Electronic Supplementary Information

Carbene Catalyzed [3+2+1] Annulation via C-N Radical Coupling of Iminyl Radicals and Ketyl radicals

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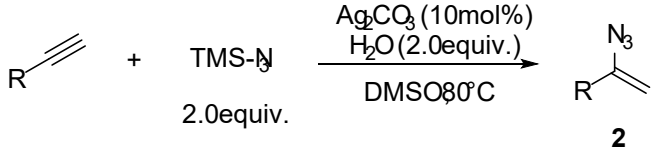
1. General information

Unless otherwise stated, all reagent-grade chemicals were obtained from commercial suppliers and were used as received without further purification. CH_2Cl_2 and acetonitrile were distilled from CaH_2 immediately prior to use. THF used in reactions was freshly distilled from sodium. The other solvents used in the experiments were all purchased anhydrous solvents and used directly. Unless otherwise noted, all reactions were carried out under an atmosphere of N_2. All reactions were carried out with oven-dried glassware. Analytical thin layer chromatography was performed on 0.20 mm silica gel plates and visualized under 254 nm UV light. Flash column chromatography was performed using silica gel (200-300 mesh).

^1H NMR, ^{13}C NMR and ^{19}F NMR spectra were measured on a 400 MHz or 600 MHz Bruker AVANCE III spectrometer, using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at ambient temperature. Chemical shifts were reported in ppm. ^1H NMR spectra were referenced to $CDCl_3$ (7.26 ppm) and ^{13}C NMR spectra were referenced to $CDCl_3$ (77.16 ppm). Peak multiplicities were designated by the following abbreviations: s, singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublets; m, multiplets and etc. Chemical shifts are given in δ relative to TMS, the coupling constants J are given in Hz. High resolution mass spectra of new compounds were recorded on LTQ Orbitrap Elite LC/MS (ESI or APCI) or MAT 95XP (Thermo, EI). Infrared (IR) spectra were recorded on PerkinElmer Frontier spectrometer and reported in wave numbers (cm^{-1}).

2. General Procedure for the preparation of substrates

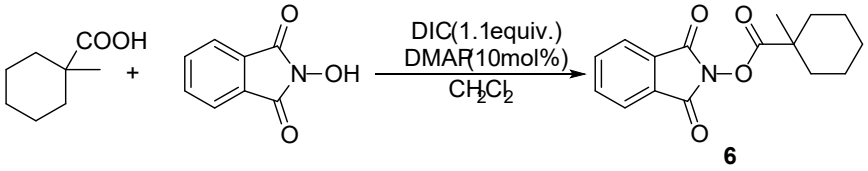
2.1 General procedure for the synthesis of Vinyl Azides 2.



2

According to the reported procedure,[1] to a solution of alkyne (5 mmol, 1.0 equiv.), TMS-N_3 (1152.1 mg, 10 mmol, 2.0 equiv.) and H_2O (180.1 mg, 10 mmol, 2.0equiv.) in anhydrous DMSO (20 mL) at 80 ℃, Ag_2CO_3 (137.9 mg, 0.5 mmol, 0.1 equiv.) was added. The mixture was then stirred for 2-3 h until alkyne was consumed as indicated by TLC. The resulting mixture was diluted with DCM (80 mL) and then washed with brine (3×50 mL), dried over Na_2SO_4 and then concentrated. The crude product was purified by flash column chromatography and concentrated in vacuo to afford vinyl azide **2**.

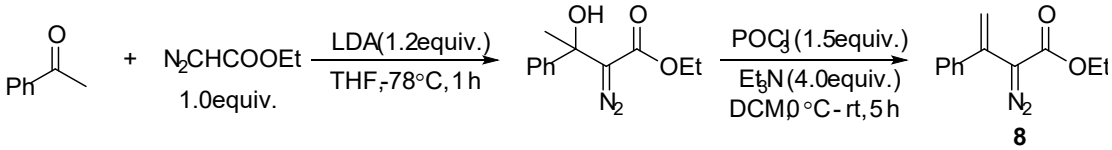
2.2 General procedure for the synthesis of redox-ester 6.



6

According to the reported procedure,[2] a round-bottom flask was charged with carboxylic acid (1.0 equiv.), N-hydroxy-phthalimide (1.0 equiv.) and DMAP (10 mol%). Dichloromethane was added (0.2 M), and the mixture was stirred vigorously. DIC (1.1 equiv.) was then added dropwise via syringe, and the mixture was allowed to stir until the acid was consumed (determined by TLC). The mixture was filtered over silica gel and rinsed with additional CH_2Cl_2/Et_2O. The solvent was removed under reduced pressure, and purification by column chromatography, afforded the redox-active ester **6**.

2.3 General procedure for the synthesis of alkenyldiazo ester 8.



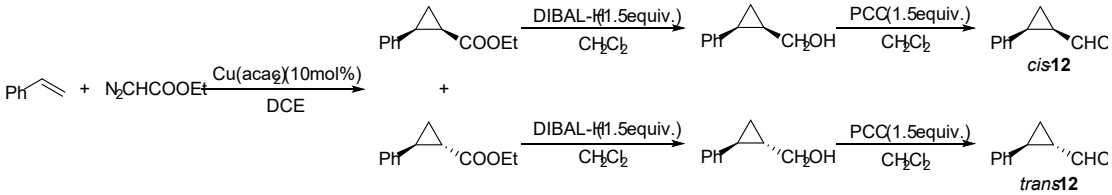
8

According to the reported procedure,[3] to a solution of ethyl diazoacetate (1.0 equiv.) in anhydrous THF at -78 °C, was added LDA (1.2 equiv.) over 30 minutes. After that acetophenone (1.0 equiv.) was added and resulting solution was stirred at -78 °C, then warmed slowly to room temperature and stirred for 1 h and quenched by addition saturated aqueous NH_4Cl. The reaction mixture was extracted with ether two times and dried over anhydrous Na_2SO_4. After the solvent was evaporated, the crude product was purified by column chromatography to give ethyl 2-diazo-3-hydroxy-3-phenylbutanoate as a yellow oil.

To a solution of ethyl 2- diazo-3-hydroxy-3-phenylbutanoate and Et_3N (4.0 equiv.) in DCM

(0.2 M) at 0 °C was slowly added $POCl_3$ (1.5 equiv.) over 30 minutes. The resulting solution was warmed to room temperature and stirred for 5 h. The solution was quenched by ice water, and washed with water two times. The organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated. The crude product was purified by flash chromatography to give alkenyldiazo ester **8** as a yellow oil.

2.4 General procedure for the synthesis of *trans*-12 and *cis*-12.



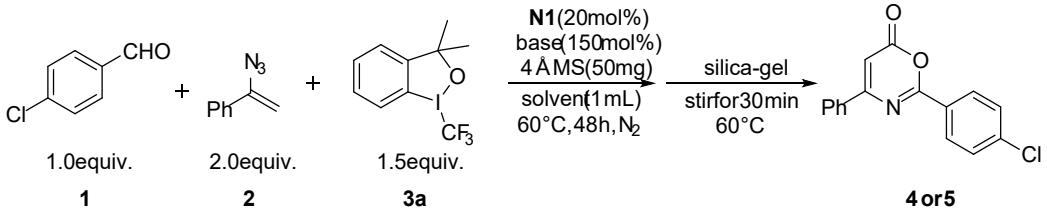
According to the reported procedure,[4] to a suspension of styrene (1.0 equiv.) and $Cu(acac)_2$ (10 mol%) in DCE at room temperature was added ethyl diazoacetate (1.5 equiv.) via syringe pump and over the course of 24 hours. Once the addition was complete, the reaction mixture was stirred for another 24 hours, and then filtered through a short pad of silica gel to afford the desired cyclopropane derivative as a mixture of diastereoisomers (*trans* isomer and *cis* isomer). The mixture was separated by flash chromatography to give desired *cis* ethyl 2-phenylcyclopropane carboxylate and *trans* ethyl 2-phenylcyclopropane carboxylate.

To a solution of ethyl 2-phenylcyclopropane carboxylate in CH_2Cl_2 at 0 °C was added DIBAL-H (1.5 equiv.) slowly, and the reaction mixture was stirred overnight at room temperature. Saturated aqueous NH_4Cl was added and the mixture was vigorously stirred at room temperature for 20 min. Solid was filtered through a pad of celite and the filtrate was evaporated under reduced pressure. The crude product was purified by flash chromatography on silica gel to give the corresponding isomer of (2-phenylcyclopropyl)methanol.

To a solution of (2-phenylcyclopropyl)methanol in CH_2Cl_2 at 0 °C was added PCC slowly, and the reaction mixture was stirred overnight at room temperature. The reaction mixture was filtered through a short pad of silica gel and the filtrate was evaporated under reduced pressure. The crude product was purified by flash chromatography on silica gel to give the corresponding isomer of 2-phenylcyclopropane-1-carbaldehyde **12**.

3. Optimization of reaction conditions

Table S1. Screening of base.

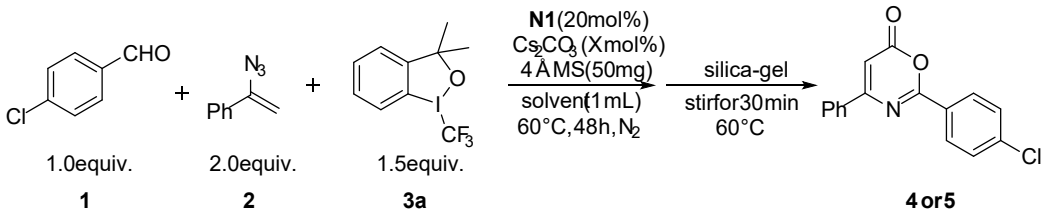


1.0equiv. **1** | 2.0equiv. **2** | 1.5equiv. **3a** | **4 or 5**

Entry	Base	Yield (%)[a]
1	K_2CO_3	53
2	K_3PO_4	14
3	CsOAc	trace
4	Cs_2CO_3	65
5	DBU	27
6	DABCO	trace
7	DIEA	43
8	KHMDS	6

[a]The yield was determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as an internal standard.

Table S2. Screening of base equivalent

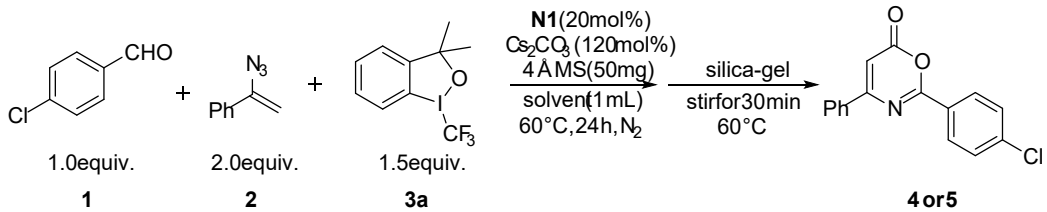


1.0equiv. **1** | 2.0equiv. **2** | 1.5equiv. **3a** | **4 or 5**

Entry	Base	Yield (%)[a]
1	80 mol%	69
2	100 mol%	69
3	120 mol%	72
4	150 mol%	65
5	200 mol%	51
6	300 mol%	42

[a]The yield was determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as an internal standard.

Table S3. Screening of solvent.



1.0equiv. 2.0equiv. 1.5equiv.

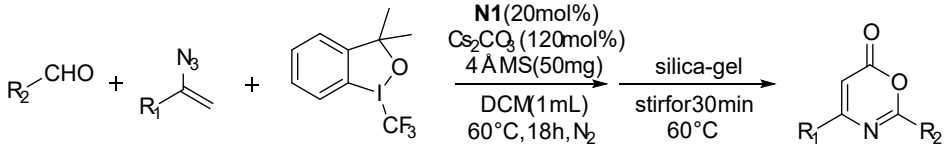
1 **2** **3a** **4 or 5**

Entry	Solvent	Yield (%)[a]
1	THF	28
2	toluene	50
3	DMF	7
4	DMA	22
5	DMSO	trace
6	CH_3CN	20
7	1,2-dichloroethane	46
8	1,4-dioxane	43
9	$PhCF_3$	57
10	$CH_3OC(CH_3)_3$	36

[a]The yield was determined by ^1H NMR using 1,3,5-trimethoxybenzene as an internal standard.

4. General Procedure for the synthesis of products

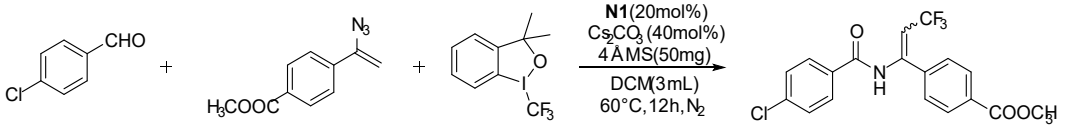
4.1 General procedure for the synthesis of products 4 and 5 using 3a.



1 **2** **3a** **4 or 5**

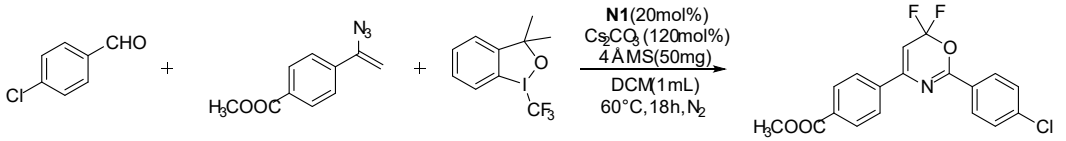
Aldehydes **1** (0.15 mmol), vinyl azides **2** (0.10 mmol), thiazolium salt **N1** (8.3 mg, 0.02 mmol), Togni reagent **3a** (49.5 mg, 0.15 mmol), 4 Å MS (50 mg) and Cs_2CO_3 (39.1 mg, 0.12 mmol) were placed in a 15 mL Schlenk-type pressure tube containing a magnetic stirring bar. The top and the branch of the tube was sealed with Teflon® septum, and then evacuated and filled with N_2 atmosphere through the branch. Finally, DCM (1 mL) was added using a syringe through the branch (*The liquid aldehydes or vinyl azides were dissolved in DCM and then added via a syringe*). After 18 h stirring at 60 °C, silica-gel was added to the reaction mixture after cooling to room temperature, then the mixture was stirred at 60 °C for 30 min after sealing with a Teflon® septum. After cooling down, the mixture was transferred to another round-bottom flask and concentrated under reduced pressure, then purified by flash column chromatography (PE/EA) to afford the products **4** or **5**. For most substrates, the by-product 2-(2-iodophenyl)propan-2-ol could not be removed completely by flash column chromatography, further purification by washing the mixture with cold petroleum ether (-20 °C) gave the pure product.

4.2 General procedure for the synthesis of 4ga and 4gb.



1a 1.5equiv. **2g** 1.0equiv. 0.3mmol **3a** 1.5equiv. **4ga**(31%)

4-chlorobenzaldehyde **1a** (63.2 mg, 0.45 mmol, 1.5 equiv.), vinyl azides **2g** (61.0 mg, 0.30 mmol, 1.0 equiv.), thiazolium salt **N1** (24.8 mg, 0.06 mmol, 20 mol%), Togni reagent **3a** (148.5 mg, 0.45 mmol, 1.5 equiv.), 4 Å MS (50 mg) and Cs_2CO_3 (39.1 mg, 0.12 mmol, 40 mol%) were placed in a Schlenk-type pressure tube containing a magnetic stirring bar. The top and the branch of the tube was sealed with Teflon® septum, and then evacuated and filled with N_2 atmosphere through the branch. DCM (3 mL) was added using a syringe through the branch and then sealed. After **12 h** stirring at 60 °C, the reaction mixture was cooled down, and then filtered. The filtrate was concentrated under reduced pressure and the mixture was added cold *n*-hexane (2 mL), filtered and washed with cold *n*-hexane (1 mLx3). The collected white solid was dried under reduced pressure to afford the product **4ga** in 31% yield (30.8 mg).

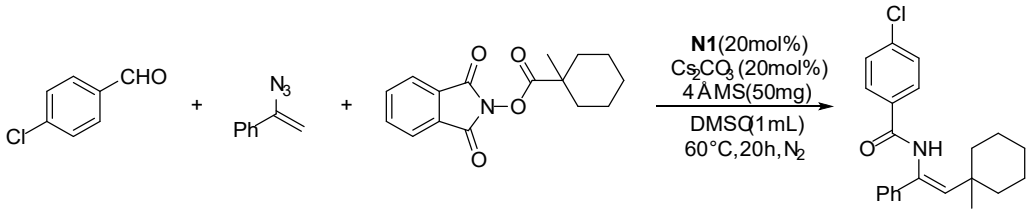


1a 1.5equiv. **2g** 1.0equiv. **3a** 1.5equiv. **4gb**(70%)

4-chlorobenzaldehyde **1a** (21.1 mg, 0.15 mmol, 1.5 equiv.), vinyl azides **2g** (20.3 mg, 0.1

mmol, 1.0 equiv.), thiazolium salt **N1** (8.3 mg, 0.02 mmol, 20 mol%), Togni reagent **3a** (49.5 mg, 0.15 mmol), 4 Å MS (50 mg) and Cs_2CO_3 (39.1 mg, 0.12 mmol) were placed in a Schlenk-type pressure tube containing a magnetic stirring bar. The top and the branch of the tube was sealed with Teflon® septum，and then evacuated and filled with N_2 atmosphere through the branch. DCM (1 mL) was added using a syringe through the branch and then sealed. After 18 h stirring at 60 °C, the reaction mixture was cooled down and then concentrated under reduced pressure. The mixture was purified by silica gel column chromatography using deactivated silica gel (by Et_3N), and 1% Et_3N in petroleum ether and ethyl acetate as eluent to afford the product **4gb** in 70% yield (25.5 mg).

4.3 General procedure for the synthesis of product 7 using the redox-ester 6.



1a **2a** **6** **7**

4-Chlorobenzaldehyde **1a** (21.1 mg, 0.15 mmol), thiazolium salt **N1** (8.3 mg, 0.02 mmol), redox-ester **6** (43.1 mg, 0.15 mmol), 4 Å MS (50 mg) and Cs_2CO_3 (6.5 mg, 0.02 mol) were placed in a Schlenk tube containing a magnetic stirring bar. The tube was sealed with a rubber septum, and then evacuated and filled with N_2 atmosphere. Vinyl azides **2a** (14.5 mg, 0.10 mmol) in DMSO (1 mL) was added via a syringe. After 20 h stirring at 60 °C, EtOAc (4 mL) was added, then the reaction mixture was washed by H_2O (4 mLx3) and dried over anhydrous Na_2SO_4. After that, the organic phase was concentrated under reduced pressure and purified by flash column chromatography (PE/EA) to afford the product **7** in 30% yield (10.6 mg).

Some unsuccessful examples with NHPI esters as radical precursors were shown in Figure S1.

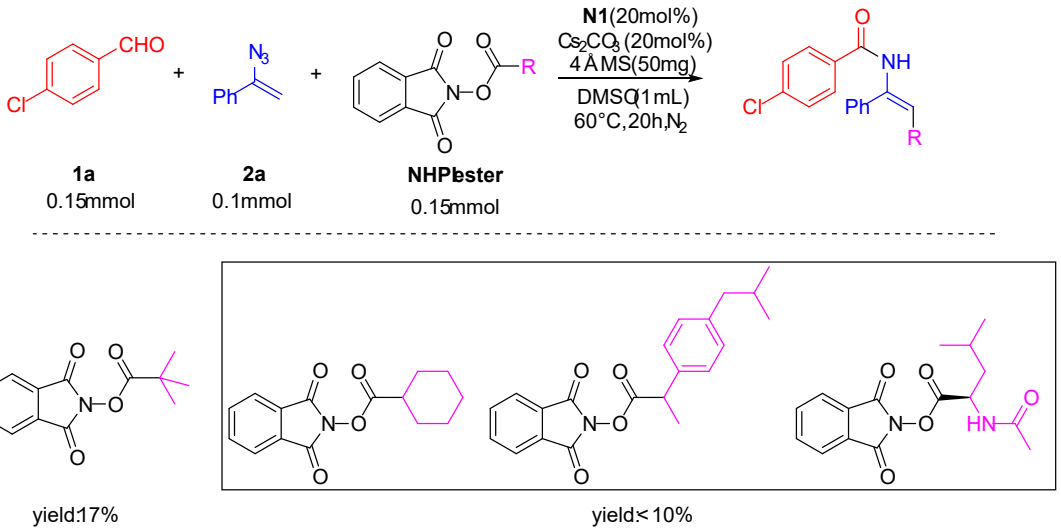
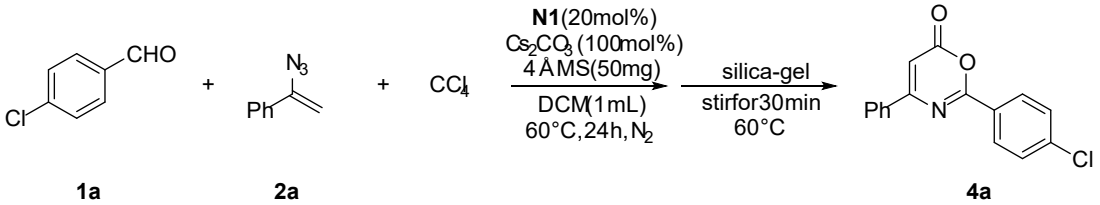


Figure S1 Examples with NHPI esters as radical precursors.

4.4 General procedure for the synthesis of product 4a using CCl_4.



1a **2a** **4a**

4-chlorobenzaldehyde **1a** (14.1 mg, 0.1 mmol), thiazolium salt **N1** (8.3 mg, 0.02 mmol), 4 Å MS (50 mg) and Cs_2CO_3 (32.6 mg, 0.1 mmol) were placed in a 15mL Schlenk-type pressure tube containing a magnetic stirring bar. The top and the branch of the tube was sealed with Teflon® septum, and then evacuated and filled with N_2 atmosphere through the branch. CCl_4 (0.2 mmol) and vinyl azides **2a** (21.8 mg, 0.15 mmol) in DCM (1 mL) was added using a syringe through the branch and then sealed. After 24 h stirring at 60 °C, silica-gel was added to the reaction mixture after cooling to room temperature, then the mixture was stirred at 60 °C for 30 min after sealing with a Teflon® septum. After cooling down, the mixture was transferred to another round-bottom flask and concentrated under reduced pressure, and then purified by flash column chromatography (PE/EA) to afford the product **4a** in 51% yield (14.5 mg).

Reactions with $BrCCl_3$ or other vinyl azides all gave low to moderate yields, the results were shown in Figure S2.

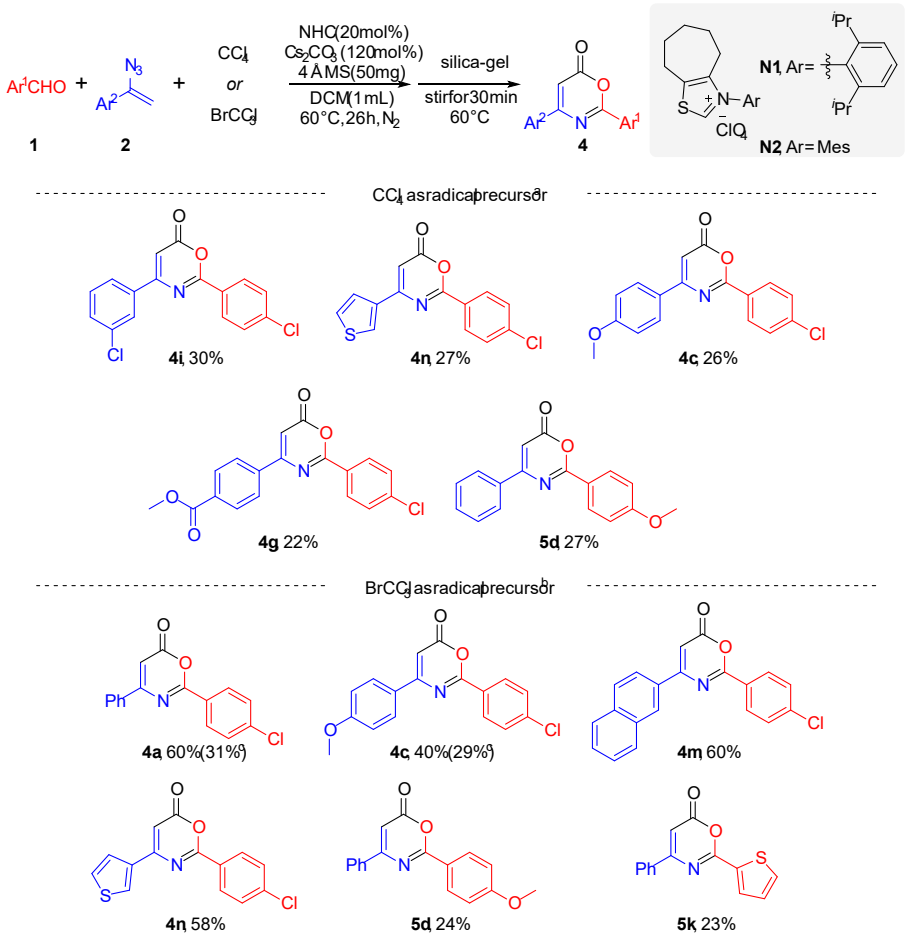
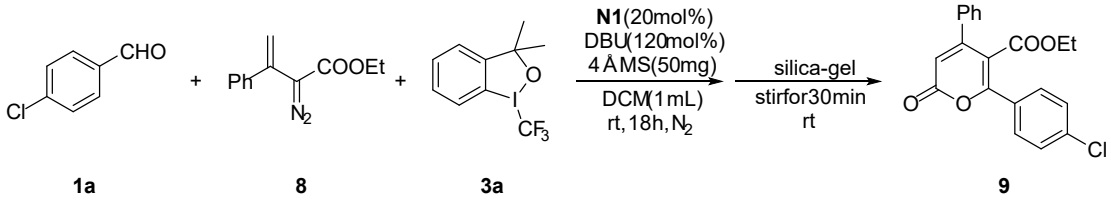


Figure S2 synthesis of product **4** or **5** using CCl_4 or $BrCCl_3$. [a]Reaction was carried out with **1** (0.1 mmol), **2** (0.15 mmol), CCl_4 (0.2 mmol), **N1** (20 mol%), Cs_2CO_3 (120 mol%), 4 Å MS (50 mg) in

anhydrous DCM (1 mL) at 60 °C for 48 h. [b] Reaction was carried out with **1** (0.15 mmol), **2** (0.1 mmol), $BrCCl_3$ (0.2 mmol), **N2** (20 mol%), Cs_2CO_3 (120 mol%), 4 Å MS (50 mg) in anhydrous DCM (1 mL) at 60 °C for 26 h. [c]**N1** (20 mol%) was used as pre-catalyst.

4.5 General procedure for the synthesis of product 9 using the alkenyldiazo ester 8.



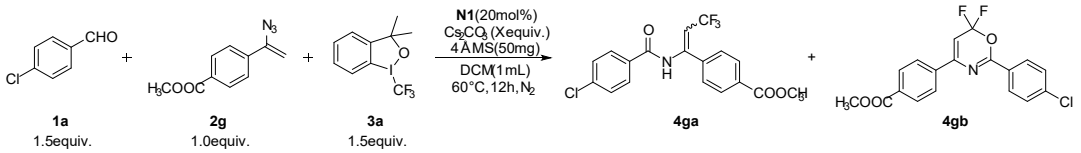
1a **8** **3a** **9**

4-chlorobenzaldehyde **1a** (14.1 mg, 0.1 mmol), thiazolium salt **N1** (8.3 mg, 0.02 mmol), Togni reagent **3a** (49.5 mg, 0.15 mmol) and 4 Å MS (50 mg) were placed in a Schlenk tube containing a magnetic stirring bar. The tube was sealed with a rubber septum, and then evacuated and filled with N_2 atmosphere. Alkenyldiazo ester **8** (43.2 mg, 0.2 mmol) in 0.5 mL DCM was added, followed by the addition of DBU (18.2 mg, 0.12 mmol) in DCM (0.5 mL) via a syringe. After 18 h stirring at room temperature, silica-gel was added to the reaction mixture, then the mixture was stirred at room temperature for 30 min. After that, the mixture was concentrated under reduced pressure and purified by flash column chromatography (PE/EA) to afford the product **9** in 9% yield (3.3 mg).

*Note: No product **9** was detected when the reaction was heat at 60 °C for 18 hours. The reaction was messy and no 8 was detected after the reaction finished.*

5. Mechanistic Experiments

5.1 The effect of base equivalent.



1a 1.5equiv. **2g** 1.0equiv. **3a** 1.5equiv. **4ga** **4gb**

4-chlorobenzaldehyde **1a** (21.1 mg, 0.15 mmol, 1.5 equiv.), vinyl azides **2g** (20.3 mg, 0.1 mmol, 1.0 equiv.), thiazolium salt **N1** (8.3 mg, 0.02 mmol, 20 mol%), Togni reagent **3a** (49.5 mg, 0.15 mmol), 4 Å MS (50 mg) and Cs_2CO_3 (X equiv.) were placed in a Schlenk-type pressure tube containing a magnetic stirring bar. The top and the branch of the tube was sealed with Teflon® septum, and then evacuated and filled with N_2 atmosphere through the branch. DCM (1 mL) was added using a syringe through the branch and then sealed. After 12 h stirring at 60 °C, the reaction mixture was concentrated under reduced pressure, then DMSO-d_6 was added. The crude mixture was tested by ^{19}F NMR.

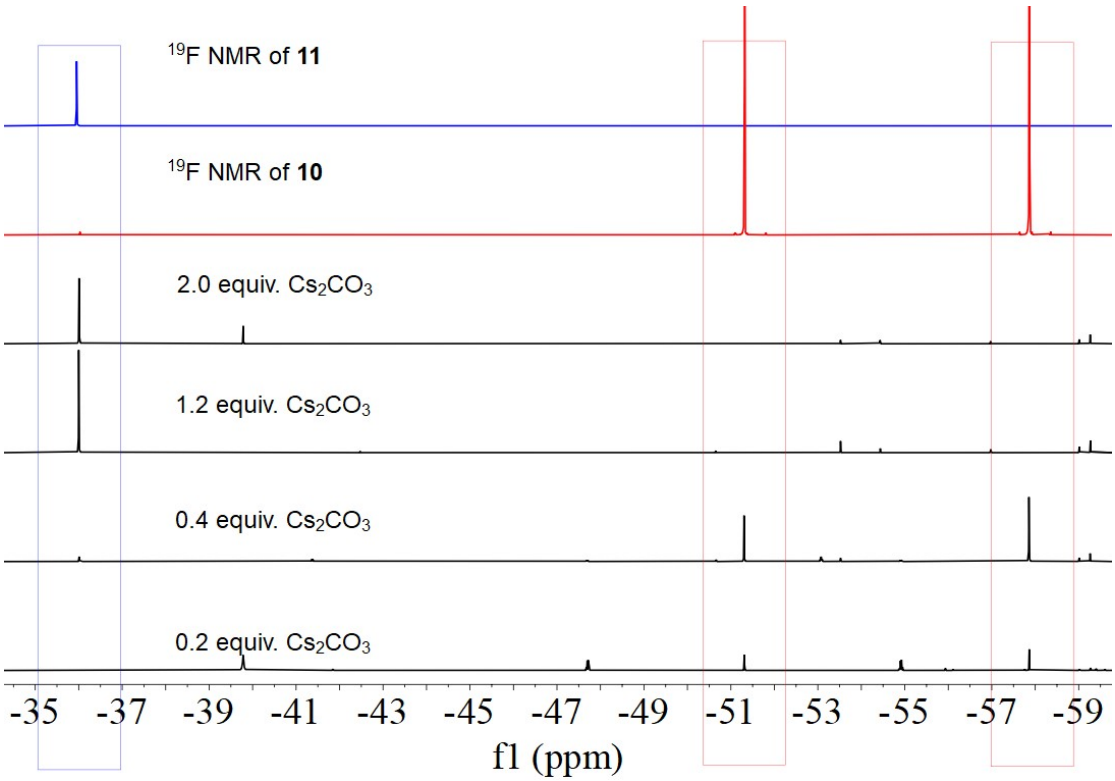
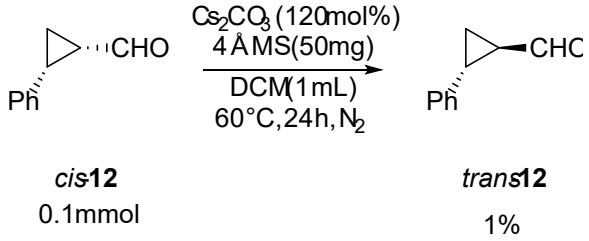


Figure S3 Combined ^{19}F NMR of **4ga**, **4gb** and the reaction mixture with different base amount.

5.2 Radical clock experiments.



4 Å MS (50 mg) and Cs_2CO_3 (39.1 mg, 0.12 mmol) were placed in a Schlenk-type pressure tube containing a magnetic stirring bar. The top and the branch of the tube was sealed with Teflon® septum, and then evacuated and filled with N_2 atmosphere through the branch. Aldehydes ***cis*-12** (14.6 mg, 0.1 mmol, 1.0 equiv.) in DCM (1 mL) was added via a syringe through the branch and then sealed. Stirred at 60 °C for 24 h. Filtered after cooling down. The filtrate was concentrated under reduced pressure. $CDCl_3$ was added and ^1H NMR was tested. Conversion of ***trans*-12** from ***cis*-12** was detected to be about 1%.

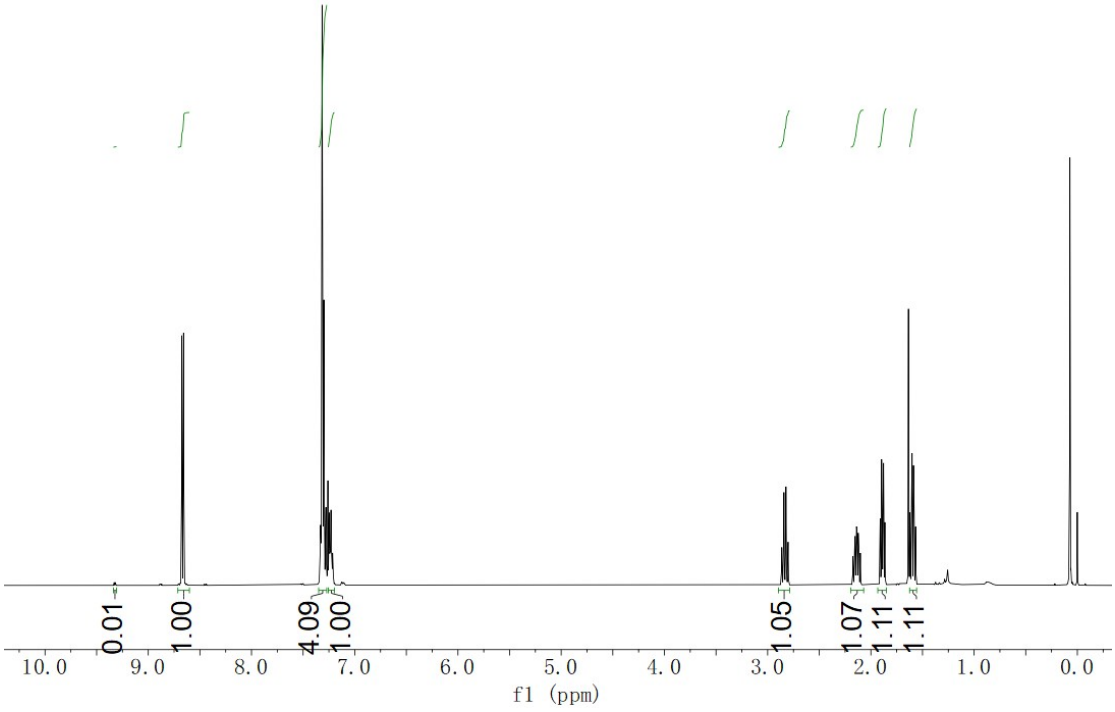
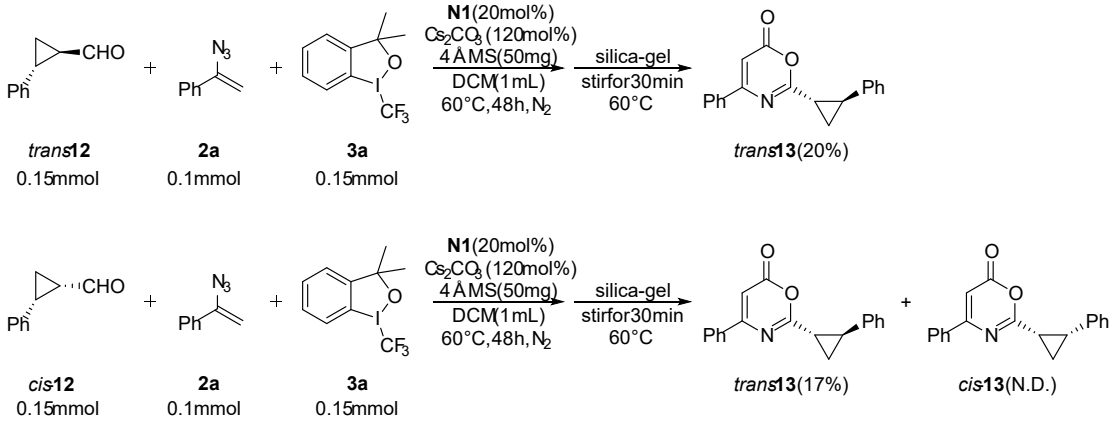
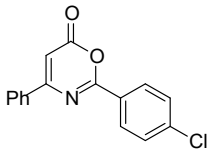


Figure S4 Crude ^1H NMR of *cis*-**12** after treated with Cs_2CO_3.



Thiazolium salt **N1** (8.3 mg, 0.02 mmol, 20 mol%), Togni reagent **3a** (49.5 mg, 0.15 mmol), 4 Å MS (50 mg) and Cs_2CO_3 (39.1 mg, 0.12 mmol) were placed in a Schlenk-type pressure tube containing a magnetic stirring bar. The top and the branch of the tube was sealed with Teflon® septum, and then evacuated and filled with N_2 atmosphere through the branch. Aldehydes **12** (21.9 mg, 0.15 mmol, 1.5 equiv.) and vinyl azides **2a** (14.5 mg, 0.10 mmol, 1.0 equiv.) in DCM (1 mL) was added via a syringe through the branch and then sealed. After 48 h stirring at 60 °C, silica-gel was added to the reaction mixture after cooling to room temperature, then the mixture was stirred at 60 °C for 30 min after sealing with a Teflon® septum. After cooling down, the mixture was transferred to another round-bottom flask and concentrated under reduced pressure, then purified by flash column chromatography (PE/EA) to afford the crude products contained 2-(2-iodophenyl)propan-2-ol. The mixture was added petroleum ether (1 mL) and kept in -20°C for over an hour. Then the mixture was filtered and the solid was collected, dried under reduced pressure to afford exclusively the product ***trans*-13. *Trans*-12** gave the ***trans*-13** in 20% yield (5.9 mg); ***Cis*-12** gave the ***trans*-13** in 17% yield (5.0 mg).

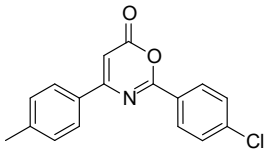
6. Characterization Data



4a

2-(4-chlorophenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (4a)[5]

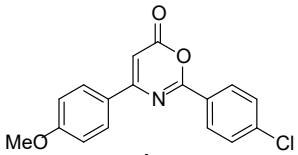
Compound **4a** was obtained as a white solid in 65% yield (18.4 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 – 8.23 (m, 2H), 8.08 – 8.02 (m, 2H), 7.58 – 7.45 (m, 5H), 6.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 161.9, 159.7, 140.1, 134.4, 132.2, 130.1, 129.4, 129.1, 128.6, 127.5, 102.0.



4b

2-(4-chlorophenyl)-4-(*p*-tolyl)-6*H*-1,3-oxazin-6-one (4b)

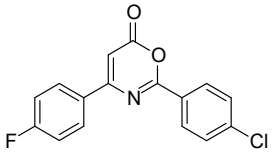
Compound **4b** was obtained as a white solid in 46% yield (13.6 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.21 (m, 2H), 7.97 – 7.91 (m, 2H), 7.50 – 7.43 (m, 2H), 7.29 (d, J = 8.0 Hz, 2H), 6.51 (s, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 161.7, 159.7, 142.9, 139.9, 131.5, 130.0, 129.8, 129.3, 128.6, 127.4, 101.0, 21.7; HRMS (ESI) for $C_{17}H_{13}ClNO_2^+$ ($[M+H]^+$): calcd 298.0629, found 298.0626; IR (film) ν_{max}: 3062, 2920, 1751, 1606, 1556, 1488, 1367, 1092, 815, 750.



4c

2-(4-chlorophenyl)-4-(4-methoxyphenyl)-6*H*-1,3-oxazin-6-one (4c)

Compound **4c** was obtained as a white solid in 48% yield (14.9 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 – 8.24 (m, 2H), 8.08 – 8.01 (m, 2H), 7.52 – 7.46 (m, 2H), 7.04 – 6.98 (m, 2H), 6.47 (s, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0, 162.1, 161.4, 159.9, 139.9, 130.1, 129.4, 129.3, 128.8, 126.7, 114.5, 99.7, 55.6; HRMS (ESI) for $C_{17}H_{13}ClNO_3^+$ ($[M+H]^+$): calcd 314.0579, found 314.0571; IR (film) ν_{max}: 3083, 2836, 1748, 1603, 1578, 1363, 1260, 1183, 1032, 838, 827, 755.

