
77.16
76.91
55.50
53.02
MeO
ppm

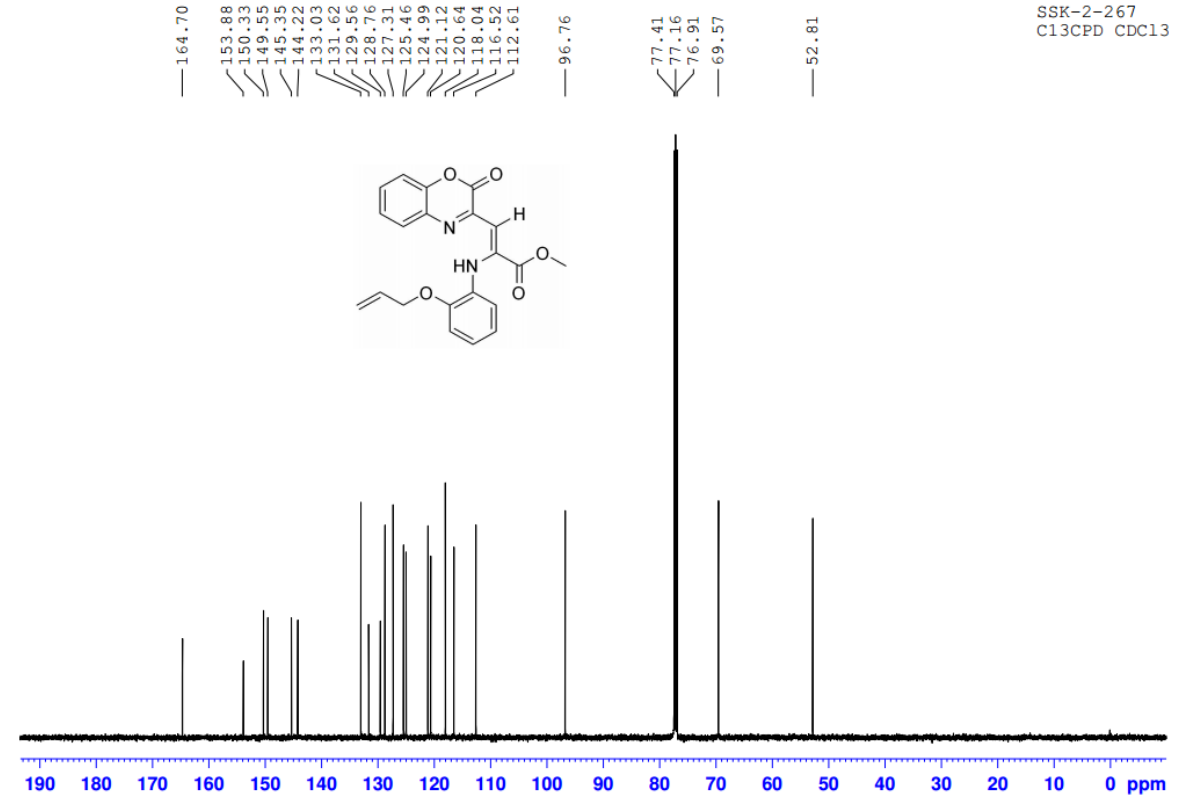
Compound **4h**


SSK-2-207
PROTON CDCl3
11.858
7.509
7.506
7.493
7.490
7.368
7.365
7.354
7.350
7.338
7.334
7.313
7.310
7.297
7.294
7.282
7.279
7.266
7.263
7.260
7.250
7.247
7.177
7.175
7.163
7.160
7.147
7.145
7.106
7.104
7.091
7.089
7.076
7.074
6.850
6.848
6.834
6.833
6.646
3.766
2.494
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 ppm
1.01 1.08 1.21 2.16 1.08 1.04 1.00
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.95 1.01 1.08 1.21 2.16 1.08 1.04 1.00 0.88 3.04 3.06

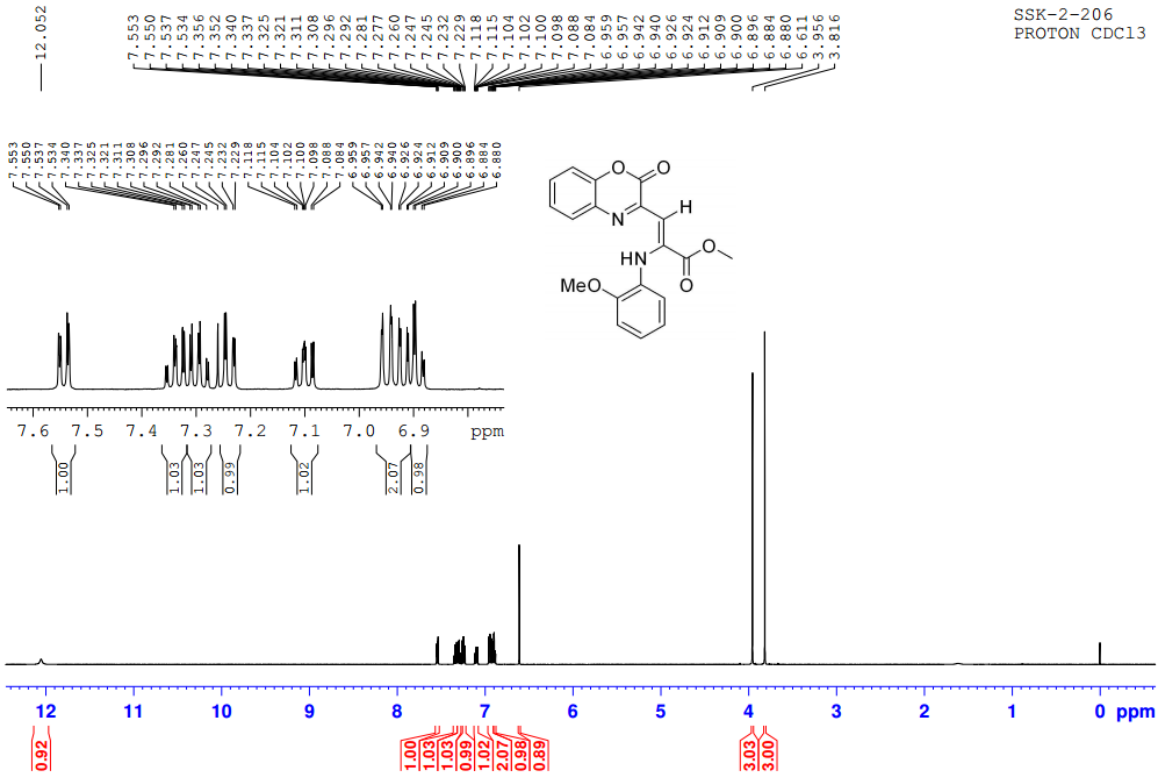

164.61
153.86
150.53
145.48
145.42
138.97
131.50
130.94
129.71
128.83
126.89
126.77
125.68
125.21
121.45
116.74
96.80
77.41
77.16
76.91
52.91
18.41
SSK-2-207
C13CPD CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