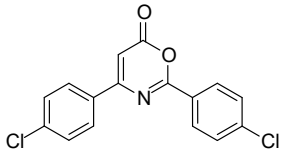


4d

2-(4-chlorophenyl)-4-(4-fluorophenyl)-6*H*-1,3-oxazin-6-one (4d)

Compound **4d** was obtained as a white solid in 50% yield (15.0 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (dd, J = 8.6, 1.6 Hz, 2H), 8.13 – 8.06 (m, 2H), 7.51 (dd, J = 8.6, 1.6 Hz, 2H), 7.24 – 7.18 (m,

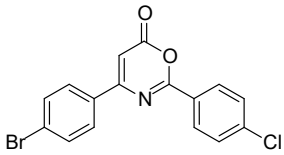
2H), 6.54 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.3 (J = 252 Hz), 162.6, 160.9, 159.5, 140.2, 130.6 (J = 4.5 Hz), 130.2, 129.8 (J = 9.0 Hz), 129.4, 128.5, 116.3 (J = 21 Hz), 101.5; ^{19}F NMR (377 MHz, $CDCl_3$) δ -107.0; HRMS (ESI) for $C_{16}H_{10}ClFNO_2^+$ ([M+H]$^+$): calcd 302.0379, found 302.0376; IR (film) ν_{max}: 2848, 1749, 1595, 1504, 1304, 1180, 1106, 834, 755.



4e

2,4-bis(4-chlorophenyl)-6*H*-1,3-oxazin-6-one (4e)

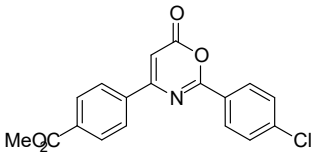
Compound **4e** was obtained as a white solid in 75% yield (24.0 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 – 8.25 (m, 2H), 8.04 – 8.00 (m, 2H), 7.53 – 7.47 (m, 4H), 6.57 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.7, 160.8, 159.4, 140.3, 138.5, 132.9, 130.2, 129.5, 129.4, 128.8, 128.5, 102.0; HRMS (ESI) for $C_{16}H_{10}Cl_2NO_2^+$ ([M+H]$^+$): calcd 318.0083, found 302.0096; IR (film) ν_{max}: 2920, 2850, 1751, 1661, 1552, 1488, 1410, 1092, 1011, 825, 753.



4f

4-(4-bromophenyl)-2-(4-chlorophenyl)-6*H*-1,3-oxazin-6-one (4f)

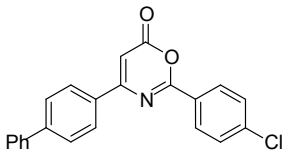
Compound **4f** was obtained as a white solid in 85% yield (30.7 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 – 8.24 (m, 2H), 7.97 – 7.91 (m, 2H), 7.69 – 7.63 (m, 2H), 7.54 – 7.48 (m, 2H), 6.58 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.7, 160.9, 159.4, 140.3, 133.3, 132.4, 130.2, 129.4, 129.0, 128.5, 127.1, 102.0; HRMS (ESI) for $C_{16}H_{10}ClBrNO_2^+$ ([M+H]$^+$): calcd 361.9578, found 361.9571; IR (film) ν_{max}: 3071, 2920, 2850, 1751, 1611, 1592, 1485, 1404, 1077, 1011, 825, 752.



4g

Methyl 4-(2-(4-chlorophenyl)-6-oxo-6*H*-1,3-oxazin-4-yl)benzoate (4g)

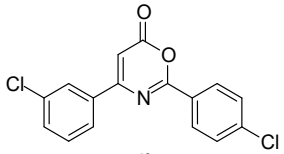
Compound **4g** was obtained as a white solid in 69% yield (23.4 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (d, J = 8.3 Hz, 2H), 8.21 – 8.10 (m, 4H), 7.52 (d, J = 8.3 Hz, 2H), 6.66 (s, 1H), 3.97 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.4, 162.8, 160.8, 159.3, 140.4, 138.4, 133.2, 130.3, 130.2, 129.5, 128.4, 127.5, 103.4, 52.6; HRMS (ESI) for $C_{18}H_{13}ClNO_4^+$ ([M+H]$^+$): calcd 342.0528, found 342.0522; IR (film) ν_{max}: 2920, 2849, 1758, 1727, 1609, 1487, 1423, 1402, 1275, 1119, 858, 752.



4h

4-([1,1'-biphenyl]-4-yl)-2-(4-chlorophenyl)-6*H*-1,3-oxazin-6-one (4h)

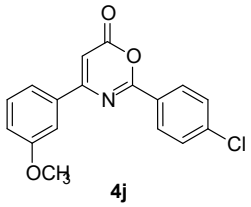
Compound **4h** was obtained as a white solid in 65% yield (23.5 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.3 Hz, 2H), 8.13 (d, *J* = 8.1 Hz, 2H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.67 – 7.63 (m, 2H), 7.52 – 7.46 (m, 4H), 7.44 – 7.40 (m, 1H), 6.60 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.4, 161.4, 159.6, 144.9, 140.0, 139.9, 133.1, 130.1, 129.3, 129.1, 128.6, 128.3, 128.0, 127.7, 127.3, 101.6; HRMS (ESI) for $C_{22}H_{14}ClNO_2Na^+$ ([M+Na]$^+$): calcd 382.0605, found 382.0614; IR (film) ν_{max}: 2770, 1751, 1603, 1561, 1488, 1097, 1007, 838, 750, 694.



4i

4-(3-chlorophenyl)-2-(4-chlorophenyl)-6*H*-1,3-oxazin-6-one (4i)

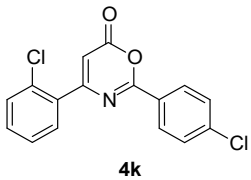
Compound **4i** was obtained as a white solid in 79% yield (25.1 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.23 (m, 2H), 8.06 (t, *J* = 1.9 Hz, 1H), 7.90 (dt, *J* = 7.8, 1.5 Hz, 1H), 7.55 – 7.41 (m, 4H), 6.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8, 160.5, 159.2, 140.3, 136.2, 135.4, 132.0, 130.4, 130.2, 129.4, 128.4, 127.6, 125.4, 102.7; HRMS (ESI) for $C_{16}H_{10}Cl_2NO_2^+$ ([M+H]$^+$): calcd 318.0083, found 318.0090; IR (film) ν_{max}: 2780, 1757, 1611, 1555, 1488, 1092, 1011, 841, 753.



4j

2-(4-chlorophenyl)-4-(3-methoxyphenyl)-6*H*-1,3-oxazin-6-one (4j)

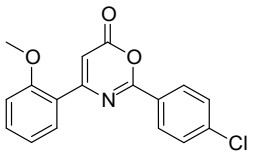
Compound **4j** was obtained as a white solid in 42% yield (13.2 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.22 (m, 2H), 7.64 – 7.58 (m, 2H), 7.51 – 7.45 (m, 2H), 7.45 – 7.38 (m, 1H), 7.10 – 7.05 (m, 1H), 6.56 (s, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 161.6, 160.1, 159.6, 140.0, 135.8, 130.1, 130.1, 129.3, 128.6, 119.8, 117.5, 113.1, 102.2, 55.6; HRMS (ESI) for $C_{17}H_{13}ClNO_3^+$ ([M+H]$^+$): calcd 314.0579, found 314.0575; IR (film) ν_{max}: 2778, 1742, 1613, 1554, 1488, 1433, 1271, 1092. 861, 843, 779, 754.



4k

4-(2-chlorophenyl)-2-(4-chlorophenyl)-6*H*-1,3-oxazin-6-one (4k)

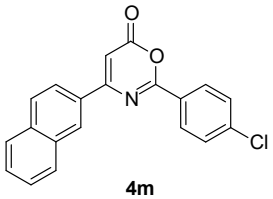
Compound **4k** was obtained as a white solid in 48% yield (15.3 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 2H), 7.78 – 7.73 (m, 1H), 7.53 – 7.46 (m, 3H), 7.45 – 7.39 (m, 2H), 6.65 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.5, 161.5, 158.9, 140.2, 134.6, 132.8, 131.7, 131.1, 131.0, 130.1, 129.4, 128.4, 127.2, 108.5; HRMS (ESI) for $C_{16}H_{10}Cl_2NO_2^+$ ([M+H]$^+$): calcd 318.0083, found 318.0084; IR (film) ν_{max}: 2784, 1767, 1605, 1550, 1488, 1279, 1092, 839, 750, 724.



4l

2-(4-chlorophenyl)-4-(2-methoxyphenyl)-6*H*-1,3-oxazin-6-one (4l)

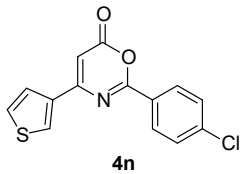
Compound **4l** was obtained as a white solid in 41% yield (12.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, *J* = 7.9, 1.7 Hz, 1H), 8.26 – 8.21 (m, 2H), 7.51 – 7.44 (m, 3H), 7.16 – 7.08 (m, 2H), 7.02 (d, *J* = 8.4 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 160.3, 159.4, 158.6, 139.6, 133.0, 131.3, 129.9, 129.2, 129.0, 123.2, 120.9, 111.7, 107.1, 55.7; HRMS (ESI) for $C_{17}H_{13}ClNO_3^+$ ([M+H]$^+$): calcd 314.0579, found 314.0573; IR (film) ν_{max}: 2837, 1748, 1611, 1558, 1486, 1246, 1160, 1093, 1015, 856, 842, 748.



4m

2-(4-chlorophenyl)-4-(naphthalen-2-yl)-6*H*-1,3-oxazin-6-one (4m)

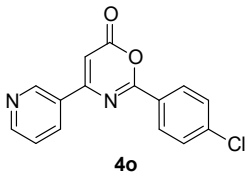
Compound **4m** was obtained as a white solid in 34% yield (11.4 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (s, 1H), 8.36 – 8.29 (m, 2H), 8.04 – 7.87 (m, 4H), 7.63 – 7.50 (m, 4H), 6.71 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 161.7, 159.7, 140.1, 135.2, 133.1, 131.6, 130.2, 129.5, 129.4, 129.0, 128.8, 128.7, 128.3, 128.0, 127.1, 123.3, 102.1; HRMS (ESI) for $C_{20}H_{13}ClNO_2^+$ ([M+H]$^+$): calcd 334.0630, found 334.0623; IR (film) ν_{max}: 3060, 1750, 1609, 1552, 1488, 1402, 1379, 1314, 1091, 1010, 840, 758.



4n

2-(4-chlorophenyl)-4-(thiophen-3-yl)-6*H*-1,3-oxazin-6-one (4n)

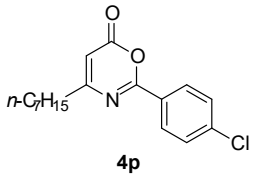
Compound **4n** was obtained as a white solid in 74% yield (21.5 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 – 8.19 (m, 3H), 7.54 – 7.50 (m, 1H), 7.50 – 7.45 (m, 2H), 7.45 – 7.40 (m, 1H), 6.36 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.5, 159.7, 157.3, 140.0, 137.8, 130.0, 129.8, 129.3, 128.5, 127.7, 125.4, 100.8; HRMS (ESI) for $C_{14}H_9ClNO_2S^+$ ([M+H]$^+$): calcd 290.0037, found 290.0033; IR (film) ν_{max}: 3086, 1749, 1610, 1564, 1488, 1421, 1403, 1307, 1092, 1012, 842, 801, 752.



4o

2-(4-chlorophenyl)-4-(pyridin-3-yl)-6*H*-1,3-oxazin-6-one (4o)

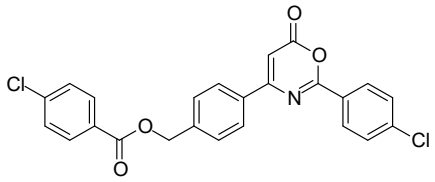
Compound **4o** was obtained as a white solid in 48% yield (13.6 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.31 (s, 1H), 8.78 (d, *J* = 4.8 Hz, 1H), 8.35 (dt, *J* = 8.0, 2.0 Hz, 1H), 8.32 – 8.26 (m, 2H), 7.55 – 7.45 (m, 3H), 6.65 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.2, 159.7, 158.9, 152.5, 148.7, 140.5, 134.9, 130.3, 130.2, 129.5, 128.3, 123.9, 103.0; HRMS (ESI) for $C_{15}H_{10}ClN_2O_2^+$ ([M+H]$^+$): calcd 285.0425, found 285.0422; IR (film) ν_{max}: 2775, 1758, 1611, 1554, 1489, 1276, 1006, 840, 753.



4p

2-(4-chlorophenyl)-4-heptyl-6*H*-1,3-oxazin-6-one (4p)

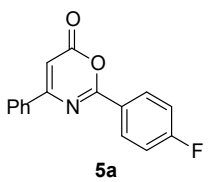
Compound **4p** was obtained as a white solid in 44% yield (13.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.6 Hz, 2H), 7.46 (d, *J* = 8.6 Hz, 2H), 6.01 (s, 1H), 2.53 (t, *J* = 7.6 Hz, 2H), 1.70 (p, *J* = 7.4 Hz, 2H), 1.43 – 1.22 (m, 8H), 0.89 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 162.2, 159.1, 139.8, 130.0, 129.2, 128.5, 105.3, 37.2, 31.8, 29.2, 29.1, 27.1, 22.7, 14.2; HRMS (ESI) for $C_{17}H_{21}ClNO_2^+$ ([M+H]$^+$): calcd 306.1255, found 306.1251; IR (film) ν_{max}: 2926, 2855, 1762, 1615, 1548, 1488, 1403, 1256, 1091, 1014, 842, 751, 725.



4q

4-(2-(4-chlorophenyl)-6-oxo-6*H*-1,3-oxazin-4-yl)benzyl 4-chlorobenzoate (4q)

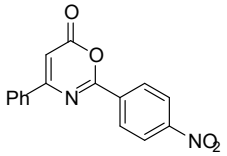
Compound **4q** was obtained as a white solid in 39% yield (17.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 – 8.25 (m, 2H), 8.14 – 8.08 (m, 2H), 8.05 – 7.99 (m, 2H), 7.62 – 7.56 (m, 2H), 7.54 – 7.48 (m, 2H), 7.46 – 7.40 (m, 2H), 6.60 (s, 1H), 5.44 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 162.6, 161.4, 159.6, 140.2, 140.1, 139.9, 134.4, 131.2, 130.2, 129.4, 129.0, 128.6, 128.6, 128.4, 127.8, 102.1, 66.3; HRMS (ESI) for $C_{24}H_{16}Cl_2NO_4^+$ ([M+H]$^+$): calcd 452.0451, found 452.0444; IR (film) ν_{max}: 2921, 2850, 1743, 1610, 1557, 1276, 1095, 838, 753, 731.



5a

2-(4-fluorophenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (5a)

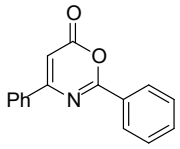
Compound **5a** was obtained as a white solid in 61% yield (15.1 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.24 (m, 2H), 8.09 – 8.03 (m, 2H), 7.58 – 7.47 (m, 3H), 7.23 – 7.15 (m, 2H), 6.56 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1 (*J* = 254 Hz), 162.3, 161.9, 159.7, 134.4, 132.1, 131.3 (*J* = 9.0 Hz), 129.1, 127.4, 126.3 (*J* = 3.0 Hz), 116.2 (*J* = 22 Hz), 101.6; ^{19}F NMR (377 MHz, $CDCl_3$) δ -104.4; HRMS (ESI) for $C_{16}H_{11}ClFNO_2^+$ ([M+H]$^+$): calcd 268.0768, found 268.0765; IR (film) ν_{max}: 2760, 1756, 1611, 1557, 1506, 1239, 1159, 850, 753, 694.



5b

2-(4-nitrophenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (5b)[5]

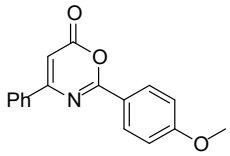
Compound **5b** was obtained as a white solid in 65% yield (17.2 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 – 8.48 (m, 2H), 8.40 – 8.33 (m, 2H), 8.12 – 8.05 (m, 2H), 7.61 – 7.50 (m, 3H), 6.66 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6, 161.1, 158.9, 150.7, 135.6, 133.9, 132.4, 129.8, 129.2, 127.5, 124.1, 102.9.



5c

2,4-diphenyl-6*H*-1,3-oxazin-6-one (5c)[5]

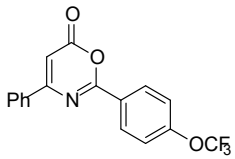
Compound **5c** was obtained as a white solid in 63% yield (18.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 – 8.32 (m, 2H), 8.14 – 8.06 (m, 2H), 7.66 – 7.58 (m, 1H), 7.58 – 7.48 (m, 5H), 6.60 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 162.0, 160.1, 134.6, 133.5, 132.1, 130.1, 129.1, 129.0, 128.9, 127.5, 101.8.



5d

2-(4-methoxyphenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (5d)[5]

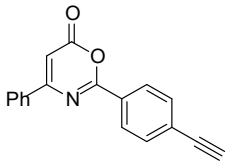
Compound **5d** was obtained as a white solid in 75% yield (20.8 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 – 8.28 (m, 2H), 8.09 – 8.06 (m, 2H), 7.55 – 7.48 (m, 3H), 7.02 – 6.98 (m, 2H), 6.52 (s, 1H), 3.90 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 164.0, 163.3, 162.3, 160.3, 134.8, 131.9, 131.0, 129.0, 127.5, 122.5, 114.4, 100.8, 55.7.



5e

4-phenyl-2-(4-(trifluoromethoxy)phenyl)-6*H*-1,3-oxazin-6-one (5e)

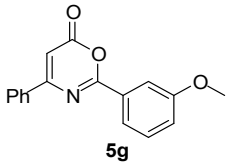
Compound **5e** was obtained as a white solid in 46% yield (15.4 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.36 (m, 2H), 8.11 – 8.04 (m, 2H), 7.60 – 7.49 (m, 3H), 7.35 (d, *J* = 8.5 Hz, 2H), 6.60 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0, 161.8, 159.6, 153.0, 134.3, 132.2, 130.8, 129.1, 128.5, 127.5, 120.8, 120.4 (q, *J* = 258 Hz), 102.0; ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.6; HRMS (ESI) for $C_{17}H_{11}F_3NO_3^+$ ($[M+H]^+$): calcd 334.0686, found 334.0681; IR (film) ν_{max}: 3073, 2850, 1754, 1615, 1558, 1506, 1277, 1213, 1147, 1100, 1009, 848, 754, 697.



5f

2-(4-ethynylphenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (5f)

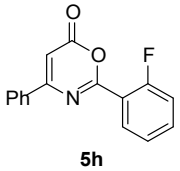
Compound **5f** was obtained as a yellow solid in 42% yield (11.6 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.34 – 8.29 (m, 2H), 8.11 – 8.07 (m, 2H), 7.66 – 7.62 (m, 2H), 7.58 – 7.50 (m, 3H), 6.61 (s, 1H), 3.30 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.6, 161.9, 159.7, 134.4, 132.6, 132.2, 130.2, 129.1, 128.7, 127.5, 127.4, 102.0, 82.9, 81.0; HRMS (ESI) for $C_{18}H_{12}NO_2^+$ ($[M+H]^+$): calcd 274.0863, found 274.0865; IR (film) ν_{max}: 3228, 1748, 1607, 1548, 1366, 1276, 1259, 867, 845, 753.



5g

2-(3-methoxyphenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (5g)

Compound **5g** was obtained as a white solid in 48% yield (13.3 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 – 8.06 (m, 2H), 7.95 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.85 – 7.82 (m, 1H), 7.56 – 7.49 (m, 3H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.15 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.58 (s, 1H), 3.90 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.1, 162.0, 160.0, 160.0, 134.5, 132.1, 131.4, 130.0, 129.1, 127.5, 121.4, 119.9, 113.3, 101.9, 55.7; HRMS (ESI) for $C_{17}H_{14}NO_3^+$ ($[M+H]^+$): calcd 280.0968, found 280.0965; IR (film) ν_{max}: 3074, 2836, 1747, 1610, 1575, 1556, 1488, 1452, 1239, 750.

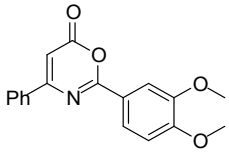


5h

2-(2-fluorophenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (5h)

Compound **5h** was obtained as a white solid in 43% yield (11.4 mg); ^{1}H NMR (400 MHz, $CDCl_3$)

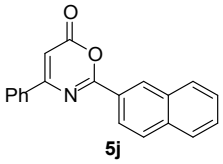
δ 8.21 (td, *J* = 7.6, 1.9 Hz, 1H), 8.12 – 8.07 (m, 2H), 7.62 – 7.49 (m, 4H), 7.34 – 7.27 (m, 1H), 7.25 – 7.21 (m, 1H), 6.63 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.0 (*J* = 261 Hz), 161.8, 160.9 (*J* = 6.0 Hz), 159.7, 134.9 (*J* = 9.0 Hz), 134.3, 132.2, 131.5, 129.1, 127.6, 124.5 (*J* = 3.0 Hz), 118.8 (*J* = 9.0 Hz), 117.6 (*J* = 21 Hz), 102.1; ^{19}F NMR (377 MHz, $CDCl_3$) δ -107.5; HRMS (ESI) for $C_{16}H_{11}FNO_2^+$ ($[M+H]^+$): calcd 268.0768, found 268.0764; IR (film) ν_{max}: 2755, 1752, 1608, 1549, 1320, 1276, 1009, 749.



5i

2-(3,4-dimethoxyphenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (5i)

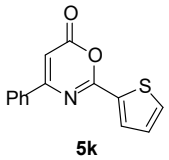
Compound **5i** was obtained as a white solid in 42% yield (13.0 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.06 (m, 2H), 8.03 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.81 (d, *J* = 2.0 Hz, 1H), 7.58 – 7.49 (m, 3H), 6.98 (d, *J* = 8.5 Hz, 1H), 6.54 (s, 1H), 4.00 (s, 3H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 162.3, 160.4, 153.8, 149.2, 134.8, 132.0, 129.1, 127.5, 123.4, 122.6, 110.9, 110.9, 101.0, 56.3, 56.3; HRMS (ESI) for $C_{18}H_{16}NO_4^+$ ($[M+H]^+$): calcd 310.1074, found 310.1069; IR (film) ν_{max}: 2838, 1744, 1606, 1508, 1347, 1275, 1141, 1021, 913, 765, 752.



5j

2-(naphthalen-2-yl)-4-phenyl-6*H*-1,3-oxazin-6-one (5j)

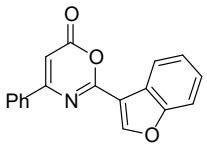
Compound **5j** was obtained as a white solid in 43% yield (12.8 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.72 (s, 1H), 8.28 (d, *J* = 8.6 Hz, 1H), 8.05 (d, *J* = 7.2 Hz, 2H), 7.93 – 7.78 (m, 3H), 7.59 – 7.46 (m, 5H), 6.50 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.0, 161.7, 159.9, 135.6, 134.4, 132.6, 131.9, 130.2, 129.5, 128.9, 128.7, 128.6, 127.8, 127.4, 127.1, 127.0, 124.2, 101.6; HRMS (ESI) for $C_{20}H_{14}NO_2^+$ ($[M+H]^+$): calcd 300.1019, found 300.1017; IR (film) ν_{max}: 3061, 1749, 1607, 1551, 1450, 1365, 1314, 1126, 759, 688.



5k

4-phenyl-2-(thiophen-2-yl)-6*H*-1,3-oxazin-6-one (5k)[5]

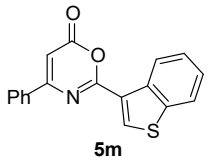
Compound **5k** was obtained as a pale yellow solid in 56% yield (14.3 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 – 7.97 (m, 3H), 7.67 – 7.63 (m, 1H), 7.55 – 7.46 (m, 3H), 7.20 – 7.15 (m, 1H), 6.49 (d, *J* = 3.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 159.7, 159.4, 134.3, 134.2, 133.7, 132.9, 132.0, 129.0, 128.7, 127.4, 100.8.



5l

2-(benzofuran-3-yl)-4-phenyl-6*H*-1,3-oxazin-6-one (5l)

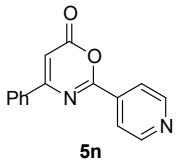
Compound **5l** was obtained as a gray white solid in 34% yield (9.9 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 – 8.39 (m, 1H), 8.36 – 8.30 (m, 1H), 8.09 – 8.01 (m, 2H), 7.60 – 7.49 (m, 4H), 7.46 – 7.38 (m, 2H), 6.51 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 159.6, 159.3, 156.0, 150.7, 134.4, 132.0, 129.1, 127.3, 125.9, 124.6, 123.7, 122.5, 114.7, 111.9, 101.7; HRMS (ESI) for $C_{18}H_{12}NO_3^+$ ($[M+H]^+$): calcd 290.0812, found 290.0809; IR (film) ν_{max}: 3073, 1744, 1613, 1582, 1449, 1356, 1286, 1127, 1103, 986, 761, 747.



5m

2-(benzo[*b*]thiophen-3-yl)-4-phenyl-6*H*-1,3-oxazin-6-one (5m)

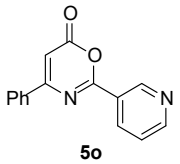
Compound **5m** was obtained as a white solid in 32% yield (9.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 – 8.92 (m, 1H), 8.61 (s, 1H), 8.11 – 8.03 (m, 2H), 7.93 – 7.86 (m, 1H), 7.61 – 7.51 (m, 4H), 7.49 – 7.41 (m, 1H), 6.55 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 159.6, 159.3, 140.5, 136.8, 135.8, 134.7, 132.0, 129.1, 127.4, 126.5, 125.9, 125.5, 125.2, 122.8, 101.9; HRMS (ESI) for $C_{18}H_{12}NO_2S^+$ ($[M+H]^+$): calcd 306.0583, found 306.0580; IR (film) ν_{max}: 3107, 2926, 1742, 1607, 1576, 1551, 1449, 1351, 1241, 1124, 1081, 972, 873, 760, 732, 701.



5n

4-phenyl-2-(pyridin-4-yl)-6*H*-1,3-oxazin-6-one (5n)

Compound **5n** was obtained as a yellow solid in 60% yield (15.0 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.87 – 8.81 (m, 2H), 8.15 – 8.11 (m, 2H), 8.08 – 8.04 (m, 2H), 7.58 – 7.49 (m, 3H), 6.66 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.4, 161.3, 158.9, 150.9, 137.5, 133.9, 132.4, 129.2, 127.5, 121.7, 103.3; HRMS (ESI) for $C_{15}H_{11}N_2O_2^+$ ($[M+H]^+$): calcd 251.0815, found 251.0813; IR (film) ν_{max}: 3074, 1749, 1615, 1551, 1491, 1414, 1331, 1256, 1110, 831, 747, 696, 683.

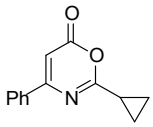


5o

4-phenyl-2-(pyridin-3-yl)-6*H*-1,3-oxazin-6-one (5o)

Compound **5o** was obtained as a pale yellow solid in 47% yield (11.8 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.54 (d, J = 2.5 Hz, 1H), 8.83 (dd, J = 4.9, 1.7 Hz, 1H), 8.57 (dt, J = 8.0, 2.0 Hz, 1H), 8.09

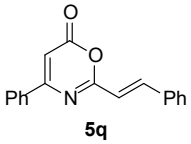
– 8.05 (m, 2H), 7.58 – 7.47 (m, 4H), 6.63 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.6, 161.6, 159.1, 153.5, 150.0, 136.1, 134.1, 132.3, 129.2, 127.5, 126.3, 123.7, 102.5; HRMS (ESI) for $C_{15}H_{11}N_2O_2^+$ ([M+H]$^+$): calcd 251.0815, found 251.0813; IR (film) ν_{max}: 3073, 1749, 1612, 1559, 1419, 1108, 828, 745, 705, 681.



5p

2-cyclopropyl-4-phenyl-6*H*-1,3-oxazin-6-one (5p)

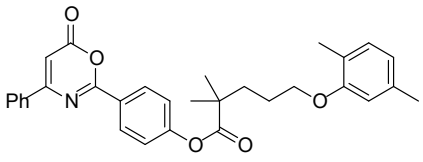
Compound **5p** was obtained as a white solid in 29% yield (6.2 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.93 (m, 2H), 7.54 – 7.44 (m, 3H), 6.45 (s, 1H), 2.01 (tt, *J* = 8.2, 4.7 Hz, 1H), 1.38 – 1.31 (m, 2H), 1.22 – 1.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 162.0, 160.4, 134.6, 131.9, 129.0, 127.4, 100.9, 15.1, 10.8; HRMS (ESI) for $C_{13}H_{12}NO_2^+$ ([M+H]$^+$): calcd 214.0863, found 214.0863; IR (film) ν_{max}: 3072, 2921, 1758, 1735, 1606, 1563, 1493, 1450, 1365, 1114, 1034, 828, 755, 687.



5q

(*E*)-4-phenyl-2-styryl-6*H*-1,3-oxazin-6-one (5q)

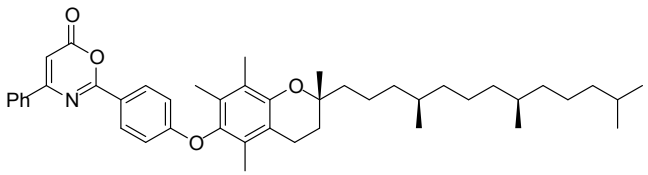
Compound **5q** was obtained as a yellow solid in 25% yield (6.9 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.97 (m, 2H), 7.92 (d, *J* = 16.1 Hz, 1H), 7.64 – 7.56 (m, 2H), 7.55 – 7.46 (m, 3H), 7.45 – 7.38 (m, 3H), 6.82 (d, *J* = 16.1 Hz, 1H), 6.51 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 162.2, 159.9, 143.8, 134.5, 134.5, 131.9, 130.8, 129.2, 129.0, 128.4, 127.4, 118.9, 101.7; HRMS (ESI) for $C_{18}H_{14}NO_2^+$ ([M+H]$^+$): calcd 276.1019, found 276.1015; IR (film) ν_{max}: 2694, 1744, 1635, 1596, 1577, 1544, 1366, 972, 763, 750.



5r

4-(6-oxo-4-phenyl-6*H*-1,3-oxazin-2-yl)phenyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (5r)

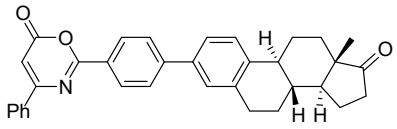
Compound **5r** was obtained as a colorless oil in 86% yield (43.0 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 – 8.35 (m, 2H), 8.12 – 8.07 (m, 2H), 7.59 – 7.51 (m, 3H), 7.24 – 7.19 (m, 2H), 7.02 (d, *J* = 7.4 Hz, 1H), 6.68 (d, *J* = 7.5 Hz, 1H), 6.64 (s, 1H), 6.60 (s, 1H), 4.01 (t, *J* = 5.6 Hz, 2H), 2.32 (s, 3H), 2.19 (s, 3H), 1.96 – 1.86 (m, 4H), 1.41 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.9, 162.6, 162.0, 159.9, 156.9, 155.3, 136.6, 134.5, 132.1, 130.5, 130.4, 129.1, 127.5, 123.7, 122.2, 121.0, 112.1, 101.8, 67.8, 42.8, 37.2, 25.4, 25.2, 21.5, 15.9; HRMS (ESI) for $C_{31}H_{32}NO_5^+$ ([M+H]$^+$): calcd 498.2275, found 498.2277; IR (film) ν_{max}: 2925, 1752, 1611, 1557, 1505, 1206, 1159, 1097, 752, 697.



5s

4-phenyl-2-(4-(((*R*)-2,5,7,8-tetramethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chroman-6-yl)oxy)phenyl)-6*H*-1,3-oxazin-6-one (5s)

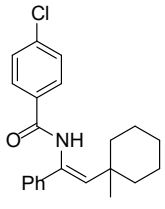
Compound **5s** was obtained as a beige solid in 62% yield (41.9 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 – 8.25 (m, 2H), 8.11 – 8.06 (m, 2H), 7.56 – 7.48 (m, 3H), 6.88 (d, *J* = 8.6 Hz, 2H), 6.54 (s, 1H), 2.63 (t, *J* = 6.8 Hz, 2H), 2.14 (s, 3H), 2.01 (s, 3H), 1.97 (s, 3H), 1.85 (dp, *J* = 28.1, 6.9 Hz, 2H), 1.67 – 1.24 (m, 18H), 1.17 – 1.02 (m, 6H), 0.91 – 0.83 (m, 12H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.5, 163.4, 162.3, 160.4, 149.3, 143.0, 134.9, 131.9, 131.2, 129.0, 127.9, 127.5, 126.0, 123.7, 122.9, 118.2, 115.3, 100.8, 75.3, 40.2, 39.5, 37.6, 37.5, 37.4, 33.0, 32.8, 31.4, 28.1, 25.0, 24.6, 24.0, 22.9, 22.8, 21.2, 20.8, 19.9, 19.8, 13.0, 12.1, 12.0; HRMS (ESI) for $C_{45}H_{60}NO_4^+$ ([M+H]$^+$): calcd 678.4517, found 678.4511; IR (film) ν_{max}: 2925, 2866, 1753, 1604, 1552, 1502, 1318, 1239, 1155, 1098, 845, 757, 697.



5t

2-(4-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)phenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (5t)

Compound **5t** was obtained as a yellow solid in 56% yield (28.0 mg), ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.37 (m, 2H), 8.16 – 8.07 (m, 2H), 7.78 – 7.71 (m, 2H), 7.60 – 7.50 (m, 3H), 7.50 – 7.39 (m, 3H), 6.61 (s, 1H), 3.08 – 2.99 (m, 2H), 2.59 – 2.44 (m, 2H), 2.43 – 2.33 (m, 1H), 2.24 – 1.96 (m, 4H), 1.73 – 1.58 (m, 4H), 1.55 – 1.45 (m, 2H), 0.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ^{13}C NMR (101 MHz, $CDCl_3$) δ 220.9, 163.3, 162.1, 160.1, 146.1, 140.4, 137.4, 137.3, 134.7, 132.1, 129.4, 129.1, 128.7, 127.9, 127.5, 127.4, 126.2, 124.8, 101.7, 50.7, 48.1, 44.6, 38.3, 36.0, 31.7, 29.7, 26.6, 25.9, 21.8, 14.0; HRMS (ESI) for $C_{34}H_{32}NO_3^+$ ([M+H]$^+$): calcd 502.2377, found 502.2382; IR (film) ν_{max}: 2924, 2853, 1736, 1605, 1545, 1491, 1367, 1276, 1099, 758, 699.

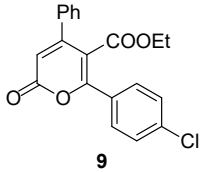


7

(*Z*)-4-chloro-N-(2-(1-methylcyclohexyl)-1-phenylvinyl)benzamide (7)

Compound **7** was obtained as a white solid in 30% yield (10.6 mg), ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.0 Hz, 2H), 7.51 – 7.36 (m, 5H), 7.34 – 7.24 (m, 3H), 5.74 (s, 1H), 1.82 (d, *J* = 13.1

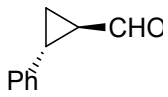
Hz, 2H), 1.64 – 1.57 (m, 2H), 1.53 – 1.44 (m, 2H), 1.40 – 1.24 (m, 4H), 1.19 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 164.8, 139.3, 138.4, 134.7, 133.6, 132.7, 129.2, 128.7, 128.5, 127.8, 125.8, 39.5, 36.8, 27.6, 26.1, 23.0; HRMS (ESI) for $C_{22}H_{24}ClNONa^+$ ([M+Na]$^+$): calcd 376.1439, found 376.1436; IR (film) ν_{max}: 3279, 2924, 2852, 1645, 1596, 1516, 1480, 1276, 1092, 1015, 757, 694; The stereochemistry of the product was determined by 2D-NMR analysis.



9

Ethyl 6-(4-chlorophenyl)-2-oxo-4-phenyl-2*H*-pyran-5-carboxylate (9)

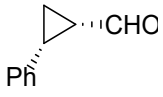
Compound **9** was obtained as a yellow oil in 9% yield (3.3 mg)Yellow oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.58 (m, 2H), 7.50 – 7.40 (m, 5H), 7.38 – 7.34 (m, 2H), 6.30 (s, 1H), 3.93 (q, *J* = 7.1 Hz, 2H), 0.88 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 160.4, 159.8, 156.2, 137.6, 136.3, 130.2, 129.9, 129.7, 129.1, 128.9, 127.1, 114.0, 113.2, 62.2, 13.5; HRMS (ESI) for $C_{20}H_{16}ClNO_4^+$ ([M+Na]$^+$): calcd 355.0732, found 355.0735; IR (film) ν_{max}: 3248, 2928, 1708, 1605, 1501, 1464, 1276, 1261, 1033, 764, 750.



*trans***12**

***trans*-2-phenylcyclopropane-1-carbaldehyde (*trans*-12)**[6]

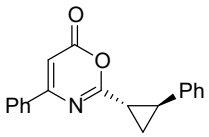
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (d, *J* = 4.6 Hz, 1H), 7.33 – 7.27 (m, 2H), 7.25 – 7.20 (m, 1H), 7.14 – 7.08 (m, 2H), 2.63 (ddd, *J* = 9.3, 6.7, 4.0 Hz, 1H), 2.18 (ddt, *J* = 8.5, 5.1, 4.2 Hz, 1H), 1.73 (dt, *J* = 9.2, 5.1 Hz, 1H), 1.53 (ddd, *J* = 8.3, 6.7, 4.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 139.1, 128.8, 127.0, 126.4, 33.9, 26.7, 16.6.



*cis***12**

***cis*-2-phenylcyclopropane-1-carbaldehyde (*cis*-12)**[6]

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 6.8 Hz, 1H), 7.34 – 7.27 (m, 4H), 7.26 – 7.20 (m, 1H), 2.83 (q, *J* = 8.2 Hz, 1H), 2.19 – 2.09 (m, 1H), 1.89 (dt, *J* = 7.3, 5.3 Hz, 1H), 1.63 – 1.58 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.4, 135.9, 129.3, 128.7, 127.3, 29.8, 26.5, 11.7.



*trans***13**

***trans*-4-phenyl-2-(2-phenylcyclopropyl)-6*H*-1,3-oxazin-6-one (*trans*-13)**

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.93 (m, 2H), 7.57 – 7.44 (m, 3H), 7.36 – 7.29 (m, 2H), 7.26 – 7.21 (m, 1H), 7.20 – 7.14 (m, 2H), 6.49 (s, 1H), 2.84 (ddd, *J* = 9.4, 6.7, 4.2 Hz, 1H), 2.28 (ddd, *J* = 8.6, 5.4, 4.2 Hz, 1H), 1.97 (dt, *J* = 9.3, 5.1 Hz, 1H), 1.65 (ddd, *J* = 8.5, 6.7, 4.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.0, 162.0, 160.2, 139.5, 134.5, 132.0, 129.0, 128.8, 127.4, 127.0, 126.4, 101.0, 28.9, 26.2, 18.7; HRMS (ESI) for $C_{19}H_{16}NO_2^+$ ($[M+H]^+$): calcd 290.1176, found 290.1178; IR (film) ν_{max}: 1749, 1612, 1579, 1561, 1276, 1261, 751, 698.