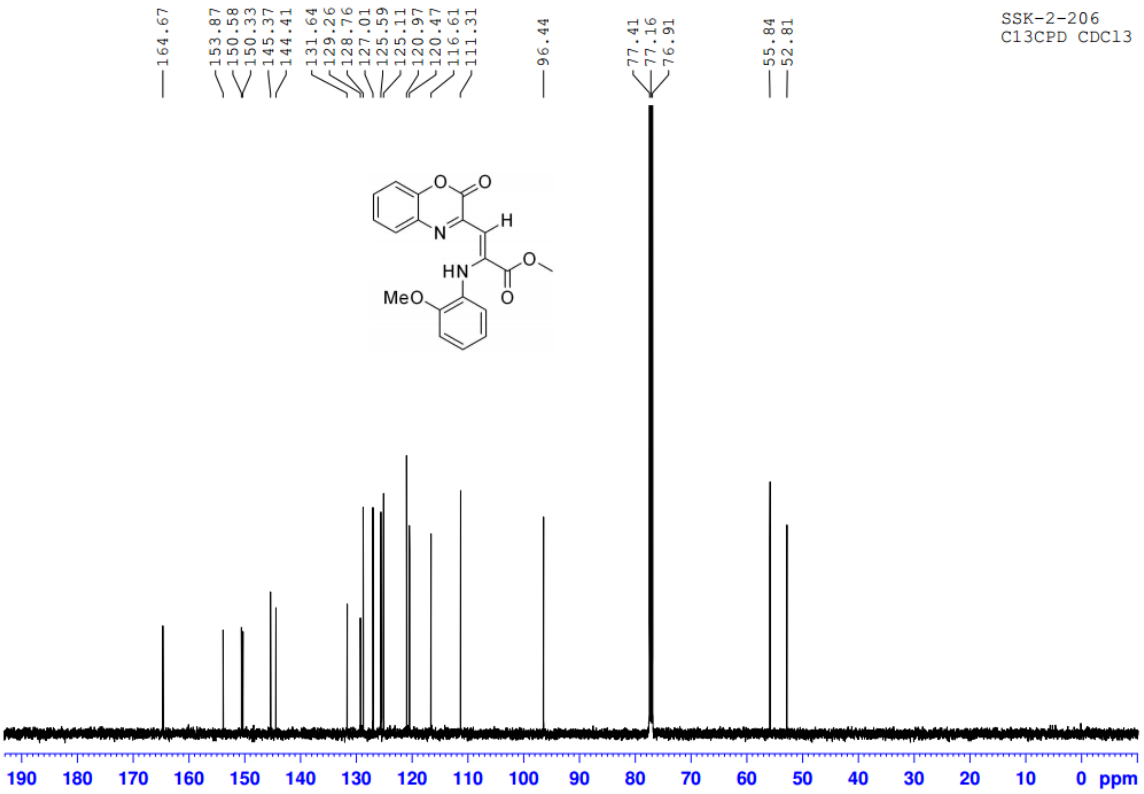
Compound **4i**



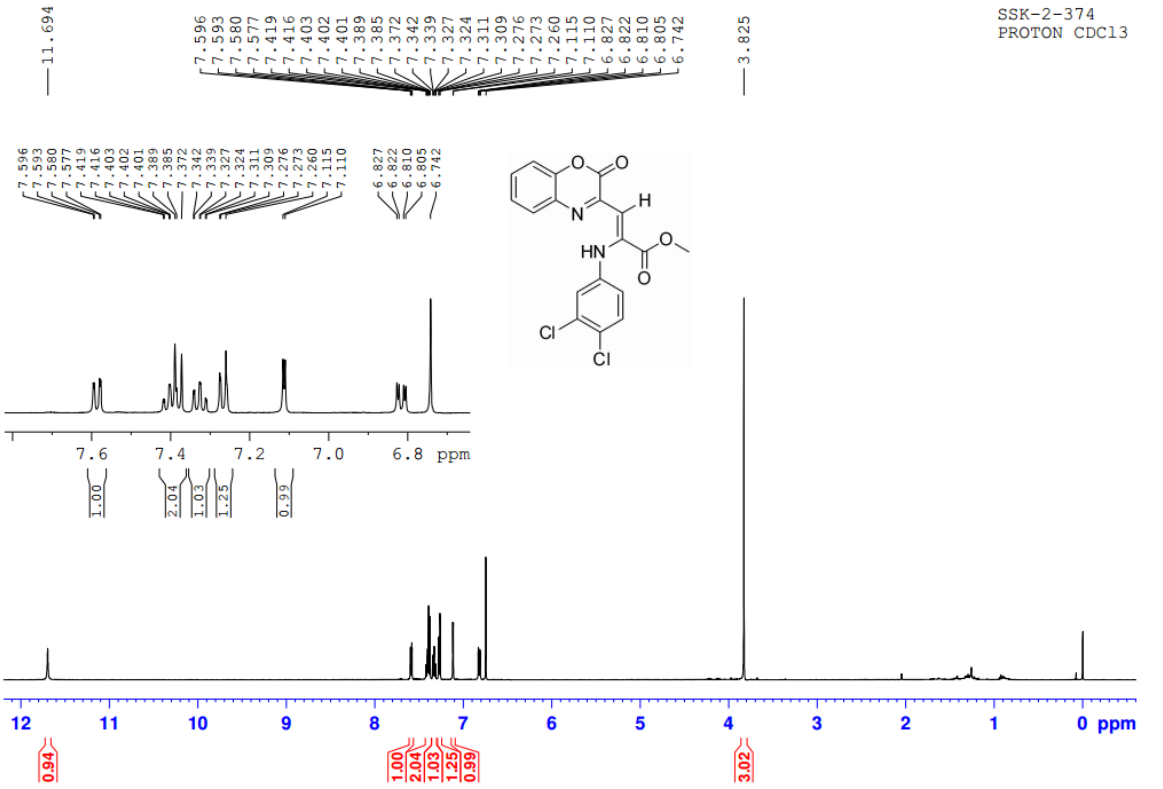


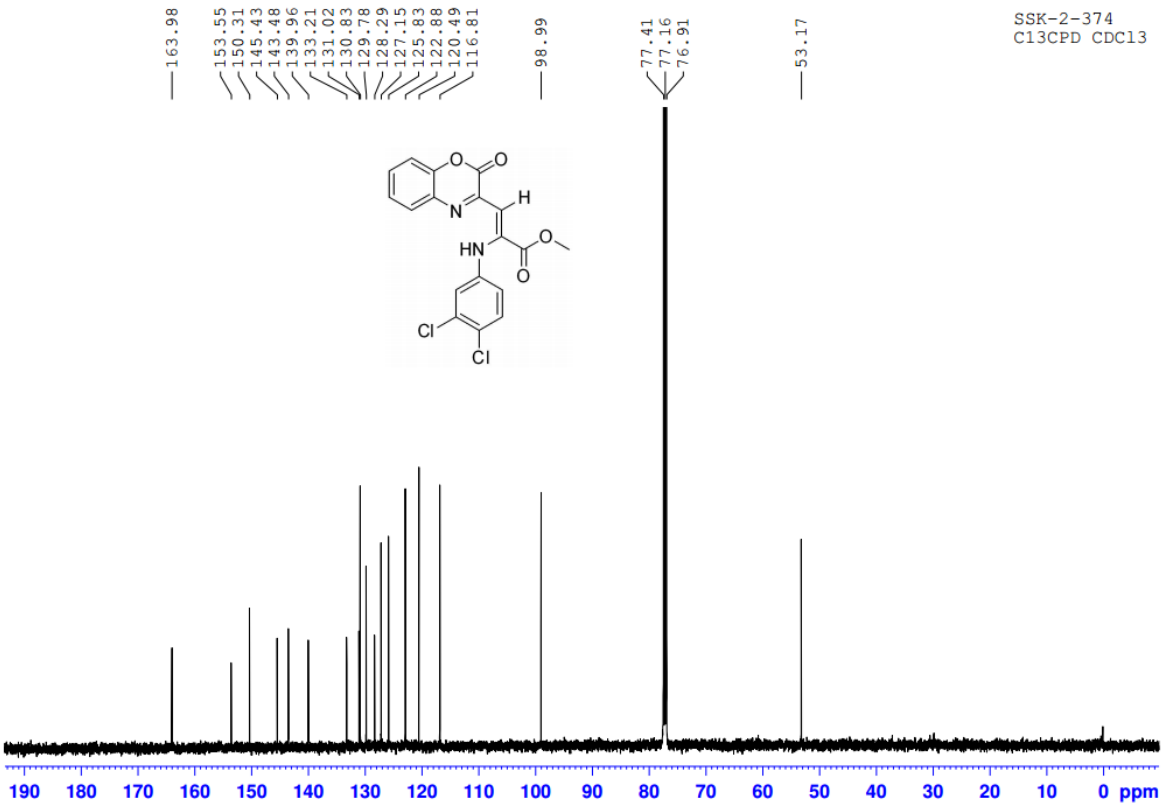
Compound **4j**


SSK-2-206
PROTON CDC13
12.052
7.553
7.550
7.537
7.534
7.356
7.352
7.340
7.337
7.325
7.321
7.311
7.308
7.296
7.292
7.281
7.277
7.260
7.247
7.245
7.232
7.229
7.118
7.115
7.104
7.102
7.100
7.098
7.088
7.084
6.959
6.957
6.942
6.940
6.926
6.924
6.912
6.909
6.900
6.896
6.884
6.880
6.611
3.956
3.816
MeO
HN
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 ppm
1.00 1.03 1.03 0.99 1.02 2.07 0.98
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.92 1.00 1.03 1.03 0.99 1.02 2.07 0.98 0.89 3.03 3.00

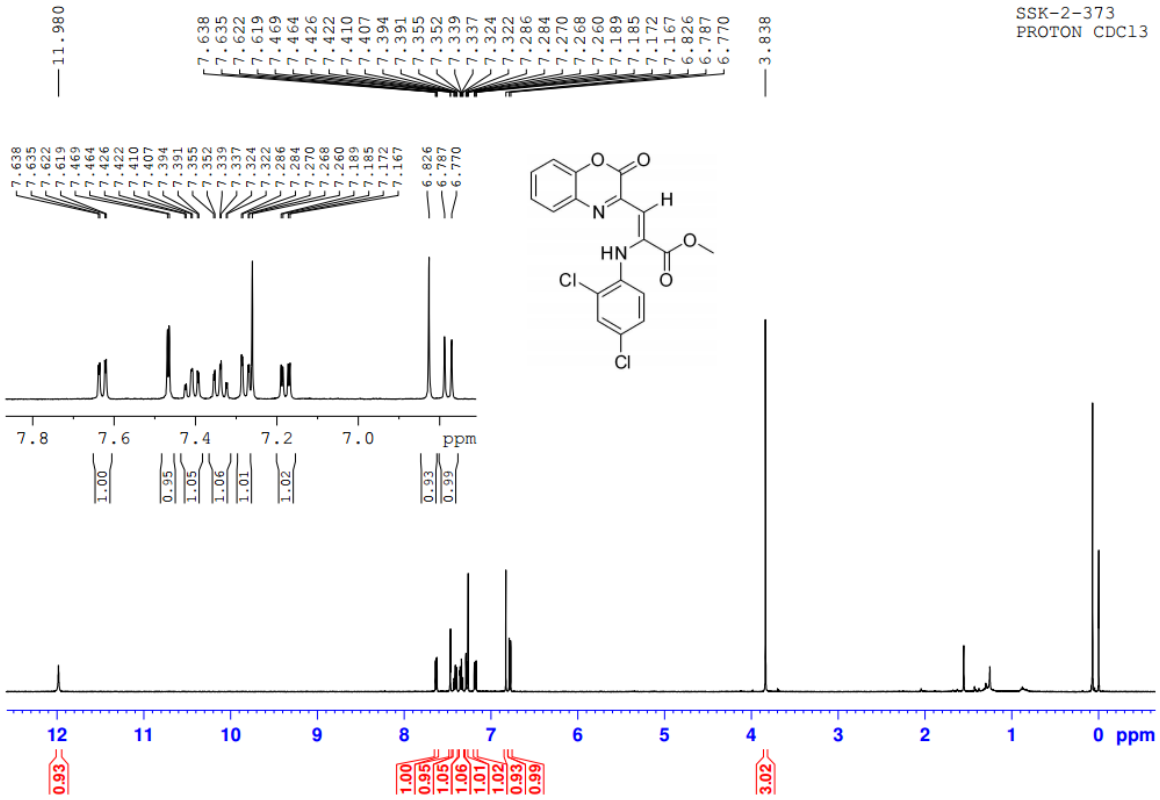

SSK-2-206
C13CPD CDC13
164.67
153.87
150.58
150.33
145.37
144.41
131.64
129.26
128.76
127.01
125.59
125.11
120.97
120.47
116.61
111.31
96.44
77.41
77.16
76.91
55.84
52.81
MeO
HN
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

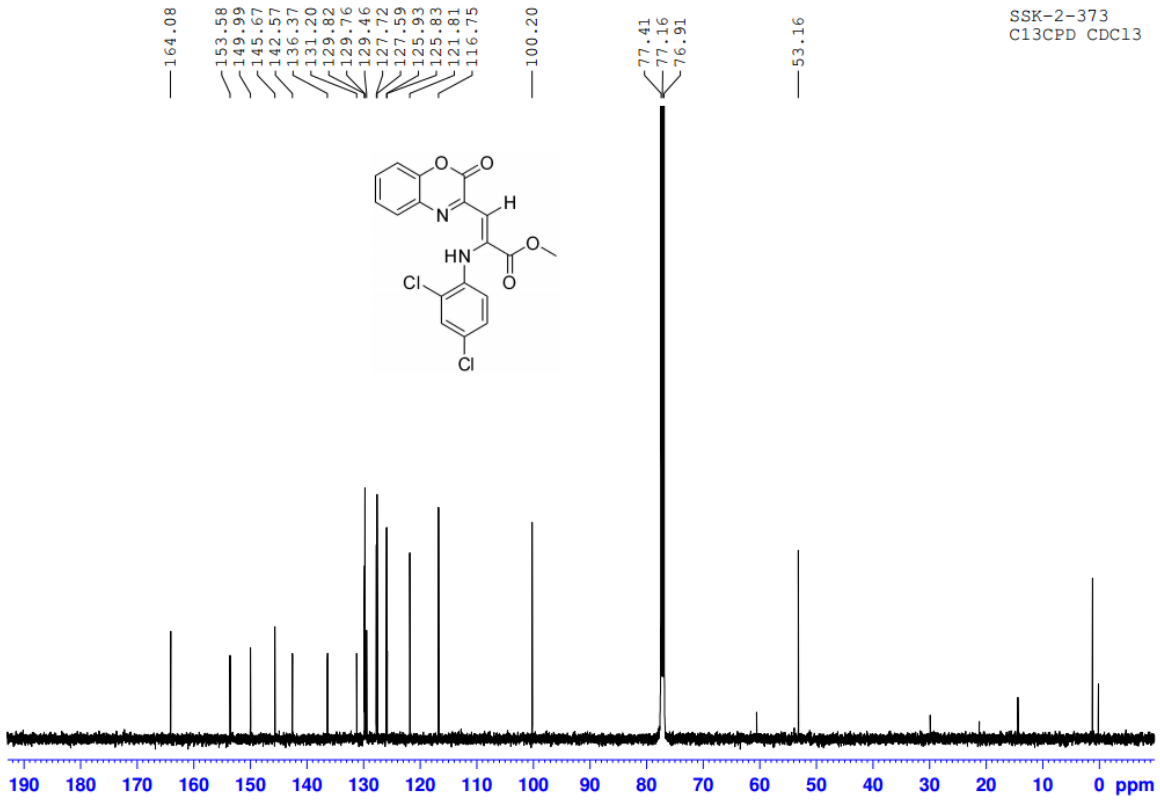
Compound **4k**


SSK-2-374
PROTON CDC13
11.694
7.596
7.593
7.580
7.577
7.419
7.416
7.403
7.402
7.401
7.389
7.385
7.372
7.342
7.339
7.327
7.324
7.311
7.309
7.276
7.273
7.260
7.115
7.110
6.827
6.822
6.810
6.805
6.742
3.825
O
O
H
N
HN
O
O
Cl
Cl
7.6
7.4
7.2
7.0
6.8 ppm
1.00
2.04
1.03
1.25
0.99
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.94
1.00
2.04
1.03
1.25
0.99
3.02

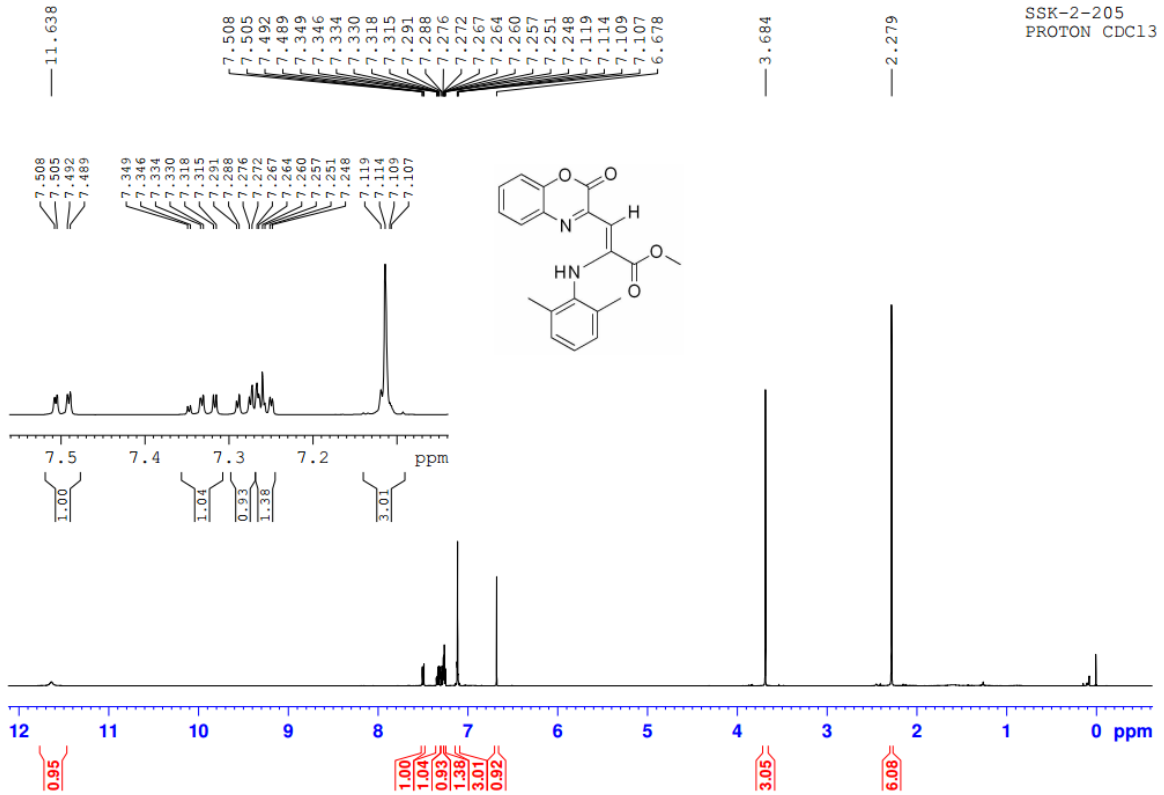

SSK-2-374
C13CPD CDC13
163.98
153.55
150.31
145.43
143.48
139.96
133.21
131.02
130.83
129.78
128.29
127.15
125.83
122.88
120.49
116.81
98.99
77.41
77.16
76.91
53.17
O
O
H
N
HN
O
O
Cl
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