7. Reference

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5. P. Song, P. Yu, J. S. Lin, Y. Li, N. Y. Yang and X. Y. Liu, *Org. Lett.*, 2017, **19**, 1330–1333.
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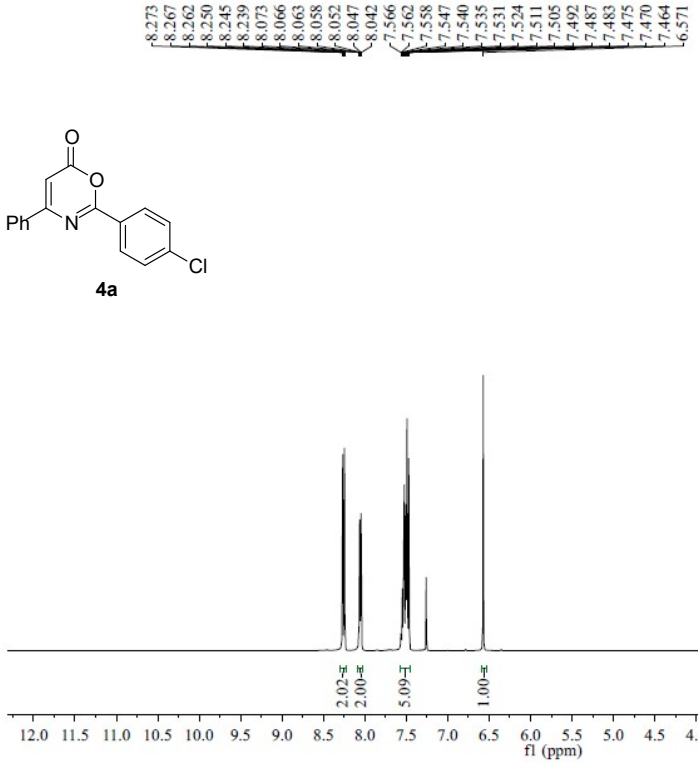
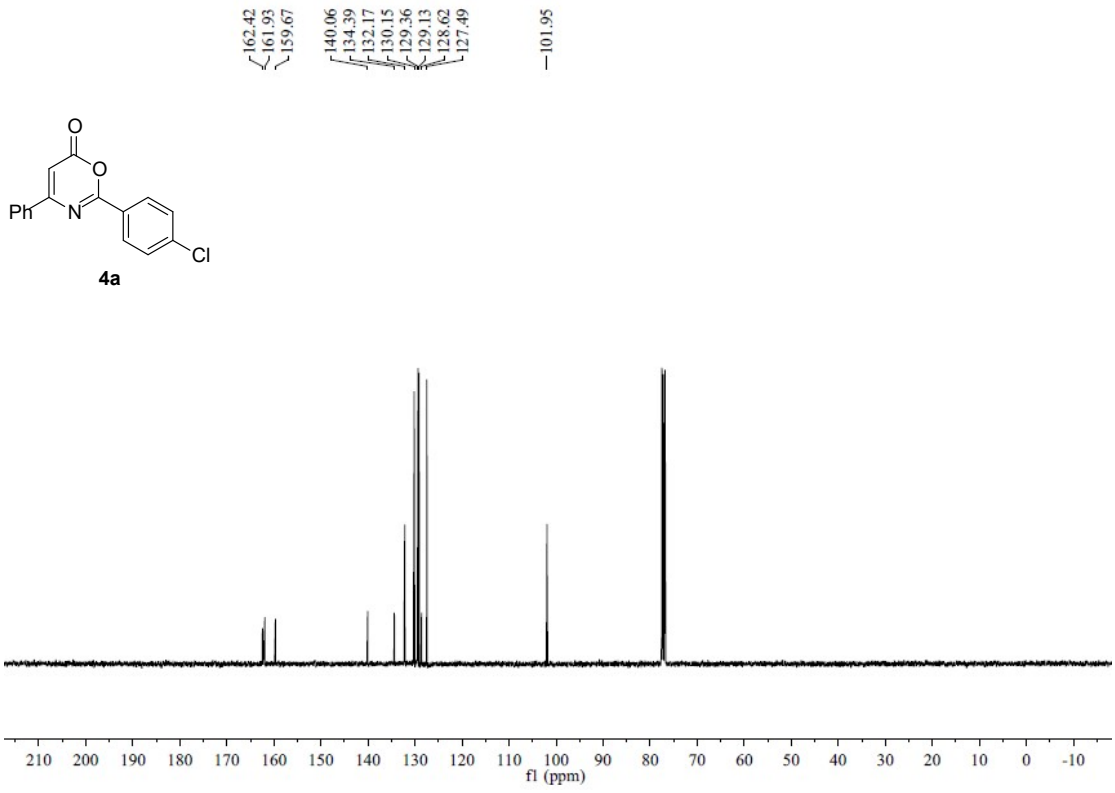
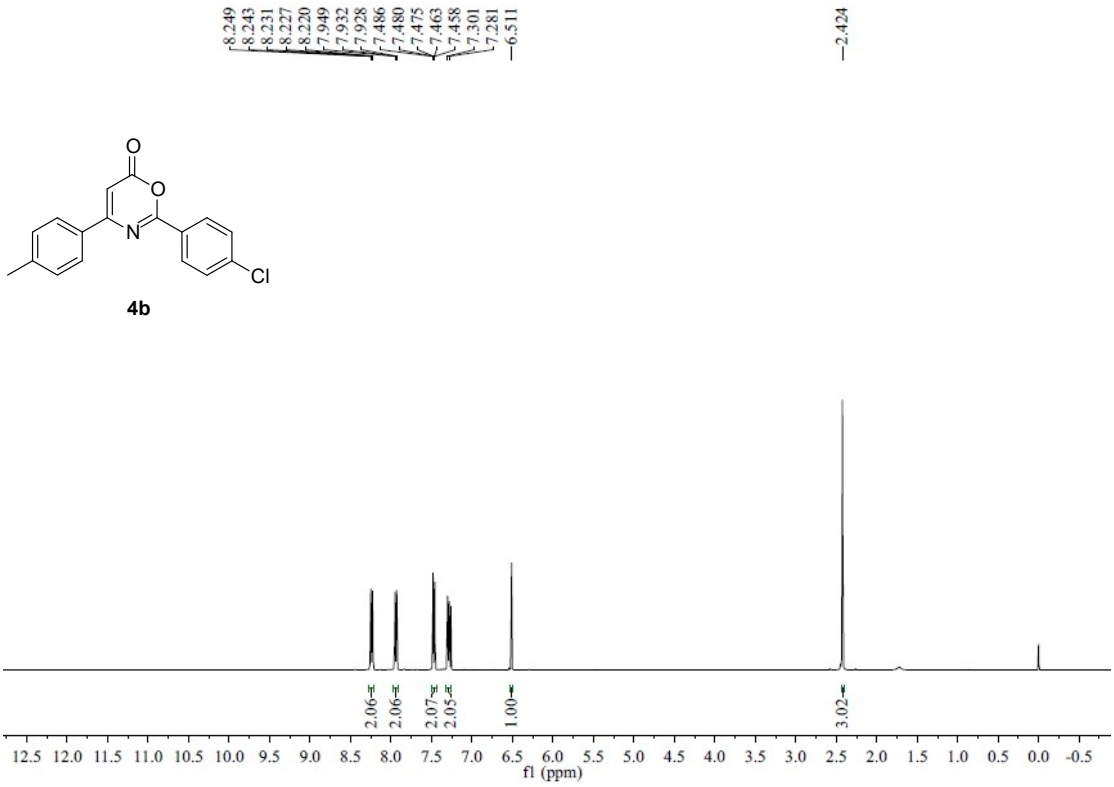
8. NMR spectra