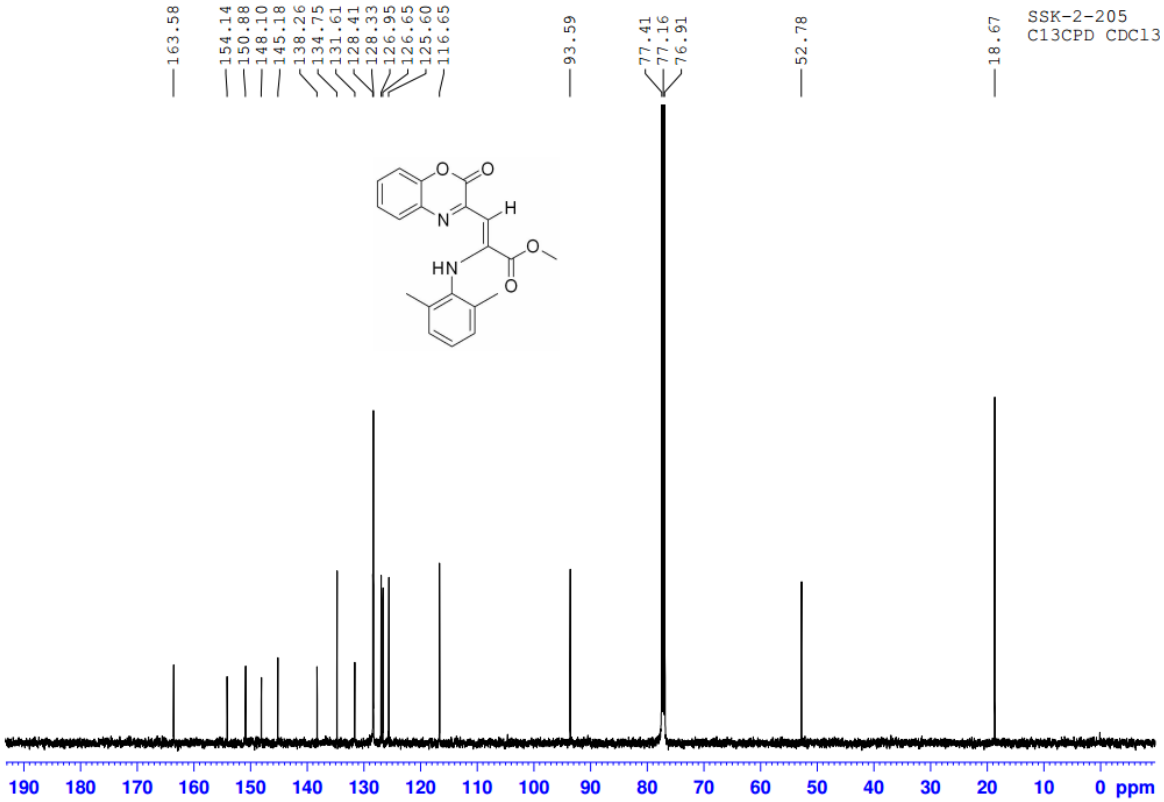
Compound **4l**


SSK-2-373
PROTON CDC13
11.980
7.638
7.635
7.622
7.619
7.469
7.464
7.426
7.422
7.410
7.407
7.394
7.391
7.355
7.352
7.339
7.337
7.324
7.322
7.286
7.284
7.270
7.268
7.260
7.189
7.185
7.172
7.167
6.826
6.787
6.770
3.838
O
O
N
H
HN
O
O
Cl
Cl
7.8
7.6
7.4
7.2
7.0
ppm
1.00
0.95
1.05
1.06
1.01
1.02
0.93
0.99
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.93
1.00
0.95
1.05
1.06
1.01
1.02
0.93
0.99
3.02

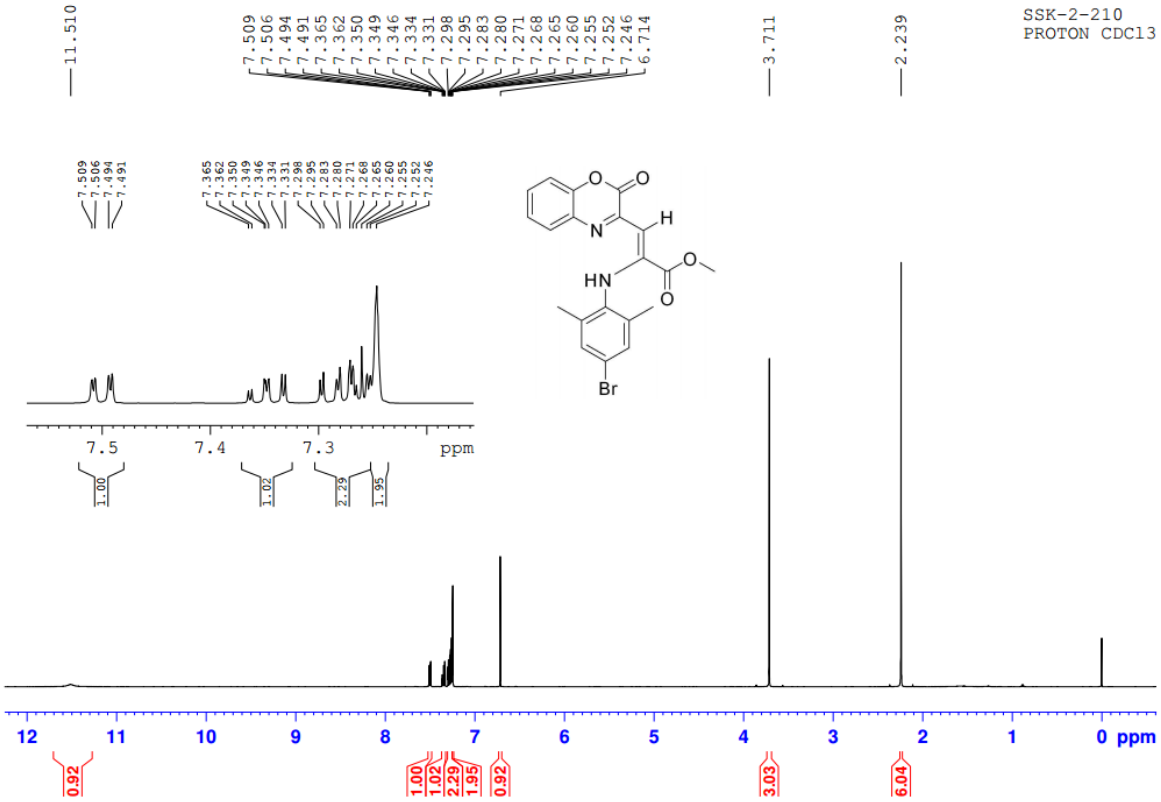

SSK-2-373
C13CPD CDC13
164.08
153.58
149.99
145.67
142.57
136.37
131.20
129.82
129.76
129.46
127.72
127.59
125.93
125.83
121.81
116.75
100.20
77.41
77.16
76.91
53.16
O
O
N
H
HN
O
O
Cl
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

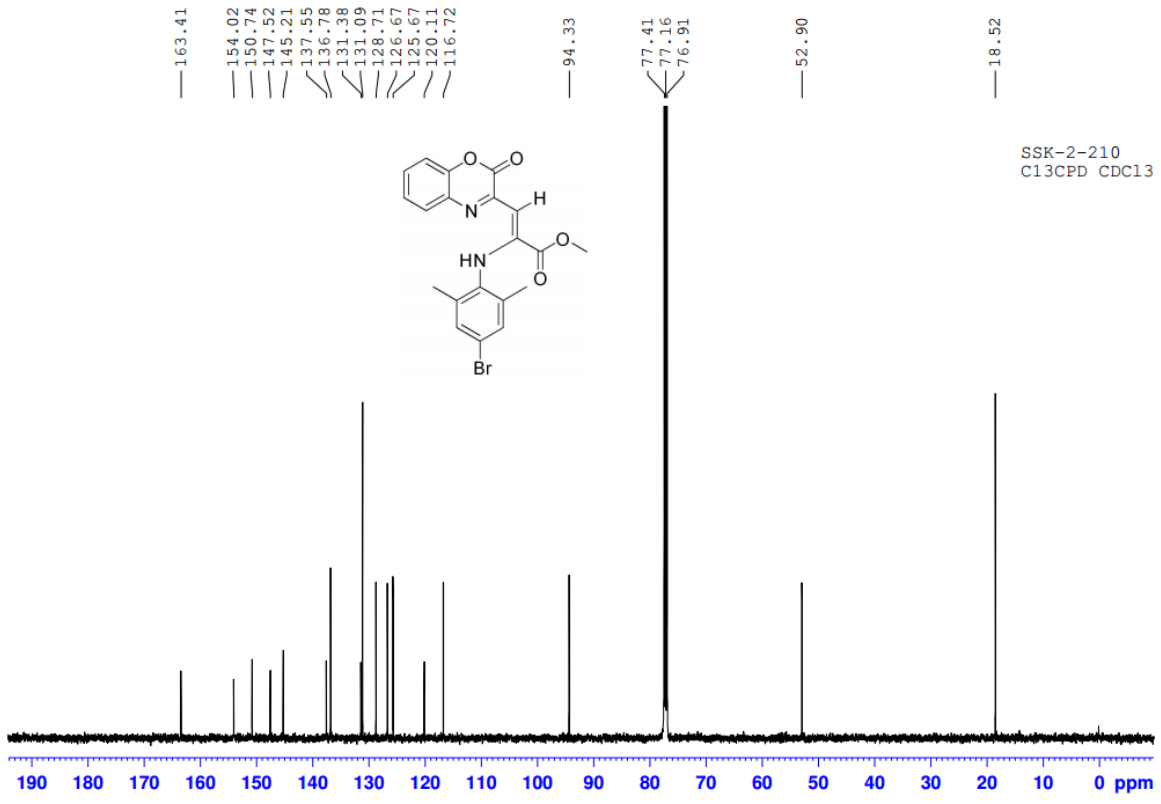
Compound **4m**


SSK-2-205
PROTON CDCl3
11.638
7.508
7.505
7.492
7.489
7.349
7.346
7.334
7.330
7.318
7.315
7.291
7.288
7.276
7.272
7.267
7.264
7.260
7.257
7.251
7.248
7.119
7.114
7.109
7.107
6.678
3.684
2.279
ppm
0.95
1.00
1.04
0.93
1.38
3.01
0.92
3.05
6.08

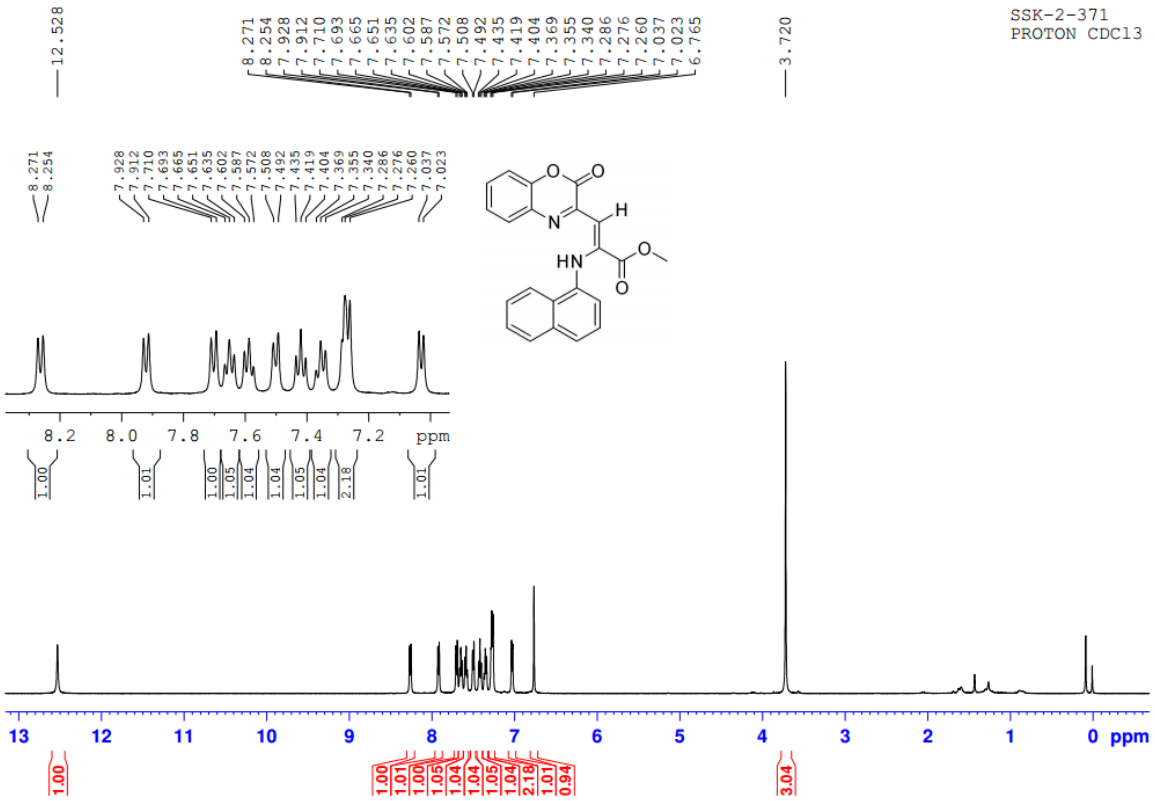

SSK-2-205
C13CPD CDCl3
163.58
154.14
150.88
148.10
145.18
138.26
134.75
131.61
128.41
128.33
126.95
126.65
125.60
116.65
93.59
77.41
77.16
76.91
52.78
18.67
ppm

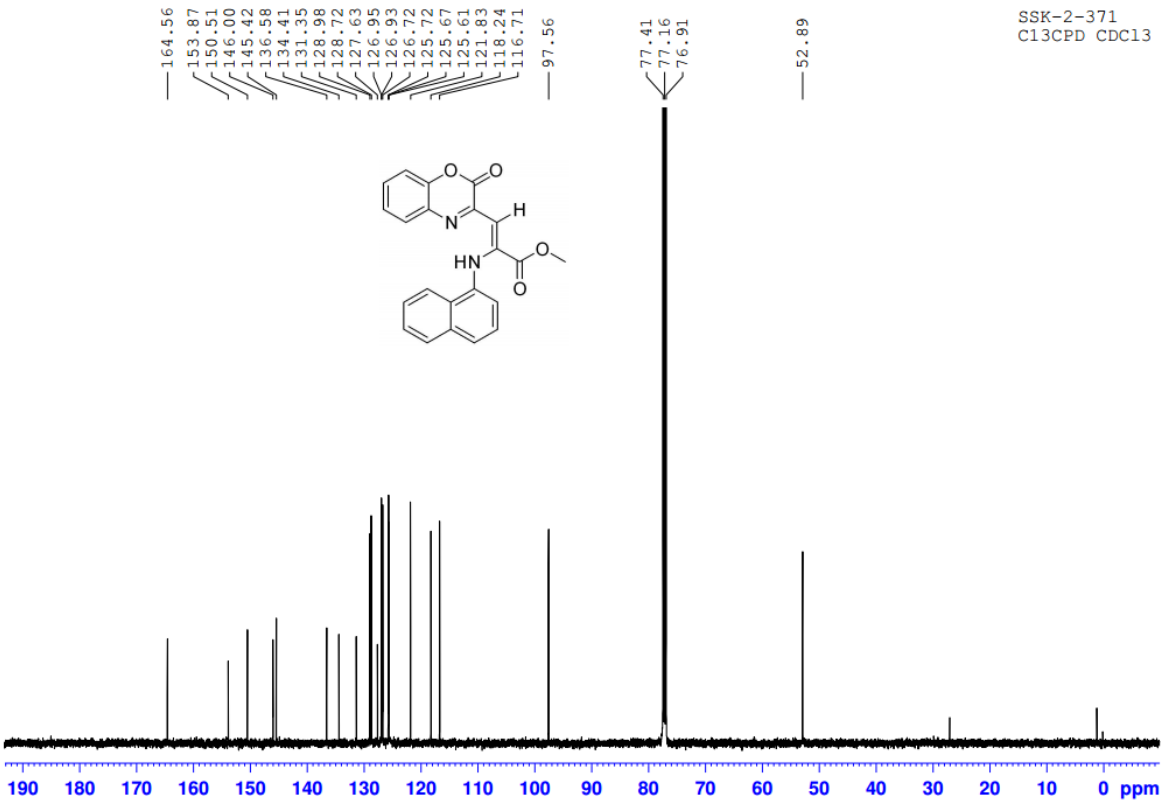
Compound **4n**


SSK-2-210
PROTON CDCl3
11.510
7.509
7.506
7.494
7.491
7.365
7.362
7.350
7.349
7.346
7.334
7.331
7.298
7.295
7.283
7.280
7.271
7.268
7.265
7.260
7.255
7.252
7.246
6.714
3.711
2.239
HN
Br
7.5
7.4
7.3
ppm
1.00
1.02
2.29
1.95
0.92
3.03
6.04
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm

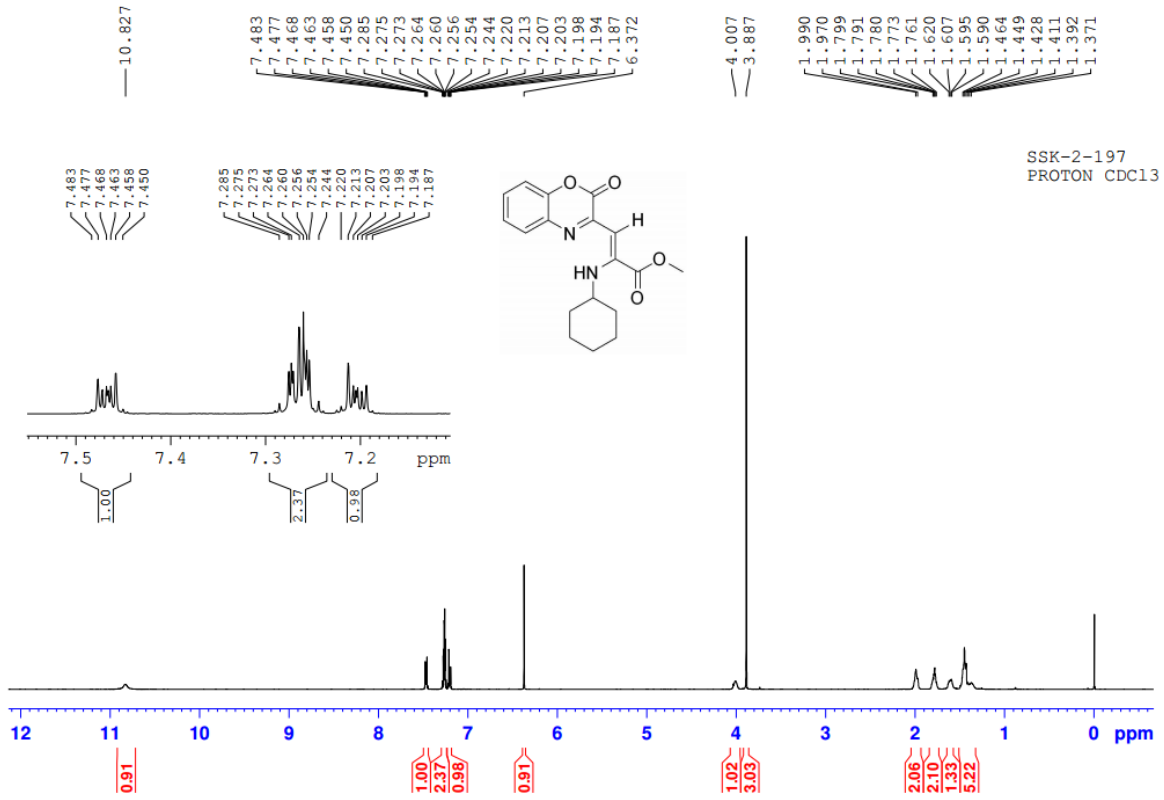

SSK-2-210
C13CPD CDCl3
163.41
154.02
150.74
147.52
145.21
137.55
136.78
131.38
131.09
128.71
126.67
125.67
120.11
116.72
94.33
77.41
77.16
76.91
52.90
18.52
HN
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

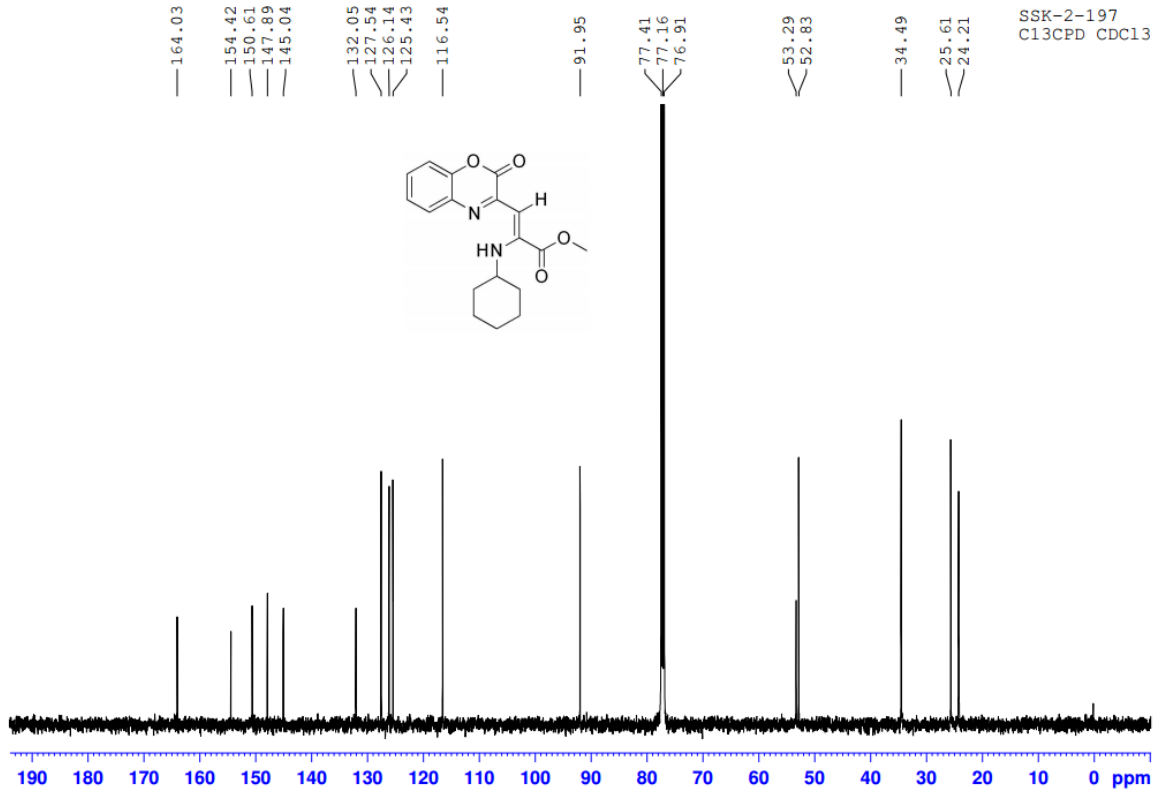
Compound **4o**


SSK-2-371
PROTON CDCl3
12.528
8.271
8.254
7.928
7.912
7.710
7.693
7.665
7.651
7.635
7.602
7.587
7.572
7.508
7.492
7.435
7.419
7.404
7.369
7.355
7.340
7.286
7.276
7.260
7.037
7.023
6.765
3.720
ppm

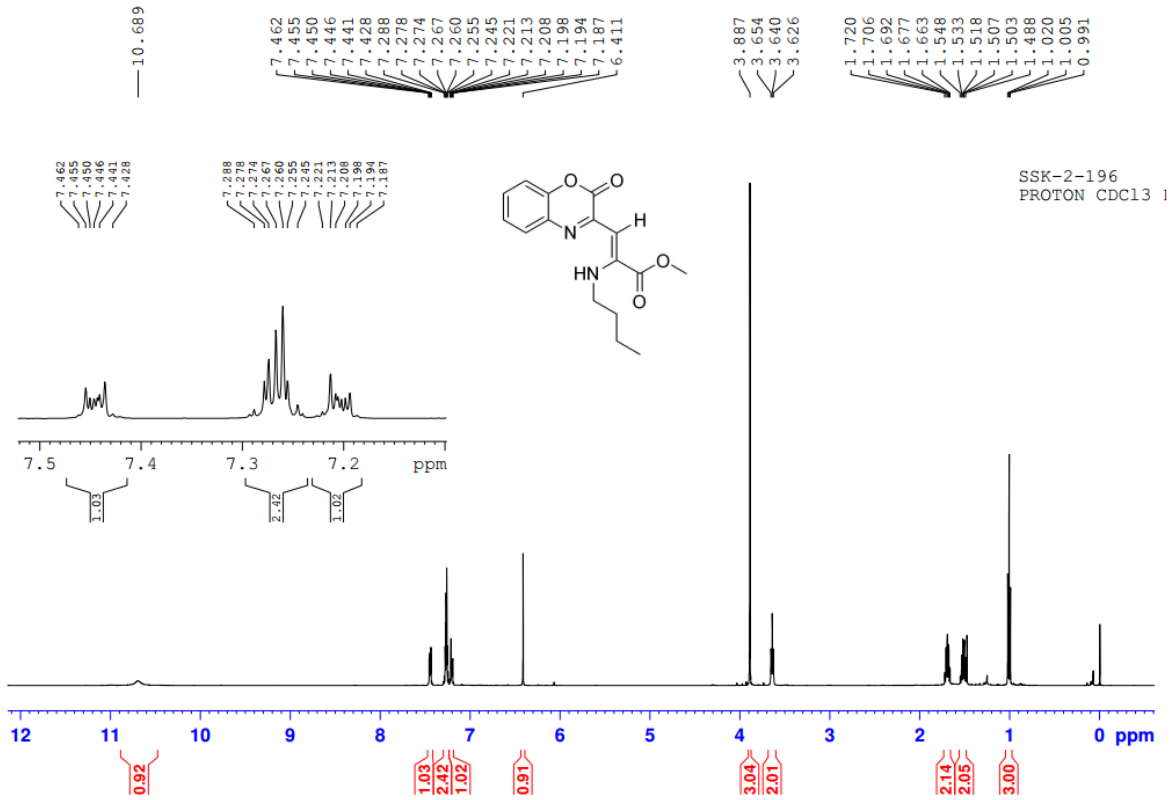

SSK-2-371
C13CPD CDCl3
164.56
153.87
150.51
146.00
145.42
136.58
134.41
131.35
128.98
128.72
127.63
126.95
126.93
126.72
125.72
125.67
125.61
121.83
118.24
116.71
97.56
77.41
77.16
76.91
52.89
ppm