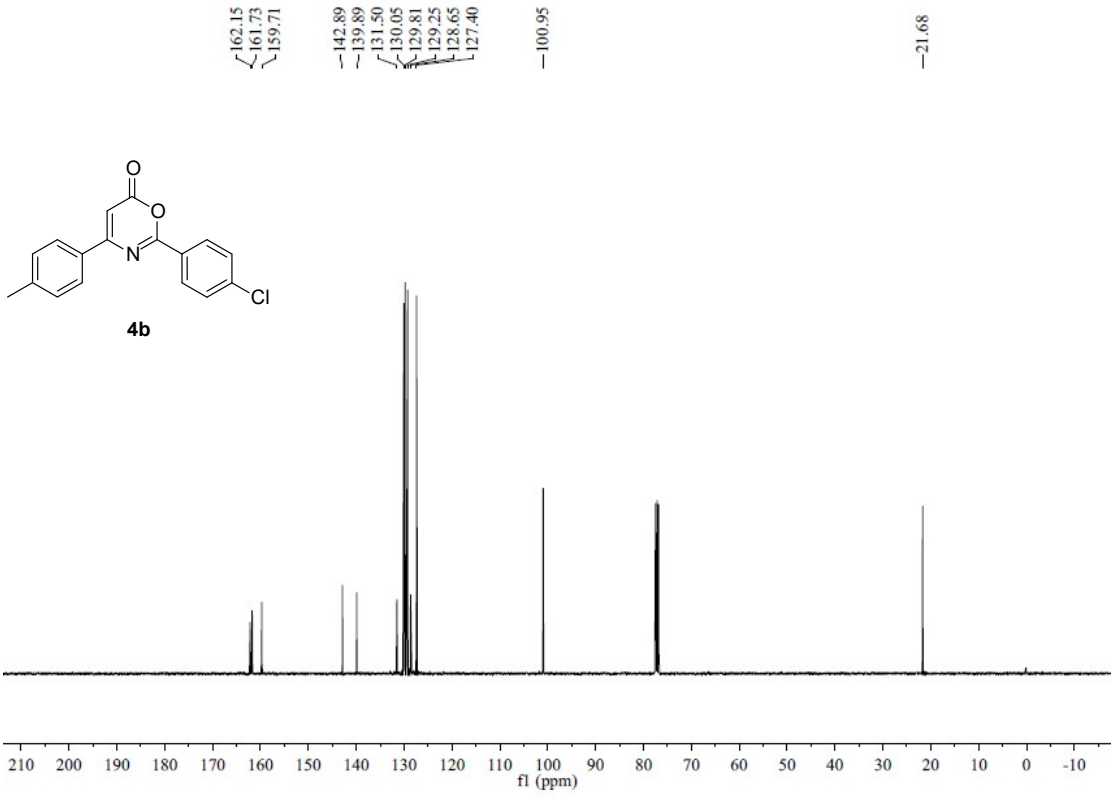
^{1}H NMR spectra for compound **4a**



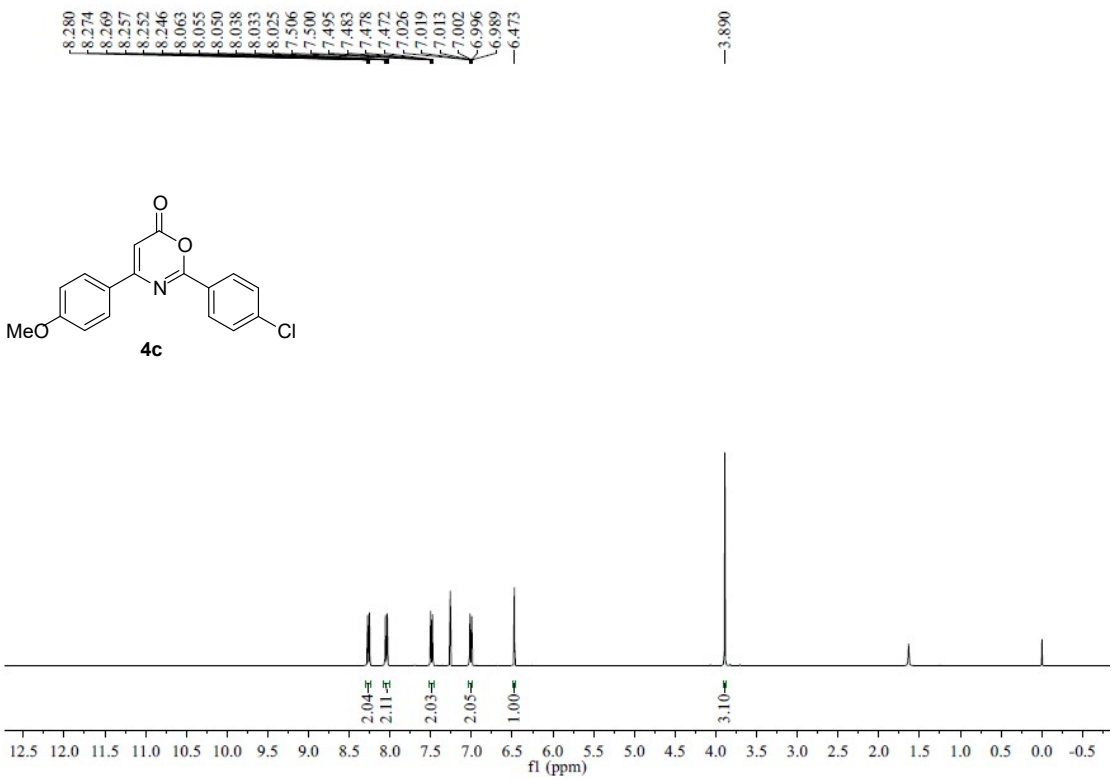
^{13}C NMR spectra for compound **4a**



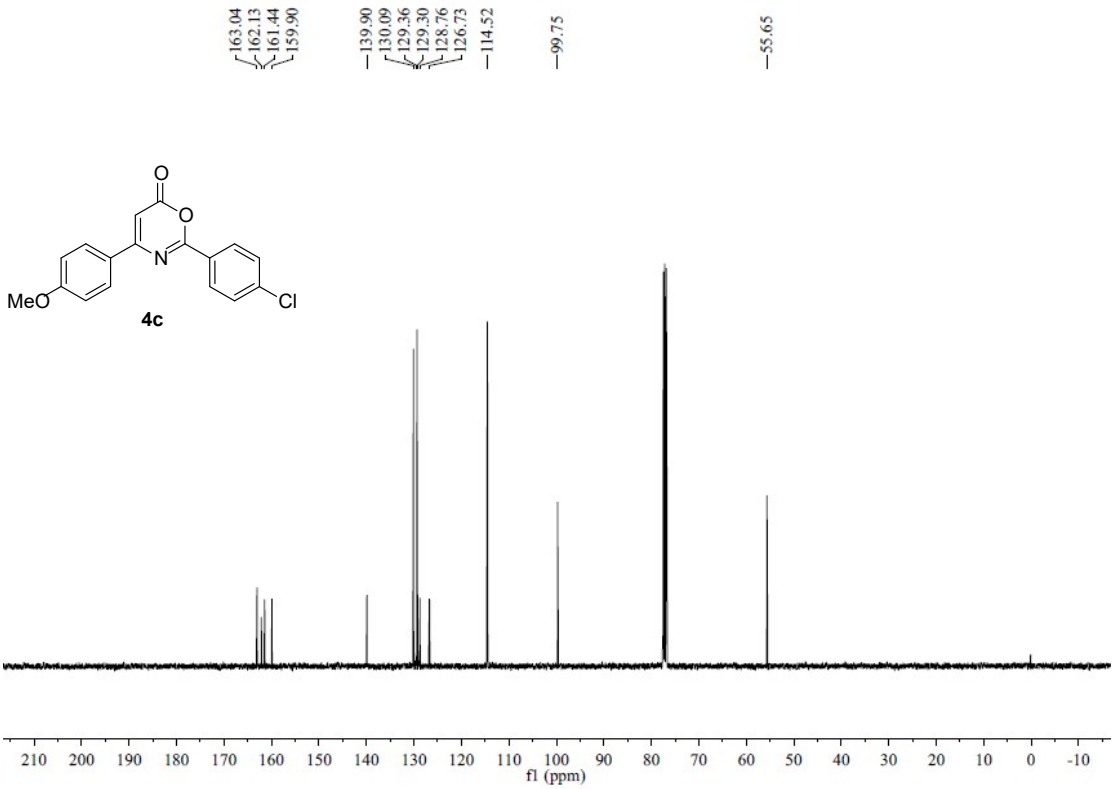
^{1}H NMR spectra for compound **4b**



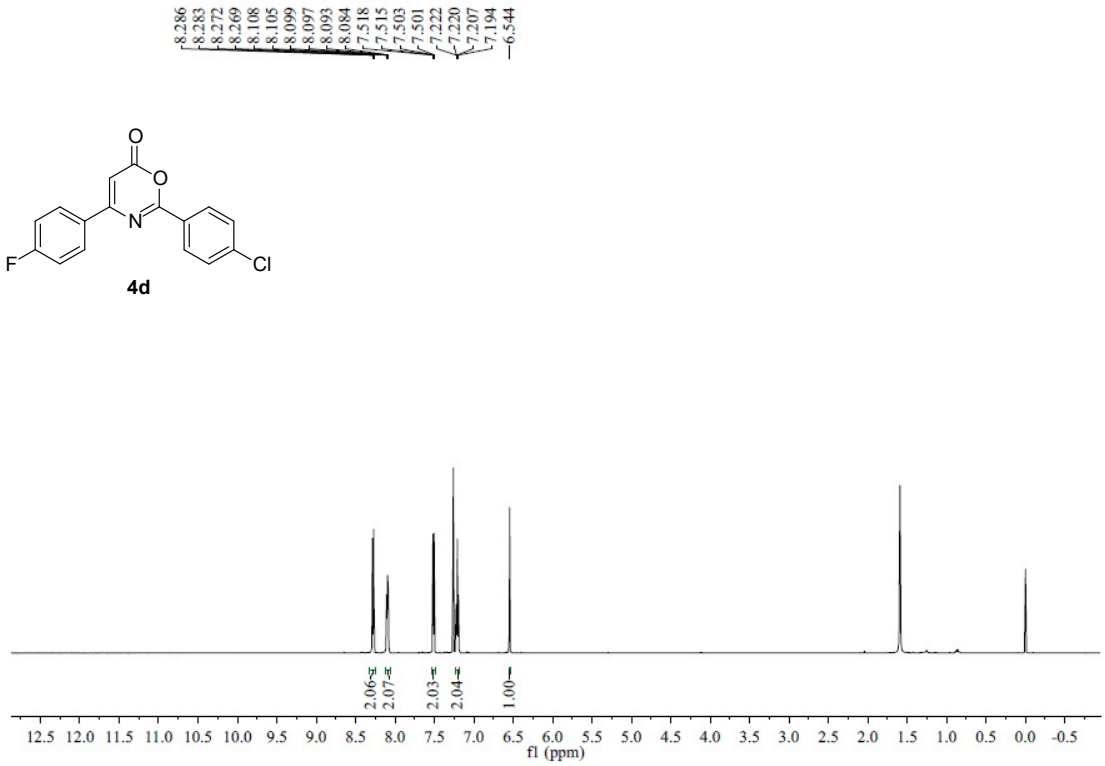
^{13}C NMR spectra for compound **4b**



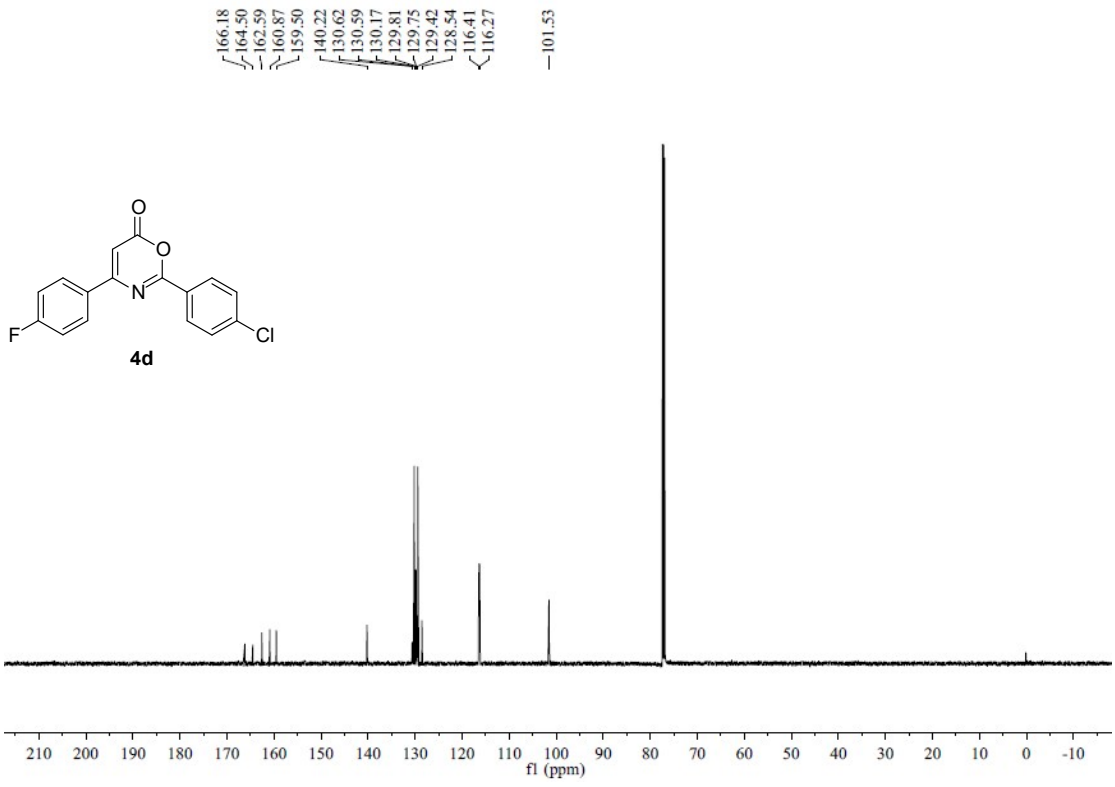
^{1}H NMR spectra for compound **4c**



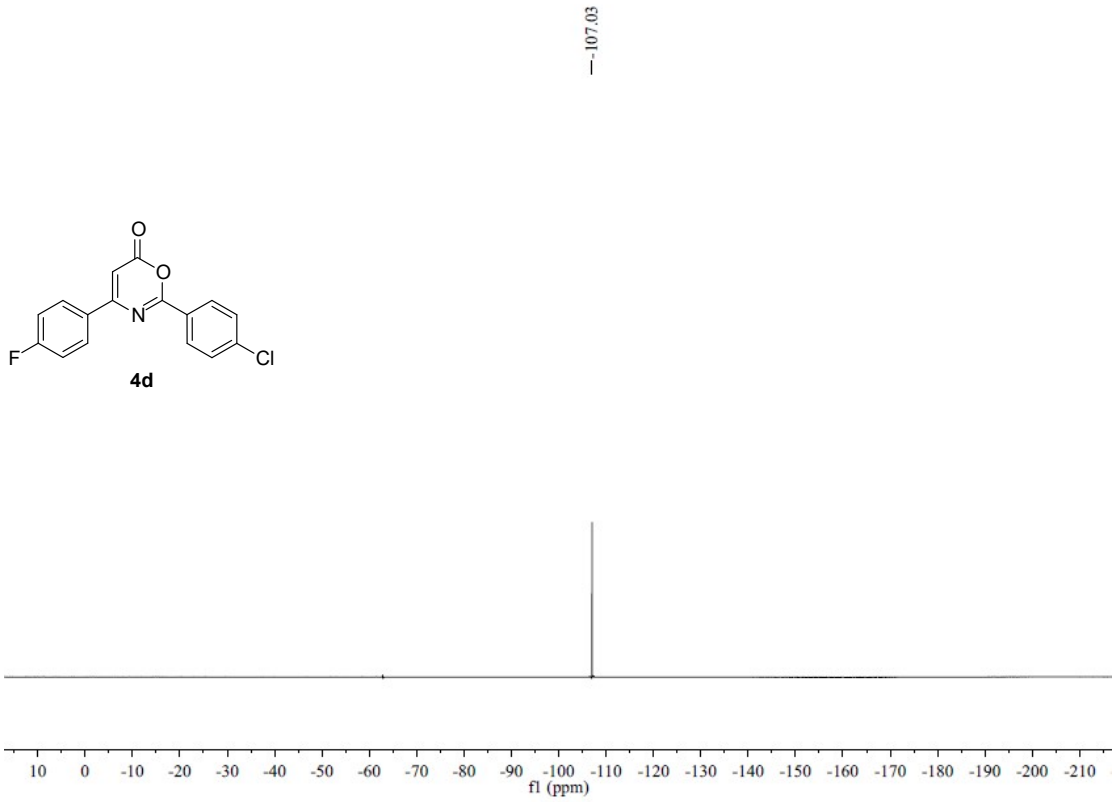
^{13}C NMR spectra for compound **4c**



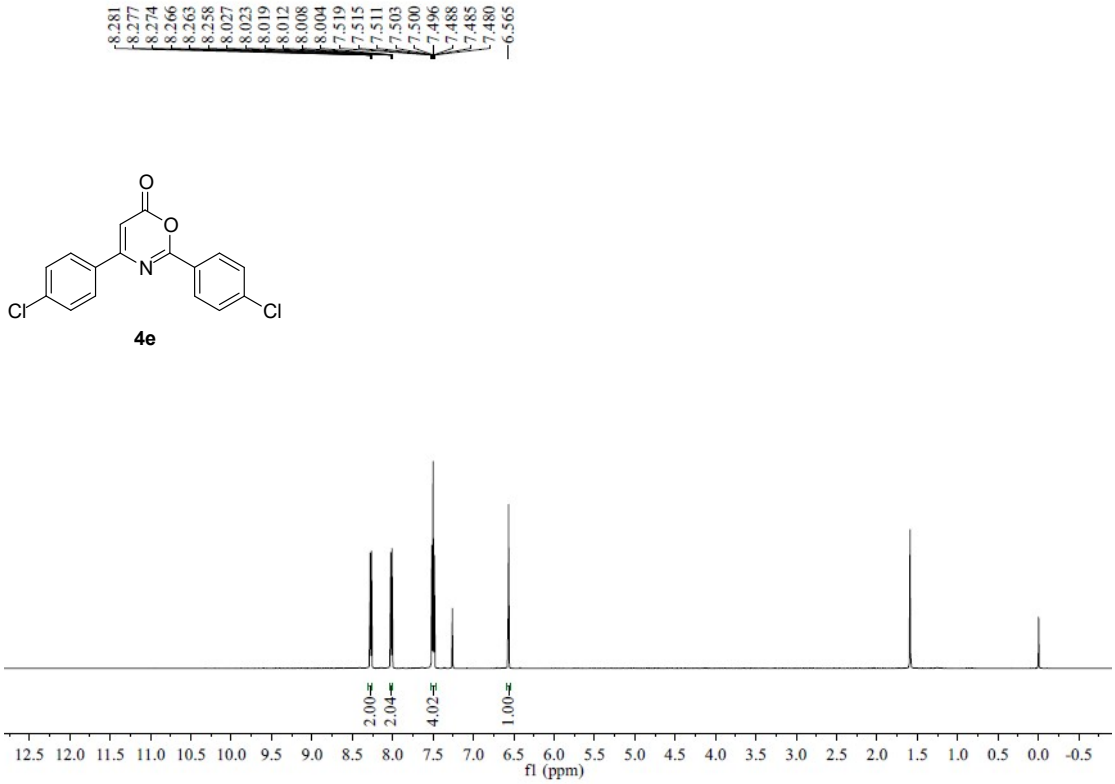
^{1}H NMR spectra for compound **4d**



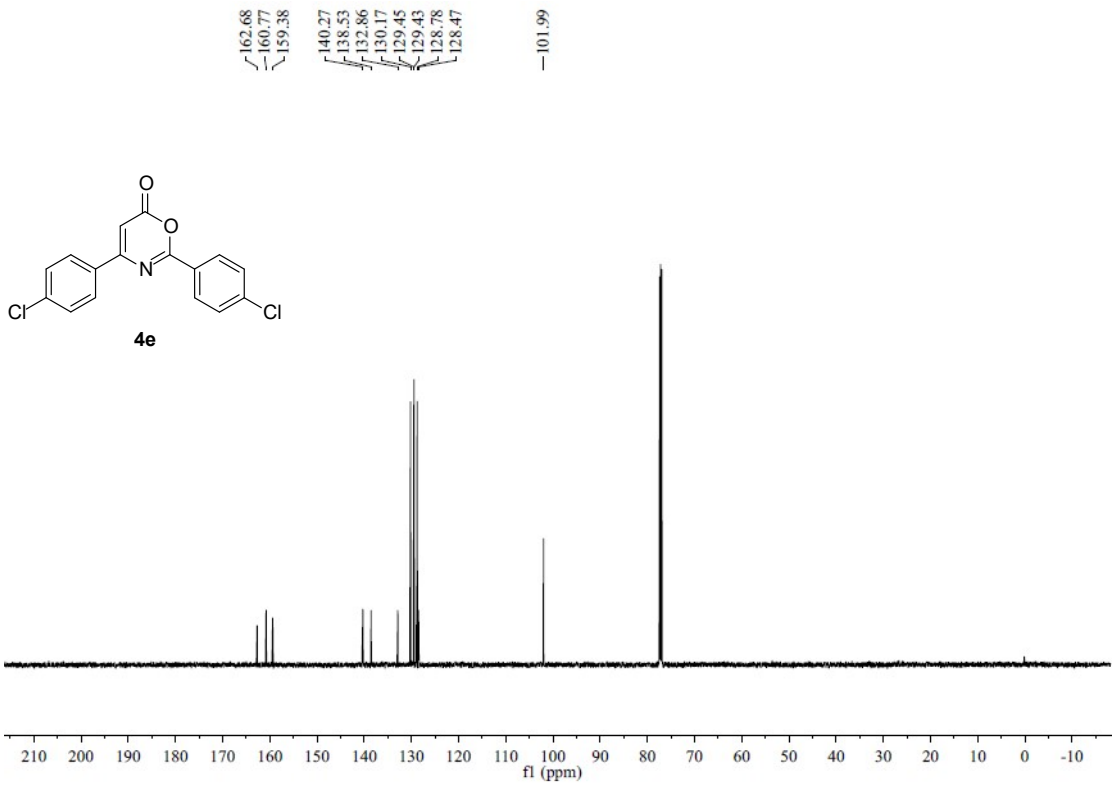
^{13}C NMR spectra for compound **4d**



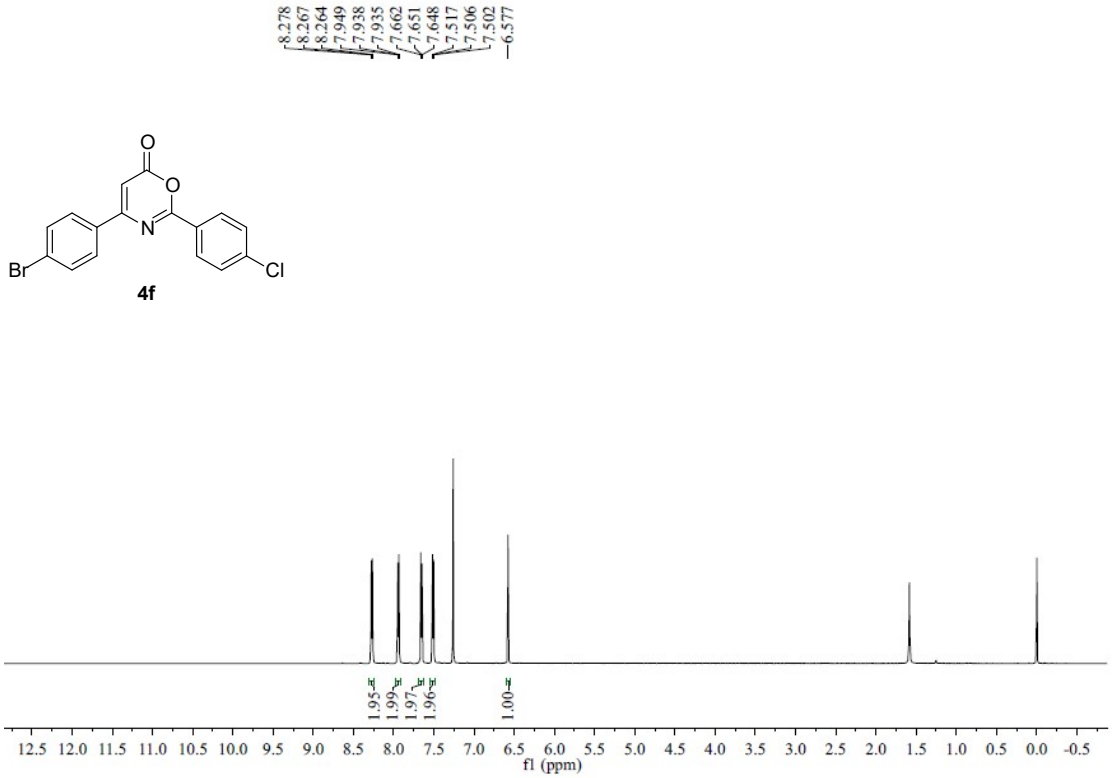
^{19}F NMR spectra for compound **4d**



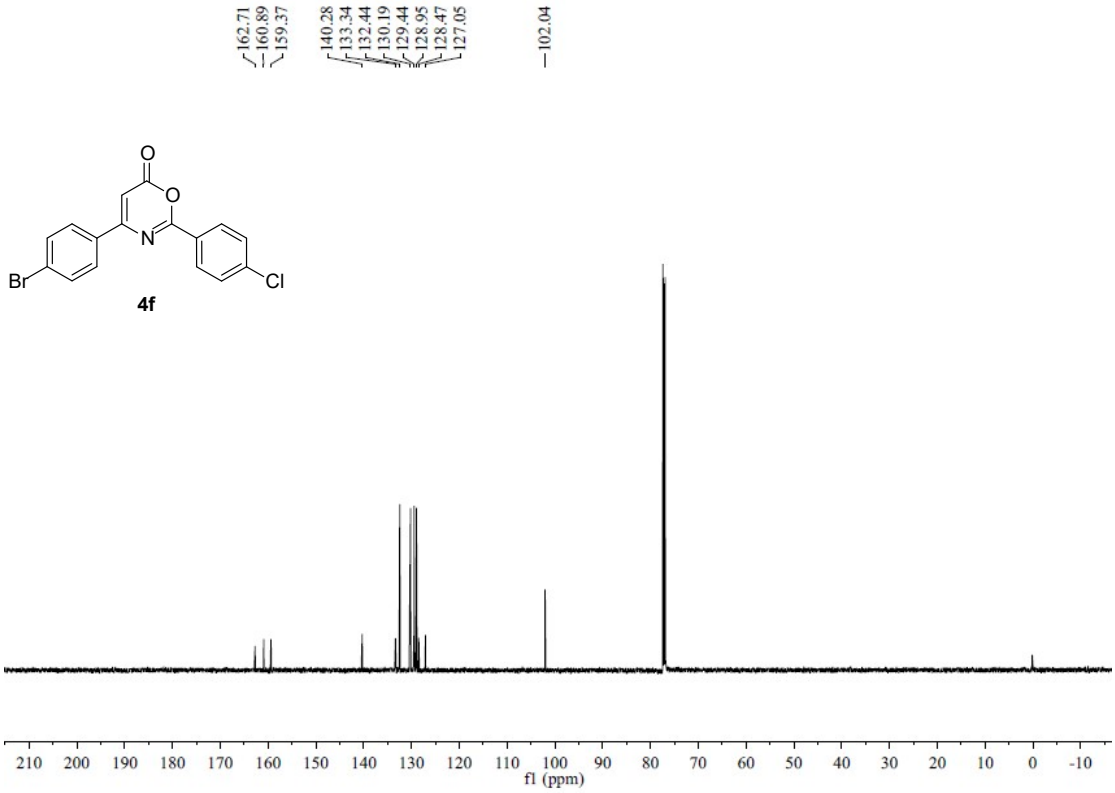
^{1}H NMR spectra for compound **4e**



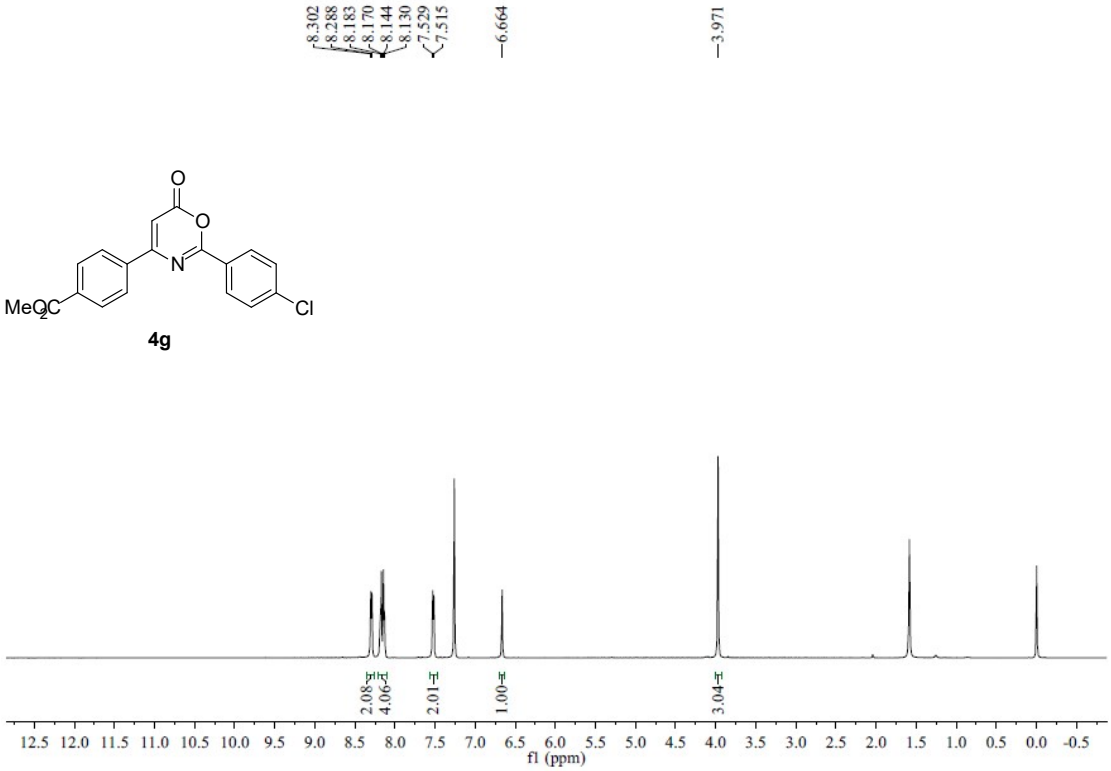
^{13}C NMR spectra for compound **4e**



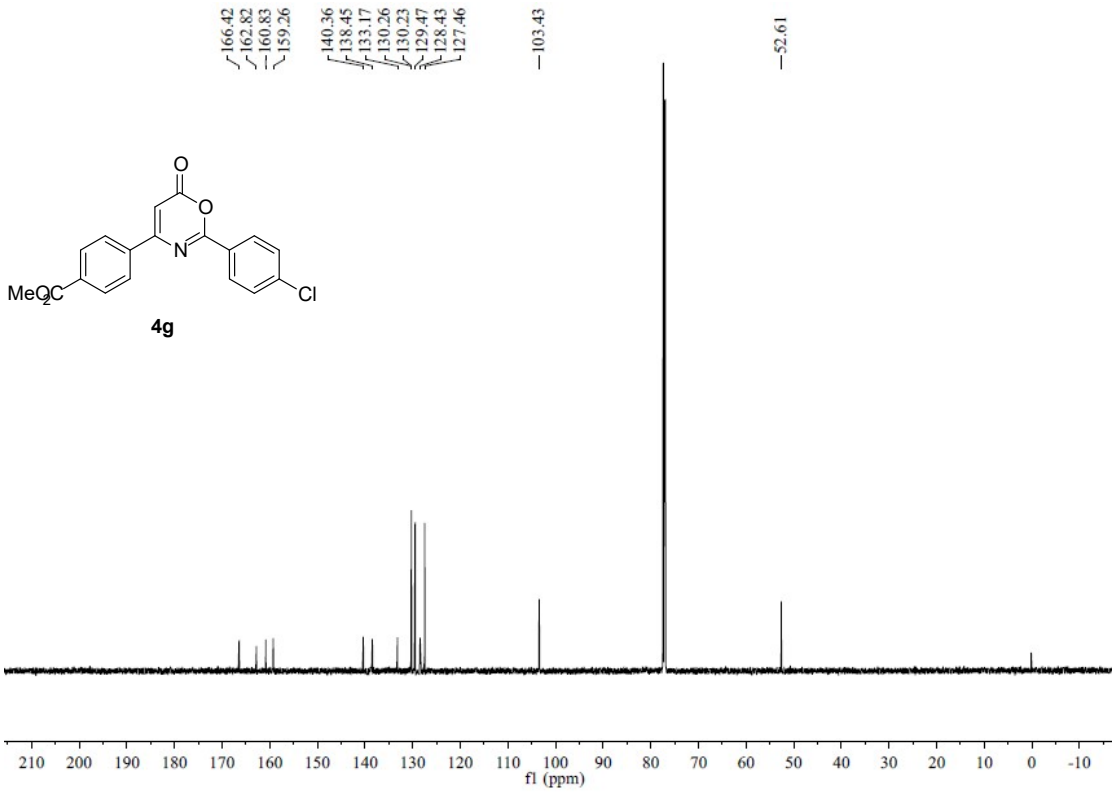
^{1}H NMR spectra for compound **4f**



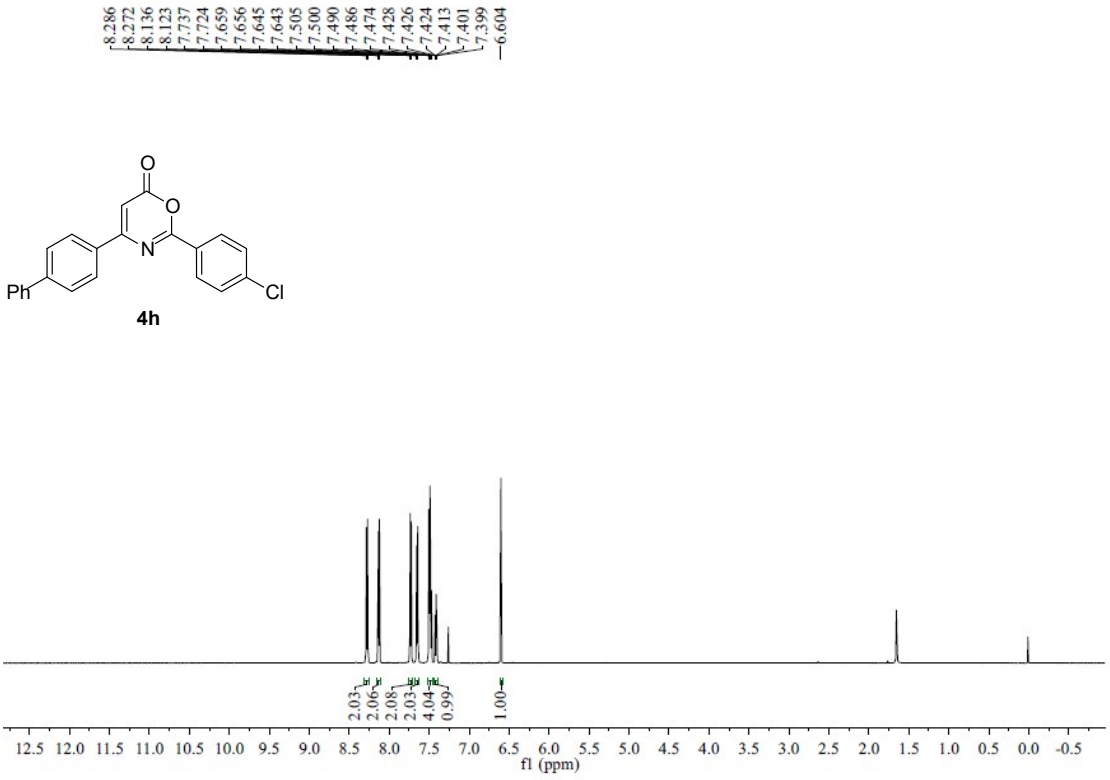
^{13}C NMR spectra for compound **4f**



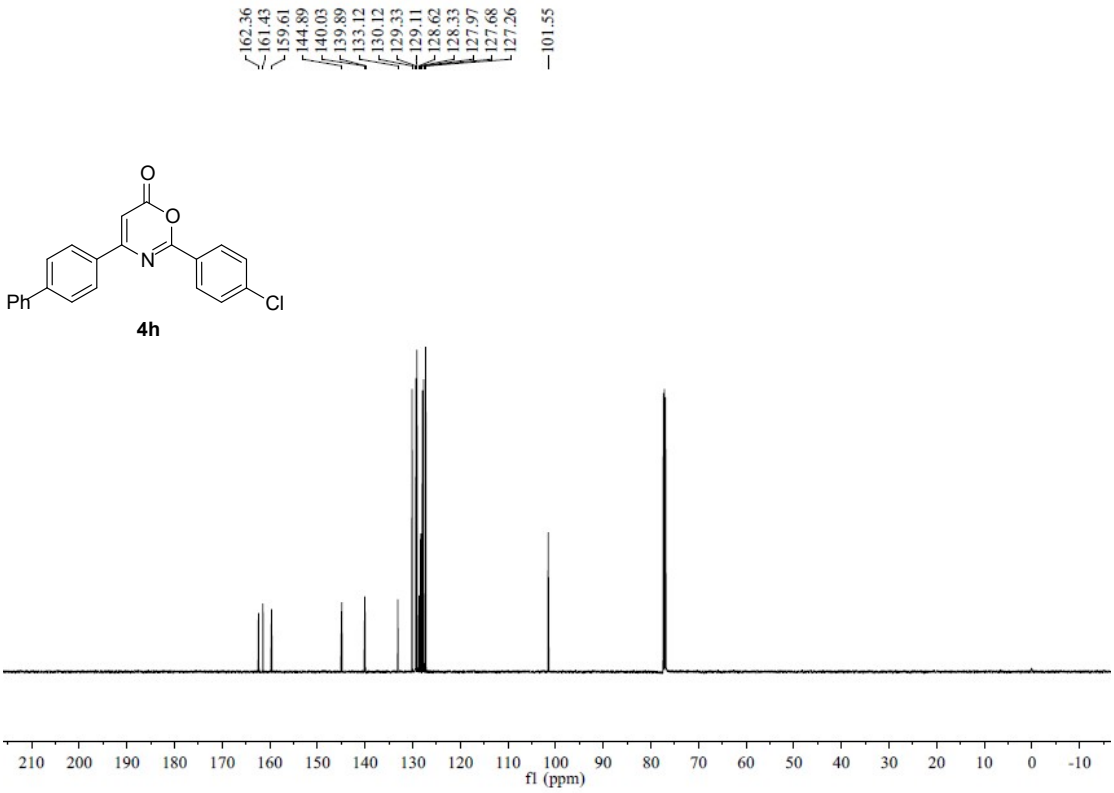
^{1}H NMR spectra for compound **4g**



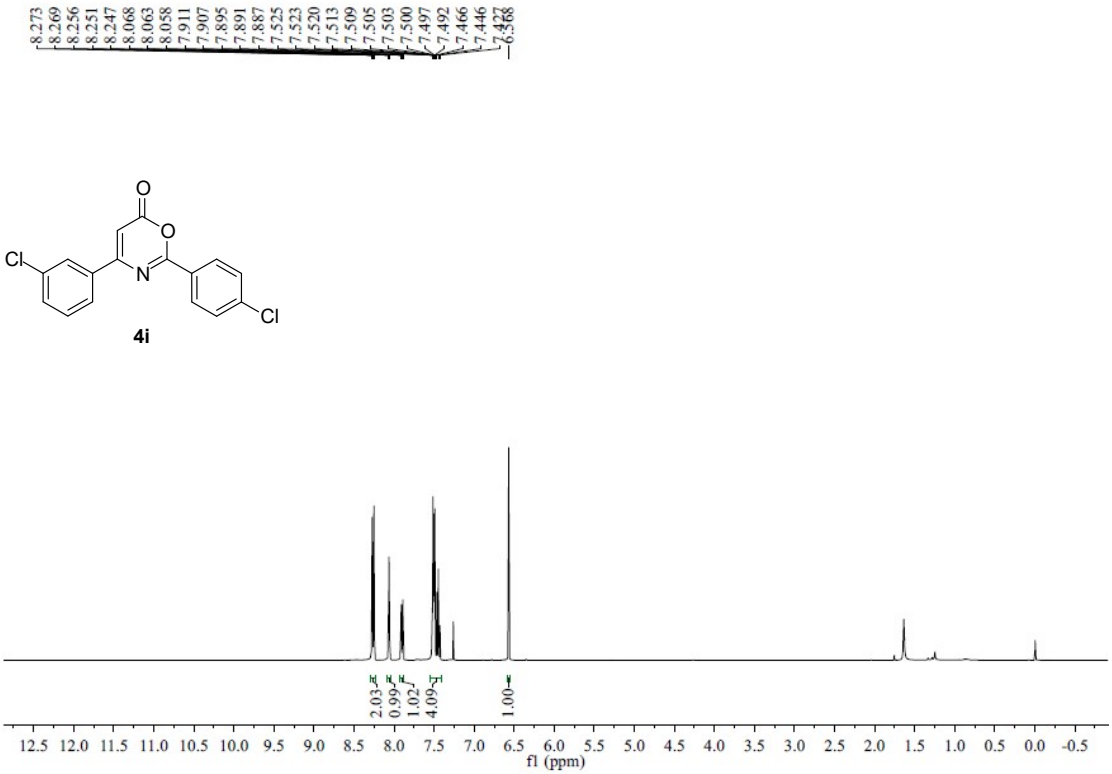
^{13}C NMR spectra for compound **4g**



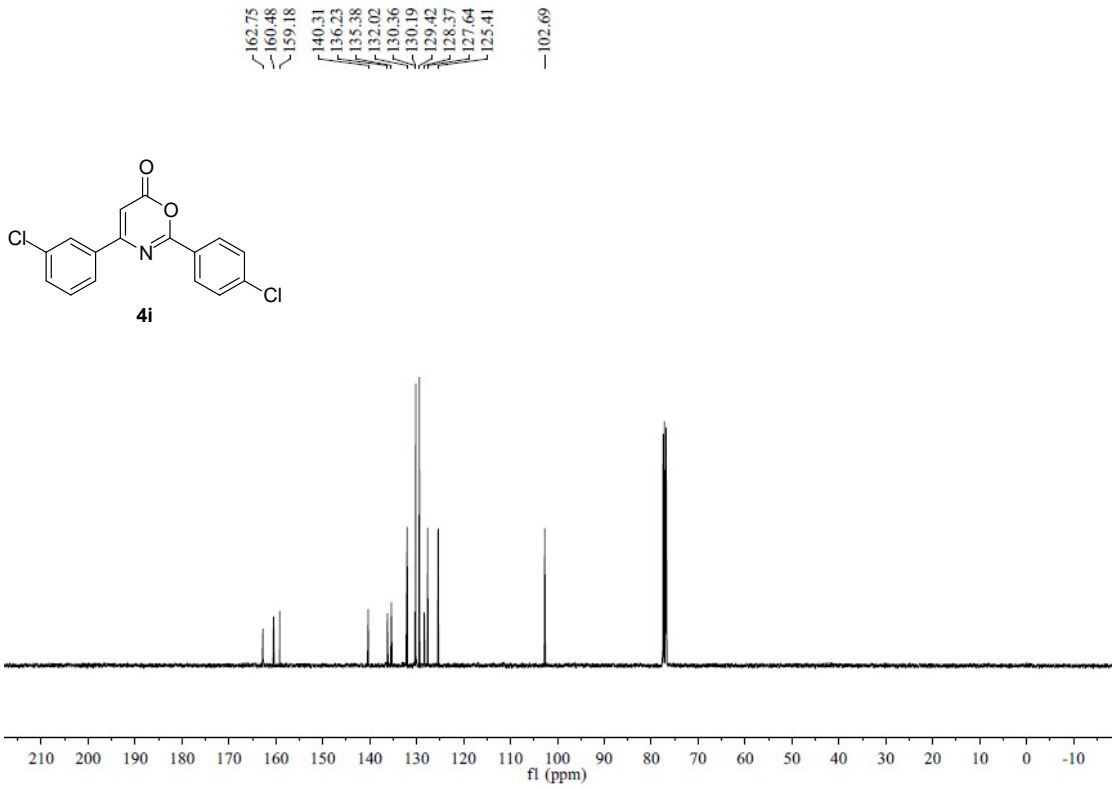
^{1}H NMR spectra for compound **4h**



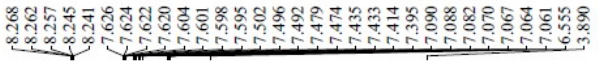
^{13}C NMR spectra for compound **4h**

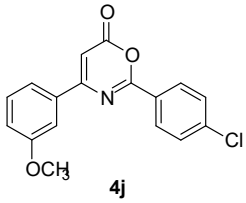


^{1}H NMR spectra for compound **4i**

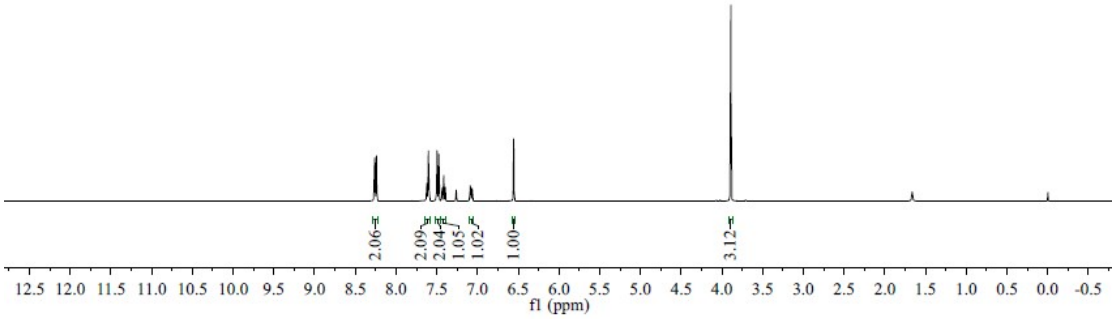


^{13}C NMR spectra for compound **4i**

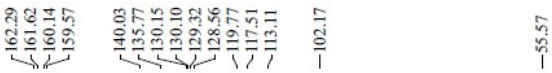


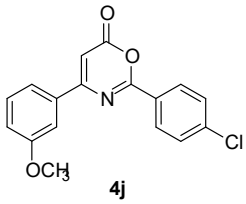


4j

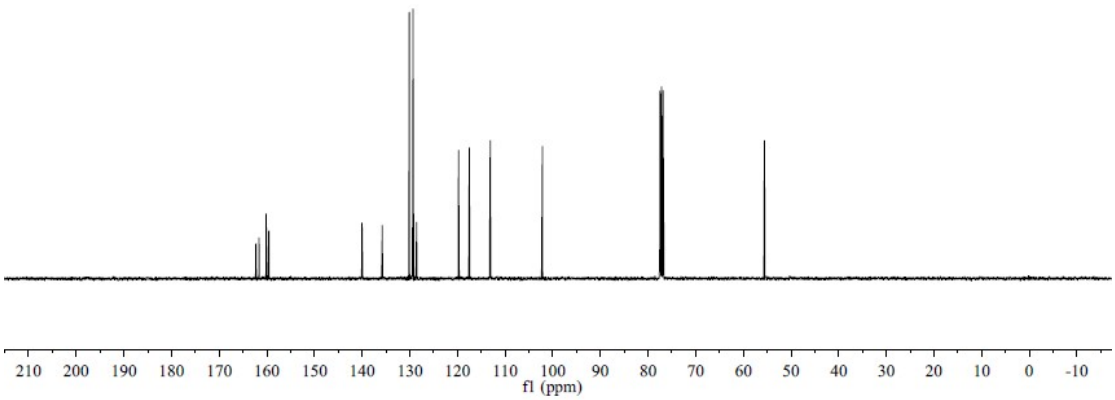