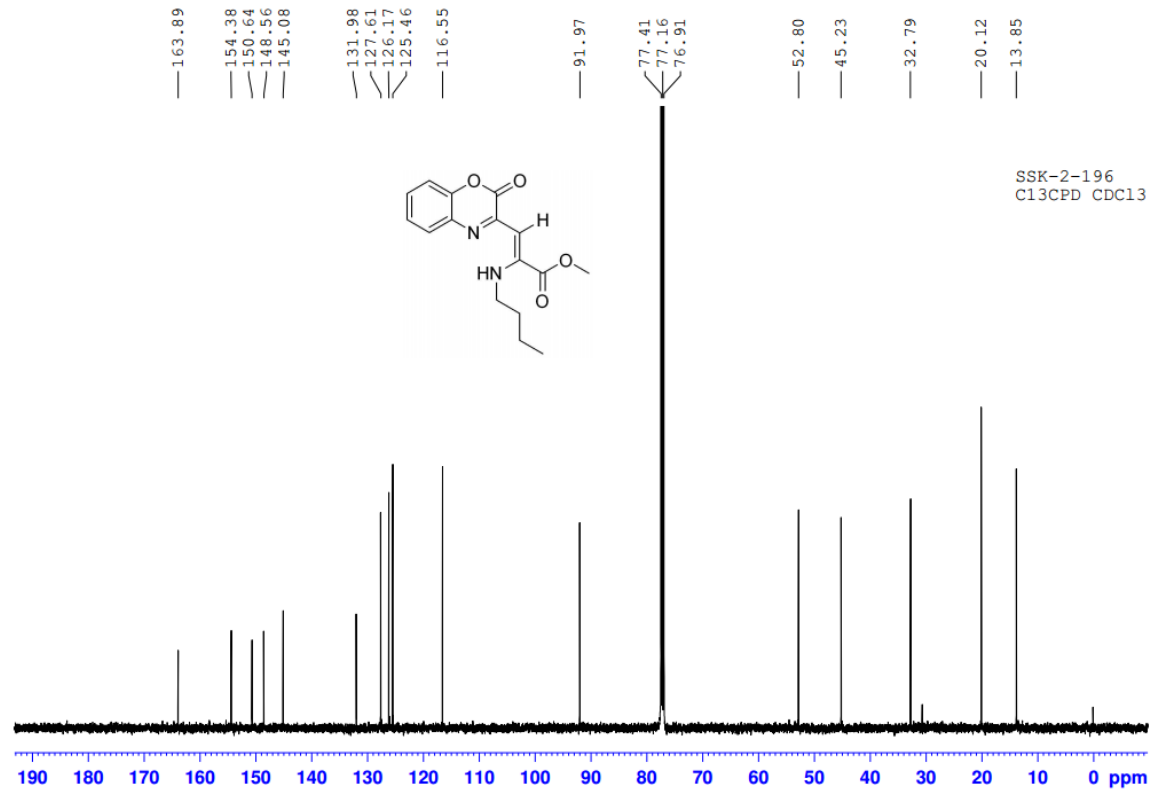
Compound **4p**


SSK-2-197
PROTON CDC13
10.827
7.483
7.477
7.468
7.463
7.458
7.450
7.285
7.275
7.273
7.264
7.260
7.256
7.254
7.244
7.220
7.213
7.207
7.203
7.198
7.194
7.187
6.372
4.007
3.887
1.990
1.970
1.799
1.791
1.780
1.773
1.761
1.620
1.607
1.595
1.590
1.464
1.449
1.428
1.411
1.392
1.371
7.5
7.4
7.3
7.2
ppm
1.00
2.37
0.98
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.91
1.00
2.37
0.98
0.91
1.02
3.03
2.06
2.10
1.33
5.22

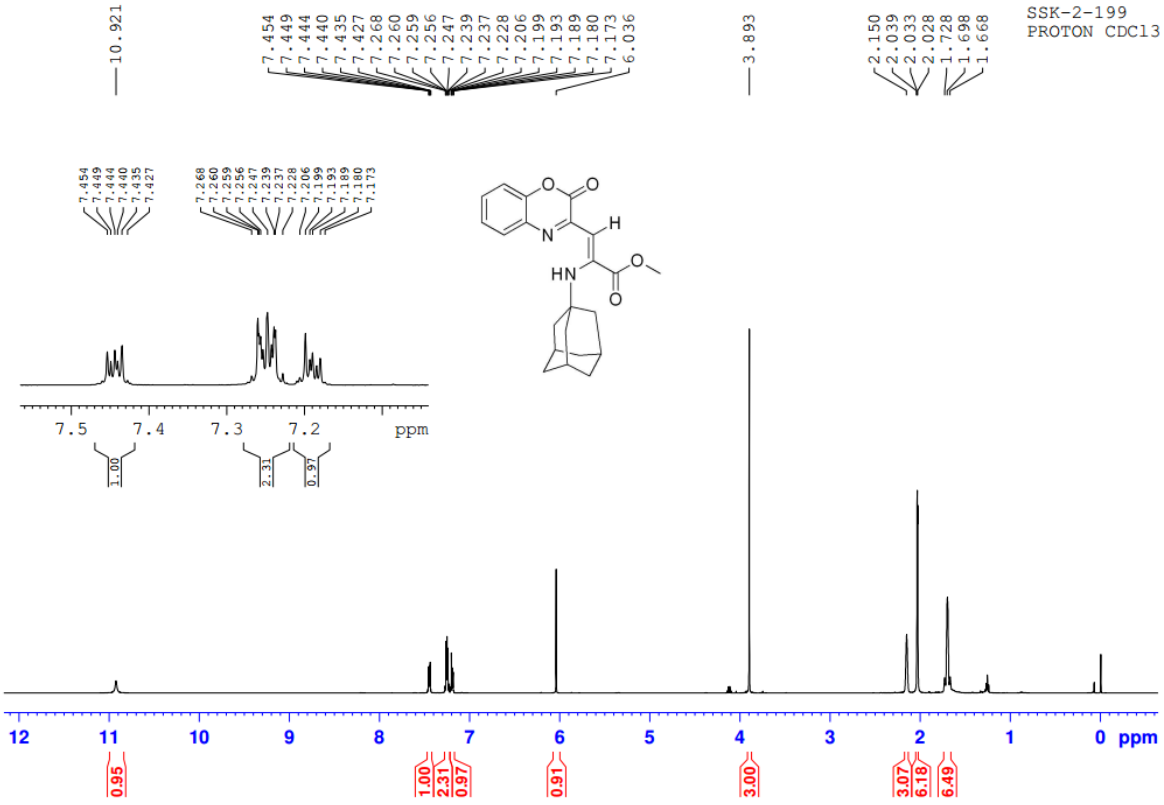

SSK-2-197
C13CPD CDC13
164.03
154.42
150.61
147.89
145.04
132.05
127.54
126.14
125.43
116.54
91.95
77.41
77.16
76.91
53.29
52.83
34.49
25.61
24.21
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