^{1}H NMR spectra for compound **4j**

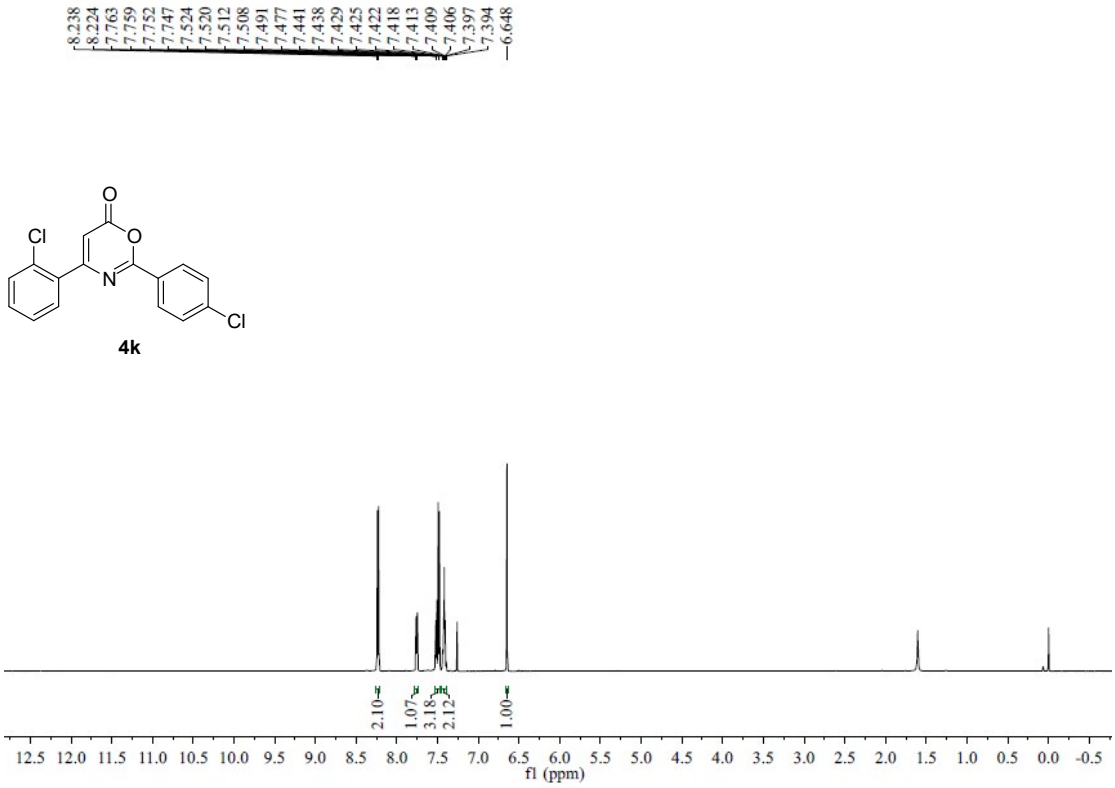




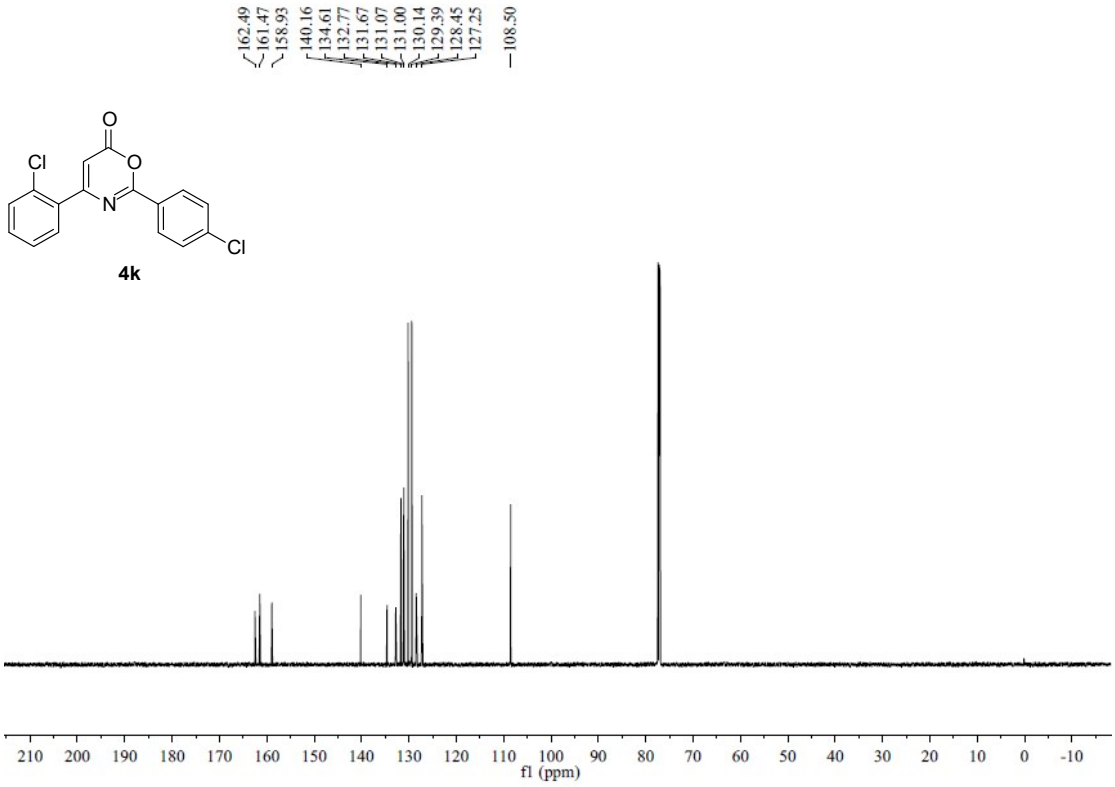
4j



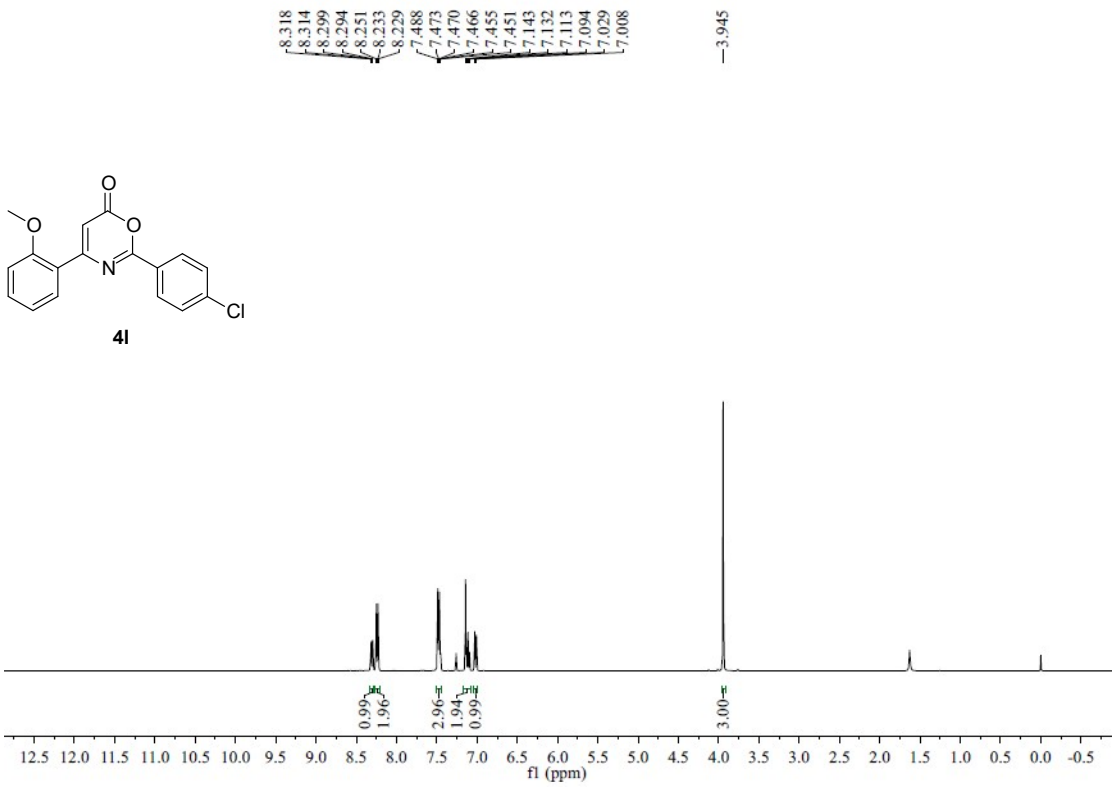
^{13}C NMR spectra for compound **4j**



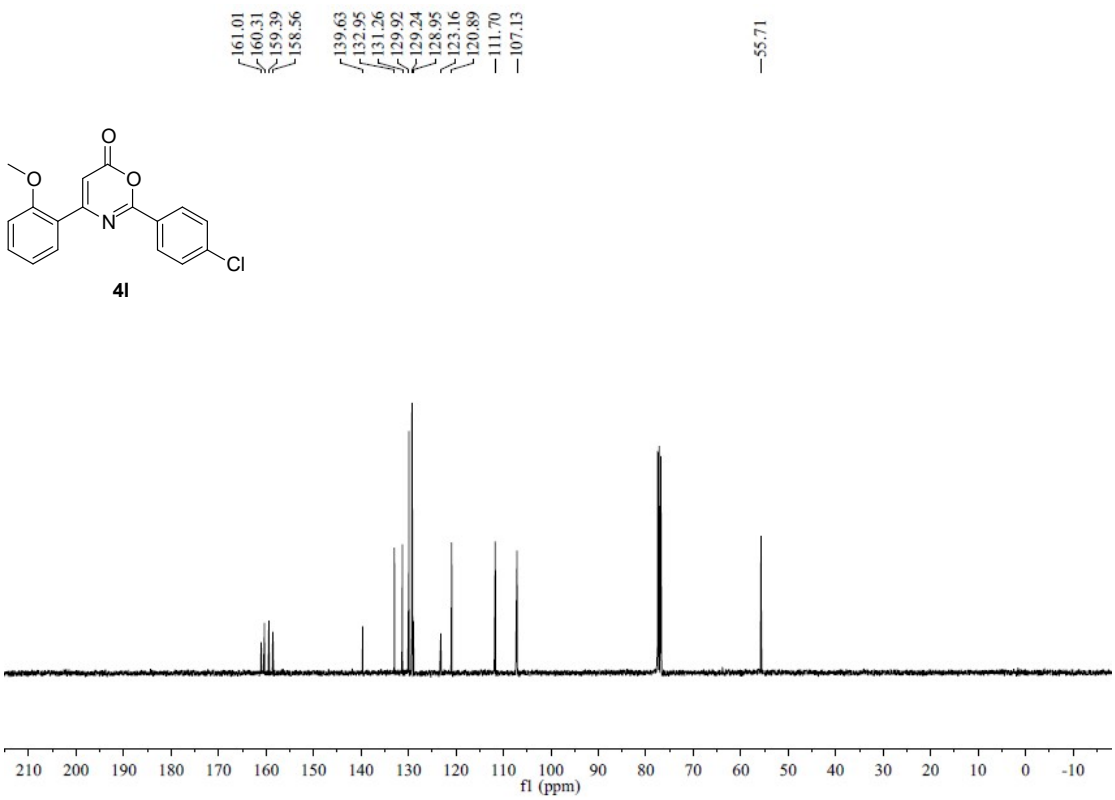
^{1}H NMR spectra for compound **4k**



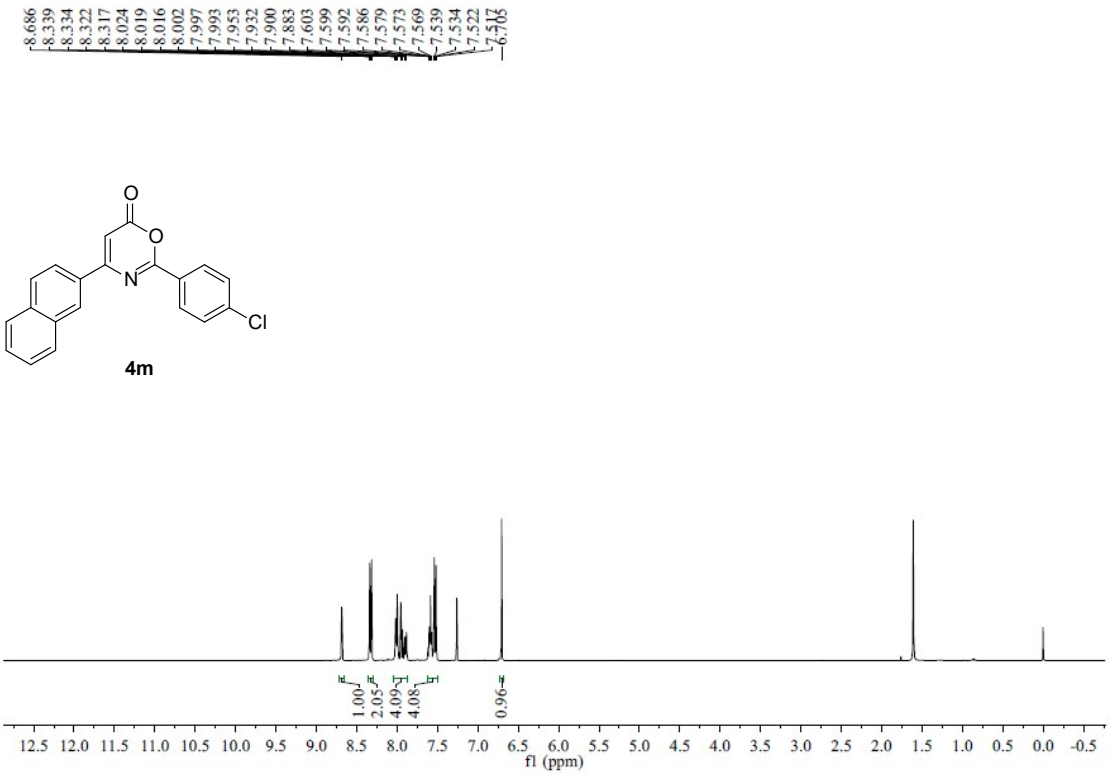
^{13}C NMR spectra for compound **4k**



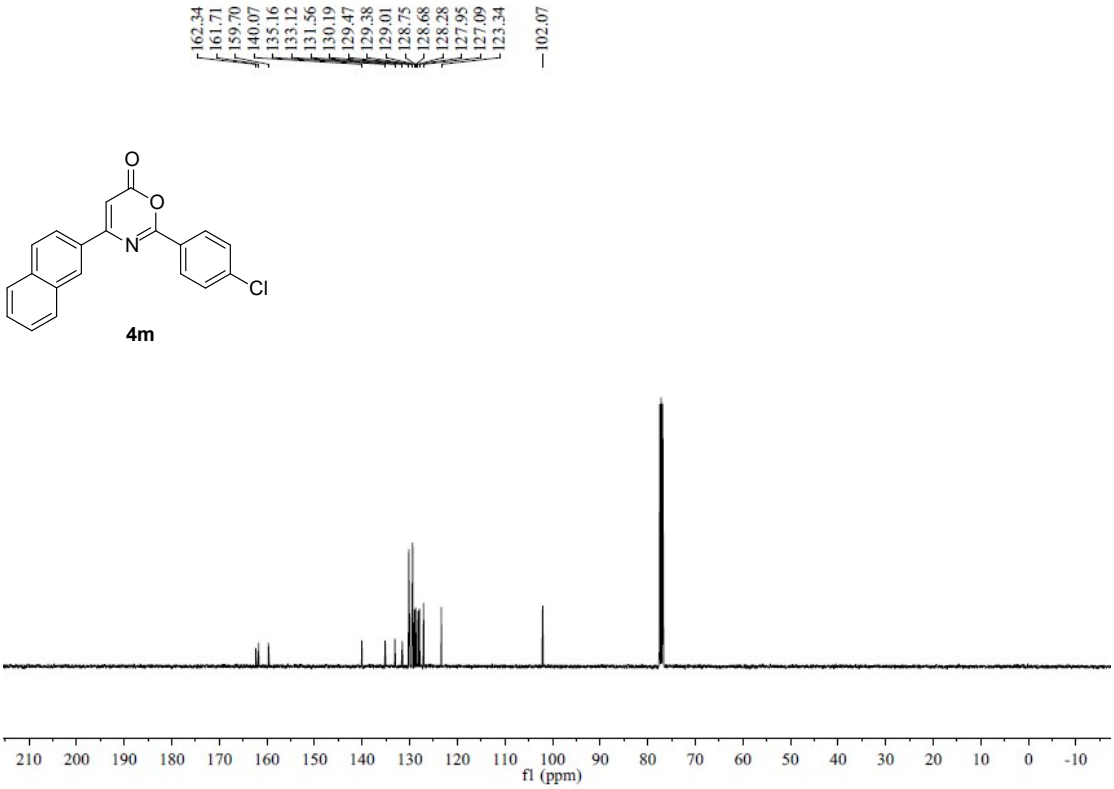
^{1}H NMR spectra for compound **4l**



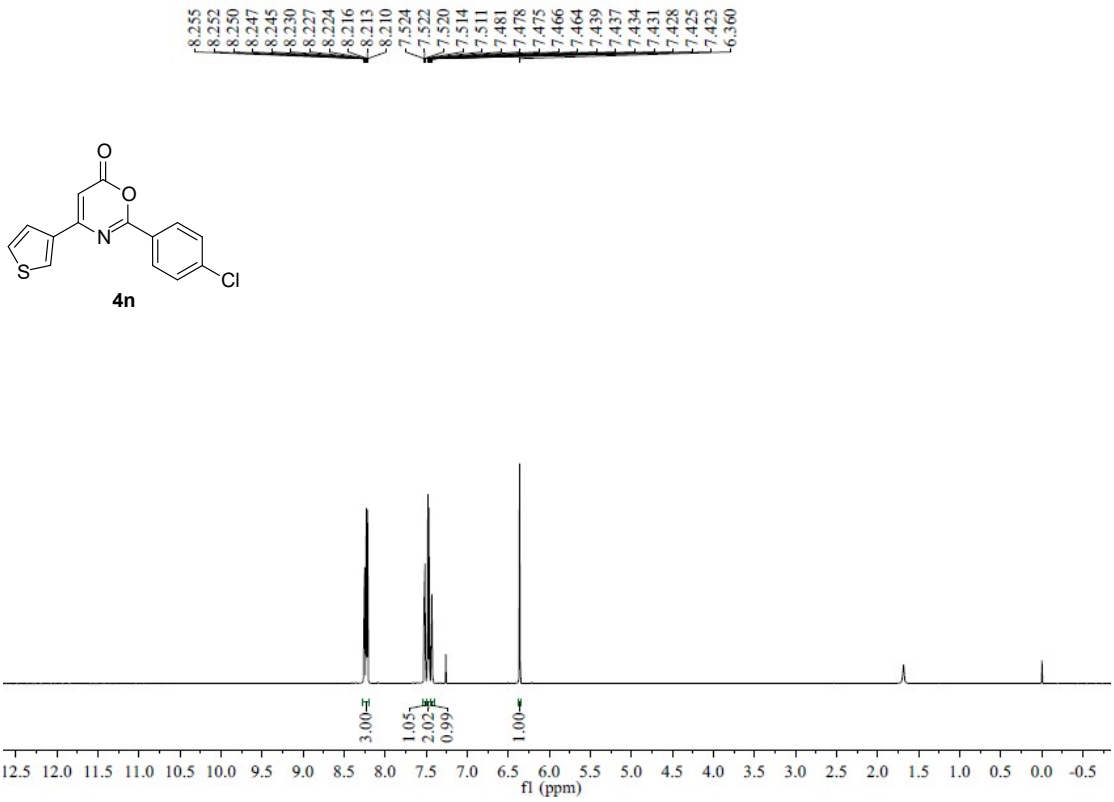
^{13}C NMR spectra for compound **4l**



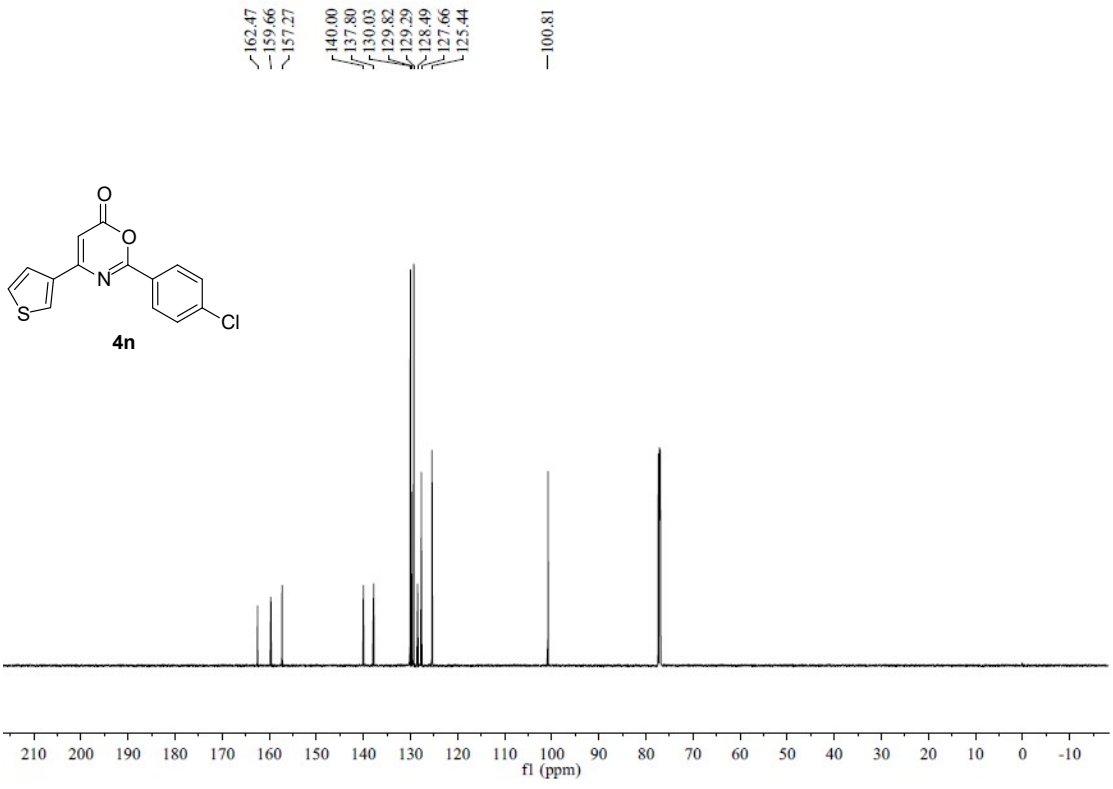
^{1}H NMR spectra for compound **4m**



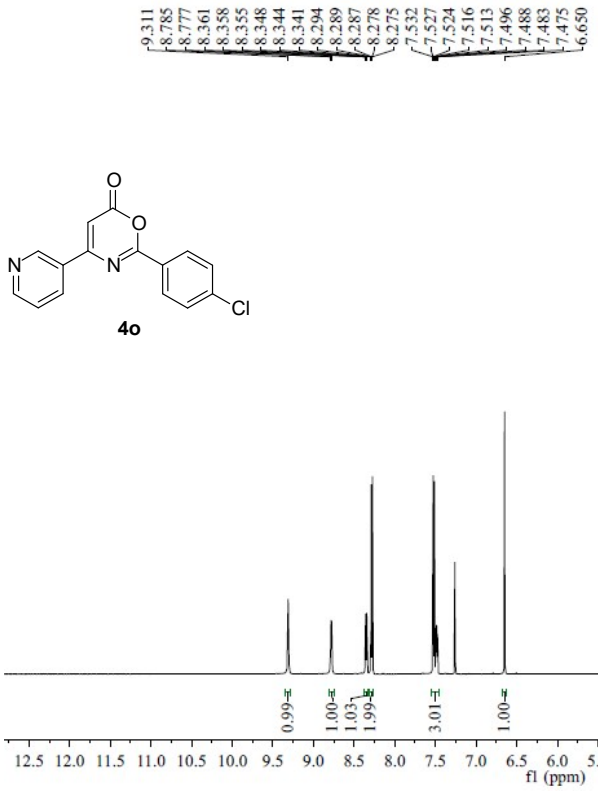
^{13}C NMR spectra for compound **4m**



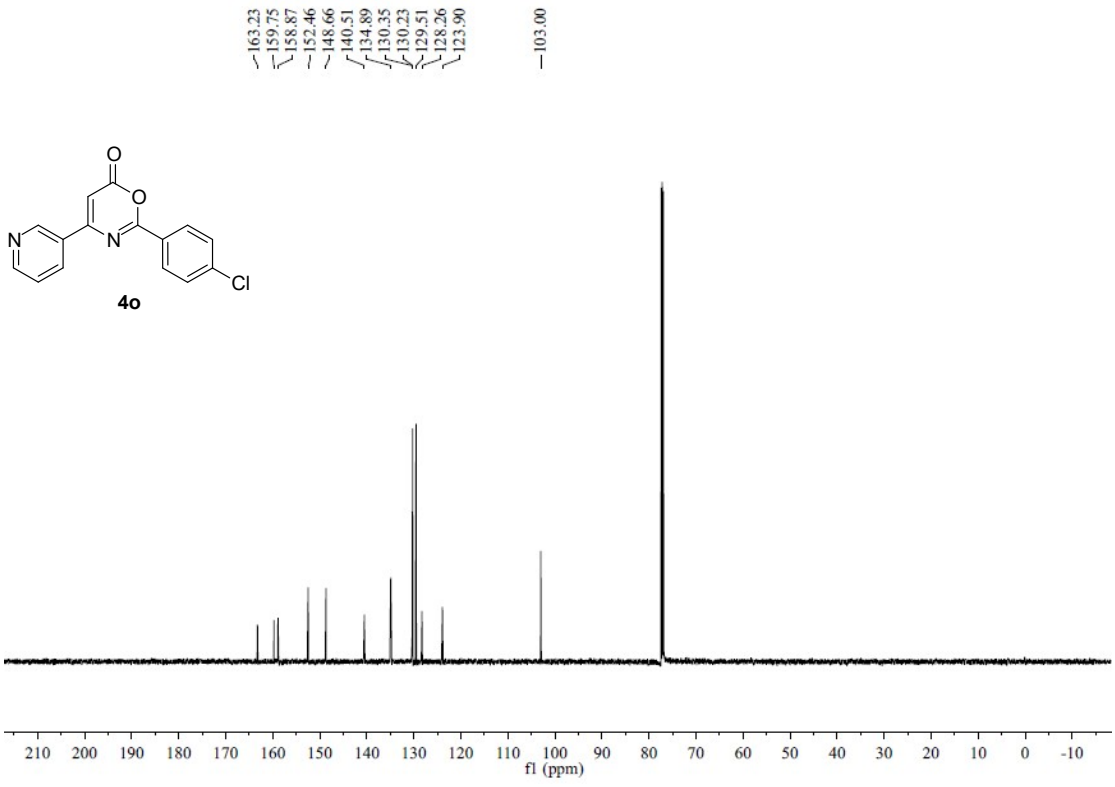
^{1}H NMR spectra for compound **4n**



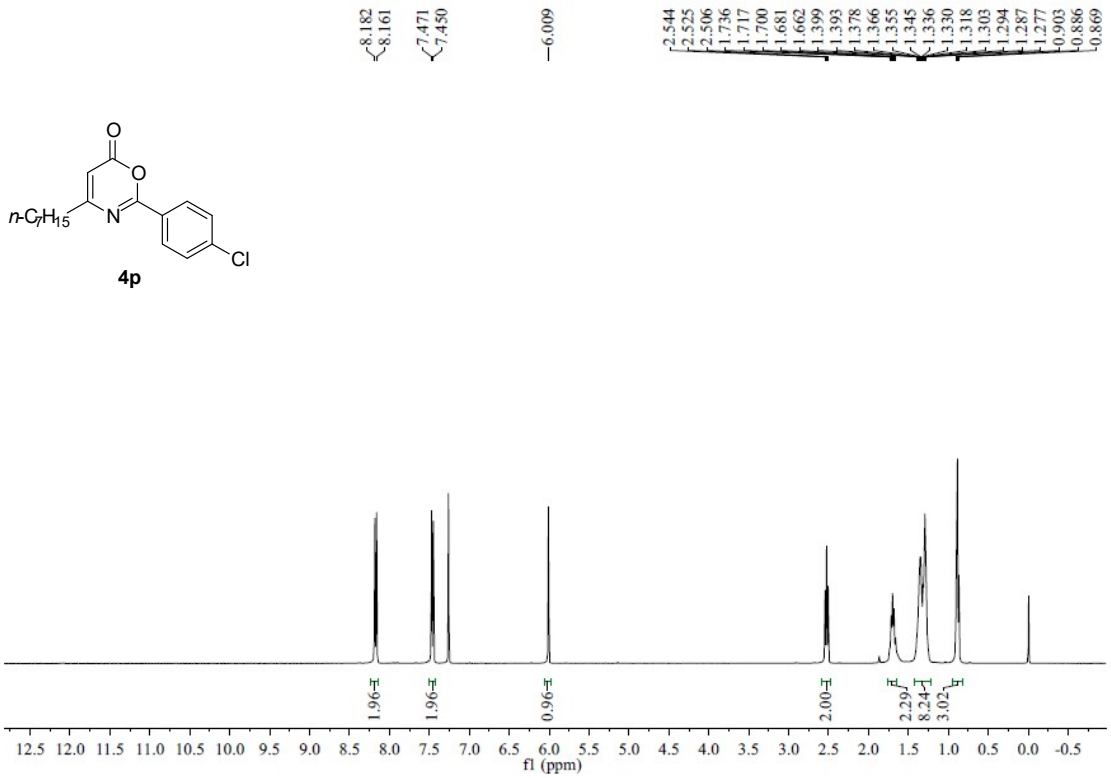
^{13}C NMR spectra for compound **4n**



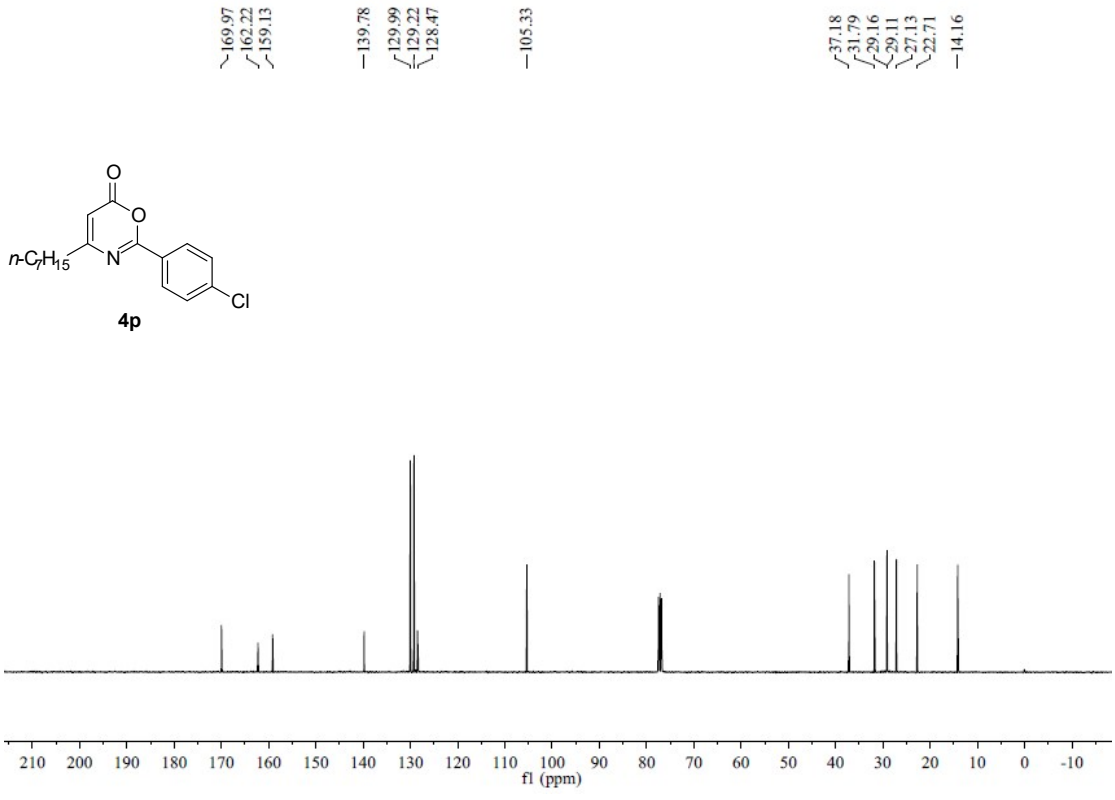
^{1}H NMR spectra for compound **4o**



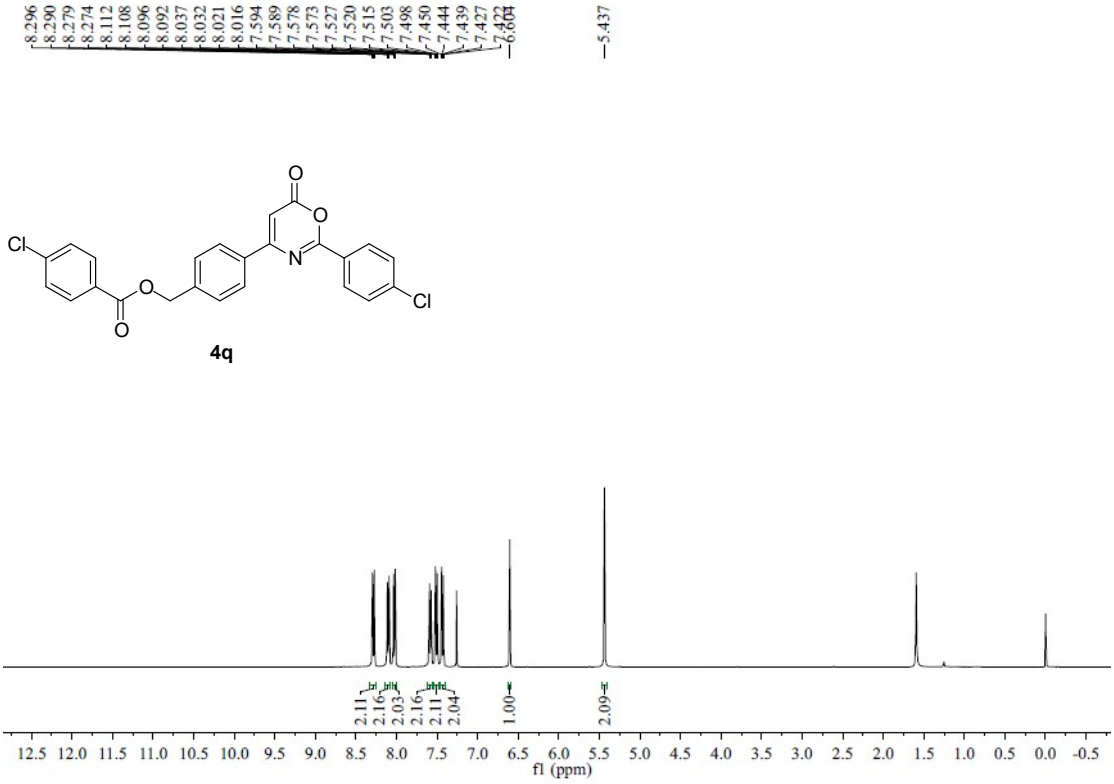
^{13}C NMR spectra for compound **4o**



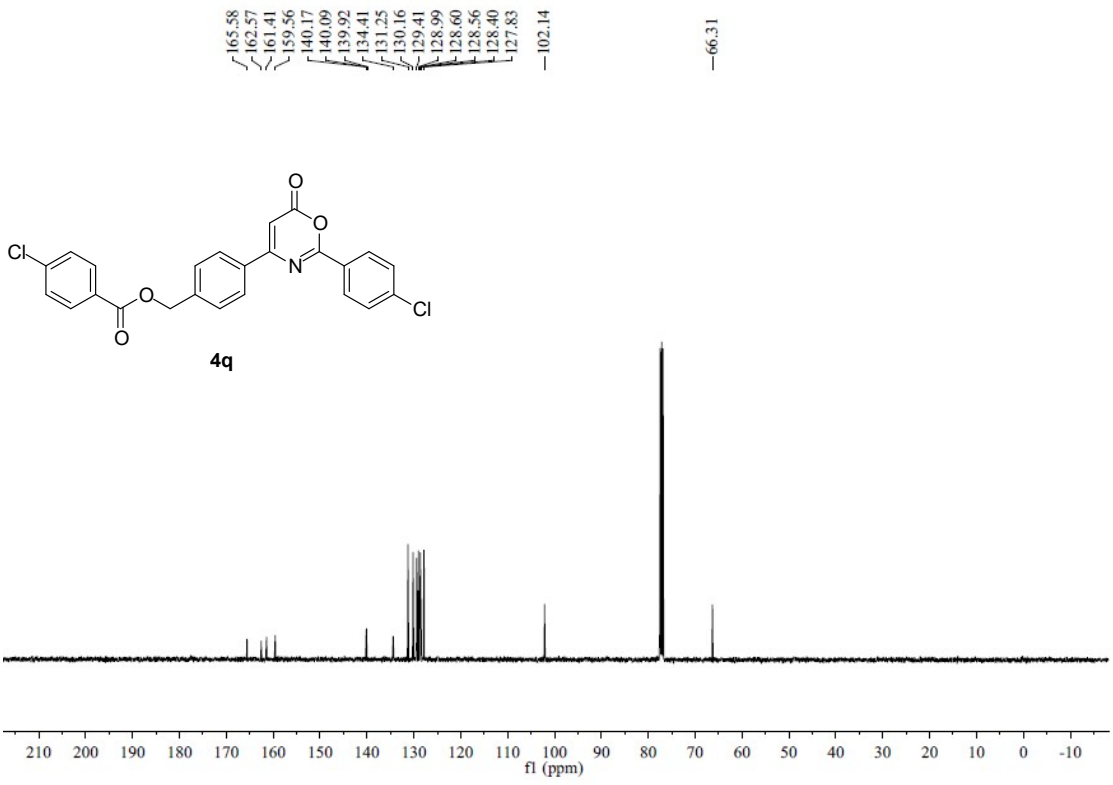
^{1}H NMR spectra for compound **4p**



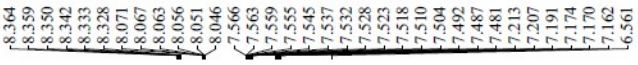
^{13}C NMR spectra for compound **4p**

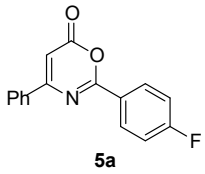


^{1}H NMR spectra for compound **4q**

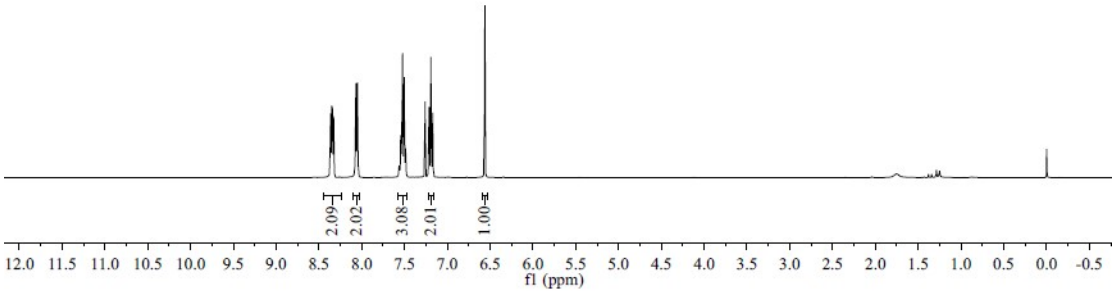


^{13}C NMR spectra for compound **4q**

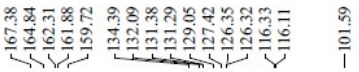


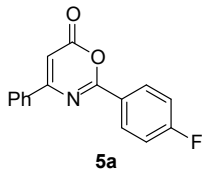


5a



^{1}H NMR spectra for compound **5a**





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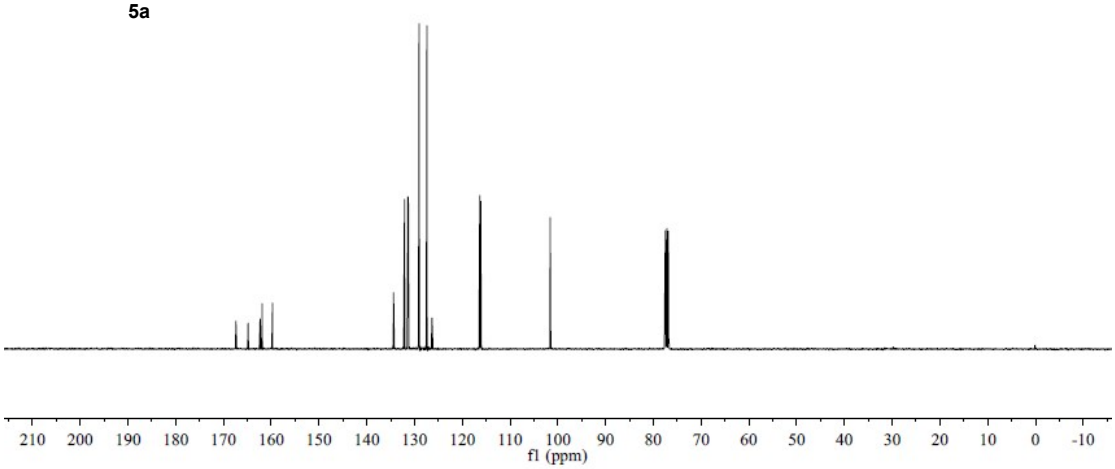
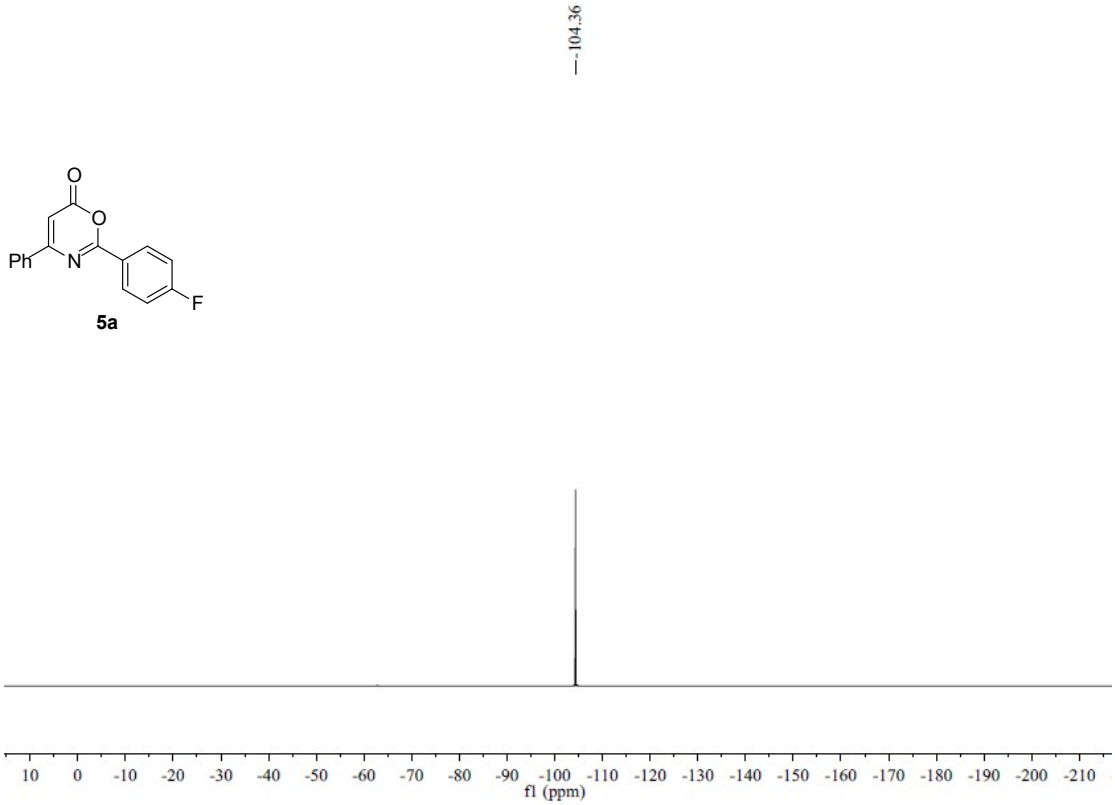
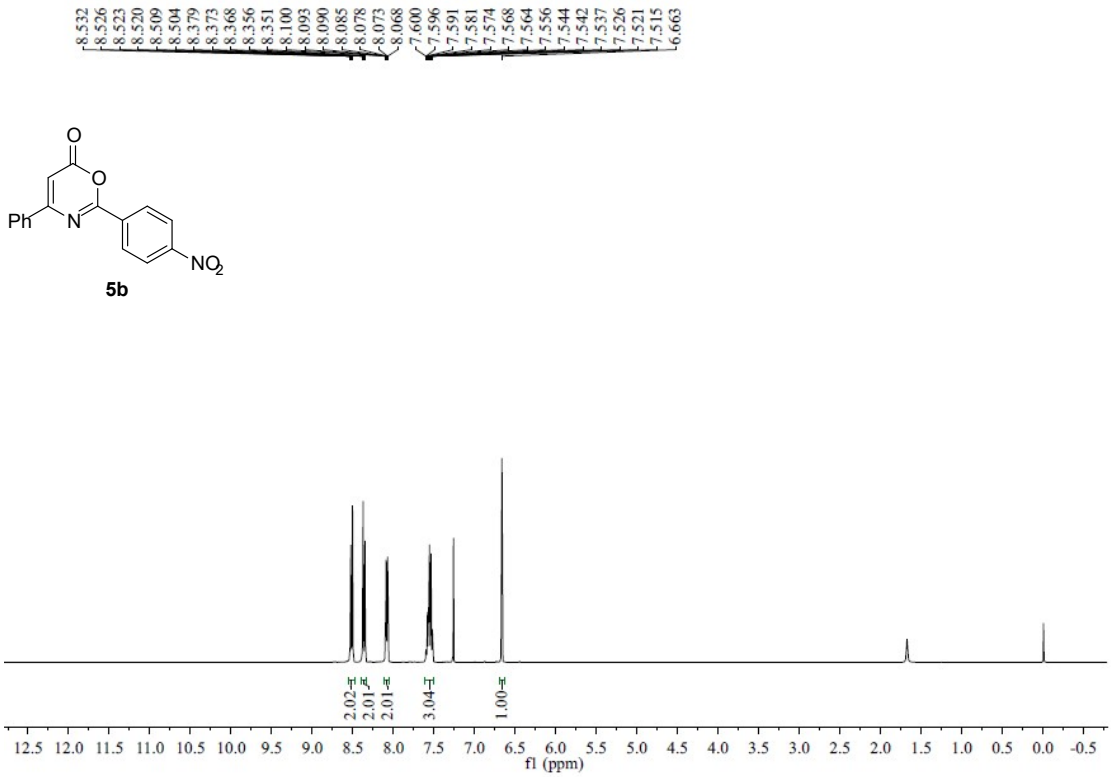


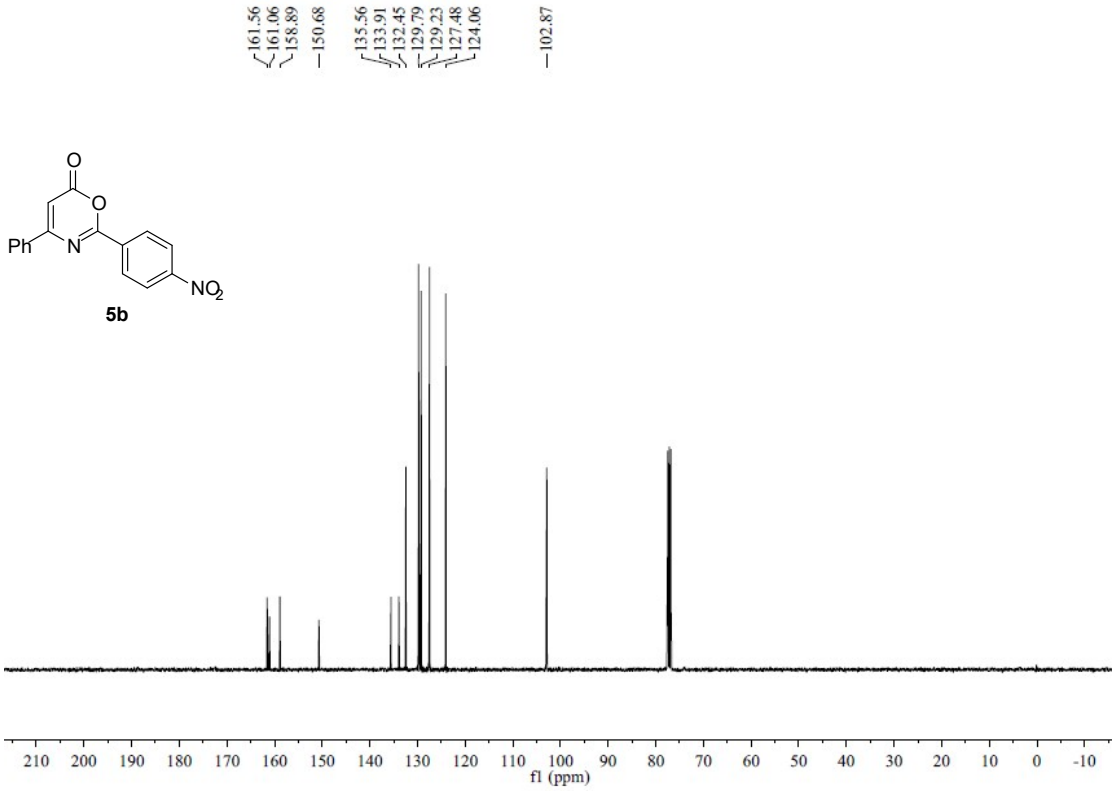
^{13}C NMR spectra for compound **5a**



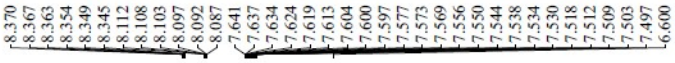
^{19}F NMR spectra for compound **5a**

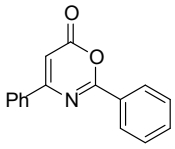


^{1}H NMR spectra for compound **5b**

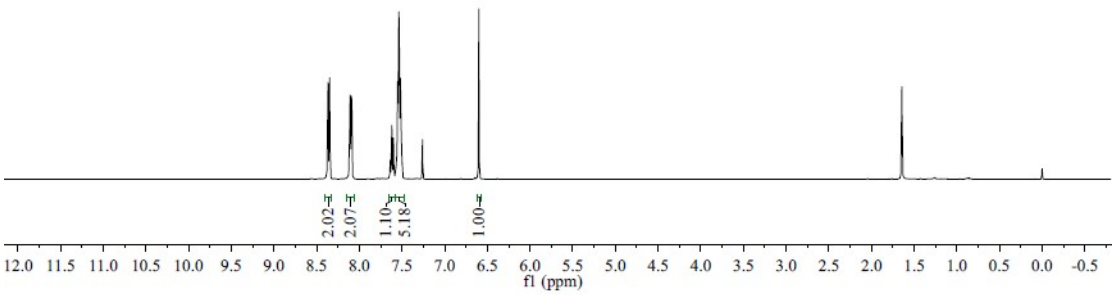


^{13}C NMR spectra for compound **5b**

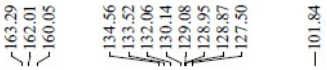


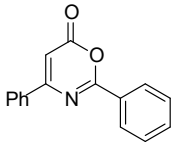


5c

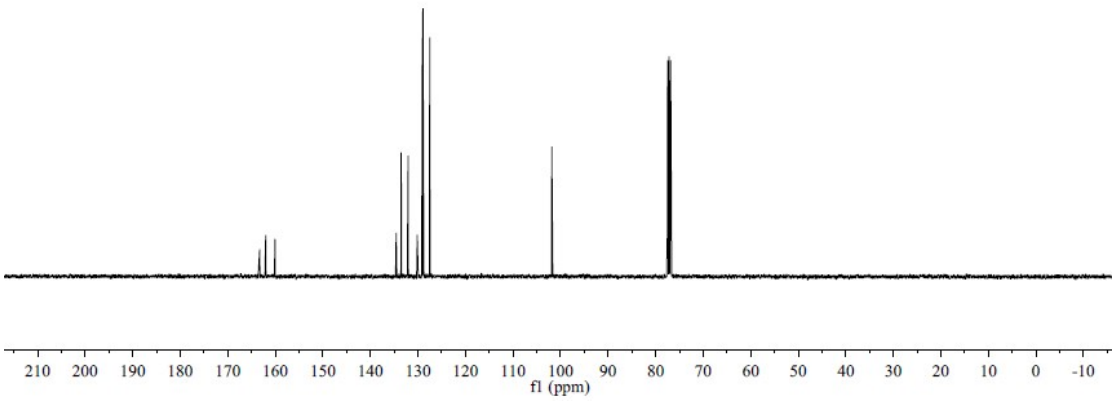


^{1}H NMR spectra for compound **5c**

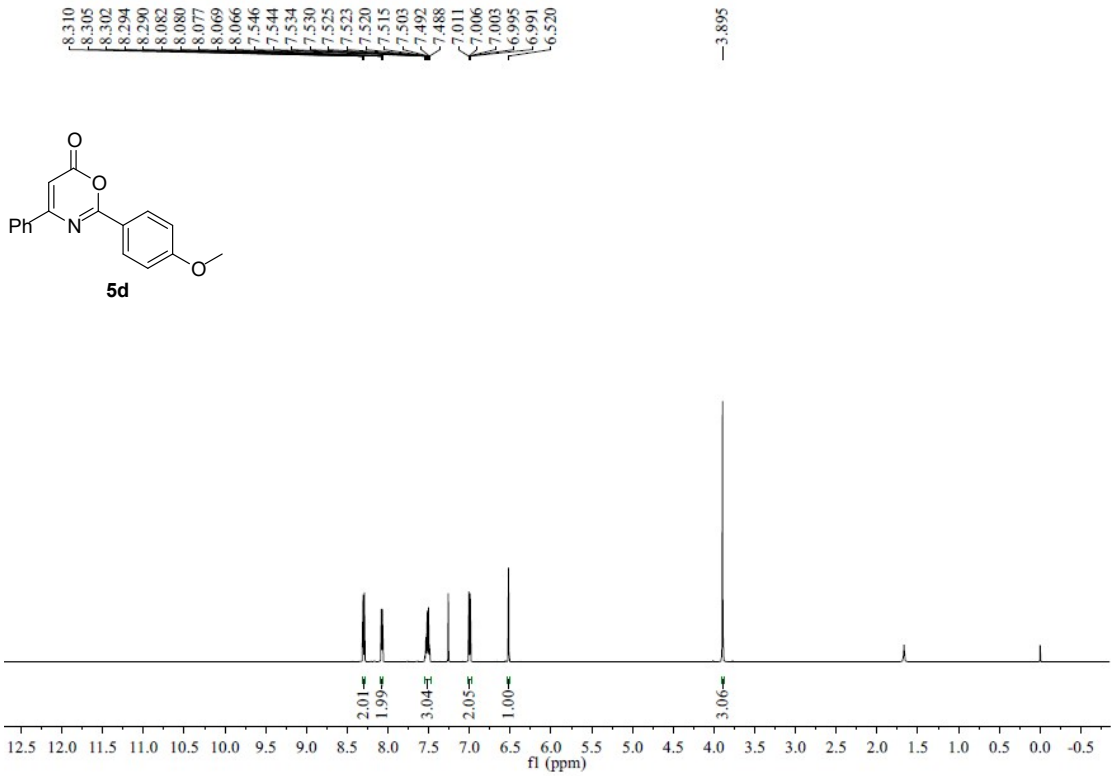




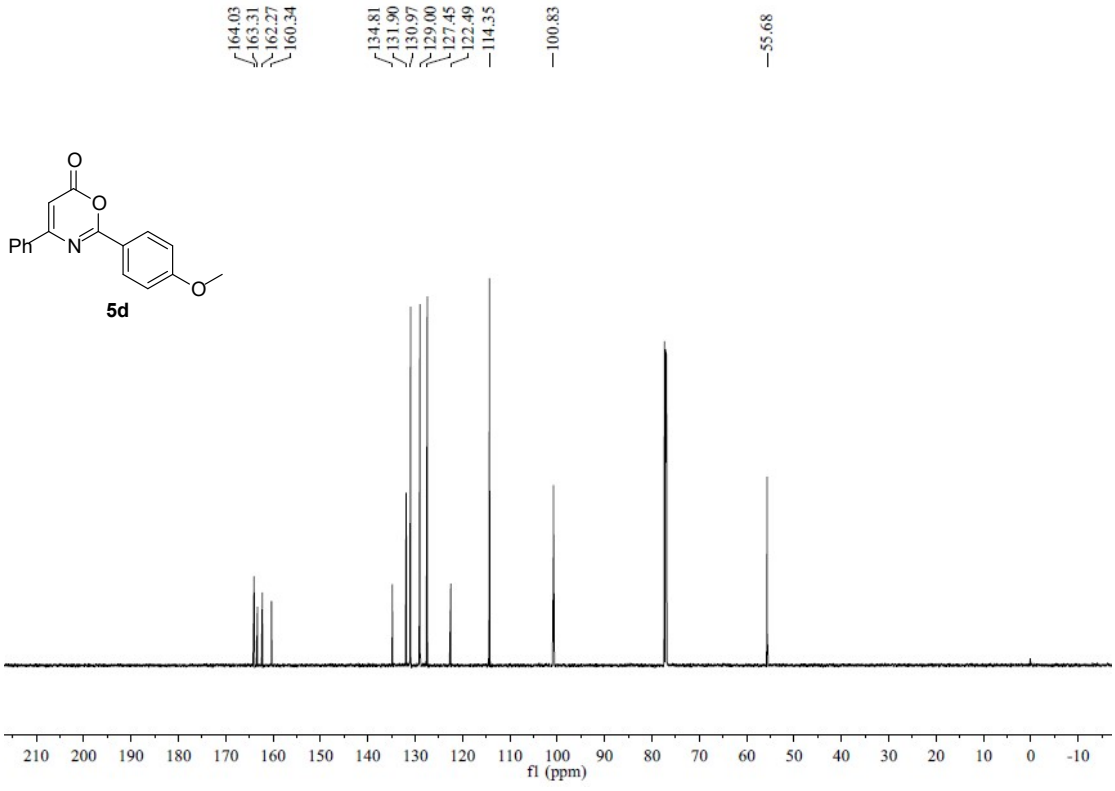
5c



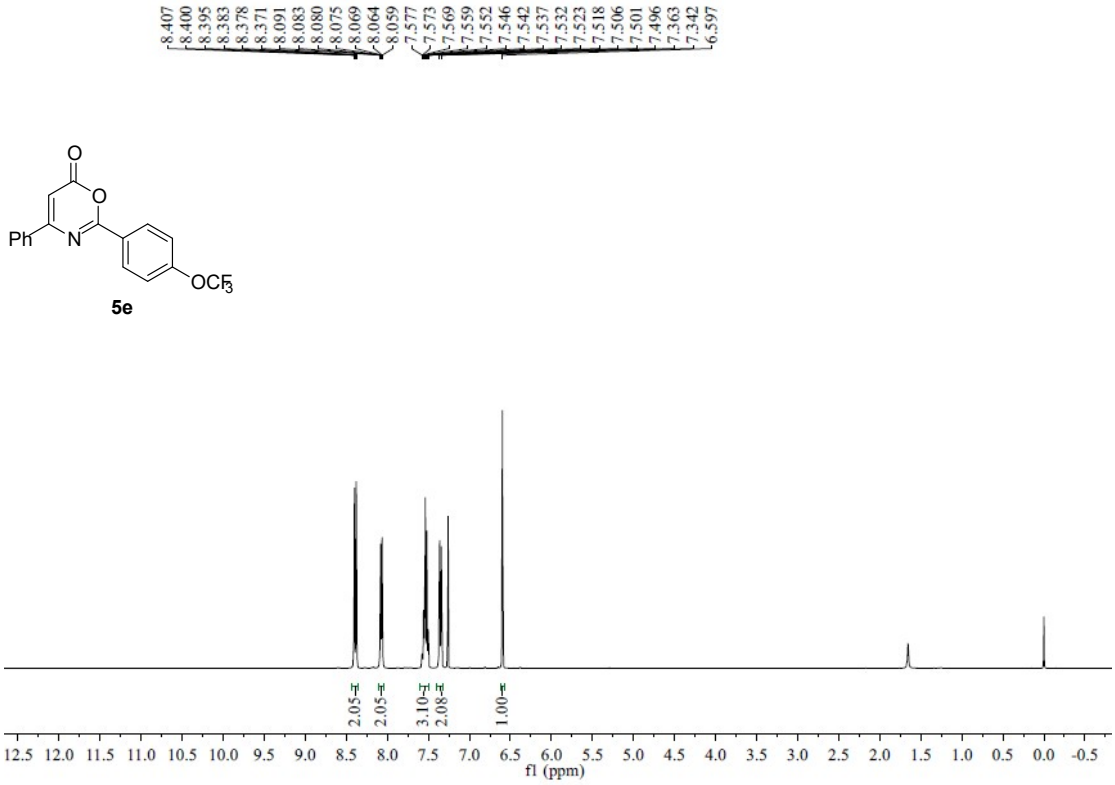
^{13}C NMR spectra for compound **5c**



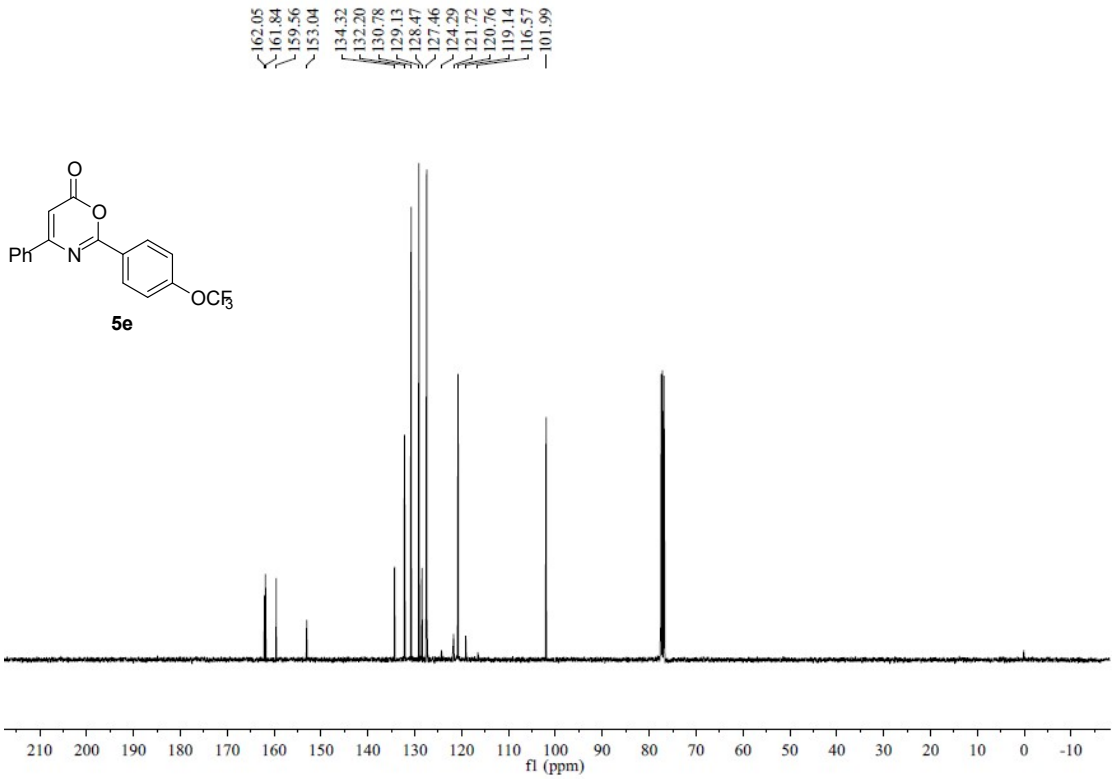
^{1}H NMR spectra for compound **5d**



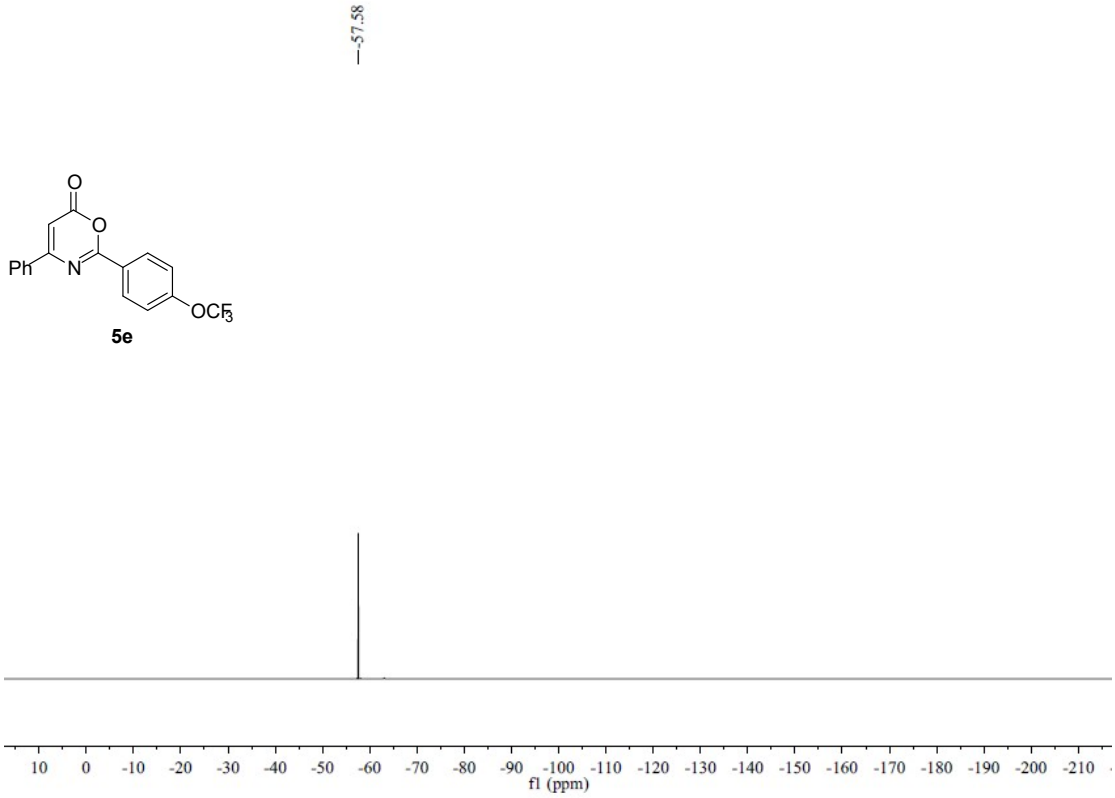
^{13}C NMR spectra for compound **5d**



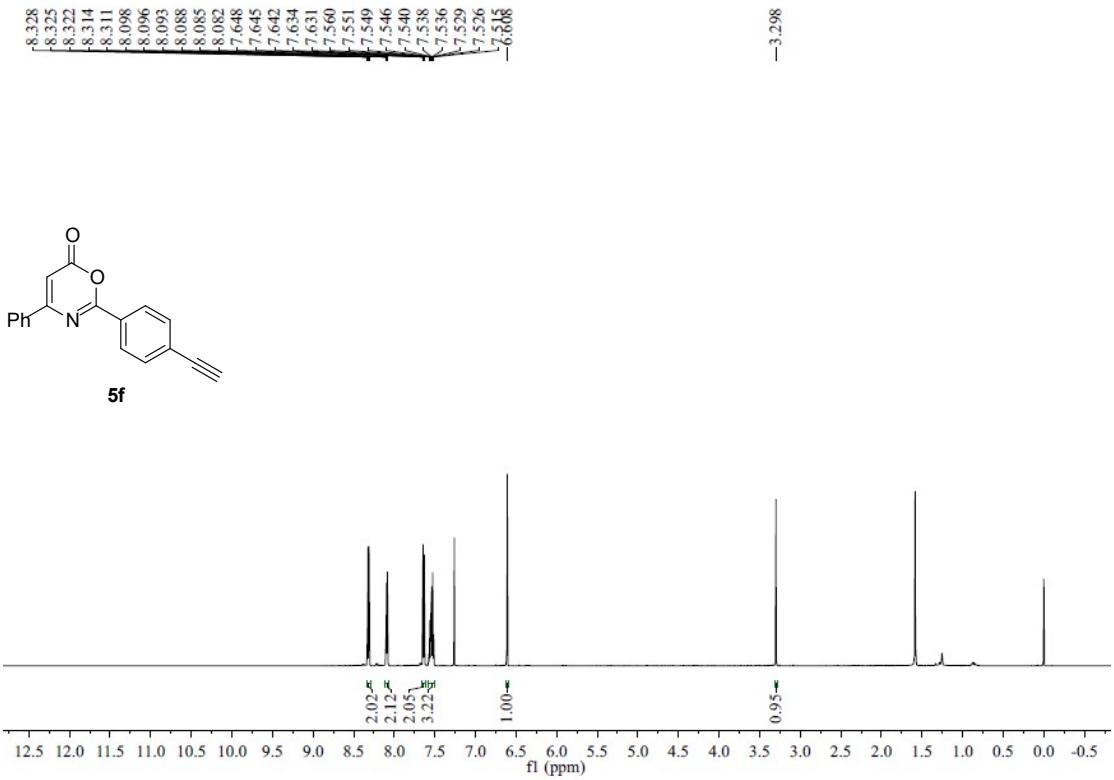
^{1}H NMR spectra for compound **5e**



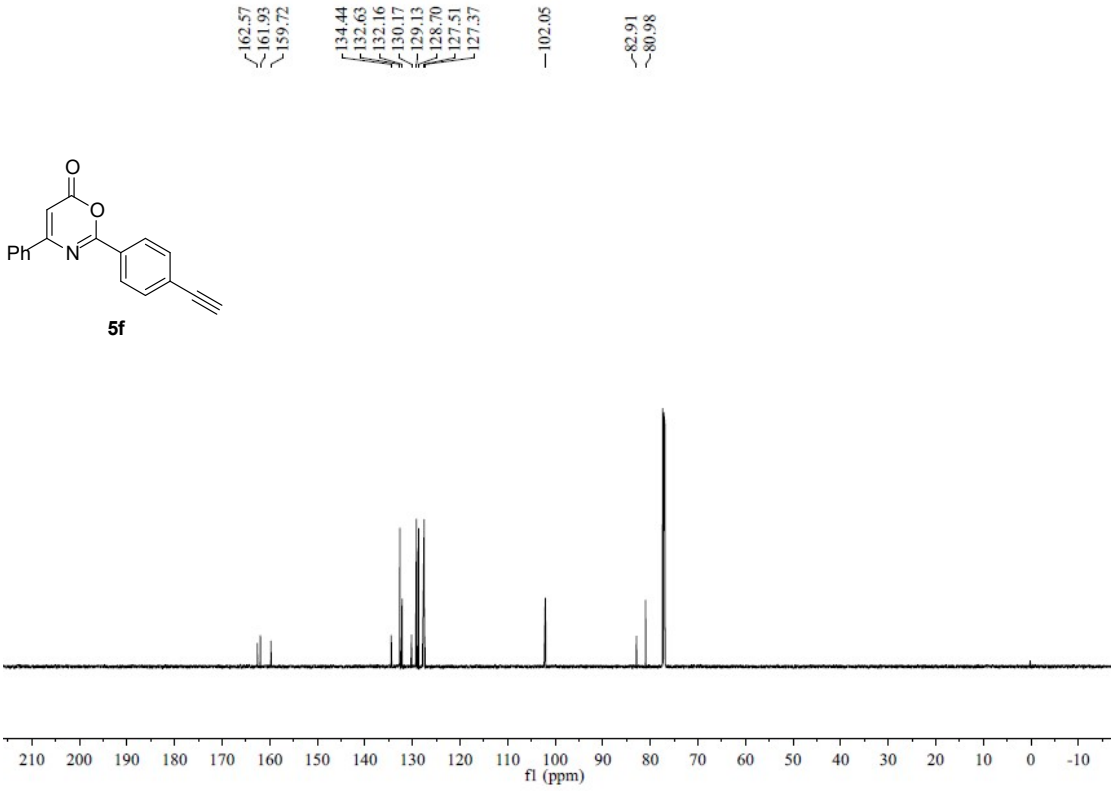
^{13}C NMR spectra for compound **5e**



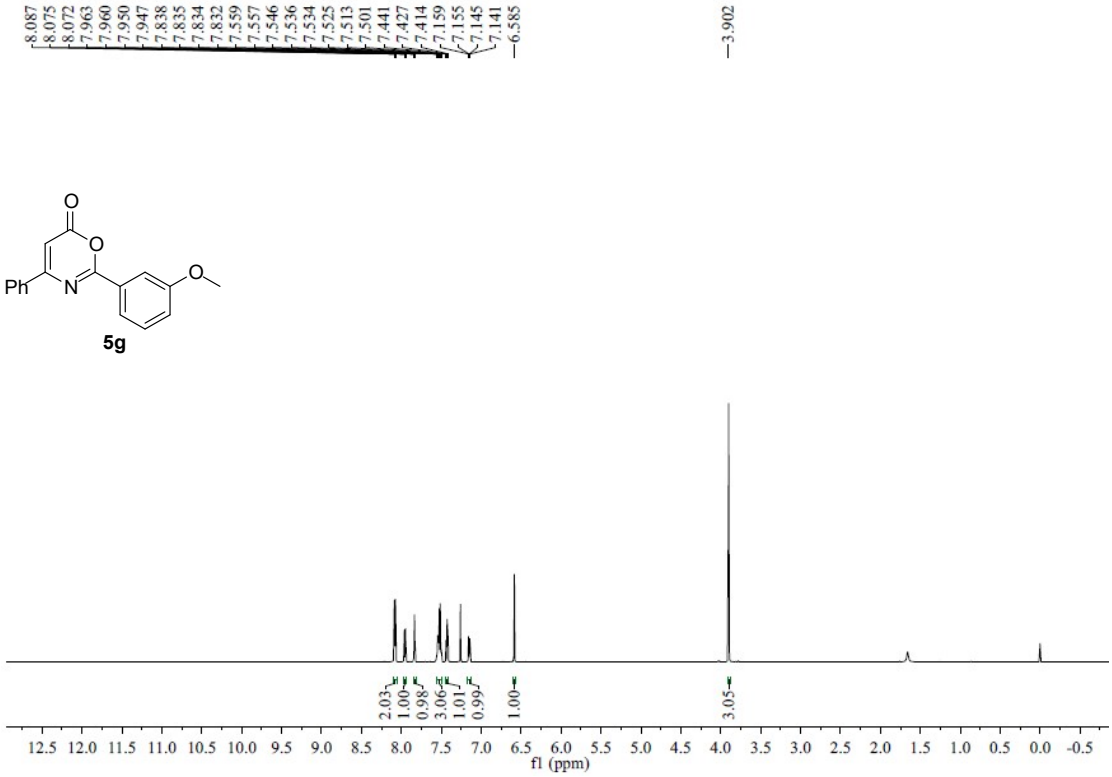
^{19}F NMR spectra for compound **5e**



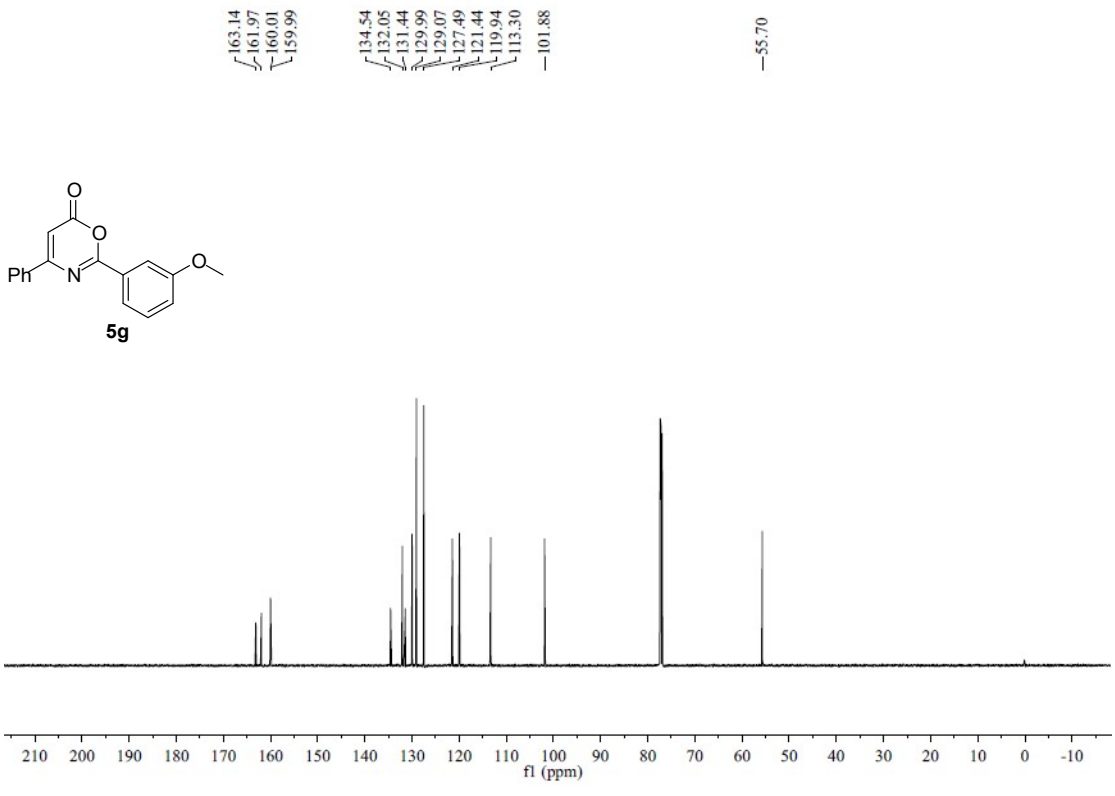
^{1}H NMR spectra for compound **5f**



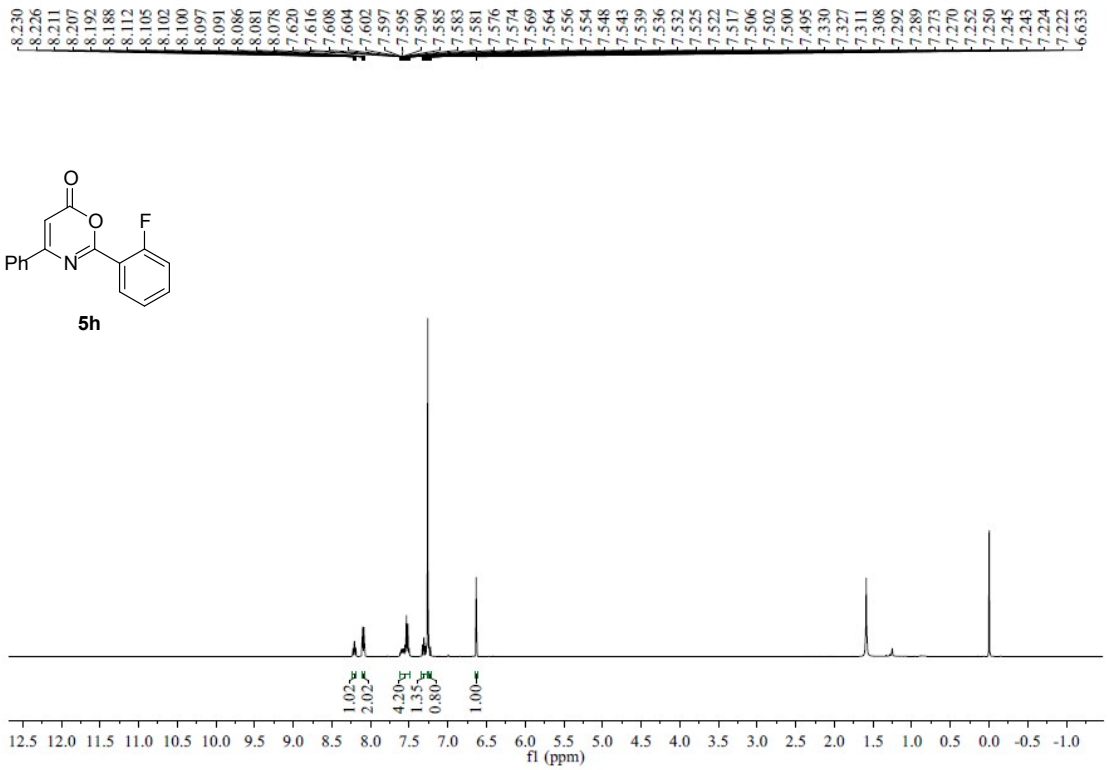
^{13}C NMR spectra for compound **5f**



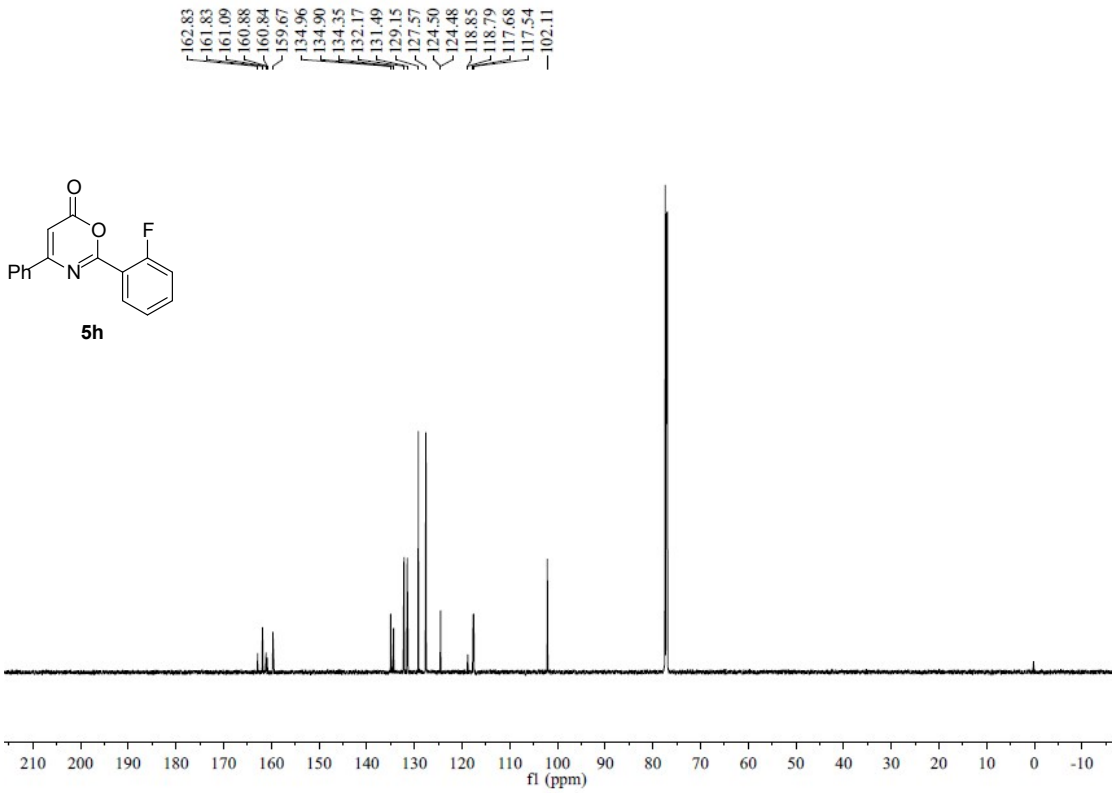
^{1}H NMR spectra for compound **5g**



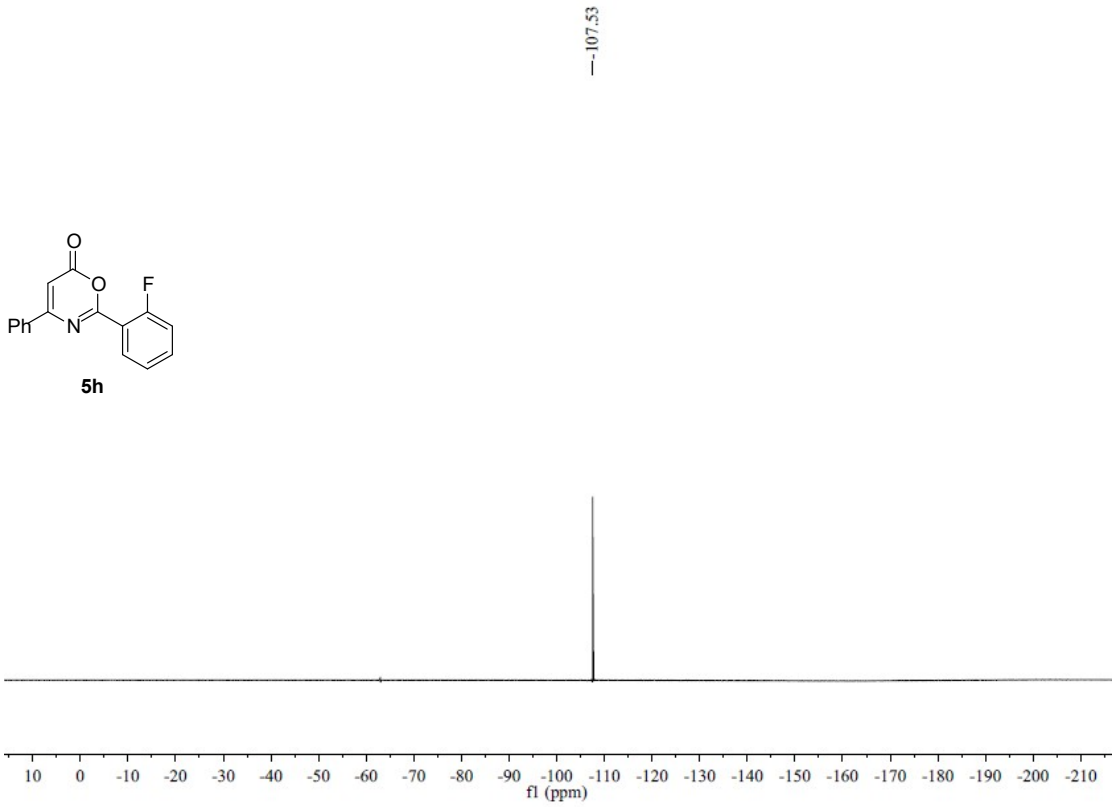
^{13}C NMR spectra for compound **5g**



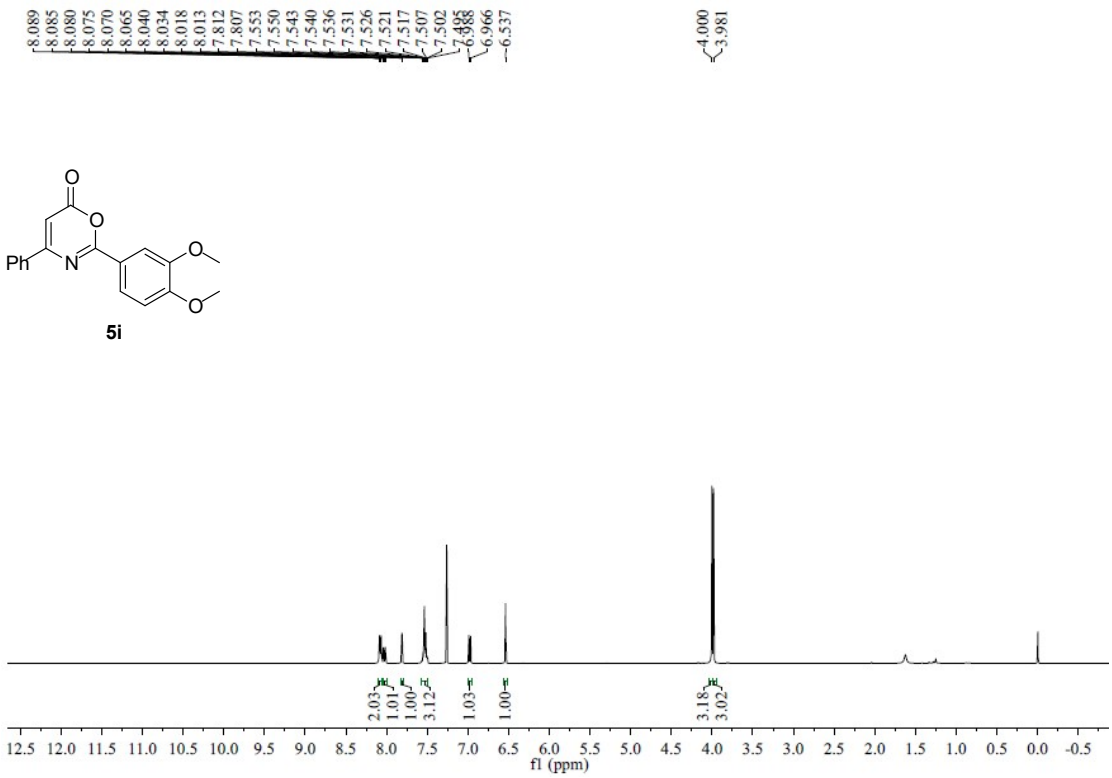
^{1}H NMR spectra for compound **5h**



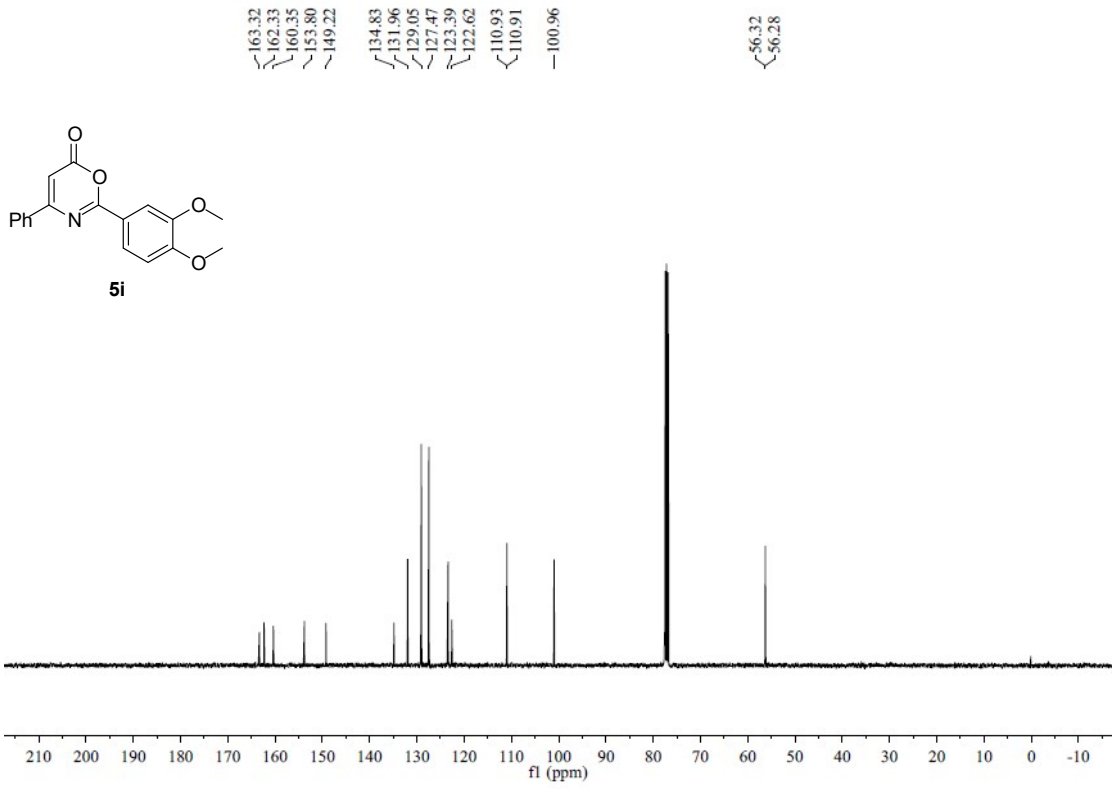
^{13}C NMR spectra for compound **5h**



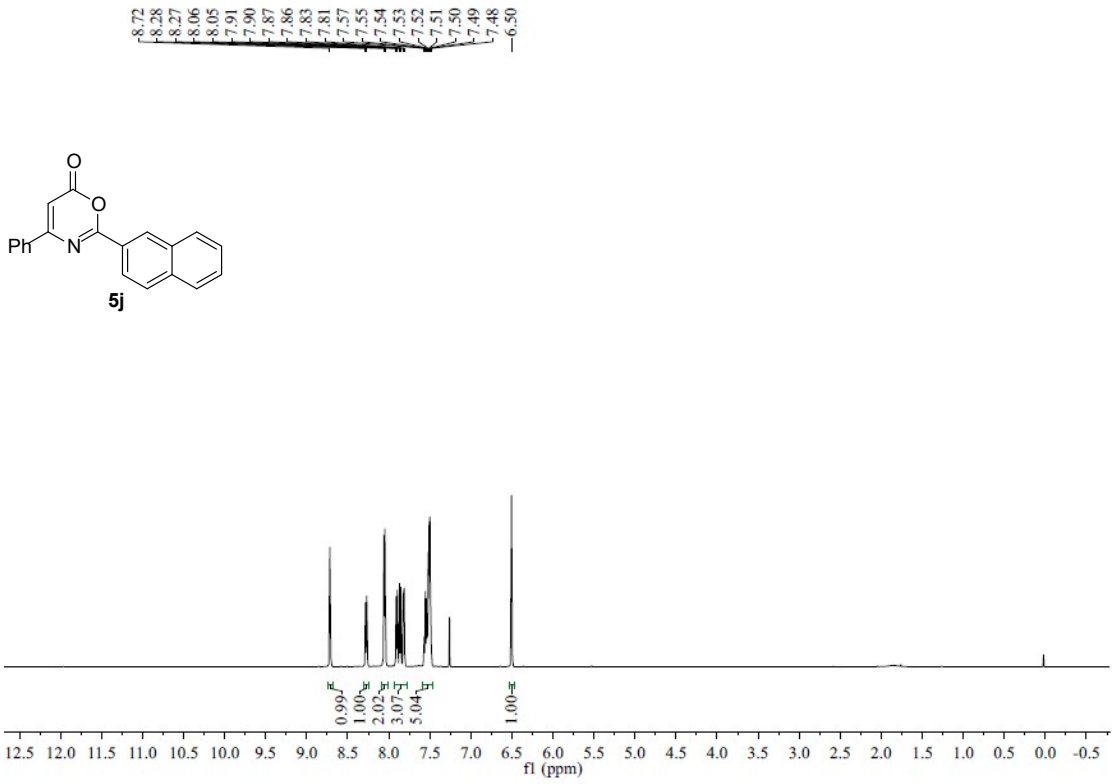
^{19}F NMR spectra for compound **5h**



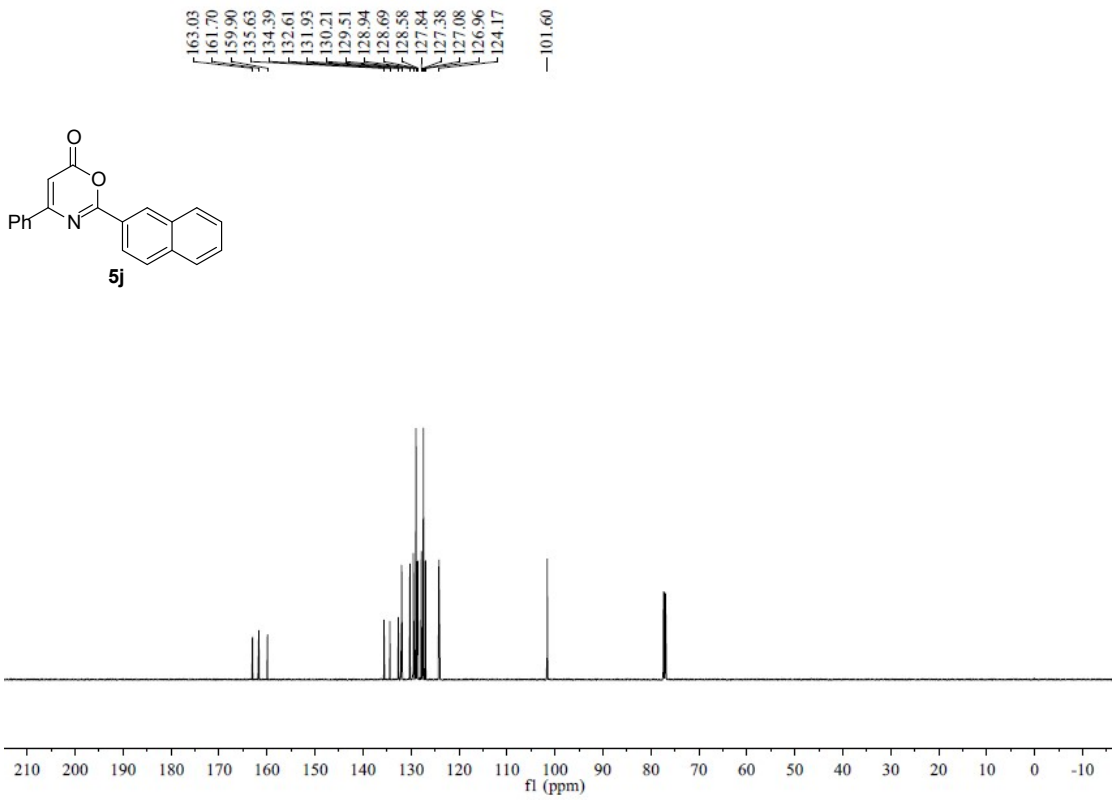
^{1}H NMR spectra for compound **5i**



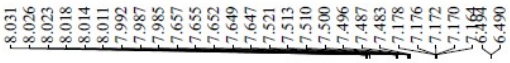
^{13}C NMR spectra for compound **5i**

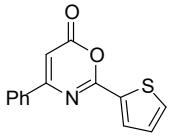


^{1}H NMR spectra for compound **5j**

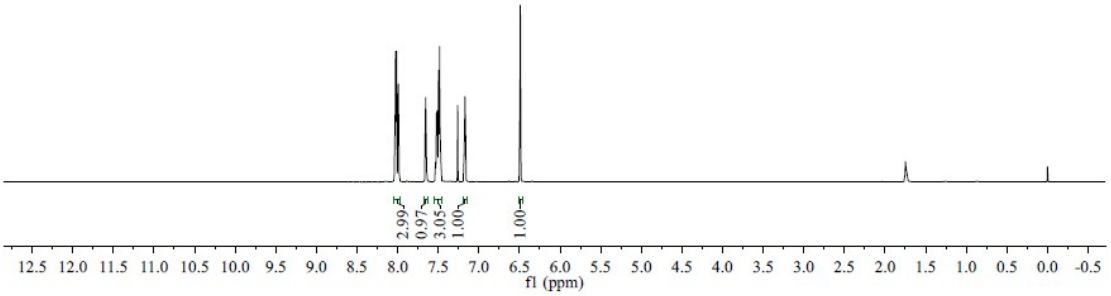


^{13}C NMR spectra for compound **5j**

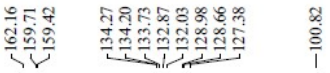


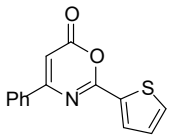


5k



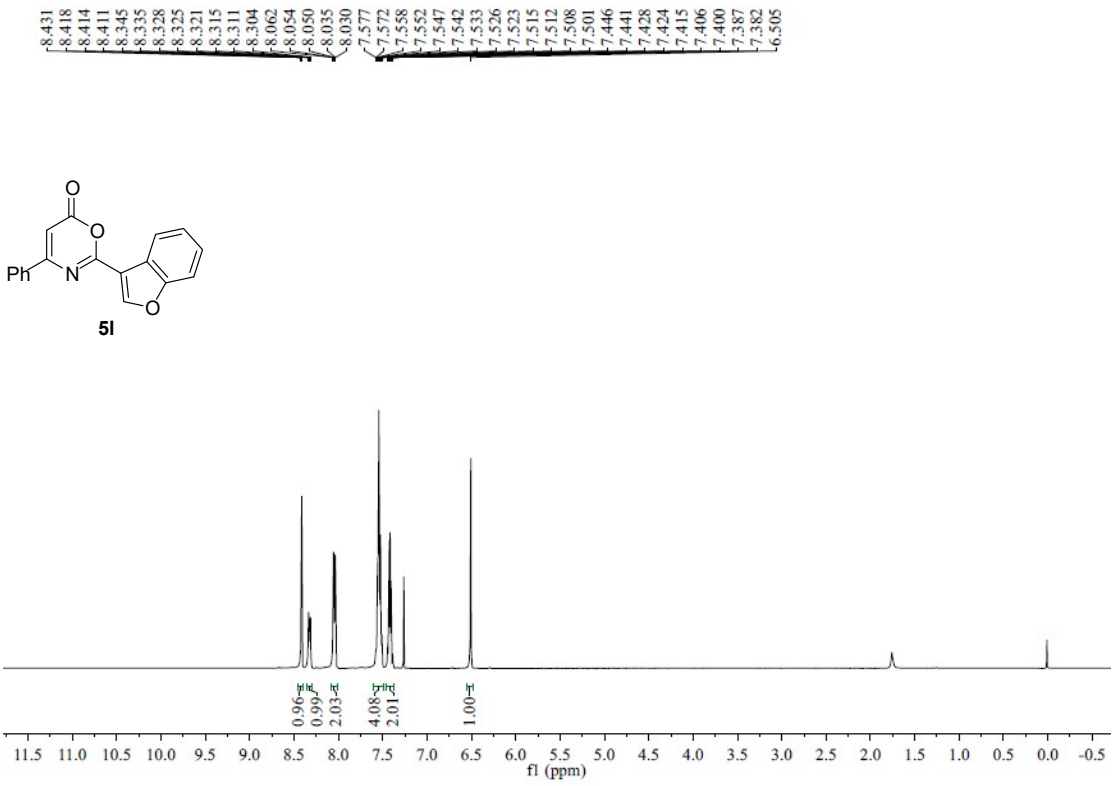
^{1}H NMR spectra for compound **5k**



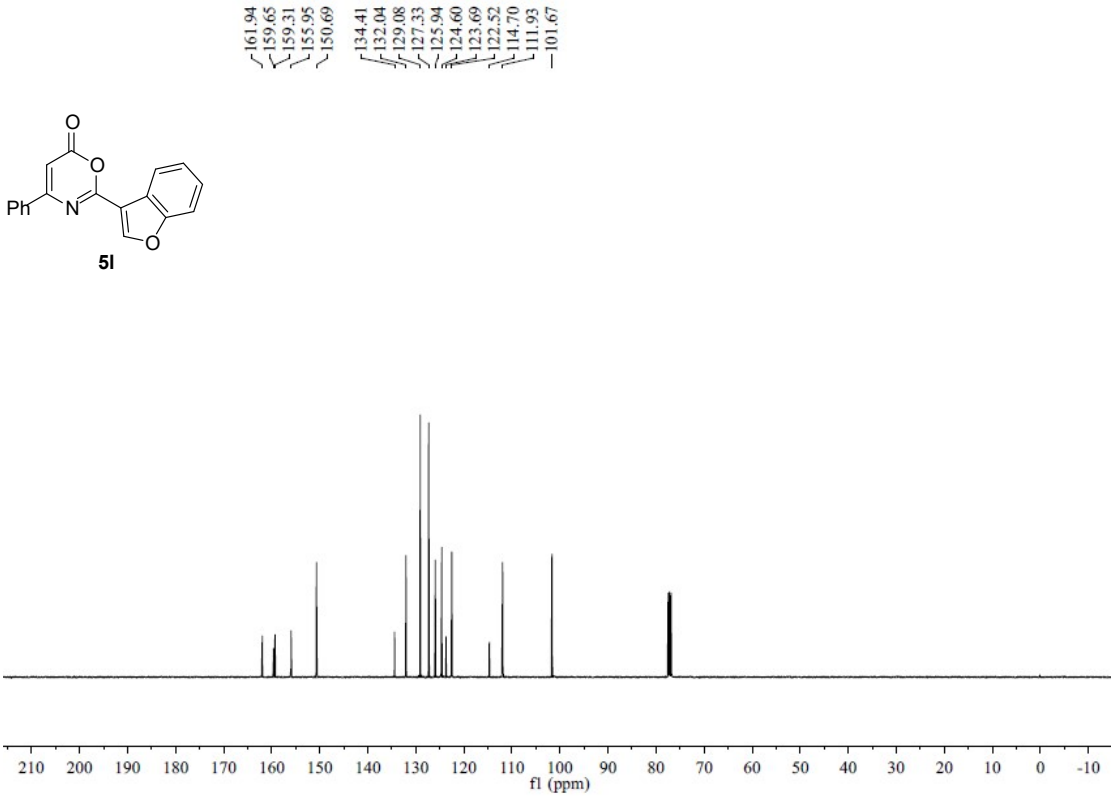


5k

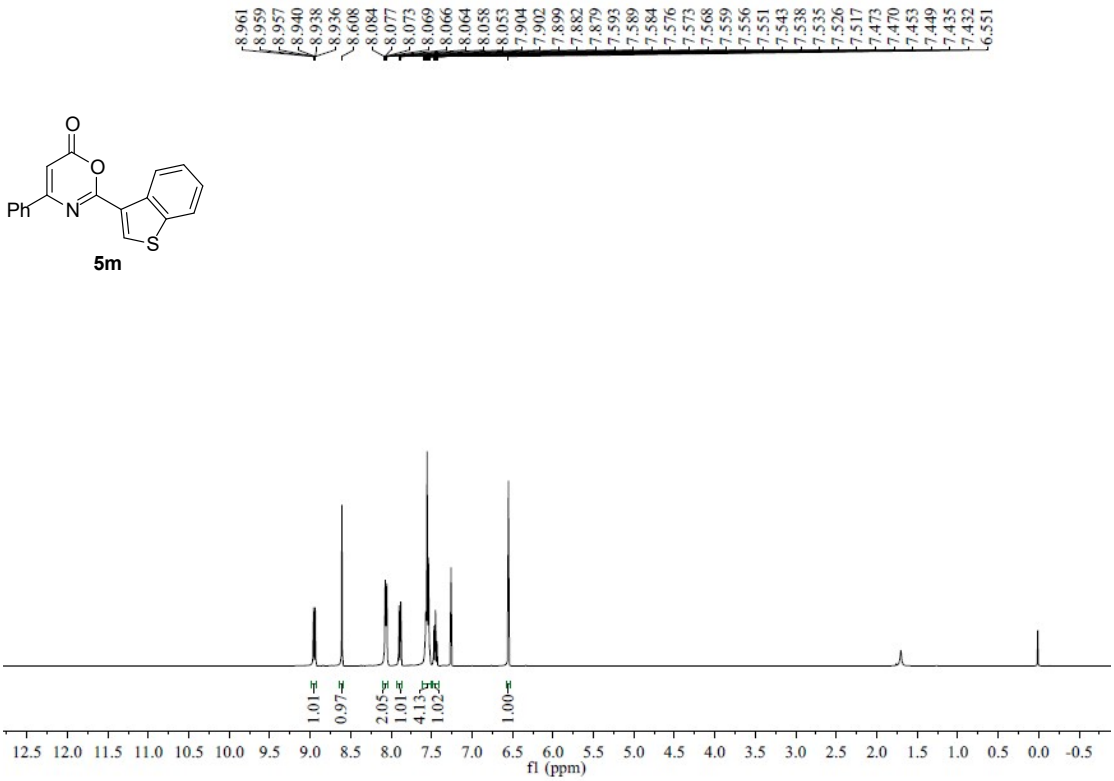
^{13}C NMR spectra for compound **5k**



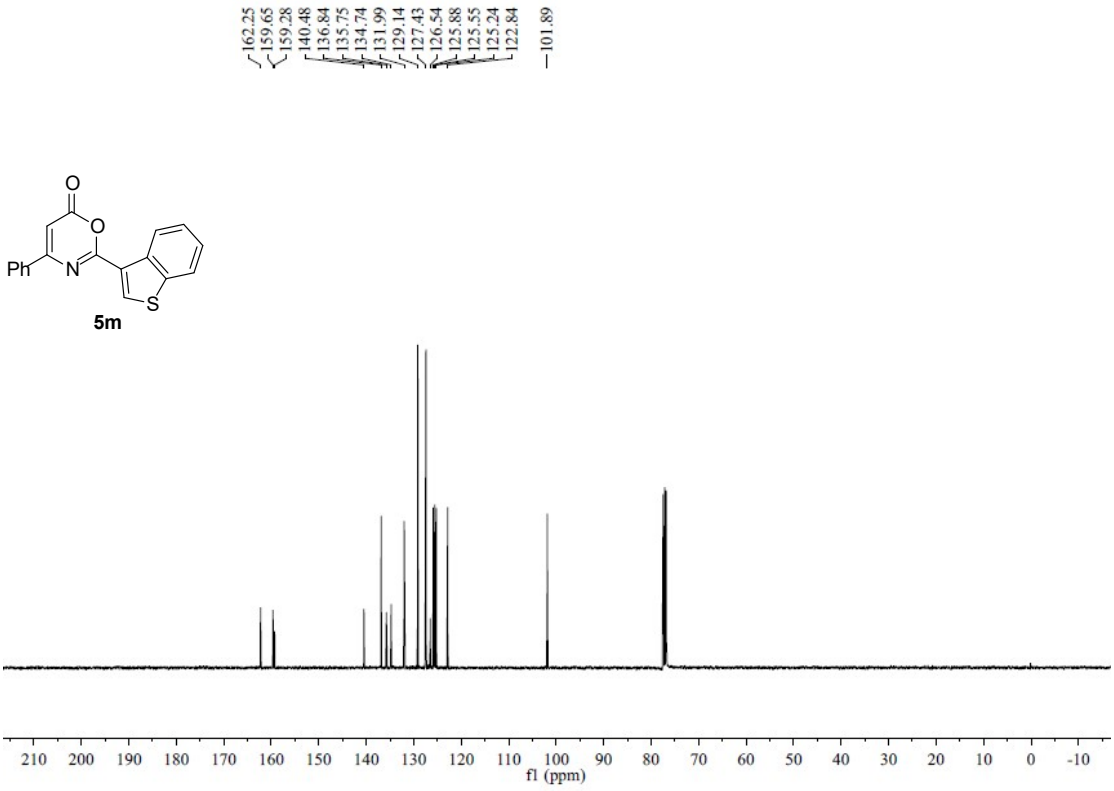
^{1}H NMR spectra for compound **5l**



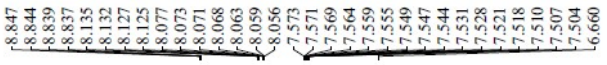
^{13}C NMR spectra for compound **5l**

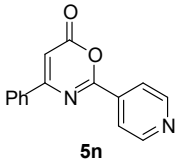


^{1}H NMR spectra for compound **5m**

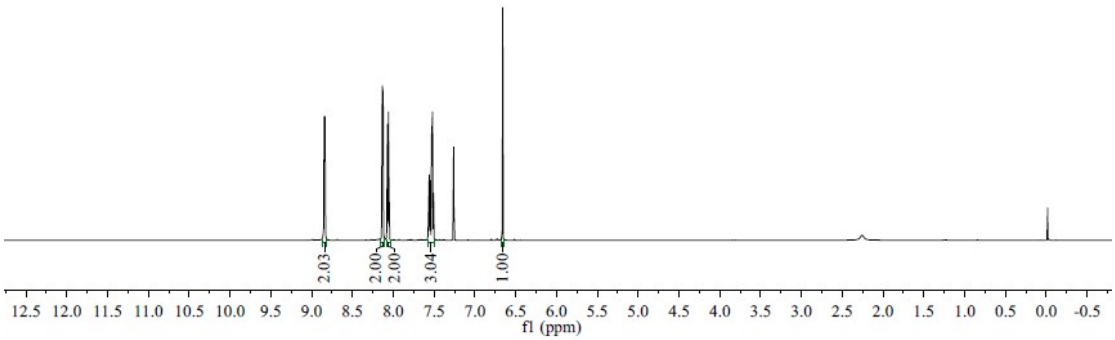


^{13}C NMR spectra for compound **5m**

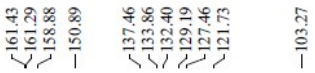


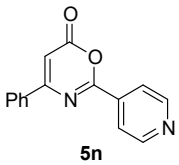


5n

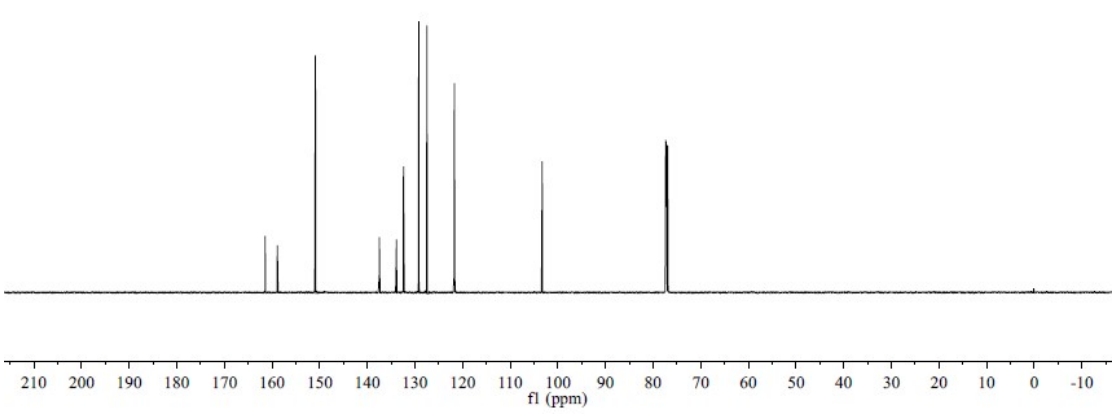


^{1}H NMR spectra for compound **5n**

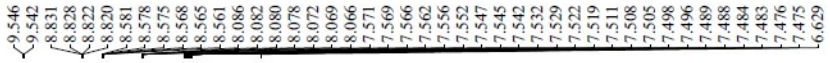


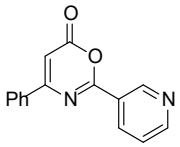


5n

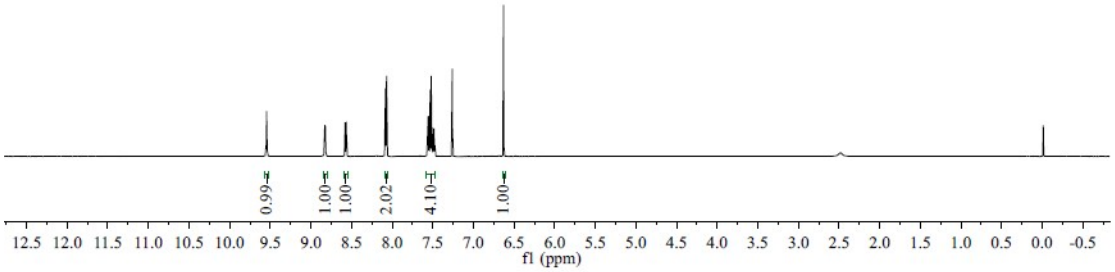


^{13}C NMR spectra for compound **5n**

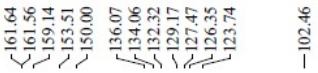


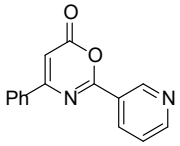


5o

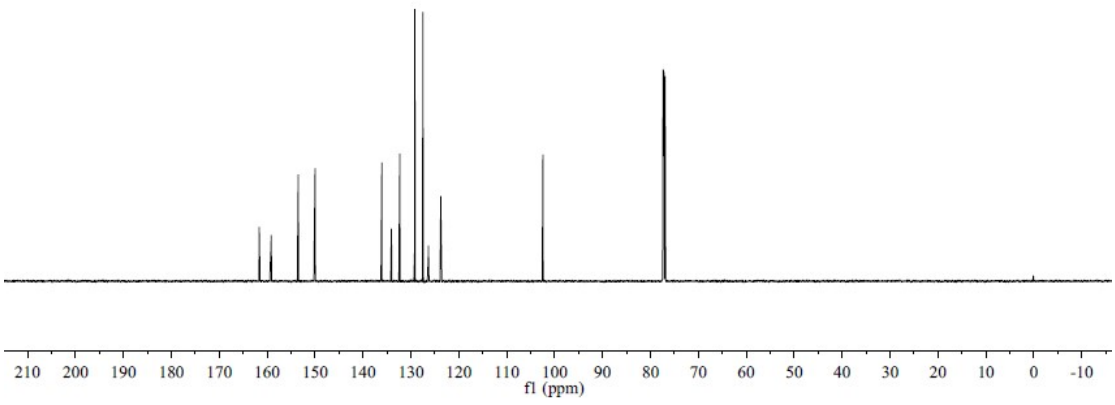


^{1}H NMR spectra for compound **5o**

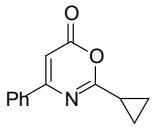




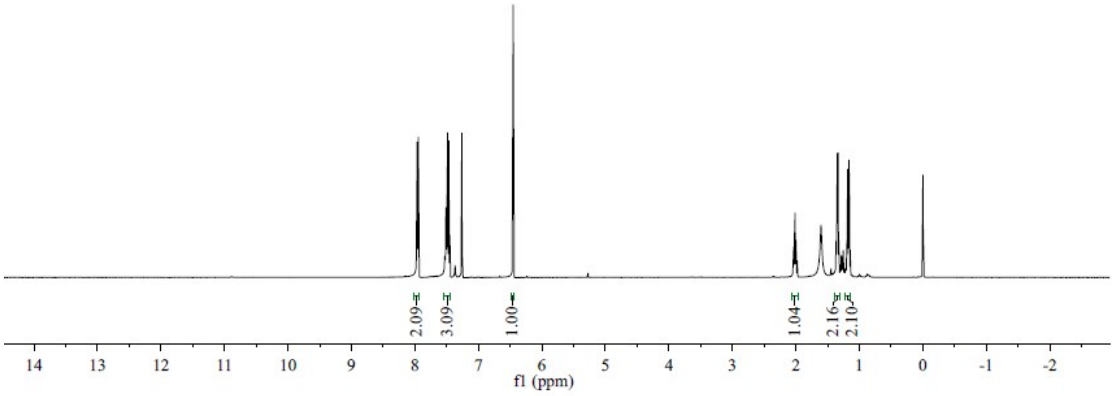
5o



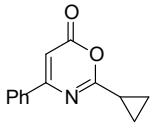
^{13}C NMR spectra for compound **5o**



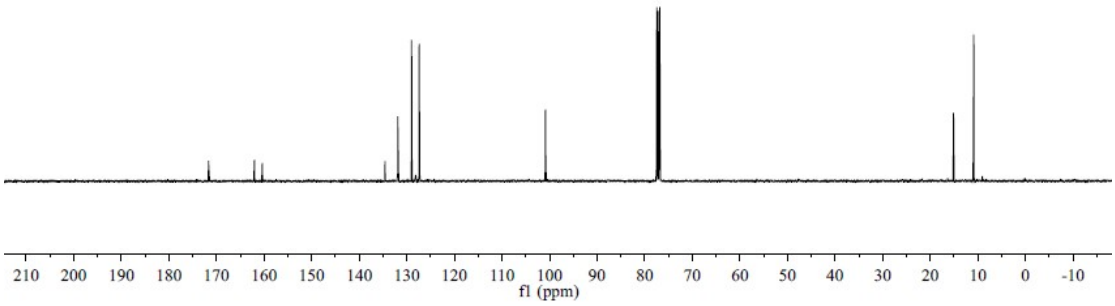
5p



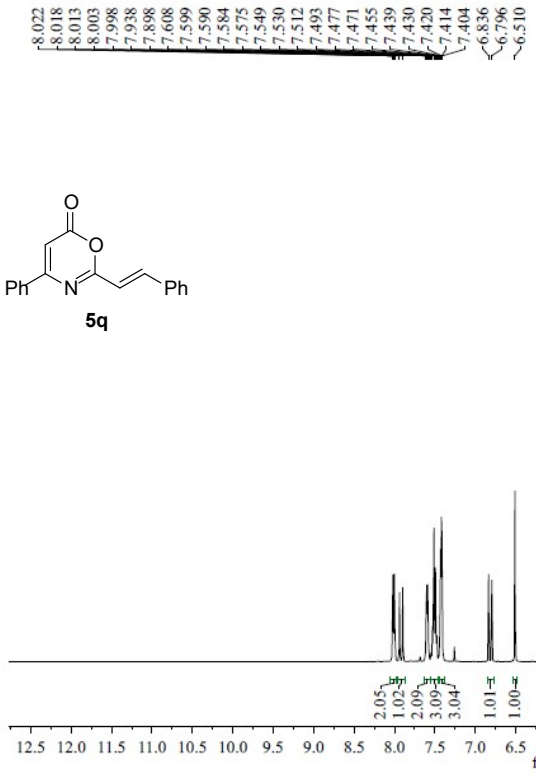
^{1}H NMR spectra for compound **5p**



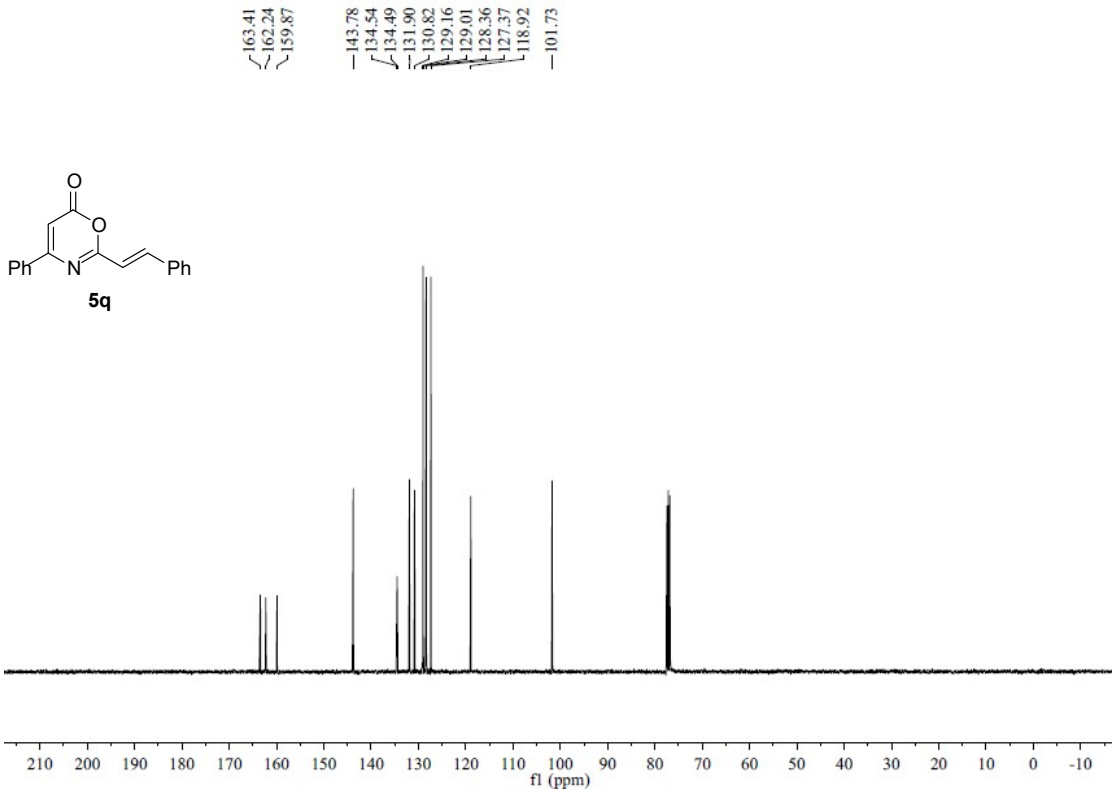
5p



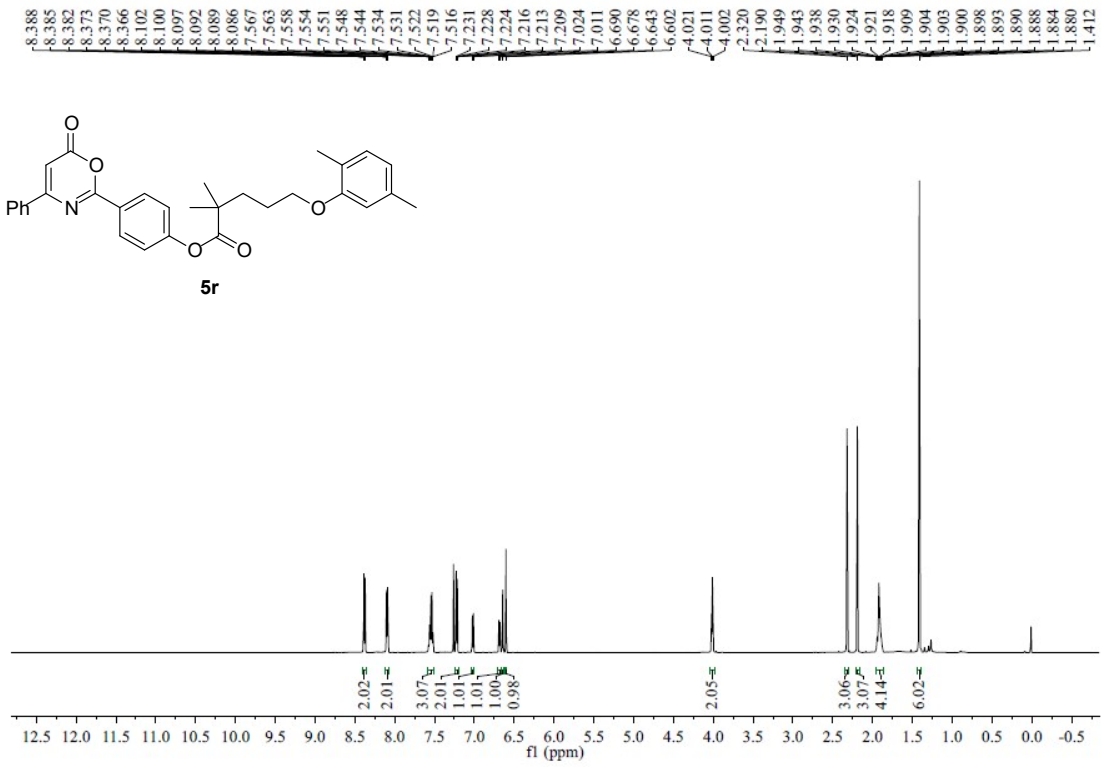
^{13}C NMR spectra for compound **5p**



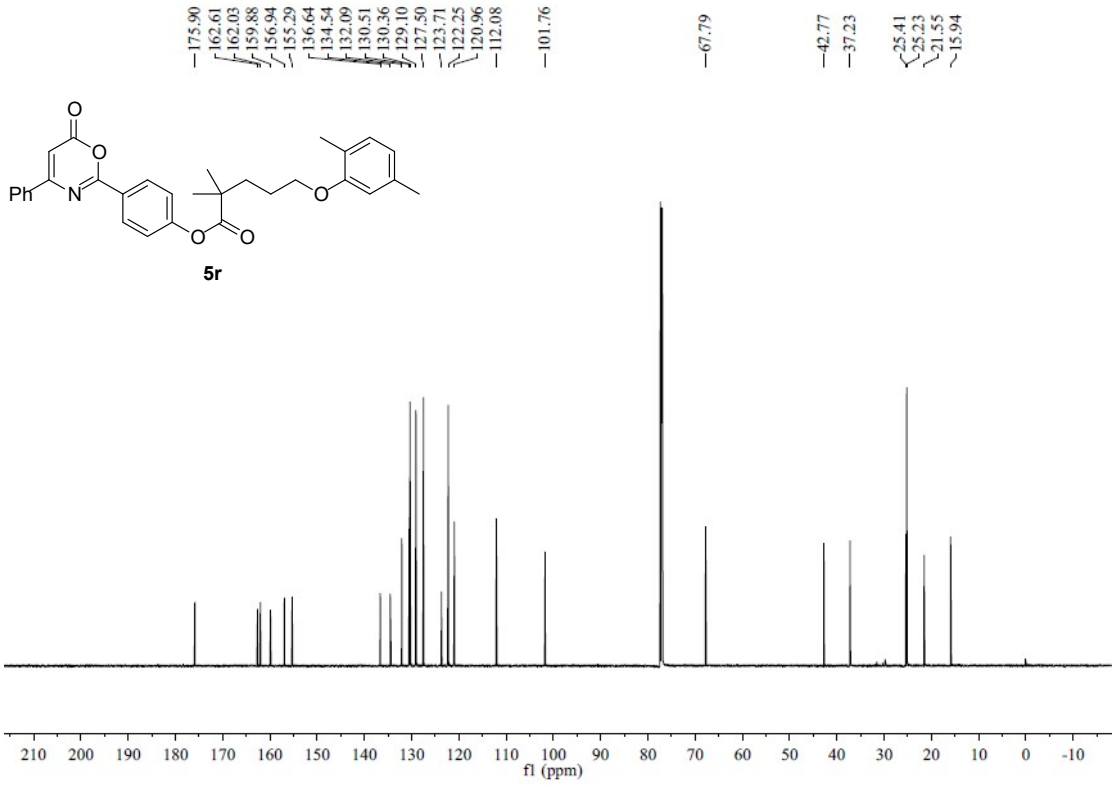
^{1}H NMR spectra for compound **5q**



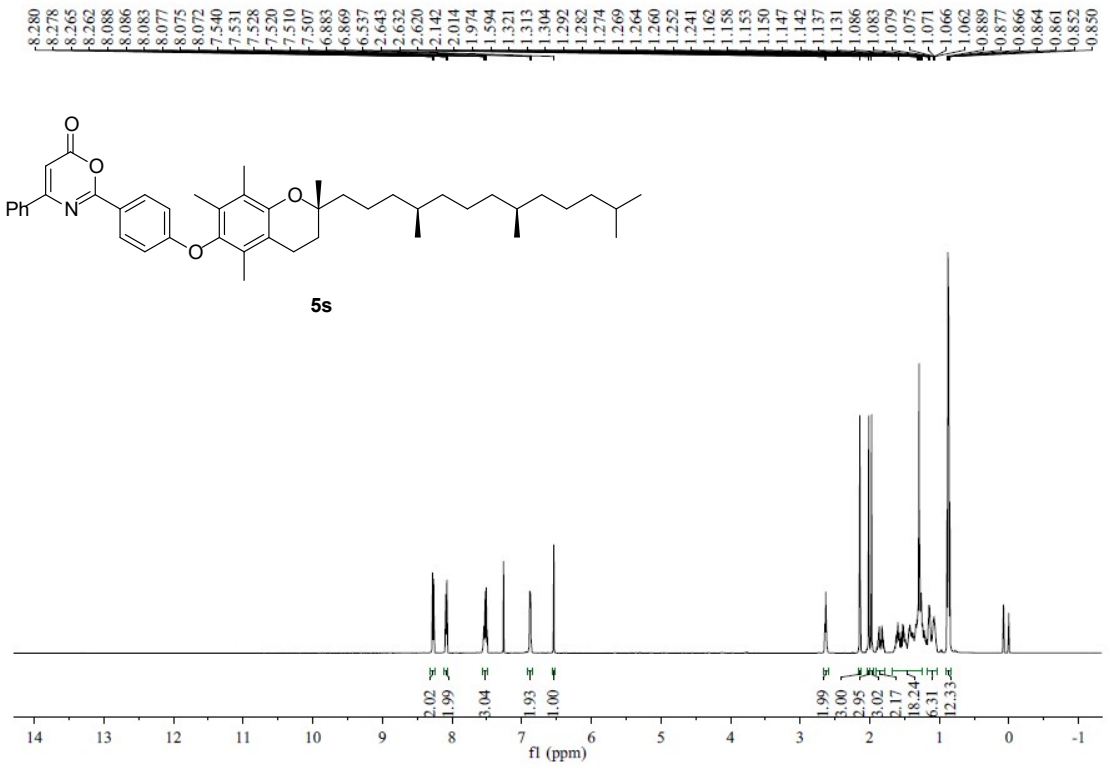
^{13}C NMR spectra for compound **5q**



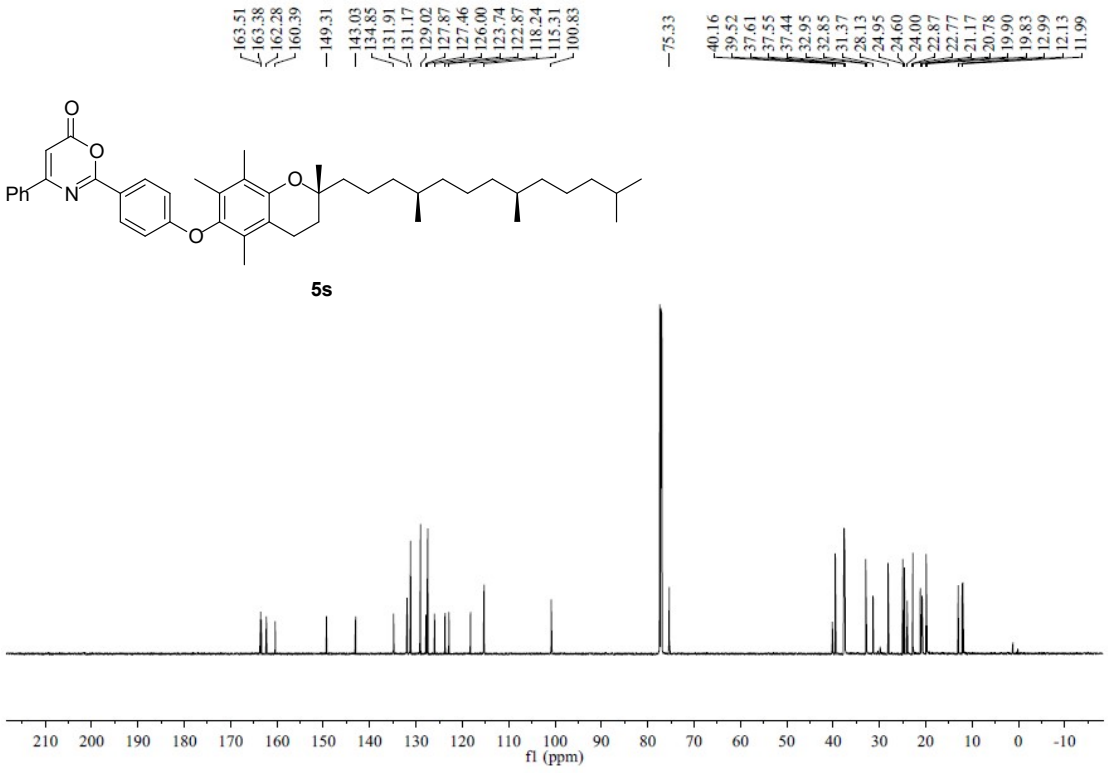
^{1}H NMR spectra for compound **5r**



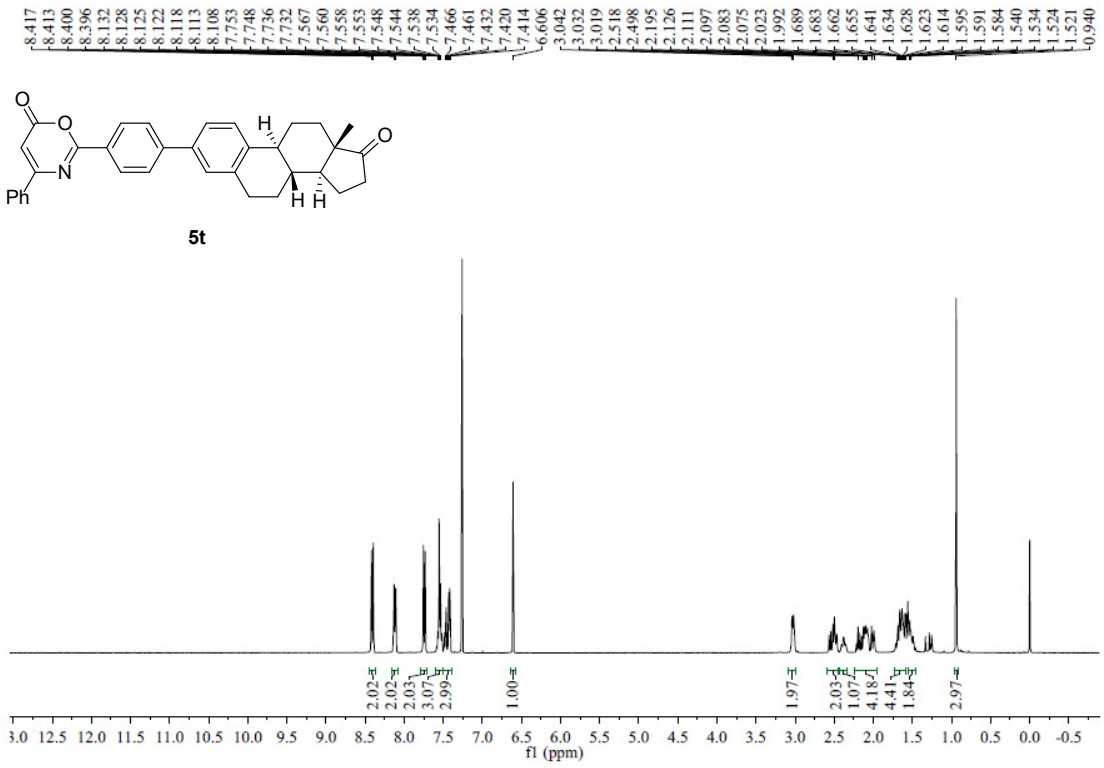
^{13}C NMR spectra for compound **5r**



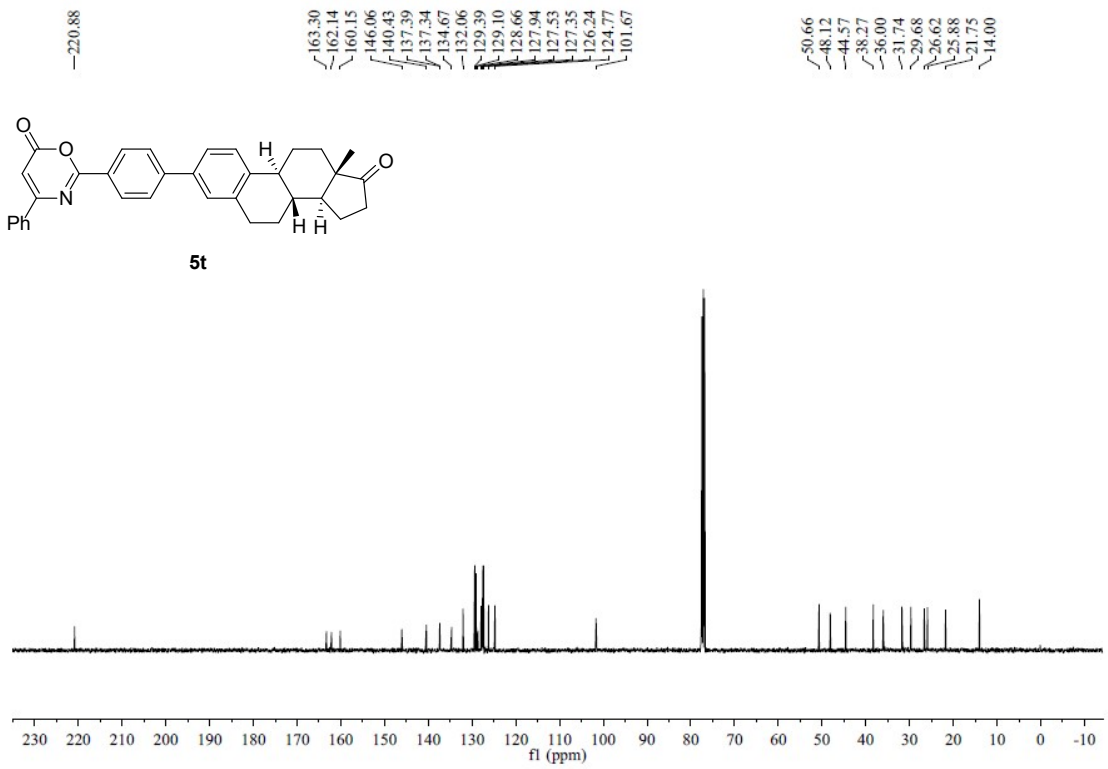
^{1}H NMR spectra for compound **5s**



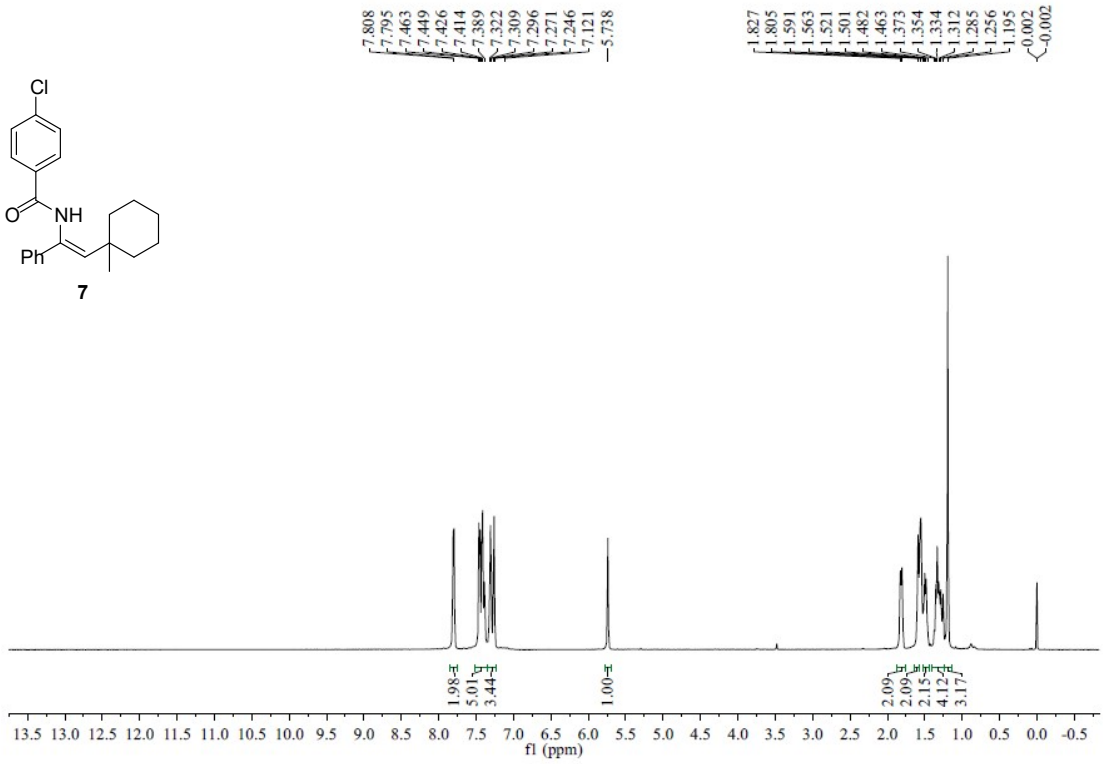
^{13}C NMR spectra for compound **5s**



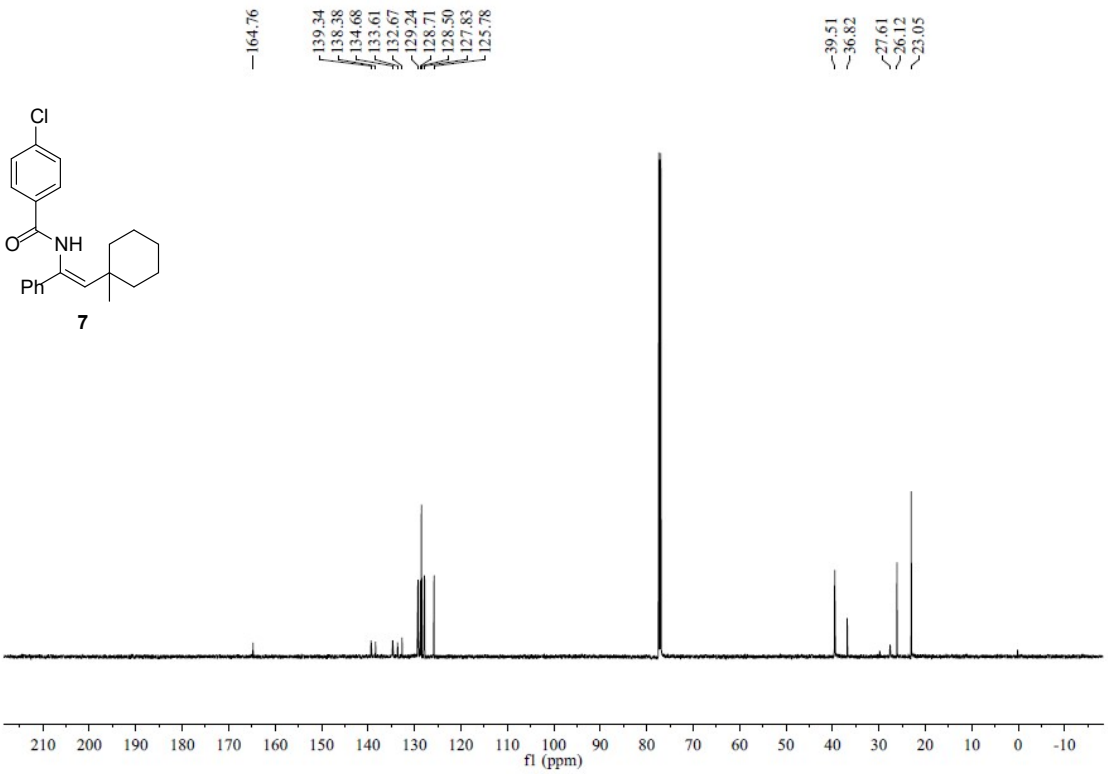
^{1}H NMR spectra for compound **5t**



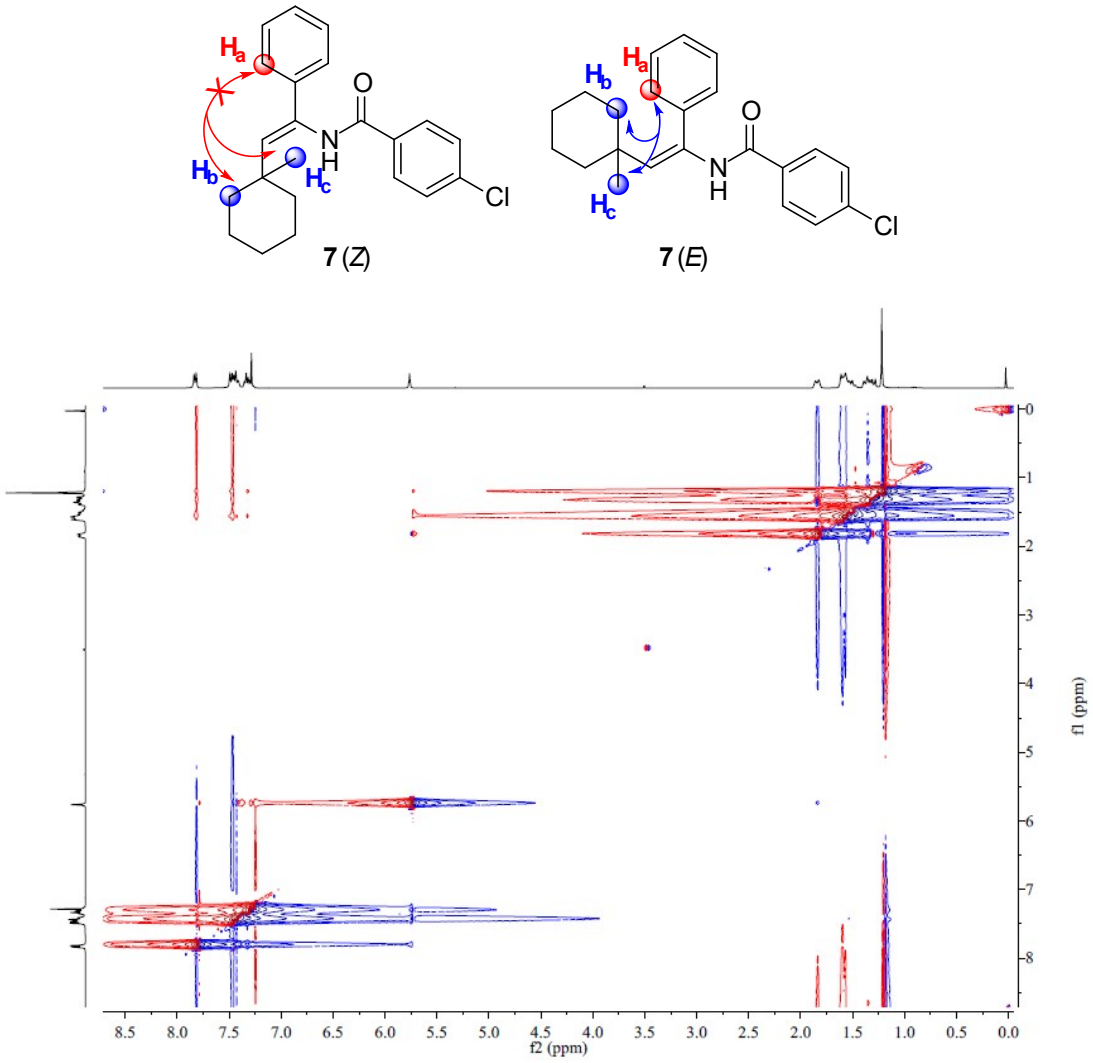
^{13}C NMR spectra for compound **5t**



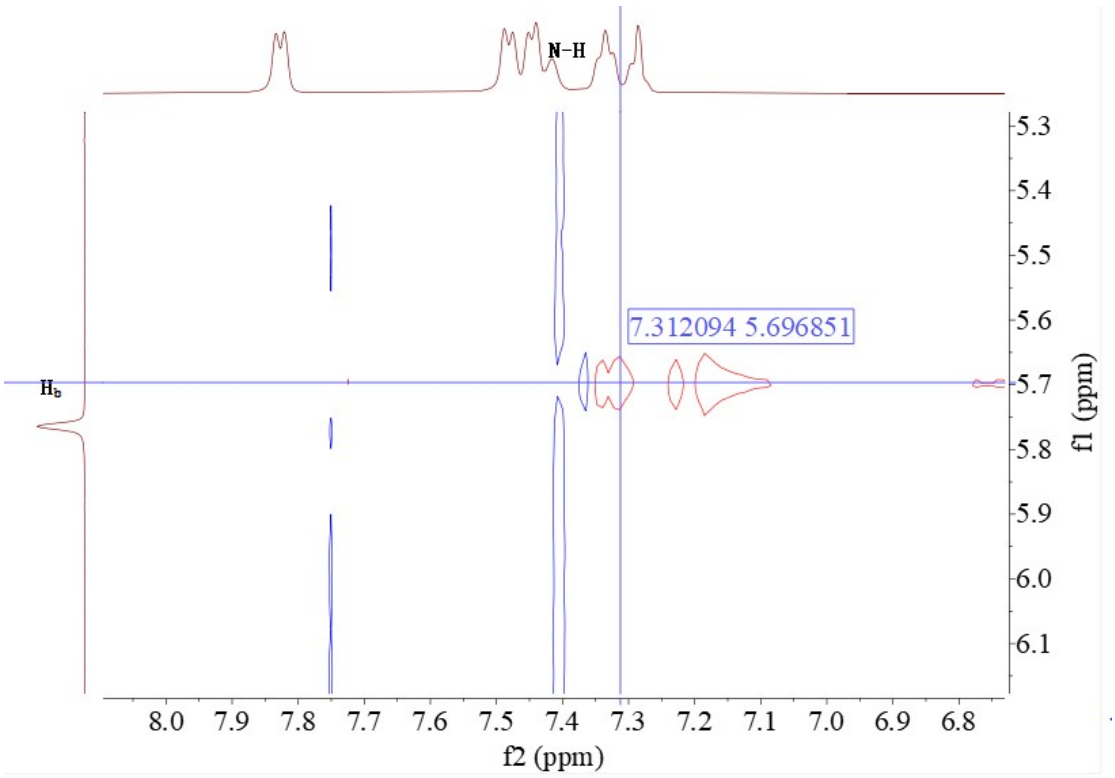
^{1}H NMR spectra for compound **7**

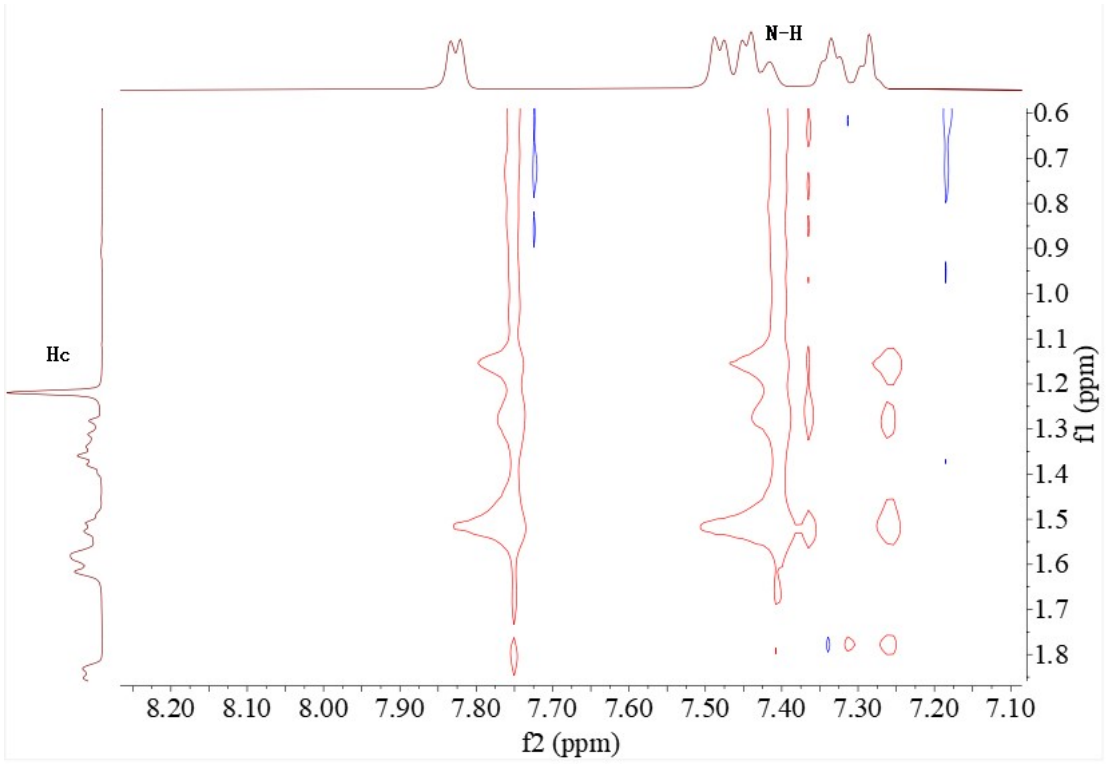


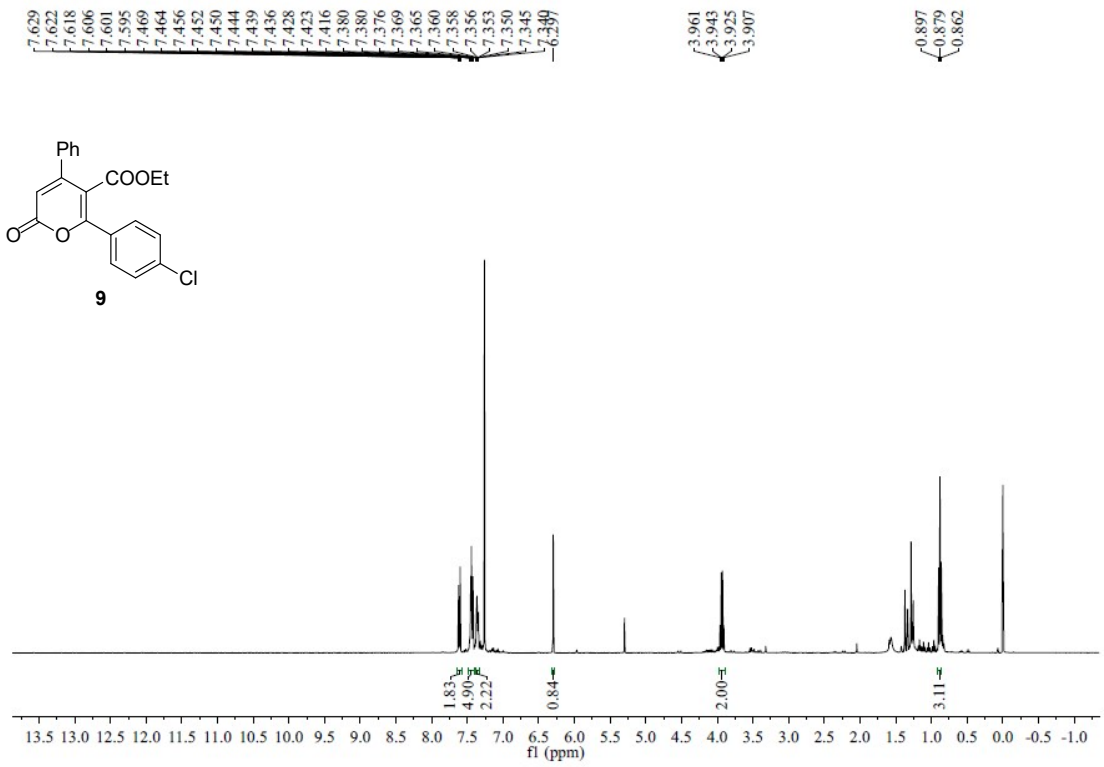
^{13}C NMR spectra for compound **7**



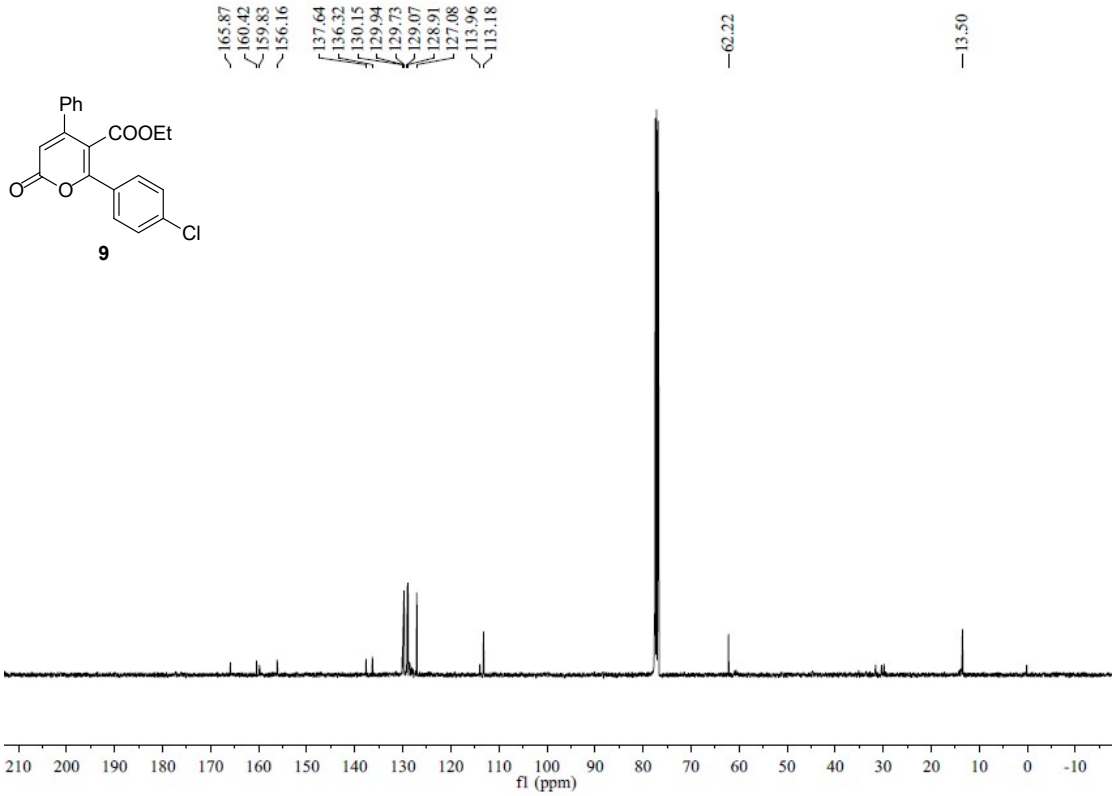
2D NOE spectra for compound **7**


N-H
7.312094 5.696851
Hb
5.3
5.4
5.5
5.6
5.7
5.8
5.9
6.0
6.1
f1 (ppm)
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f2 (ppm)

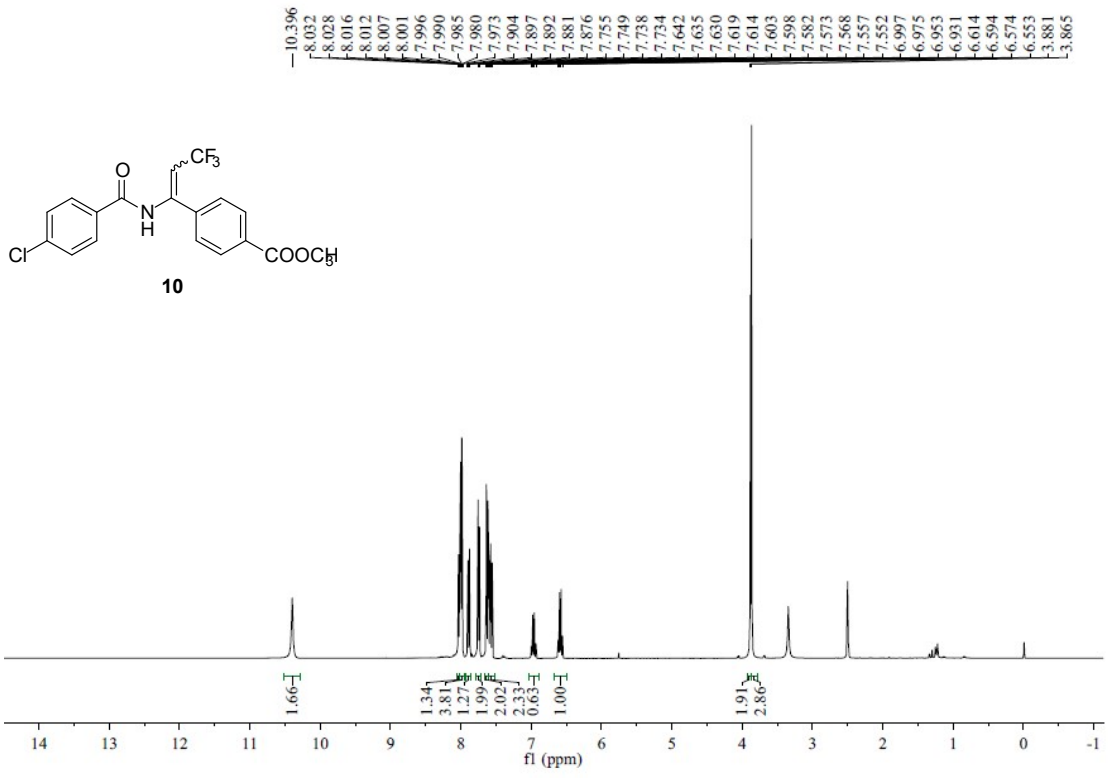

N-H
Hc
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
f1 (ppm)
8.20 8.10 8.00 7.90 7.80 7.70 7.60 7.50 7.40 7.30 7.20 7.10
f2 (ppm)



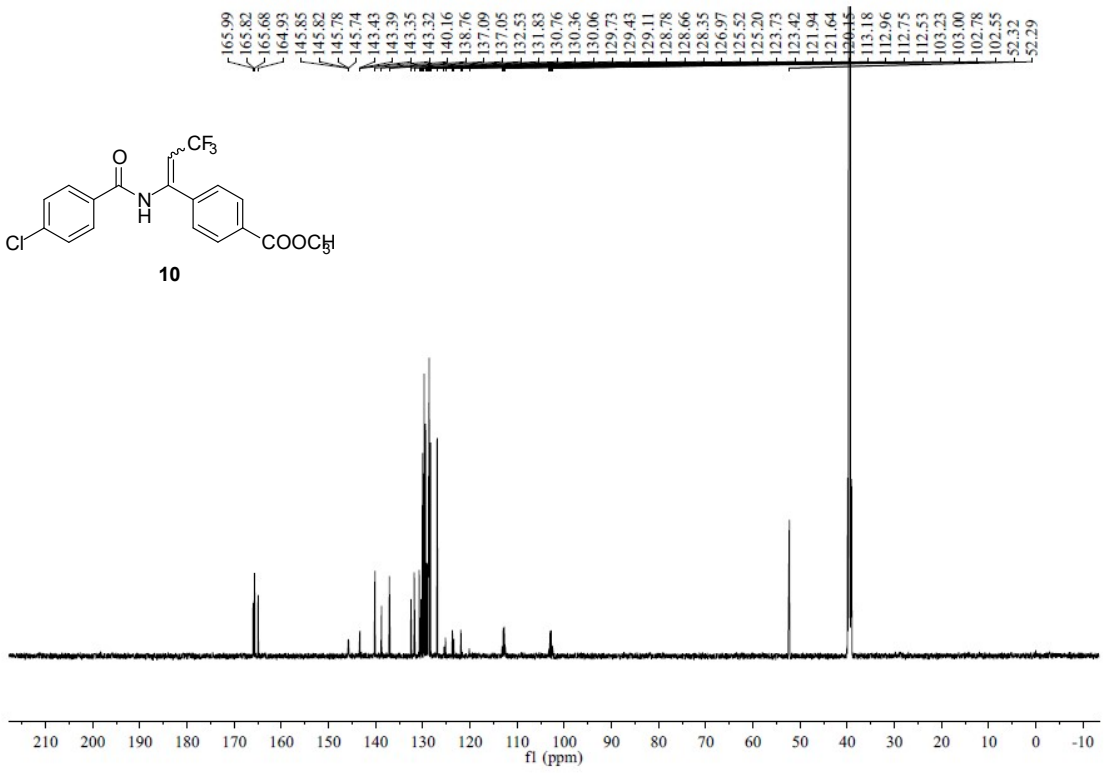
^{1}H NMR spectra for compound **9**



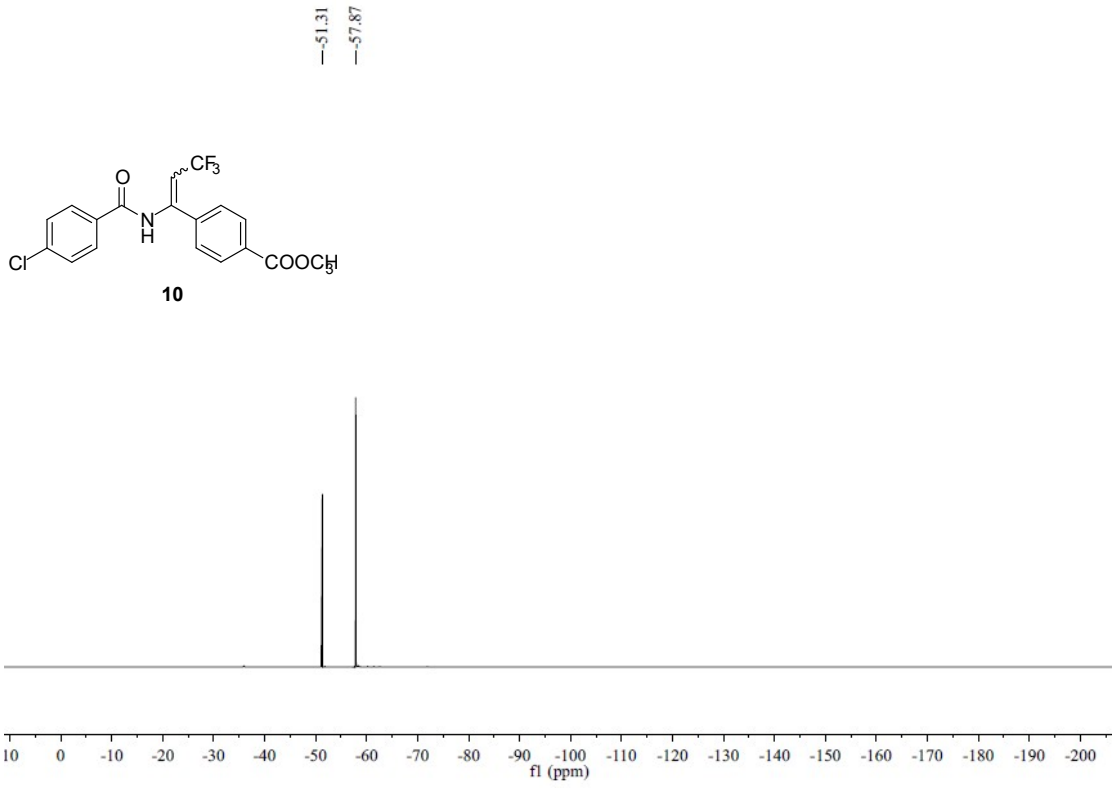
^{13}C NMR spectra for compound **9**



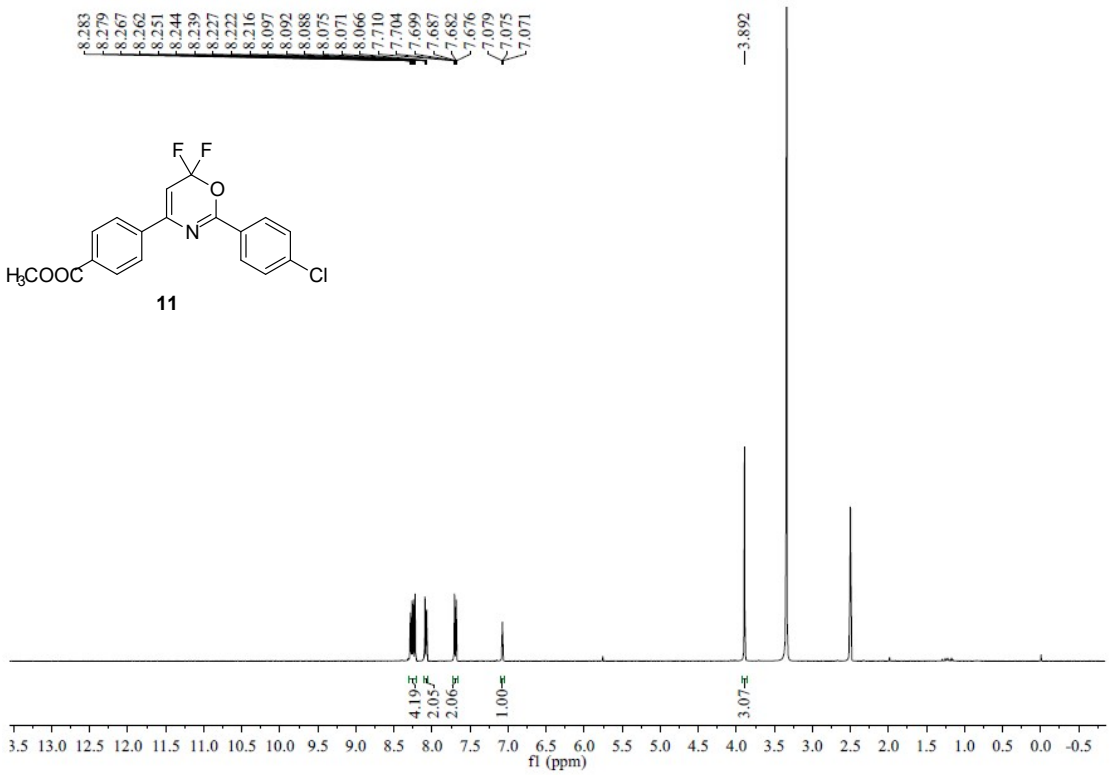
^{1}H NMR spectra for compound **10**



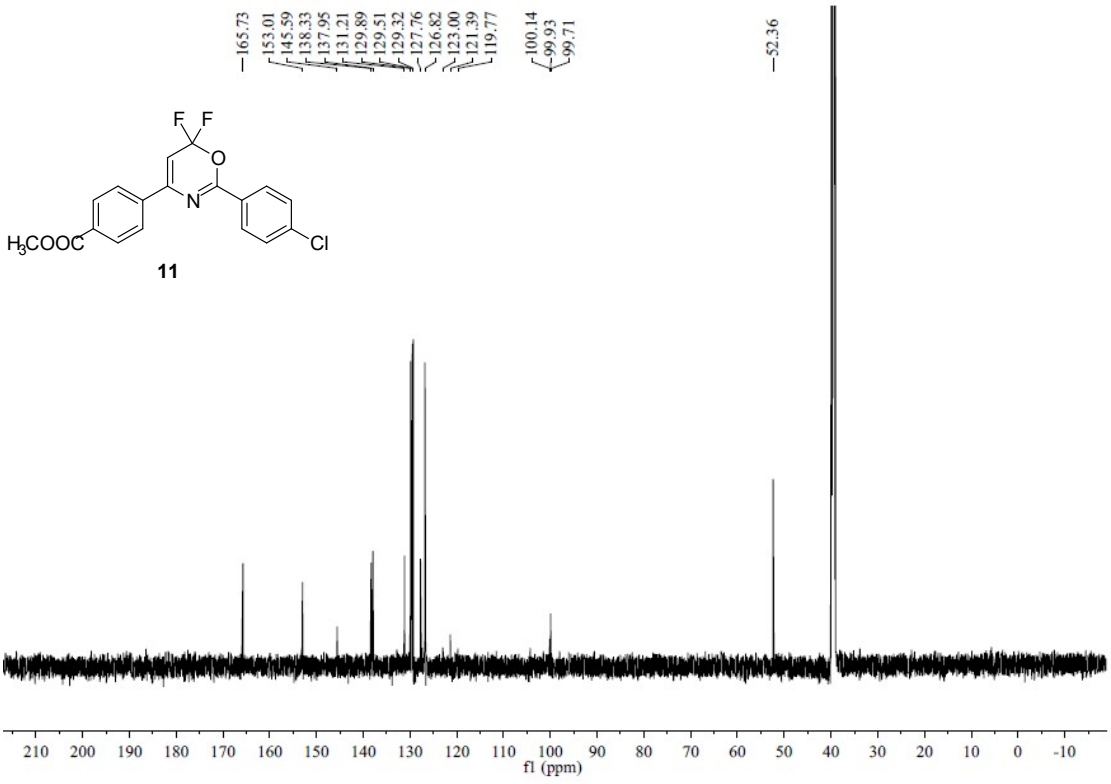
^{13}C NMR spectra for compound **10**



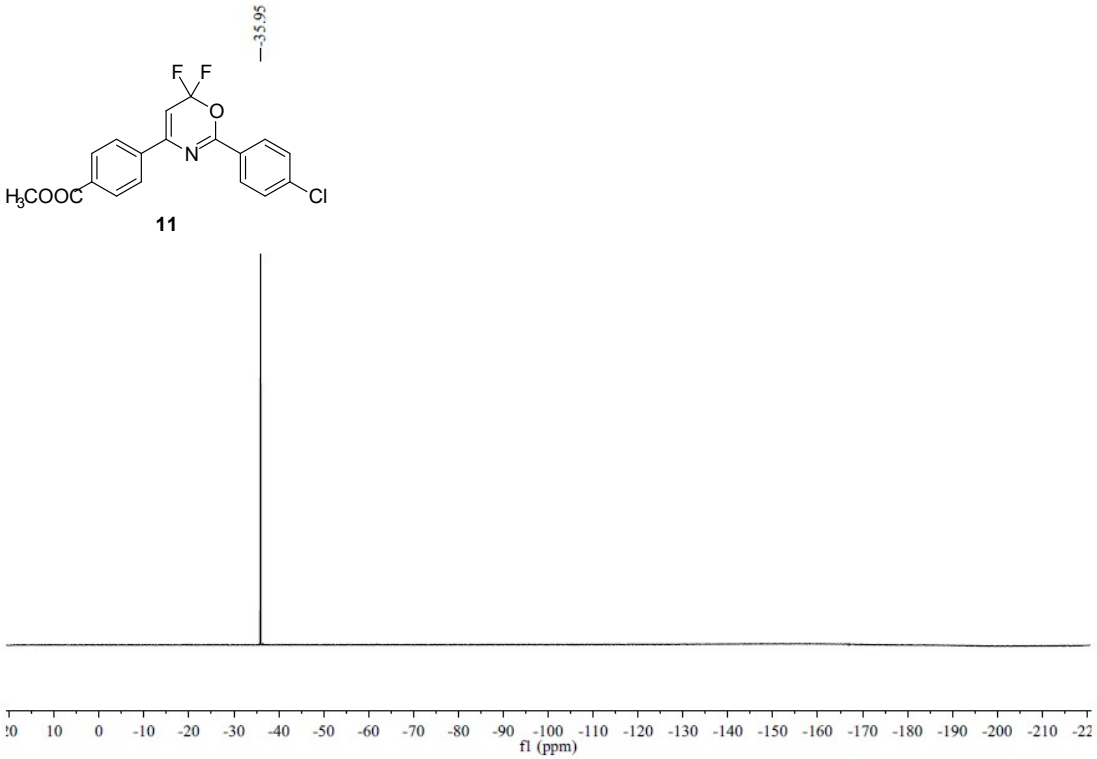
^{19}F NMR spectra for compound **10**



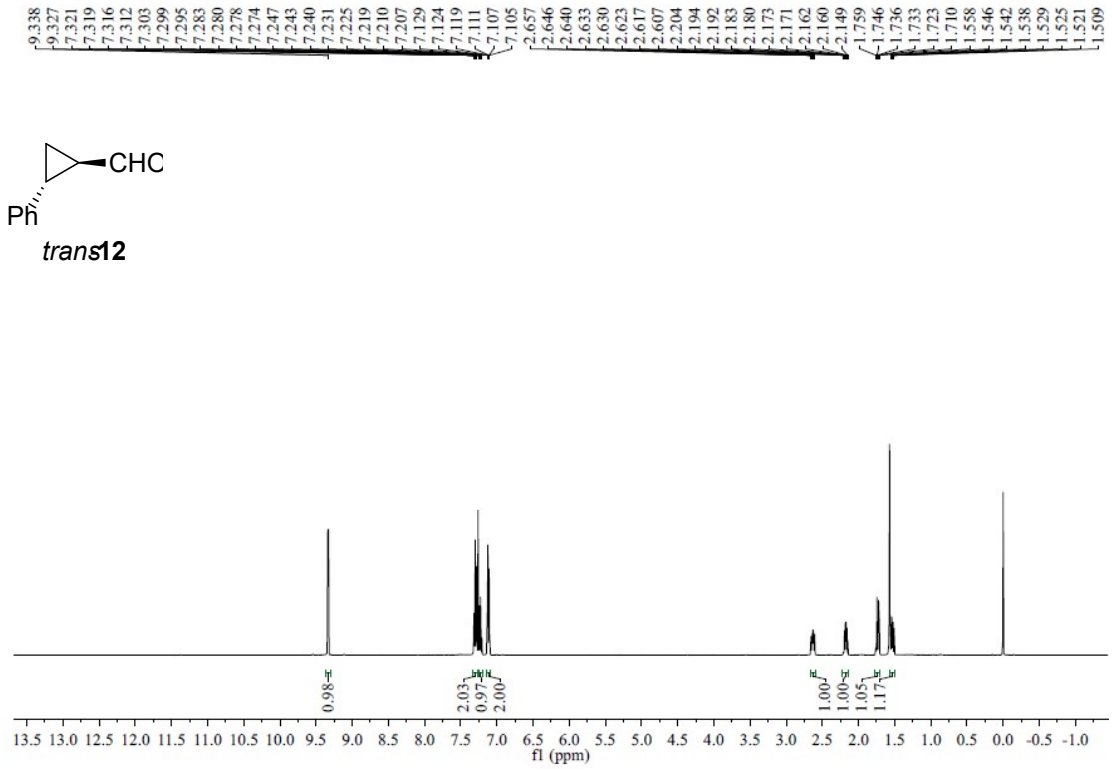
^{1}H NMR spectra for compound **11**



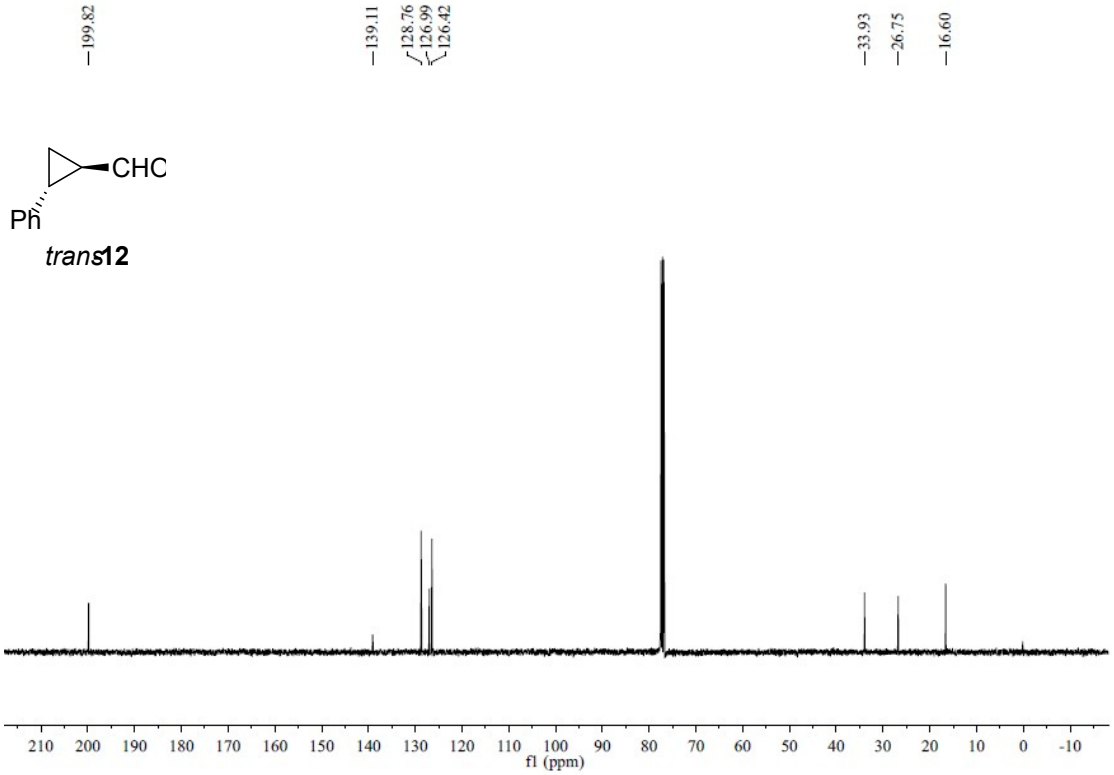
^{13}C NMR spectra for compound **11**



^{19}F NMR spectra for compound **11**

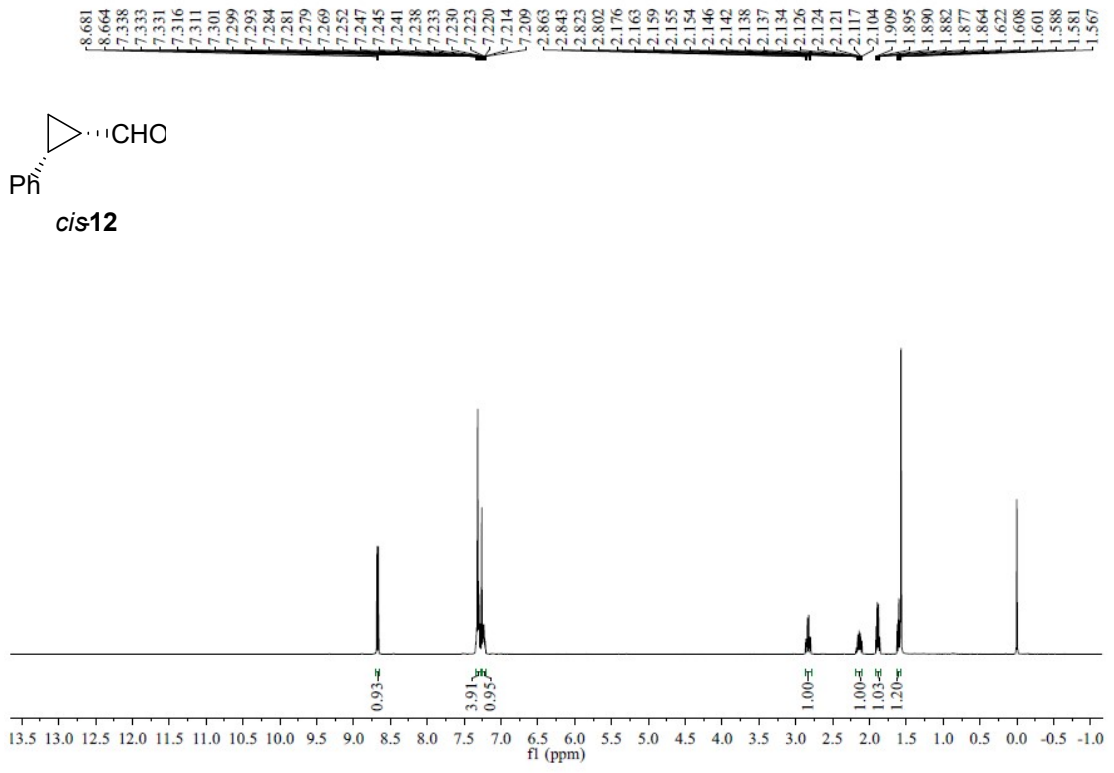


^{1}H NMR spectra for compound ***trans*-12**



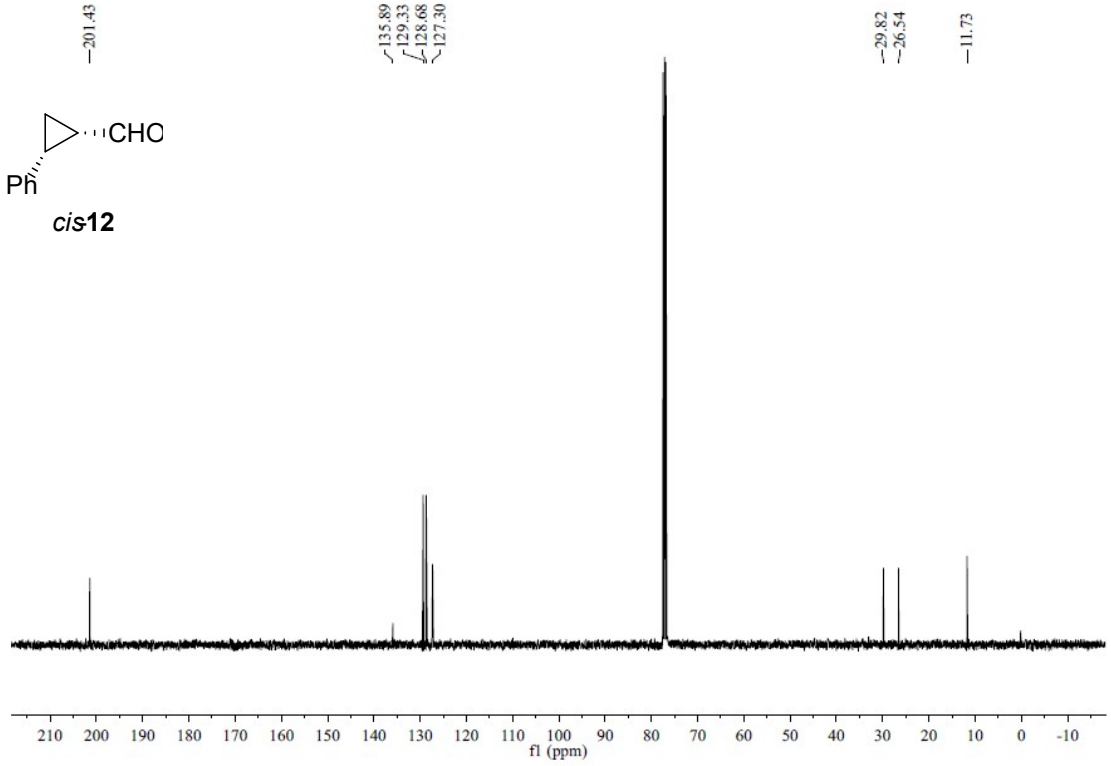
*trans***12**

^{13}C NMR spectra for compound ***trans*-12**

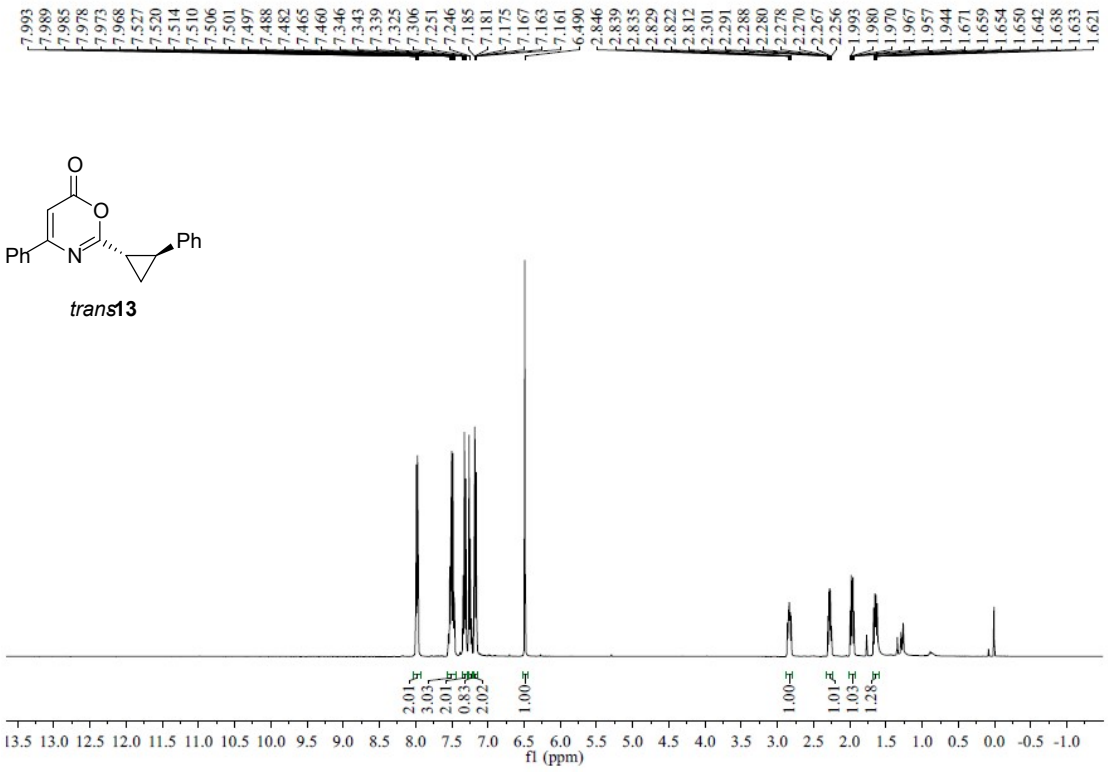


*cis***12**

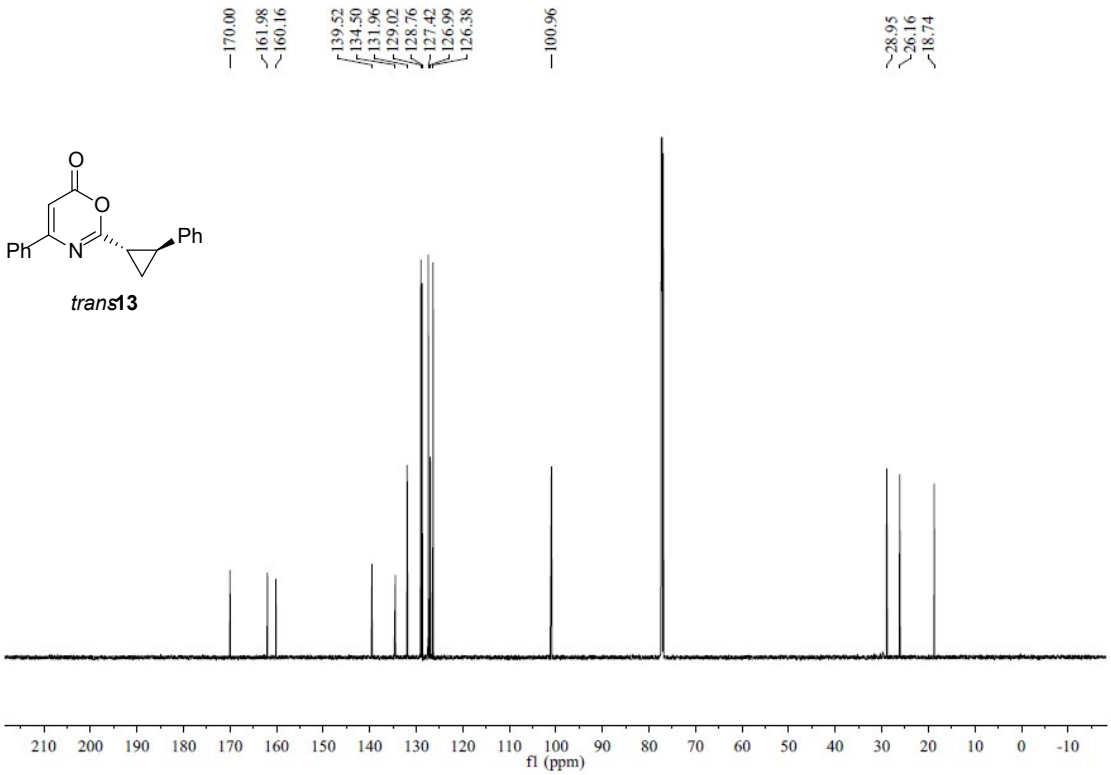
^{1}H NMR spectra for compound ***cis*-12**



^{13}C NMR spectra for compound ***cis*-12**



^{1}H NMR spectra for compound ***trans*-13**



^{13}C NMR spectra for compound ***trans*-13**