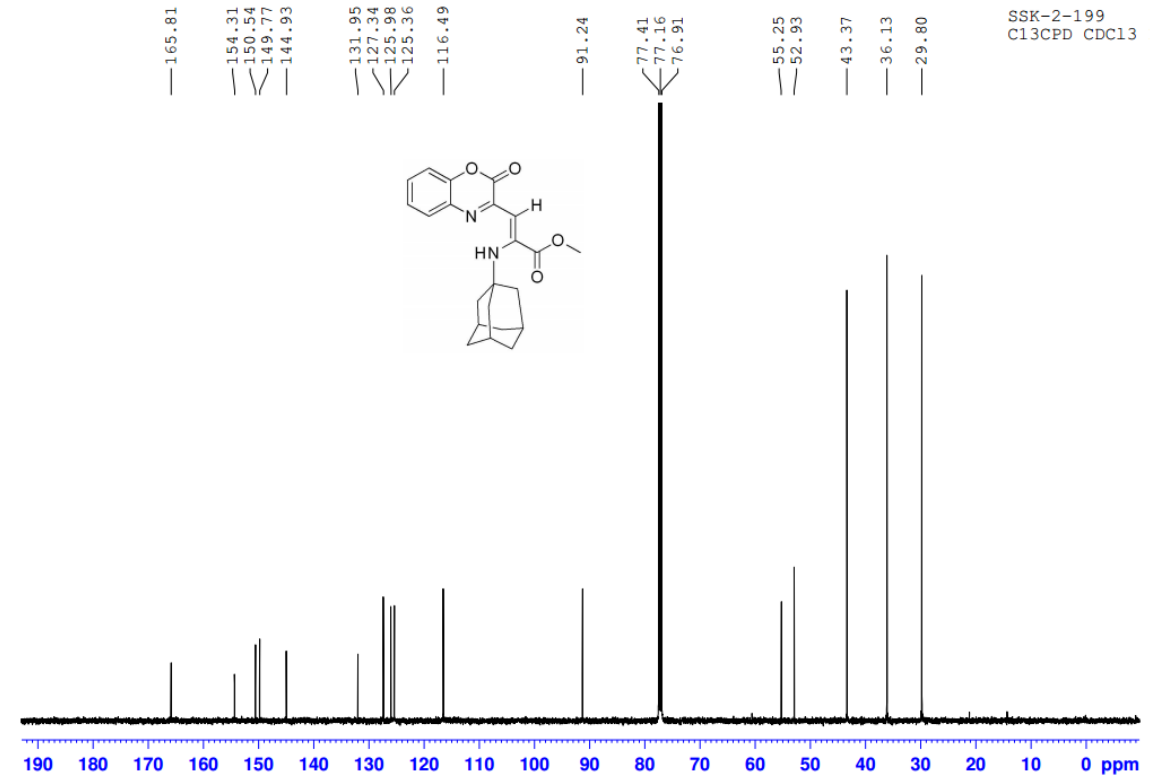
Compound **4q**


10.689
7.462
7.455
7.450
7.446
7.441
7.428
7.288
7.278
7.274
7.267
7.260
7.255
7.245
7.221
7.213
7.208
7.198
7.194
7.187
6.411
3.887
3.654
3.640
3.626
1.720
1.706
1.692
1.677
1.663
1.548
1.533
1.518
1.507
1.503
1.488
1.020
1.005
0.991
SSK-2-196
PROTON CDCl3
7.5
7.4
7.3
7.2
ppm
1.03
2.42
1.02
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.92
1.03
2.42
1.02
0.91
3.04
2.01
2.14
2.05
3.00

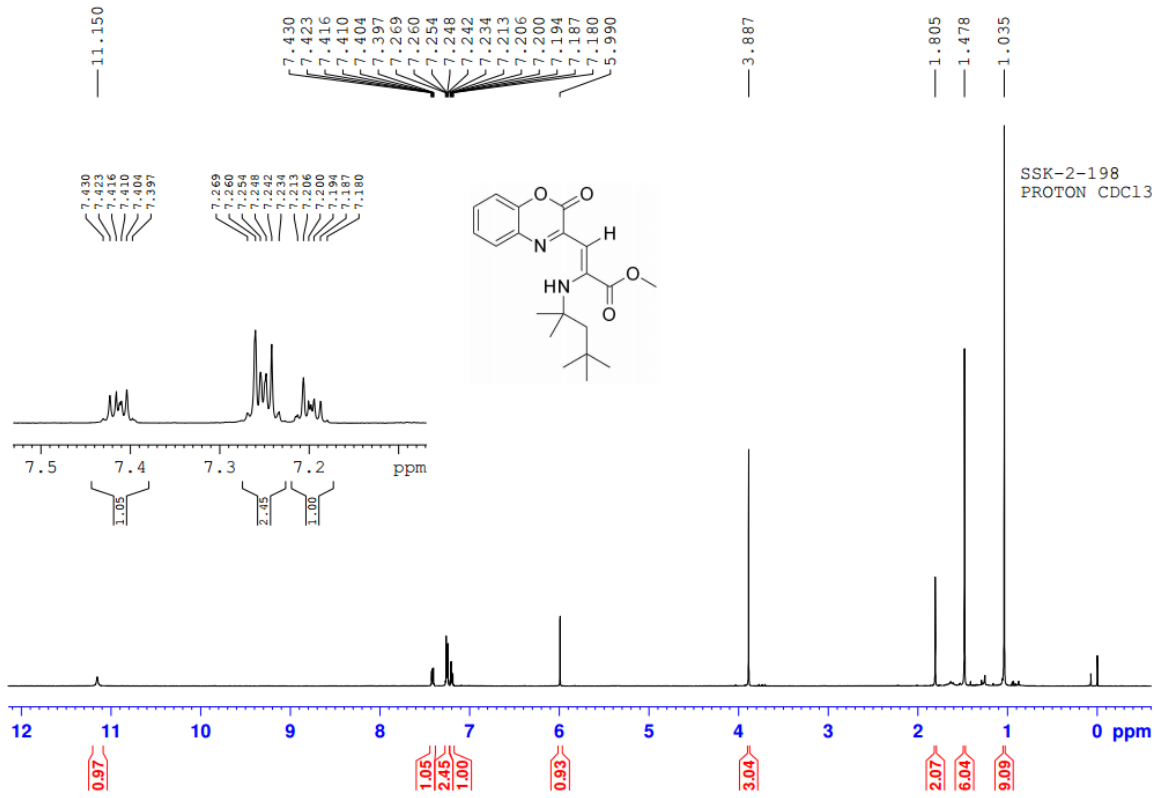

163.89
154.38
150.64
148.56
145.08
131.98
127.61
126.17
125.46
116.55
91.97
77.41
77.16
76.91
52.80
45.23
32.79
20.12
13.85
SSK-2-196
C13CPD CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

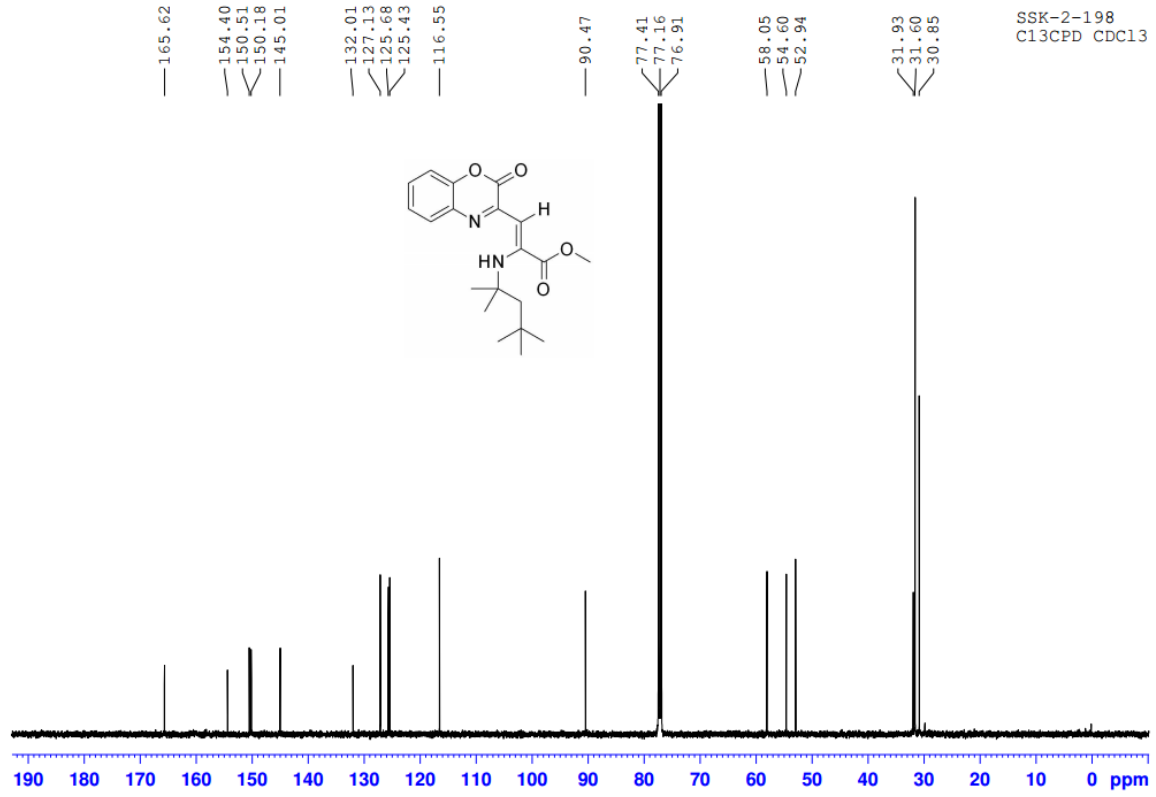
Compound **4r**


SSK-2-199
PROTON CDCl3
10.921
7.454
7.449
7.444
7.440
7.435
7.427
7.268
7.260
7.259
7.256
7.247
7.239
7.237
7.228
7.206
7.199
7.193
7.189
7.180
7.173
6.036
3.893
2.150
2.039
2.033
2.028
1.728
1.698
1.668
ppm
0.95
1.00
2.31
0.97
0.91
3.00
3.07
6.18
6.49


SSK-2-199
C13CPD CDCl3
165.81
154.31
150.54
149.77
144.93
131.95
127.34
125.98
125.36
116.49
91.24
77.41
77.16
76.91
55.25
52.93
43.37
36.13
29.80
ppm

Compound **4s**


11.150
7.430
7.423
7.416
7.410
7.404
7.397
7.269
7.260
7.254
7.248
7.242
7.234
7.213
7.206
7.200
7.194
7.187
7.180
5.990
3.887
1.805
1.478
1.035
SSK-2-198
PROTON CDCl3
7.5
7.4
7.3
7.2
ppm
1.05
2.45
1.00
0.97
0.93
3.04
2.07
6.04
9.09
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm


165.62
154.40
150.51
150.18
145.01
132.01
127.13
125.68
125.43
116.55
90.47
77.41
77.16
76.91
58.05
54.60
52.94
31.93
31.60
30.85
SSK-2-198
C13CPD CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm