Supporting Information

for

Difluorocarbene Enabled to Access 1,3-oxazin-6-ones from Enamides

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Table of Content

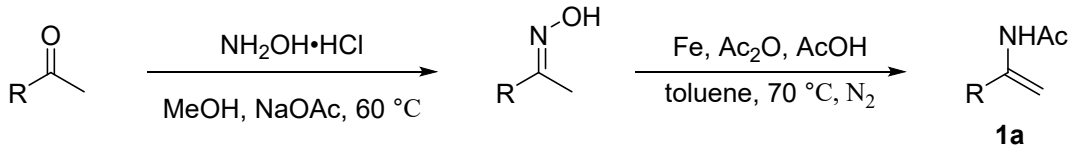
1. General Information

All chemicals were purchased from Adamas Reagent, Ltd, Energy chemical company, J&K Scientific Ltd, Alfa Aesa chemical company and so forth. Anhydrous solvents are commercially available (energy) and stored in a glove box. Unless otherwise stated, all experiments were conducted in a seal tube under air atmosphere. Reactions were monitored by TLC or GC-MS analysis. Flash column chromatography was performed over silica gel (200-300 mesh).

^{1}H-NMR and ^{13}C-NMR spectra were recorded in $CDCl_3$ on a Bruker Avance 500 spectrometer (500 MHz ^{1}H, 126 MHz ^{13}C, 471 MHz ^{19}F) at room temperature. Chemical shifts were reported in ppm on the scale relative to $CDCl_3$ (δ = 7.26 for ^{1}H-NMR, δ = 77.00 for ^{13}C-NMR) as an internal reference. High resolution mass spectra were recorded using Q-TOF time-of-flight mass spectrometer. Coupling constants (*J*) were reported in Hertz (Hz). Oil bath was used as heating source.

2. Experimental Details

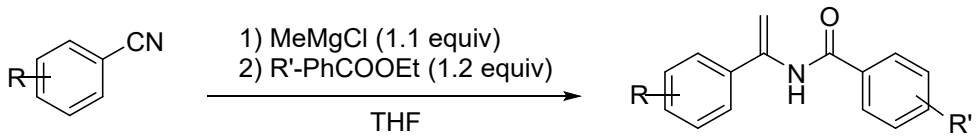
General procedure for synthesis of 1a-1t [1-2]



1a

Synthetic procedure: a) A mixture of ketone (1 equiv.), NaOAc (1.2 equiv.) and hydroxylamine hydrochloride (1.2 equiv.) in methanol (0.5M) was stirred for 2 h at 60 ℃. Add water after cooling down to room temperature, then the mixture was extracted with ethyl acetate twice. The organic layer was collected, dried over $MgSO_4$ and vacuo to afford the ketoxime pure enough for next step. b) To an oven-dried 50 mL two-neck RBF assembled with condenser was added the before-metioned ketoxime. The flask was vacuumed and back filled with N_2 for three times. Anhydrous toluene (0.5 M) was added followed by acetic anhydride (3 equiv.), acetic acid (3 equiv.) and iron powder (2 equiv.). The reaction flask was put into a 70 ℃ preheated oil bath and allowed to stir under nitrogen atomsphere. After reaction completed and cooling to room temperature, ethyl acetate was added and the mixture was filtered through a short pad of celite. The solution thus obtained was evapoured to product crude enamide, which was directly purified by column chromatography.

General procedure B for synthesis of 4a-4l [3-4]

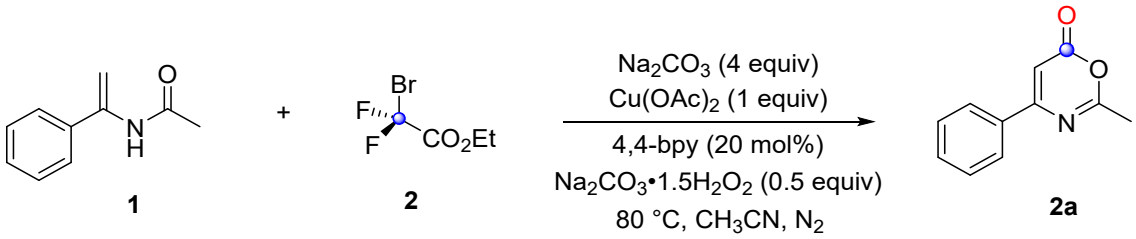


4a-4l

Synthetic procedure: Benzonitrile (15 mmol) and methyl magnesium chloride in THF (3.0 M, 5.5 mL, 16.5 mmol, Aldrich) were mixed under argon atmosphere, followed by heating to reflux for 30 min. After cooling to room temperature, the solution thus obtained was added to a solution of ethyl benzoate (2.70 g, 18 mmol) in THF (5.0 mL) at 0 °C. After 4 h, ether (20 mL) and water (10 ml) were added. After vigorous stirring for 5 min, the mixture was filtered through Celite pad. The solution were extracted with EtOAc (3× 30 mL), washed with brine, dried with anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether = 1/15-1/5) to give N-(1-Phenylvinyl)benzamide **4a-4l**.

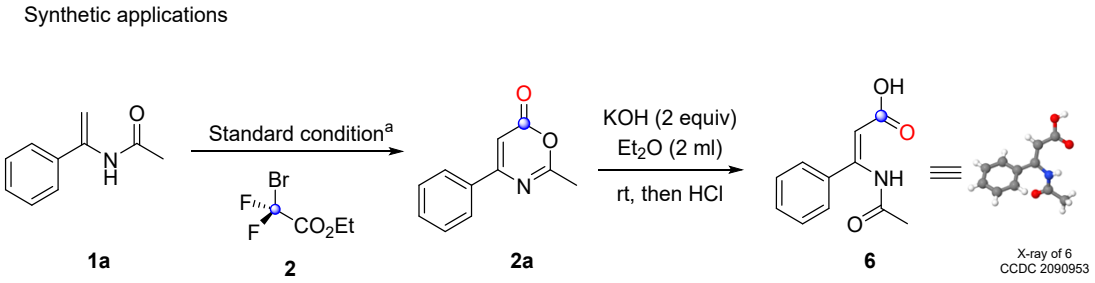
3. Experimental Procedures

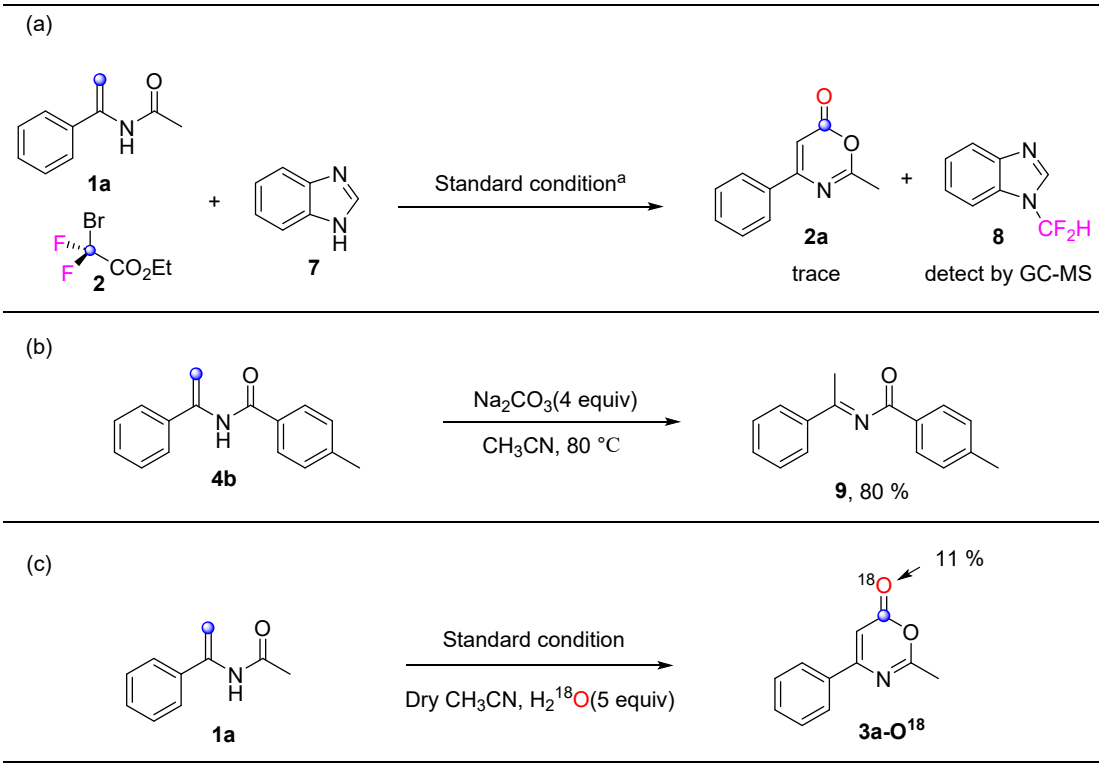
3.1 Experimental Procedures



A mixture of **1a** (0.2 mmol), $Cu(OAc)_2$ (0.2 mmol), Na_2CO_3 (0.8 mmol), 4,4-bpy (0.04 mmol), and $Na_2CO_3 \cdot 1.5H_2O_2$ (0.1 mmol) were charged into a Schleck tube, then the air was removed, N_2 was filled of Schleck tube and **2** (1.0 mmol), CH_3CN (2 mL) is added the mixture. Subsequently, the seal tube was sealed and immersed into an oil bath preheated at 80 ℃ for 12 h under N_2. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA (10:1) to afford the corresponding product.

3.2 Synthetic Applications and Control Experiments





3.2.1 Synthetic Applications

Conditions: A mixture of **1a** (0.5 mmol), $Cu(OAc)_2$ (0.5 mmol), Na_2CO_3 (2.0 mmol), 4,4-bpy (0.1 mmol), and $Na_2CO_3 \cdot 1.5H_2O_2$ (0.25 mmol) were charged into a Schleck tube, then the air was removed, N_2 was filled of Schleck tube and **2** (2.5 mmol), CH_3CN (2 mL) is added the mixture. Subsequently, the seal tube was sealed and immersed into an oil bath preheated at 80 ℃ for 12 h under N_2. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA (10:1) to afford **2a** (65 mg, 70 %).

2a (0.2 mmol, 37 mg) and KOH (0.4mmol, 22.4 mg) were weighed and to Et_2O (2 ml) placed in tube. Subsequently, the tube was sealed and immersed at 25 ℃ under air. After 6 h, ether (5 mL) and HCl (2 ml) were added. After vigorous stirring for 5 min, the mixture was filtered through Celite pad. The solution were extracted with EtOAc (3× 30 mL), washed with brine, dried with anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether = 1/2) to give **6**.

3.2.2 Control Experiments

(a) Conditions: 1a (48.8 mg, 0.2 mmol), **2** (1 mmol, 5 equiv), **7** (1 mmol, 5 equiv), $Cu(OAc)_2$ (0.5 mmol), Na_2CO_3 (2.0 mmol), 4,4-bpy (0.1 mmol) and $Na_2CO_3 \cdot 1.5H_2O_2$ (0.25 mmol) were weighed and to CH_3CN (2 mL) placed in a dried seal tube. Subsequently, the seal tube was sealed and immersed into an oil bath

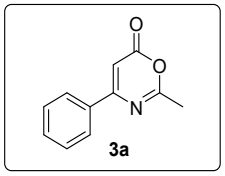
preheated at 80 °C for 12 h under N_2. After the reaction was completed, the formation of **7a** can be detected by GC-MS.

(b) Conditions: 4b (0.2 mmol, 47.4 mg), Na_2CO_3 (0.8 mmol, 4 equiv) were weighed and to CH_3CN (2 mL) placed in a dried seal tube. Subsequently, the seal tube was sealed and immersed into an oil bath preheated at 80 °C for 12 h under N_2. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA (10:1) to afford **9** (38 mg, 80 %).

(c) Conditions: 1a (0.2 mmol), $Cu(OAc)_2$ (0.2 mmol), Na_2CO_3 (0.8 mmol), 4,4-bpy (0.04 mmol), and $Na_2CO_3 \cdot 1.5H_2O_2$ (0.1 mmol) were charged into a Schleck tube, then the air was removed, N_2 was filled of Schleck tube and **2** (1.0 mmol), dry CH_3CN (2 mL) is added the mixture. Subsequently, the seal tube was sealed and immersed into an oil bath preheated at 80 °C for 12 h under N_2. After the reaction was completed, the formation of **3a-O^{18}** can be detected by GC-MS.

4. Spectal Data of Products

2-methyl-4-phenyl-6H-1,3-oxazin-6-one(3a) [CAS:76569-84-1]



3a

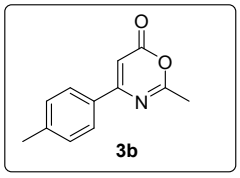
Following the general procedure 1 on 0.2 mmol scale, yield: 70% (26 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.00 – 7.94 (m, 2H), 7.50 (dt, J = 14.8, 7.1 Hz, 3H), 6.52 (s, 1H), 2.49 (s, 3H);

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.9, 161.5, 160.1, 134.2, 131.9, 129.0, 127.3, 101.7, 21.8

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{11}H_{10}NO_2^+$ 188.0706; found: 188.0705;

2-methyl-4-(p-tolyl)-6H-1,3-oxazin-6-one (3b) [CAS:1589584-10-0]



3b

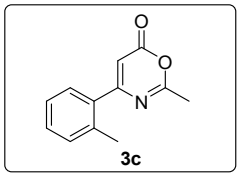
Following the general procedure 1 on 0.2 mmol scale, yield: 61 % (25 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.86 (d, J = 8.2 Hz, 2H), 7.28 (s, 2H), 6.47 (s, 1H), 2.48 (s, 3H), 2.41 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.7, 161.6, 142.6, 131.4, 129.7, 127.3, 100.8, 21.8, 21.6.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}NO_2^+$ 202.0863; found: 202.0866;

2-methyl-4-(o-tolyl)-6H-1,3-oxazin-6-one (3c)



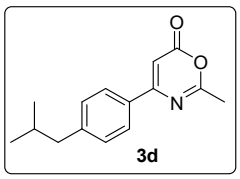
Following the general procedure 1 on 0.2 mmol scale, yellow oil, yield: 60 % (24 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.44 (dd, J = 8.0, 1.5 Hz, 1H), 7.35 (td, J = 7.4, 1.5 Hz, 1H), 7.29 – 7.26 (m, 2H), 6.22 (s, 1H), 2.48 (s, 3H), 2.44 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.6, 164.9, 159.6, 136.3, 135.6, 131.4, 130.3, 129.0, 126.2, 106.9, 21.8, 20.6.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}NO_2^+$ 202.0863; found: 202.0867;

4-(4-isobutylphenyl)-2-methyl-6H-1,3-oxazin-6-one (3d)



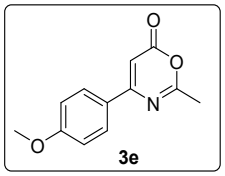
Following the general procedure 1 on 0.2 mmol scale, yellow oli, yield: 66 % (32 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 (d, J = 8.2 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 6.48 (s, 1H), 2.53 (d, J = 7.2 Hz, 2H), 2.48 (s, 3H), 1.89 (dt, J = 13.5, 6.8 Hz, 1H), 0.91 (d, J = 6.7 Hz, 6H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.7, 161.6, 160.3, 146.4, 131.7, 129.8, 127.2, 100.9, 45.3, 30.2, 22.3, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{15}H_{18}NO_2^+$ 244.1332; found: 244.1332;

4-(4-methoxyphenyl)-2-methyl-6H-1,3-oxazin-6-one (3e) [CAS:1589584-18-8]



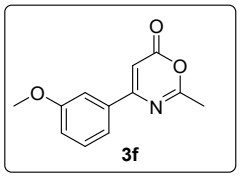
Following the general procedure 1 on 0.2 mmol scale, yield: 76% (33 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.00 – 7.87 (m, 2H), 7.02 – 6.90 (m, 2H), 6.40 (s, 1H), 3.86 (s, 3H), 2.47 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.5, 162.8, 161.1, 160.4, 129.2, 126.6, 114.4, 99.5, 55.5, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}NO_3^+$ 218.0812; found: 218.0814;

4-(3-methoxyphenyl)-2-methyl-6H-1,3-oxazin-6-one (3f) [CAS:1589584-20-2]



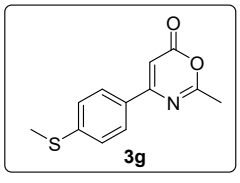
Following the general procedure 1 on 0.2 mmol scale, yield: 67 % (29 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.56 – 7.49 (m, 2H), 7.42 – 7.34 (m, 1H), 7.11 – 7.00 (m, 1H), 6.50 (s, 1H), 3.87 (s, 3H), 2.49 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.8, 161.4, 160.1, 160.1, 135.7, 130.0, 119.6, 117.7, 112.5, 102.0, 55.5, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}NO_3^+$ 218.0812; found: 218.0809;

2-methyl-4-(4-(methylthio)phenyl)-6H-1,3-oxazin-6-one (3g)



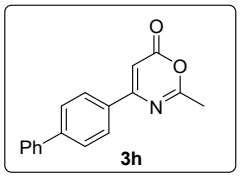
Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp:48-53 ℃ yield: 65 % (30 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.92 – 7.85 (m, 2H), 7.32 – 7.27 (m, 2H), 6.46 (s, 1H), 2.53 (s, 3H), 2.48 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.7, 161.0, 160.3, 144.4, 130.4, 127.6, 125.7, 100.5, 21.8, 15.0.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}NO_2S^+$ 234.0583; found: 234.0581;

4-([1,1'-biphenyl]-4-yl)-2-methyl-6H-1,3-oxazin-6-one (3h) [CAS:1589584-16-6]



3h

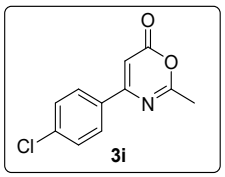
Following the general procedure 1 on 0.2 mmol scale, yield: 70 % (37 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.08 – 8.01 (m, 2H), 7.74 – 7.68 (m, 2H), 7.66 – 7.61 (m, 2H), 7.48 (t, J = 7.6 Hz, 2H), 7.41 (d, J = 7.4 Hz, 1H), 6.55 (s, 1H), 2.51 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.9, 161.2, 160.2, 144.7, 139.9, 133.0, 129.0, 128.2, 127.8, 127.6, 127.2, 101.4, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{17}H_{14}NO_2^+$ 264.1019; found: 264.1020;

4-(4-chlorophenyl)-2-methyl-6H-1,3-oxazin-6-one (3i) [CAS:1589584-28-0]



3i

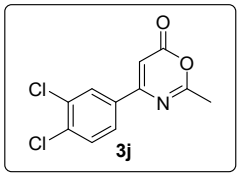
Following the general procedure 1 on 0.2 mmol scale, yield: 63% (28 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.93 – 7.89 (m, 2H), 7.44 (d, J = 8.6 Hz, 2H), 6.49 (s, 1H), 2.49 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 167.1, 160.3, 159.9, 138.2, 132.6, 129.2, 128.6, 101.8, 21.8

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{11}H_9ClNO_2^+$ 222.0316; found: 222.0320;

4-(3,4-dichlorophenyl)-2-methyl-6H-1,3-oxazin-6-one (3j)



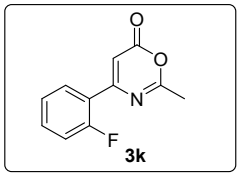
Following the general procedure 1 on 0.2 mmol scale, yellow oil, yield: 55 % (28 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.09 (d, J = 2.1 Hz, 1H), 7.76 (dd, J = 8.5, 2.1 Hz, 1H), 7.54 (d, J = 8.4 Hz, 1H), 6.49 (s, 1H), 2.50 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 167.4, 159.5, 159.1, 136.2, 134.1, 133.6, 131.0, 129.3, 126.1, 102.4, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{11}H_8Cl_2NO_2^+$ 255.9927; found: 255.9926;

4-(2-fluorophenyl)-2-methyl-6H-1,3-oxazin-6-one (3k)



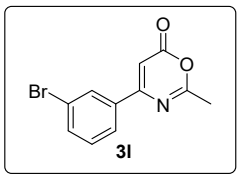
Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp: 90-95℃, yield: 61 % (25 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.13 (td, J = 7.9, 1.9 Hz, 1H), 7.50 – 7.43 (m, 1H), 7.30 – 7.24 (m, 1H), 7.16 (ddd, J = 11.9, 8.3, 1.2 Hz, 1H), 6.76 (s, 1H), 2.48 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.4, 162.8, 160.3 (d, *J* = 103.4 Hz), 156.5 (d, *J* = 3.2 Hz), 133.1 (d, *J* = 9.3 Hz), 130.8 (d, *J* = 1.8 Hz), 124.6 (d, *J* = 3.6 Hz), 122.4 (d, *J* = 9.5 Hz), 116.7 (d, *J* = 23.1 Hz), 107.1 (d, *J* = 15.9 Hz), 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{11}H_9FNO_2^+$ 206.0612; found: 206.0615;

4-(3-bromophenyl)-2-methyl-6H-1,3-oxazin-6-one (3l)



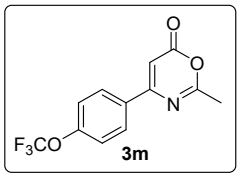
Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp: 123-127℃, yield: 55 % (29 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.14 (q, *J* = 1.6 Hz, 1H), 7.85 (dq, *J* = 7.8, 1.2 Hz, 1H), 7.63 (ddt, *J* = 7.9, 2.1, 1.0 Hz, 1H), 7.34 (td, *J* = 7.9, 1.0 Hz, 1H), 6.49 (s, 1H), 2.50 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 167.2, 160.0, 159.7, 136.2, 134.7, 130.4 (d, J = 3.1 Hz), 125.7, 123.2, 102.5, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{11}H_9BrNO_2^+$ 265.9811; found: 265.9808;

2-methyl-4-(4-(trifluoromethoxy)phenyl)-6H-1,3-oxazin-6-one (3m)



Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp: 80-84℃, yield: 60 % (33 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

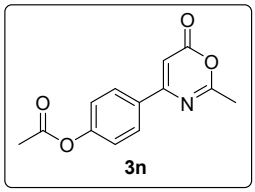
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.06 – 7.97 (m, 2H), 7.34 – 7.28 (m, 2H), 6.50 (s, 1H), 2.50 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 167.2, 160.1, 159.8, 151.8 (d, J = 2.0 Hz), 132.6, 129.1, 120.9, 120.4 (q, J = 258.6 Hz), 102.1, 21.8.

^{19}F NMR (471 MHz, Chloroform-d) δ -63.02.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{12}H_9F_3NO_3^+$ 272.0529; found: 272.0523;

4-(2-methyl-6-oxo-6H-1,3-oxazin-4-yl)phenyl acetate (3n)



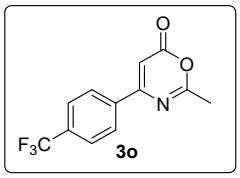
Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp: 131-135℃, yield: 55 % (27 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.04 – 7.95 (m, 2H), 7.24 – 7.18 (m, 2H), 6.48 (s, 1H), 2.48 (s, 3H), 2.32 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.0, 166.9, 160.6, 160.0, 153.5, 131.7, 128.7, 122.2, 101.6, 21.8, 21.2.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{13}H_{12}NO_4^+$ 246.0761; found: 246.0748;

2-methyl-4-(4-(trifluoromethyl)phenyl)-6H-1,3-oxazin-6-one (3o) [CAS:1951432-76-0]



3o

Following the general procedure 1 on 0.2 mmol scale, yield: 65 % (33 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

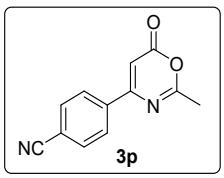
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.07 (d, J = 8.1 Hz, 2H), 7.79 – 7.67 (m, 2H), 6.57 (d, J = 2.2 Hz, 1H), 2.51 (d, J = 2.1 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 167.4, 160.0, 159.6, 137.6, 133.3 (q, J = 32.8 Hz), 127.6, 125.9 (q, J = 3.8 Hz), 124.8, 122.6, 103.3, 21.8.

^{19}F NMR (471 MHz, Chloroform-d) δ -63.02.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{12}H_9F_3NO_2^+$ 256.0580; found: 256.0580;

4-(2-methyl-6-oxo-6H-1,3-oxazin-4-yl)benzonitrile (3p)



3p

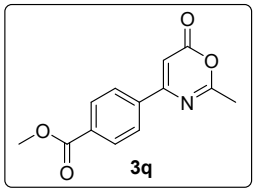
Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp: 147-152℃, yield: 30% (13 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.07 (d, J = 8.1 Hz, 2H), 7.77 (d, J = 8.1 Hz, 2H), 6.58 (s, 1H), 2.52 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 167.6, 159.3, 138.3, 132.6, 127.8, 123.6, 118.1, 115.2, 103.8, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{12}H_9N_2O_2^+$ 213.0659; found: 213.0660;

methyl 4-(2-methyl-6-oxo-6H-1,3-oxazin-4-yl)benzoate (3q)



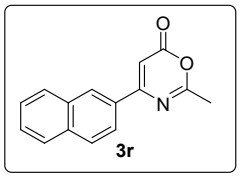
Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp:132-136 ℃, yield: 49 % (24 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.14 – 8.08 (m, 2H), 8.04 – 7.97 (m, 2H), 6.57 (s, 1H), 3.94 (s, 3H), 2.50 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) 167.2, 166.3, 160.3, 159.7, 138.2, 132.9, 130.1, 129.4, 127.3, 103.2, 52.4, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{13}H_{12}NO_4^+$ 246.0761; found: 246.0746;

2-methyl-4-(naphthalen-2-yl)-6H-1,3-oxazin-6-one (3r) [CAS:1589584-34-8]



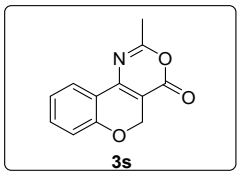
Following the general procedure 1 on 0.2 mmol scale, yield: 58 % (28 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.60 (s, 1H), 7.96 (d, J = 7.8 Hz, 1H), 7.91 (d, J = 1.3 Hz, 2H), 7.87 (d, J = 7.9 Hz, 1H), 7.57 (dq, J = 14.7, 6.8 Hz, 2H), 6.63 (s, 1H), 2.53 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.7, 161.3, 160.2, 135.0, 133.0, 131.3, 129.3, 128.8, 128.7, 128.1, 127.8, 126.9, 123.1, 101.9, 21.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{15}H_{12}NO_2^+$ 238.0863; found: 238.0858;

2-methyl-4H,5H-chromeno[4,3-d][1,3]oxazin-4-one (3s)



3s

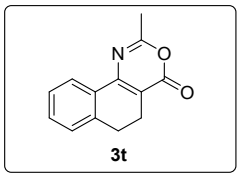
Following the general procedure 1 on 0.2 mmol scale, yellow oil, yield: 68 % (29 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.93 (dd, J = 7.8, 1.8 Hz, 1H), 7.39 (ddd, J = 8.5, 7.4, 1.7 Hz, 1H), 7.06 (td, J = 7.6, 1.1 Hz, 1H), 6.93 (dd, J = 8.2, 1.1 Hz, 1H), 5.17 (s, 2H), 2.50 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 167.1, 157.6, 157.4, 152.3, 134.1, 126.0, 122.1, 119.0, 117.0, 105.2, 62.3, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{12}H_{10}NO_3^+$ 216.0655; found: 216.0654;

2-methyl-5,6-dihydro-4H-naphtho[1,2-d][1,3]oxazin-4-one (3t) [CAS:1589584-43-9]



3t

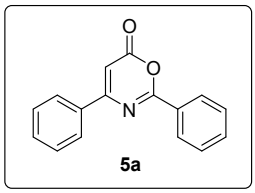
Following the general procedure 1 on 0.2 mmol scale, yield: 59 % (25 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.08 (dd, J = 7.7, 1.6 Hz, 1H), 7.38 (td, J = 7.4, 1.6 Hz, 1H), 7.33 (td, J = 7.5, 1.4 Hz, 1H), 7.22 (dd, J = 7.4, 1.3 Hz, 1H), 2.93 (dd, J = 9.0, 7.0 Hz, 2H), 2.78 (dd, J = 9.0, 7.0 Hz, 2H), 2.46 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.8, 160.9, 154.2, 138.8, 131.4, 130.8, 128.1, 127.1, 126.0, 112.4, 26.8, 21.6, 19.6.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{13}H_{12}NO_2^+$ 214.0863; found: 214.0864;

2,4-diphenyl-6H-1,3-oxazin-6-one (5a) [71898-21-0]



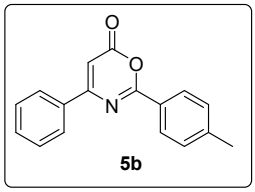
Following the general procedure 1 on 0.2 mmol scale, yield: 68 % (34 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.40 – 8.33 (m, 2H), 8.13 – 8.07 (m, 2H), 7.65 – 7.59 (m, 1H), 7.57 – 7.49 (m, 5H), 6.60 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.2, 161.9, 159.9, 134.5, 133.4, 131.9, 130.1, 129.0, 128.8, 128.8, 127.4, 101.7.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{16}H_{12}NO_2^+$ 250.0863; found: 250.0869;

4-phenyl-2-(p-tolyl)-6H-1,3-oxazin-6-one (5b) [CAS:2087490-78-4]



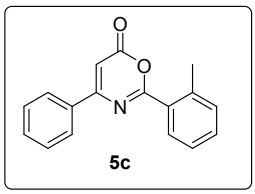
Following the general procedure 1 on 0.2 mmol scale, yield: 51 % (27 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.27 – 8.21 (m, 2H), 8.13 – 8.06 (m, 2H), 7.56 – 7.49 (m, 3H), 7.33 (d, J = 8.1 Hz, 2H), 6.57 (s, 1H), 2.45 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.4, 162.0, 160.1, 144.4, 134.6, 131.9, 129.6, 128.9, 128.8, 127.4, 127.3, 101.4, 21.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{17}H_{14}NO_2^+$ 264.1019; found: 264.1018;

4-phenyl-2-(o-tolyl)-6H-1,3-oxazin-6-one (5c)



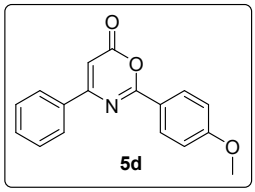
Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp: 84-88℃, yield: 51 % (27 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.15 (dd, J = 8.2, 1.5 Hz, 1H), 8.09 – 8.03 (m, 2H), 7.52 (qd, J = 8.8, 7.8, 3.7 Hz, 3H), 7.47 (td, J = 7.5, 1.5 Hz, 1H), 7.35 (t, J = 7.1 Hz, 2H), 6.61 (s, 1H), 2.80 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.1, 161.7, 160.1, 139.9, 134.6, 132.4, 132.3, 131.9, 130.6, 129.3, 129.0, 127.4, 126.3, 101.5, 22.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{17}H_{14}NO_2^+$ 264.1019; found: 264.1020;

2-(4-methoxyphenyl)-4-phenyl-6H-1,3-oxazin-6-one (5d) [CAS:2087490-79-5]



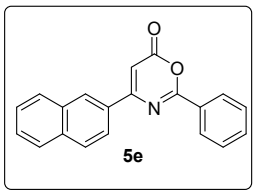
Following the general procedure 1 on 0.2 mmol scale, yield: 50 % (27 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.34 – 8.29 (m, 2H), 8.12 – 8.06 (m, 2H), 7.56 – 7.49 (m, 3H), 7.04 – 6.98 (m, 2H), 6.54 (s, 1H), 3.91 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.0, 163.2, 162.2, 160.3, 134.7, 131.8, 130.9, 128.9, 127.4, 122.4, 114.3, 100.7, 55.6.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{17}H_{14}NO_3^+$ 280.0968; found: 280.0966;

4-(naphthalen-2-yl)-2-phenyl-6H-1,3-oxazin-6-one (5e) [CAS:2232874-33-6]



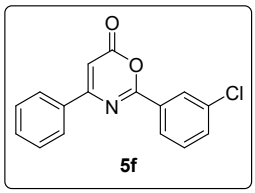
Following the general procedure 1 on 0.2 mmol scale, yield: 53 % (32 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.73 (d, *J* = 1.8 Hz, 1H), 8.44 – 8.39 (m, 2H), 8.03 (ddd, *J* = 11.8, 7.8, 2.0 Hz, 2H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.92 – 7.88 (m, 1H), 7.67 – 7.62 (m, 1H), 7.61 – 7.54 (m, 4H), 6.72 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.1, 161.6, 160.0, 135.0, 133.4, 133.0, 131.6, 130.1, 129.4, 128.9, 128.8, 128.6, 128.1, 127.8, 126.9, 123.3, 101.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{20}H_{14}NO_2^+$ 300.1019; found: 300.1022;

2-(3-chlorophenyl)-4-phenyl-6H-1,3-oxazin-6-one (5f) [CAS:381174-05-6]



5f

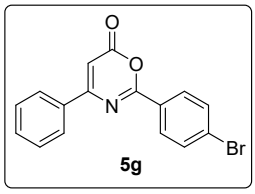
Following the general procedure 1 on 0.2 mmol scale, yield: 47 % (27 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.33 (t, *J* = 1.8 Hz, 1H), 8.26 – 8.18 (m, 1H), 8.08 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.60 – 7.57 (m, 1H), 7.54 (qd, *J* = 8.8, 8.0, 4.0 Hz, 3H), 7.47 (t, *J* = 7.9 Hz, 1H), 6.61 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 161.9, 161.7, 159.4, 135.1, 134.2, 133.4, 132.1, 131.8, 130.2, 129.0, 128.9, 128.7, 127.4, 126.8, 102.2.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{16}H_{11}ClNO_2^+$ 284.0473; found: 284.0480;

2-(4-bromophenyl)-4-phenyl-6H-1,3-oxazin-6-one (5g) [CAS:2087490-80-8]



5g

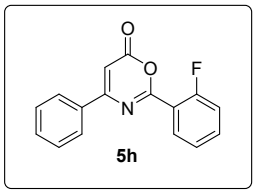
Following the general procedure 1 on 0.2 mmol scale, yield: 46 % (30 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.25 – 8.18 (m, 2H), 8.11 – 8.05 (m, 2H), 7.71 – 7.64 (m, 2H), 7.59 – 7.49 (m, 3H), 6.60 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) 162.4, 161.8, 159.5, 134.3, 132.2, 132.1, 130.1, 129.0, 129.0, 128.7, 127.4, 101.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{16}H_{11}BrNO_2^+$ 327.9968; found: 327.9973;

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



Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp:117-122 ℃, yield: 53 % (32 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

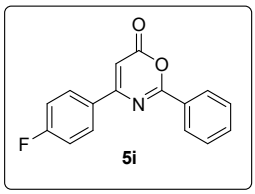
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.24 – 8.16 (m, 1H), 8.08 (d, *J* = 7.4 Hz, 2H), 7.58 (q, *J* = 7.6 Hz, 1H), 7.51 (h, *J* = 8.2, 7.5 Hz, 3H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.27 – 7.21 (m, 1H), 6.62 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 162.9, 161.7, 160.8, 160.7 (d, *J* = 5.8 Hz), 159.5, 134.8 (d, *J* = 8.9 Hz), 134.2, 132.0, 131.4, 129.0, 127.4, 124.4 (d, *J* = 3.9 Hz), 118.7 (d, *J* = 8.2 Hz), 117.6, 117.4, 102.0.

^{19}F NMR (471 MHz, Chloroform-d) δ -107.5.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{16}H_{11}FNO_2^+$ 268.0768; found: 268.0764;

4-(4-fluorophenyl)-2-phenyl-6H-1,3-oxazin-6-one (5i) [CAS:1589584-38-2]



Following the general procedure 1 on 0.2 mmol scale, yield: 60 % (32 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

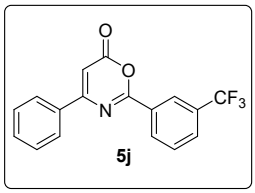
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.38 – 8.30 (m, 2H), 8.14 – 8.08 (m, 2H), 7.65 – 7.59 (m, 1H), 7.53 (dd, J = 8.5, 7.0 Hz, 2H), 7.20 (t, J = 8.5 Hz, 2H), 6.54 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 165.2 (d, J = 253.8 Hz), 163.3, 160.8, 159.7, 133.5, 130.7, 130.6, 129.9, 129.8, 129.6, 128.9, 128.8, 116.2, 116.1, 101.3.

^{19}F NMR (471 MHz, Chloroform-d) δ -107.28.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{16}H_{11}FNO_2^+$ 268.0768; found: 267.0764;

4-phenyl-2-(3-(trifluoromethyl)phenyl)-6H-1,3-oxazin-6-one (5j)



Following the general procedure 1 on 0.2 mmol scale, yellow solid, mp:94-100℃, yield: 50 % (31 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

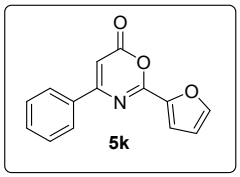
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.60 (d, J = 2.1 Hz, 1H), 8.53 (d, J = 8.1 Hz, 1H), 8.12 – 8.06 (m, 2H), 7.87 (d, J = 7.8 Hz, 1H), 7.68 (t, J = 7.9 Hz, 1H), 7.60 – 7.50 (m, 3H), 6.64 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 161.7 (d, J = 6.1 Hz), 159.2, 134.1, 132.2, 131.8, 131.0, 130.0 (d, J = 3.7 Hz), 129.5, 129.1, 127.4, 125.6 (d, J = 3.9 Hz), 124.9 – 120.1 (m), 102.3.

^{19}F NMR (471 MHz, Chloroform-d) δ -62.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{17}H_{11}F_3NO_2^+$ 318.0736; found: 318.0733;

2-(furan-2-yl)-4-phenyl-6H-1,3-oxazin-6-one (5k) [CAS:2087490-88-6]



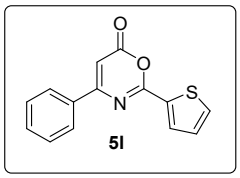
Following the general procedure 1 on 0.2 mmol scale, yield: 61 % (29 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.07 – 8.02 (m, 2H), 7.72 (dd, J = 1.7, 0.8 Hz, 1H), 7.55 – 7.48 (m, 3H), 7.45 (dd, J = 3.6, 0.8 Hz, 1H), 6.64 (dd, J = 3.6, 1.7 Hz, 1H), 6.52 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 162.3, 158.9, 155.5, 147.6, 144.7, 134.3, 132.0, 129.0, 127.4, 118.6, 112.9, 101.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{14}H_{10}NO_3^+$ 240.0655; found: 240.0657;

4-phenyl-2-(thiophen-2-yl)-6H-1,3-oxazin-6-one (5l) [CAS:2087490-87-5]



Following the general procedure 1 on 0.2 mmol scale, yield: 66 % (34 mg), R_f = 0.3 (silica gel, PE: EA = 10:1, v/v), column chromatography (silica gel, PE: DCM = 10:1, v/v).

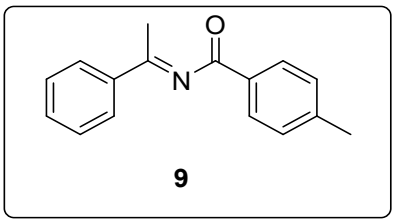
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.07 – 8.03 (m, 2H), 8.02 (dd, *J* = 3.8, 1.3 Hz, 1H), 7.67 (dd, *J*

= 5.0, 1.3 Hz, 1H), 7.55 – 7.48 (m, 3H), 7.19 (dd, *J* = 5.0, 3.8 Hz, 1H), 6.52 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 162.2, 159.7, 159.4, 134.3, 134.2, 133.7, 132.8, 132.0, 129.0, 128.6, 128.1, 127.4, 100.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{14}H_{10}NO_2S^+$ 256.0427; found: 256.0423;

4-methyl-N-(1-phenylethylidene)benzamide (9)



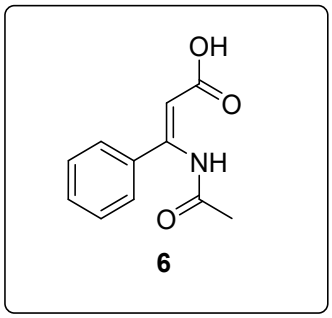
9

Following the general procedure 1 on 0.2 mmol scale, yellow oil, yield: 80 % (38 mg), R_f = 0.3 (silica gel, PE: EA = 20:1, v/v), column chromatography (silica gel, PE: DCM = 20:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.06 – 7.99 (m, 2H), 7.93 – 7.86 (m, 2H), 7.58 – 7.53 (m, 1H), 7.53 – 7.47 (m, 2H), 7.30 – 7.26 (m, 2H), 2.44 (s, 3H), 2.41 (s, 3H).
^{13}C NMR (126 MHz, Chloroform-*d*) δ 180.6, 165.5, 144.0, 137.1, 131.7, 130.5, 129.4, 129.3, 128.6, 127.7, 21.7, 19.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{16}H_{16}NO^+$ 238.1226; found: 238.1228;

(Z)-3-acetamido-3-phenylacrylic acid (6) [CAS:950919-72-9]



6

Following the general procedure 1 on 0.2 mmol scale, yield: 90 % (37 mg), R_f = 0.3 (silica gel, PE: EA = 2:1, v/v), column chromatography (silica gel, PE: DCM = 2:1, v/v).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 10.52 (s, 1H), 7.52 – 7.33 (m, 5H), 5.34 (s, 1H), 2.20 (s, 3H).
^{13}C NMR (126 MHz, Chloroform-*d*) δ 172.6, 168.8, 156.7, 135.7, 130.0, 128.2, 127.2, 100.1, 24.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{11}H_{12}NO_3^+$ 206.0812; found: 206.0808;

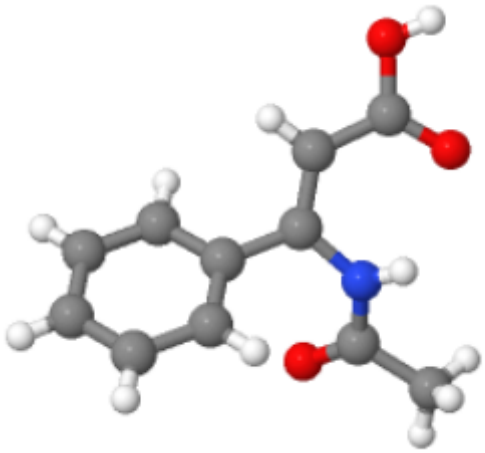
5. Crystal Data

Crystal data of 6

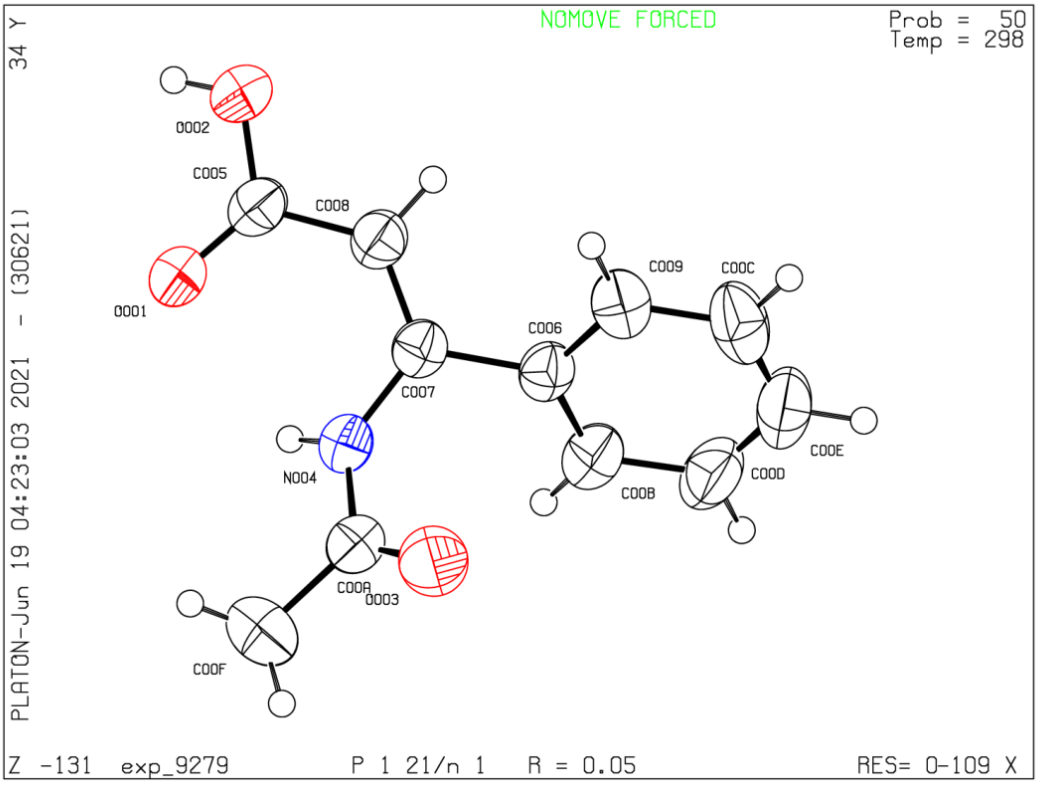
Method for single crystals cultivation: a pure solid sample (10−20 mg) was dissolved in ethyl acetate (2 mL) in a vial at room temperature, and petroleum ether/hexane (2-3 mL) was added into the above solution slowly while keeping the sample completely dissolved. The vial was properly sealed with parafilm and kept at room temperature to allow the slow evaporation of the solvents until a single crystal was obtained.

The data were collected on a Agilent Gemini E diffractometer（Mo，50kV 40mA） instrument using Mo-Kαradiation (λ = 0.71073 Å) at 296 K and reducted by CrysAlisPro (Rigaku). The crystal structures were solved and refined using the SHELXTL software package. Refinements were performed with SHELXL-2013 using fullmatrix least-squares calculations on F2, with anisotropic displacement parameters for all the nonhydrogen atoms. The crystallographic data have already been deposited at the Cambridge Crystallographic Data Centre.

Crystallographic data for compound **6** (CCDC-2090953) has been deposited with the Cambridge Crystallographic Data Centre, Copies of the data can be obtained, free of charge, on application to CCDC (Email:deposit@ccdc.cam.ac.uk). Thermal ellipsoids are drawn at 50% probability level



Datablock exp_9279 - ellipsoid plot



Bond precision: C-C = 0.0028A Wavelength=0.71073

Cell: a=13.3443(15) b=5.3107(6) c=15.7486(17)
alpha= 90 beta=105.862(12) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	1073.6(2)	1073.6(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2ybc (x-
Moiety formula	C11 H11 N O3	C11 H11 N O3
Sum formula	C11 H11 N O3	C11 H11 N O3
Mr	205.21	205.21
Dx,g cm-3	1.270	1.270
Z	4	4
Mu (mm-1)	0.093	0.093
F000	432.0	432.3
F000'	432.23	
h,k,lmax	15,6,18	15,6,18
Nref	1888	1886
Tmin,Tmax		0.503,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.503 Tmax=1.000
AbsCorr = MULTI-SCAN

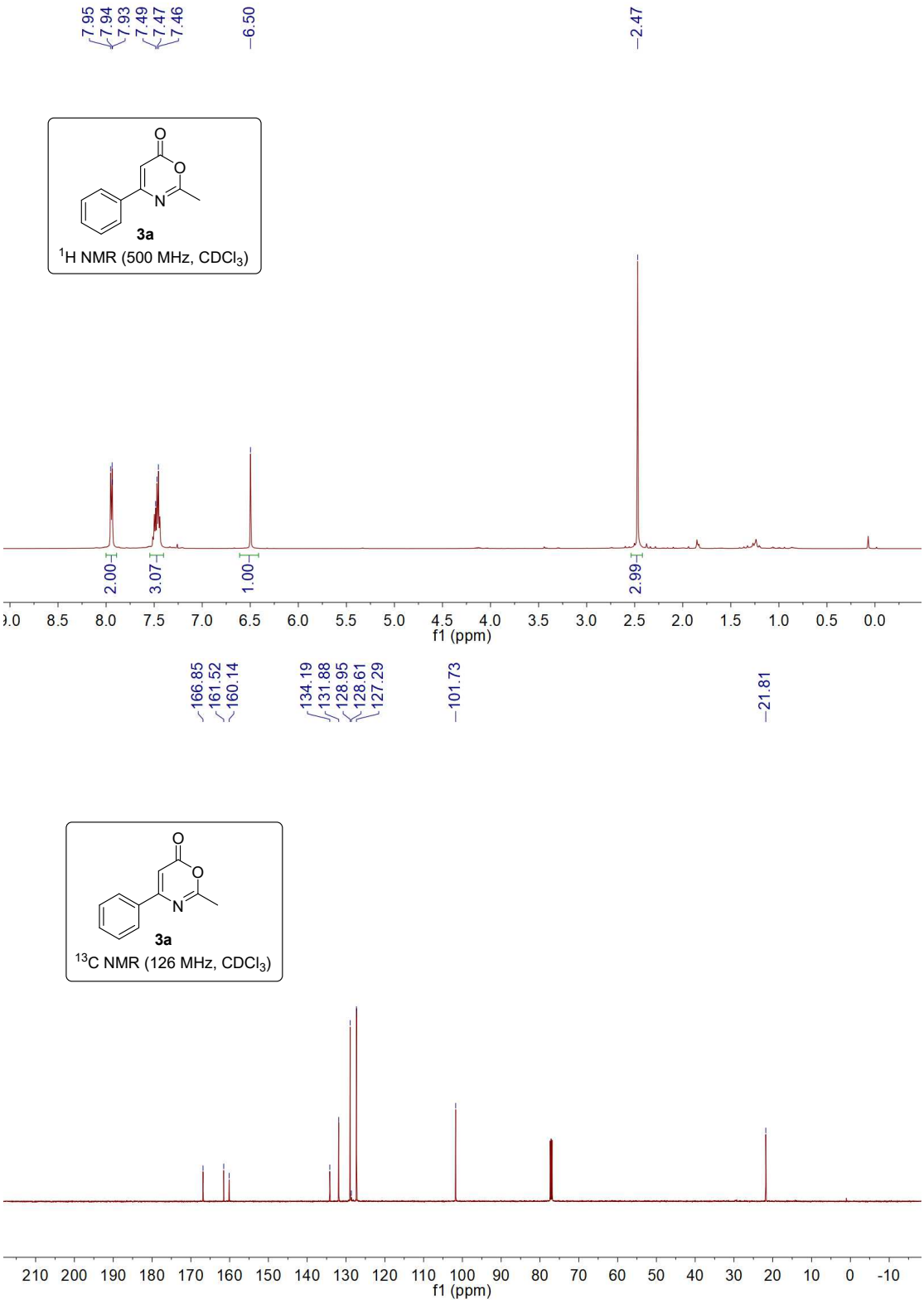
Data completeness= 0.999 Theta(max)= 24.990
R(reflections)= 0.0463 (1542) wR2(reflections)= 0.1587(1886)
S = 1.103 Npar= 137

6. References

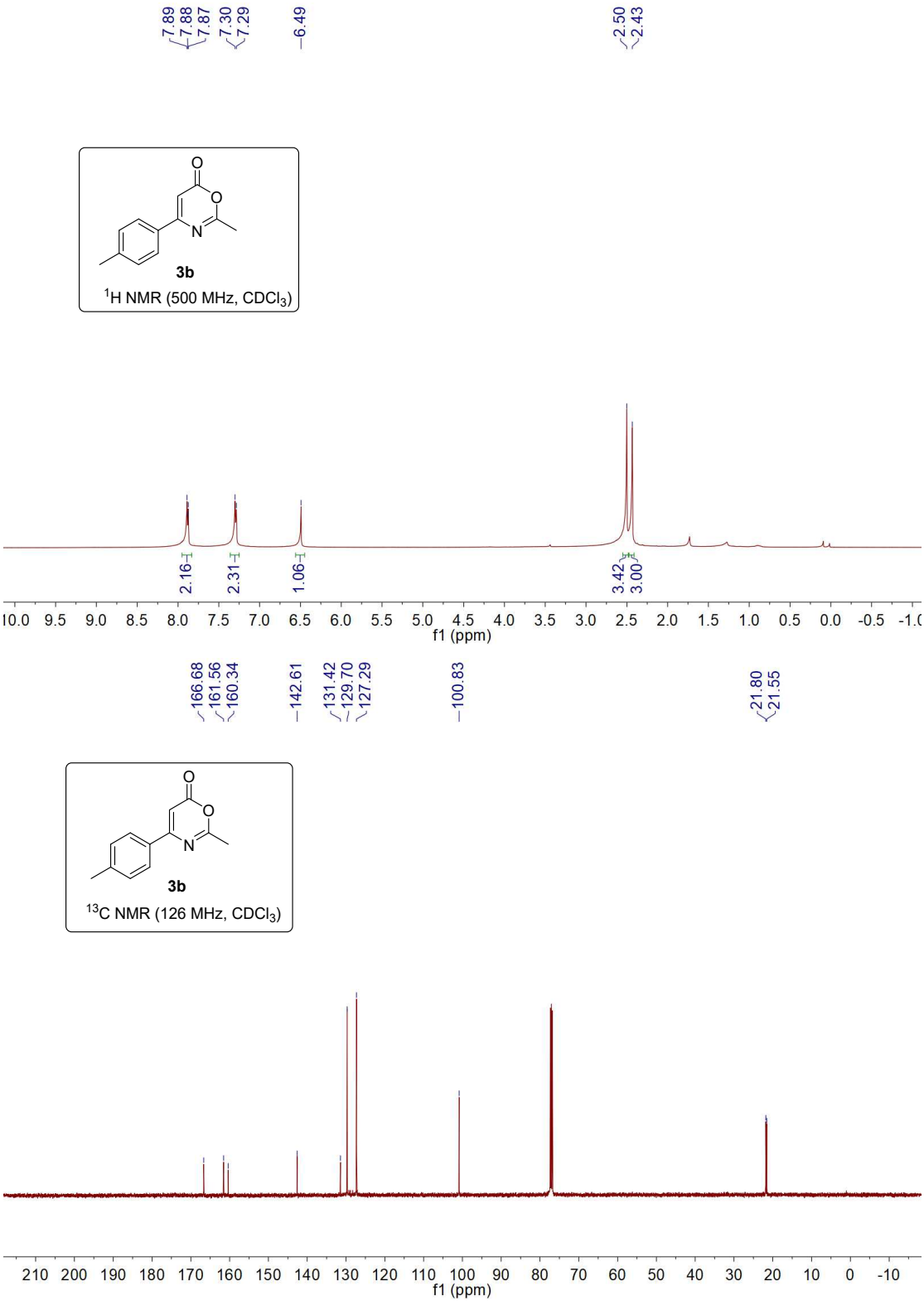
[1]J.P. Brand, J. Waser, *Angew. Chem., Int. Ed.*, **2010**, *49*, 7304.
[2]M. Berg, R. M. Haak, A. J. Minnaard, A. H. M. Vries, J. G. Vries, B. L. Feringa, *Adv. Synth. Catal.*, **2002**, *344*, 1003;
[3] H. Kiyohara, R. Matsubara and S. Kobayashi, *Org. Lett.*, **2006**, *8*, 5333.
[4] Song, P.; Yu, P.; Lin, J. S.; Liu, X. Y. *Org. Lett.* **2017**, *19*, 1330.

7. NMR Spectra

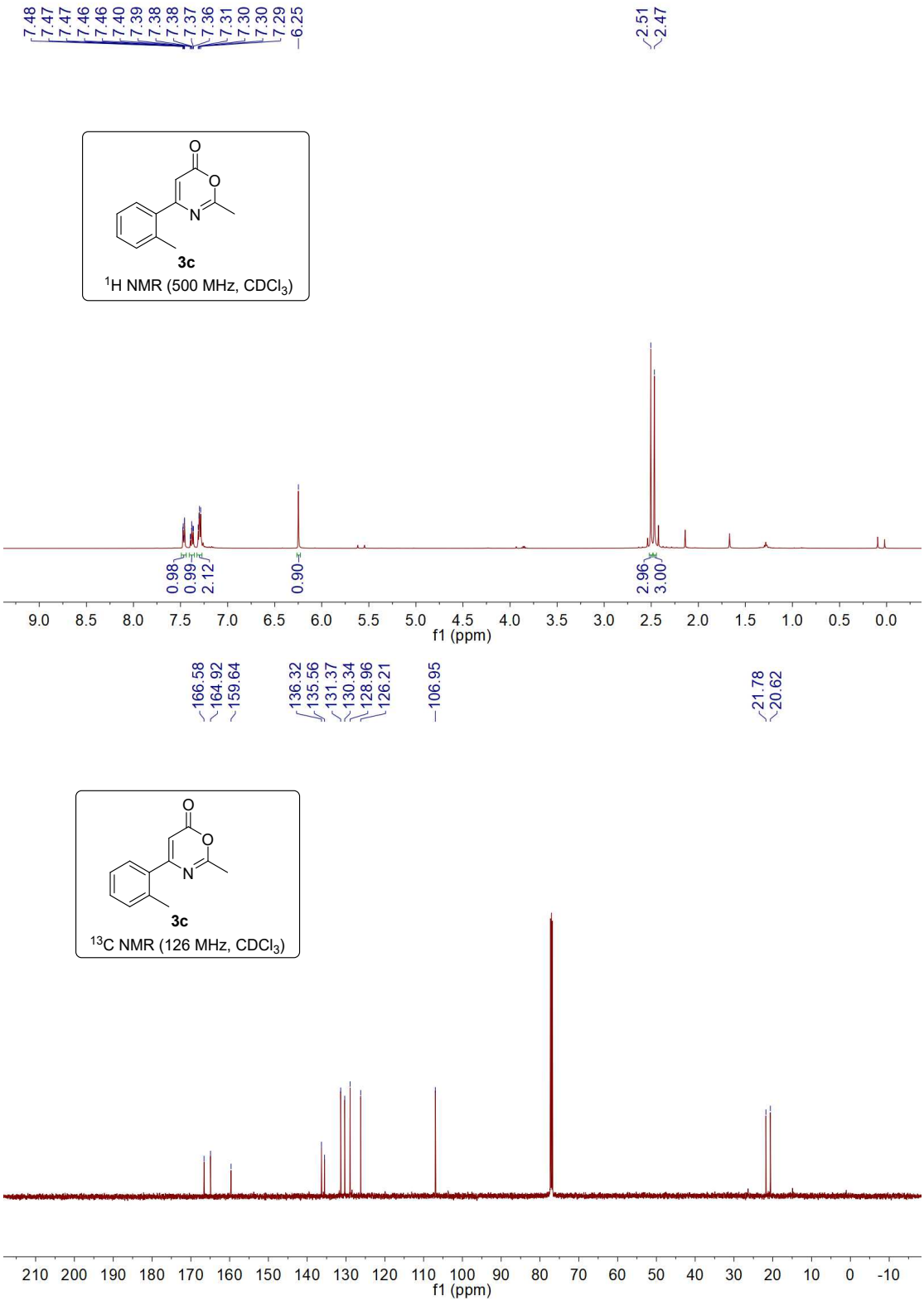
2-methyl-4-phenyl-6H-1,3-oxazin-6-one(3a)



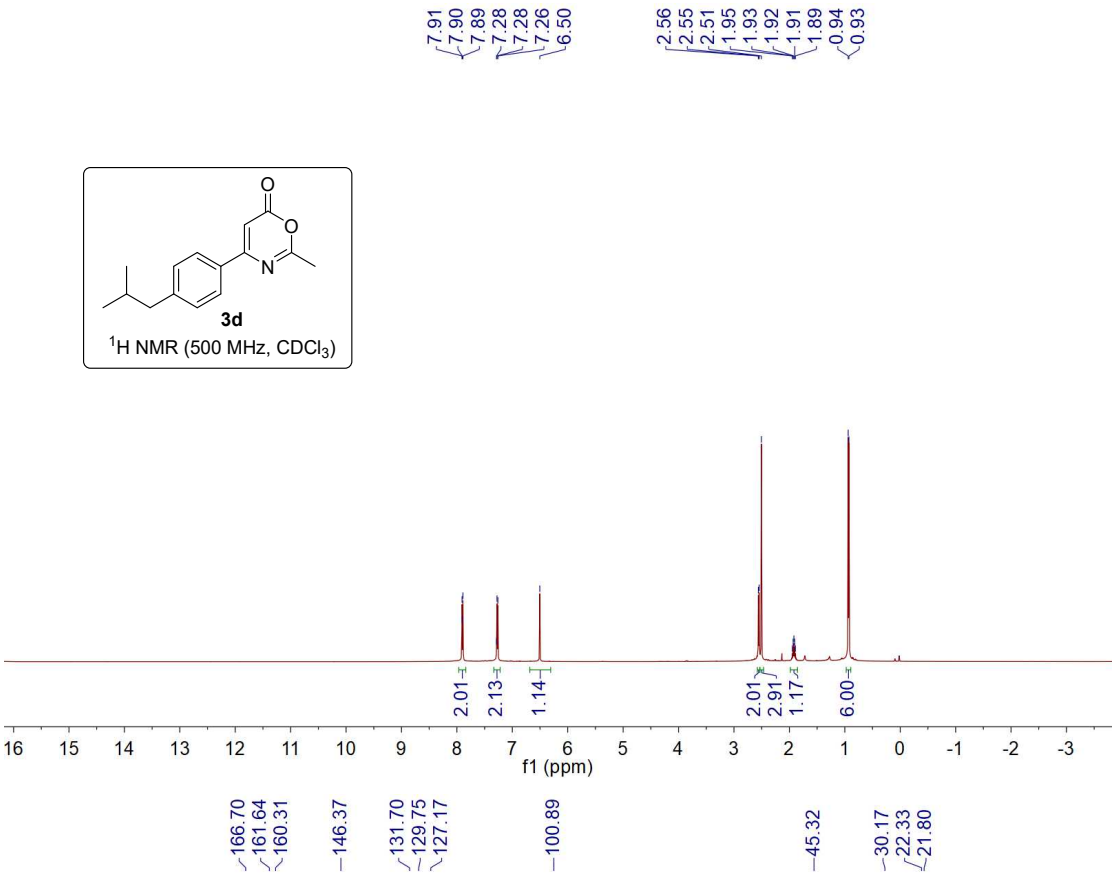
2-methyl-4-(p-tolyl)-6H-1,3-oxazin-6-one (3b)

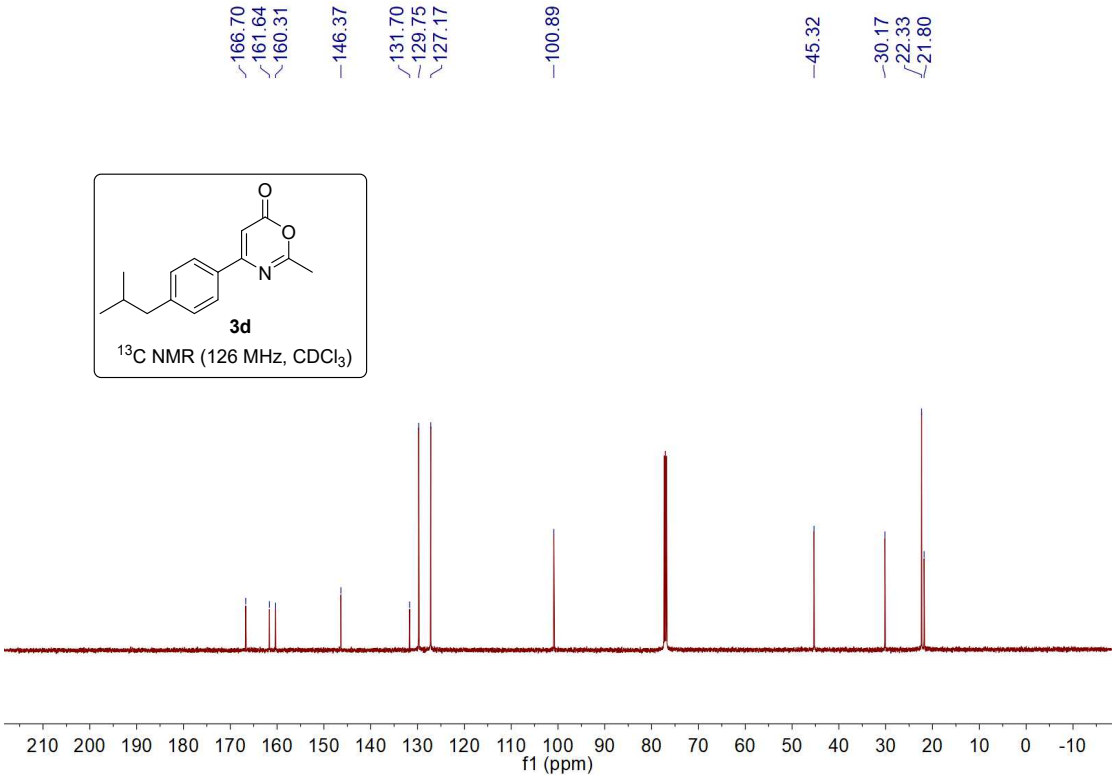


2-methyl-4-(o-tolyl)-6H-1,3-oxazin-6-one (3c)

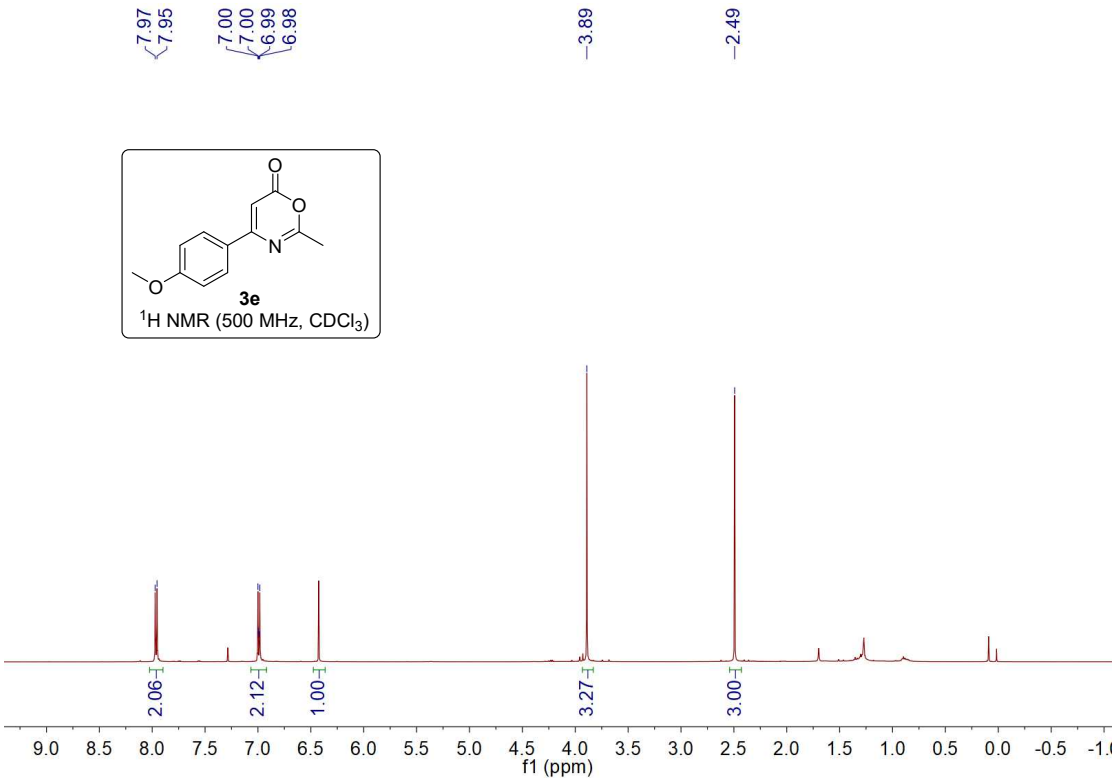


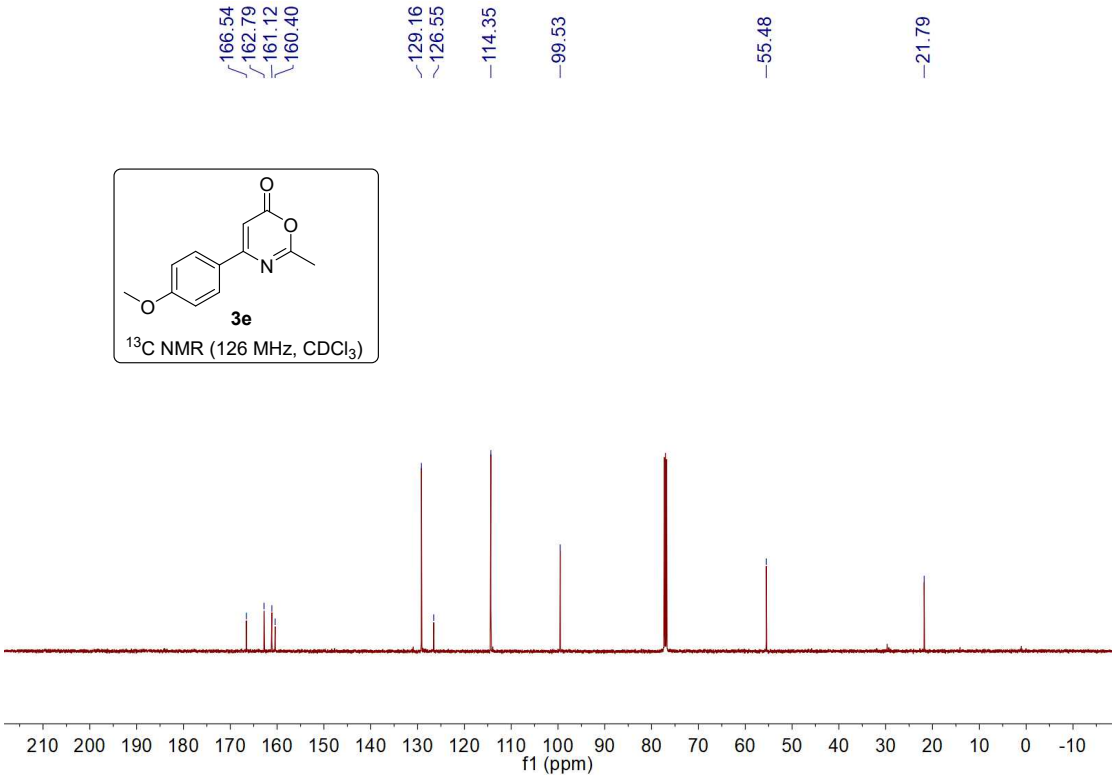
4-(4-isobutylphenyl)-2-methyl-6H-1,3-oxazin-6-one (3d)



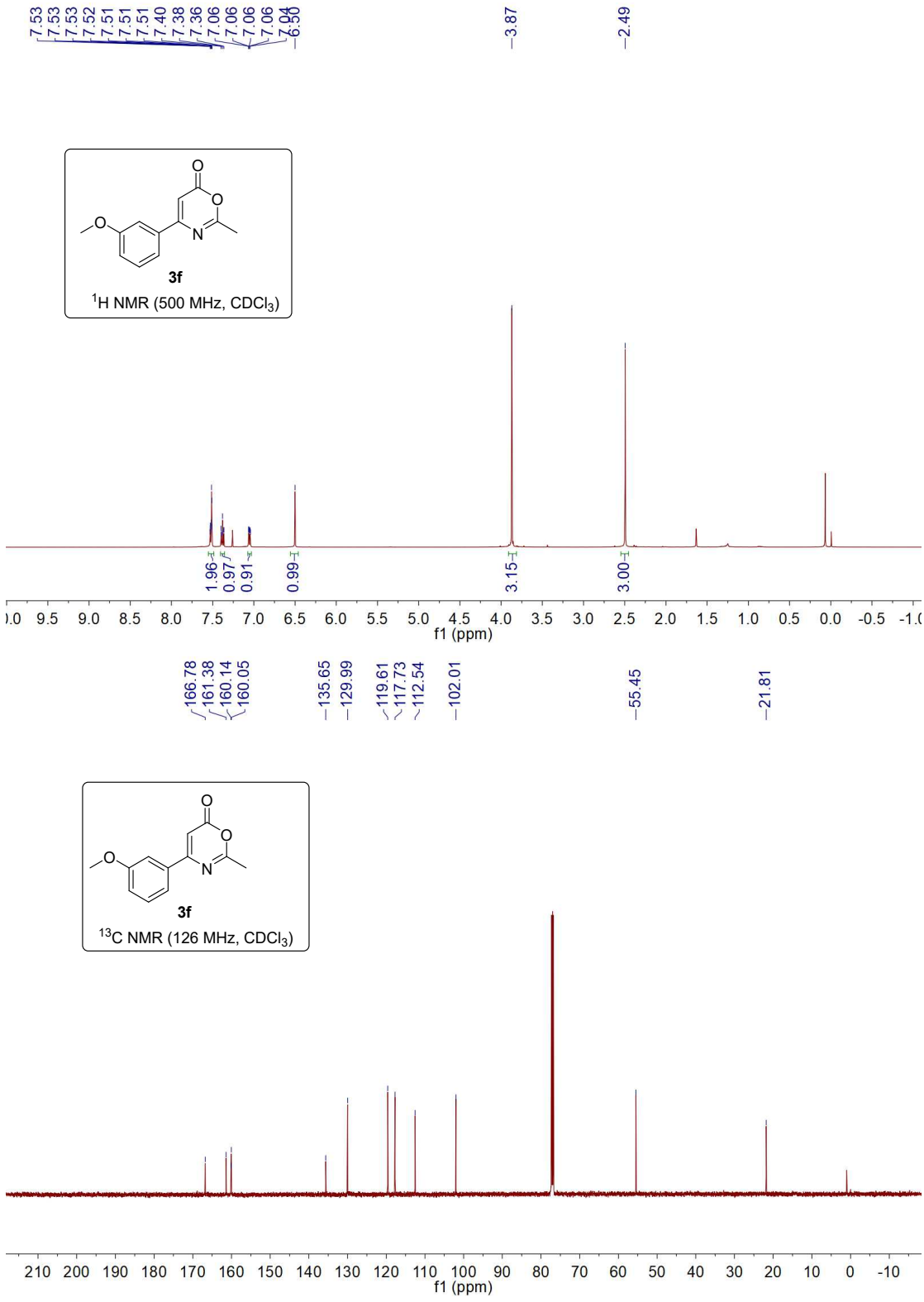


4-(4-methoxyphenyl)-2-methyl-6H-1,3-oxazin-6-one (3e)

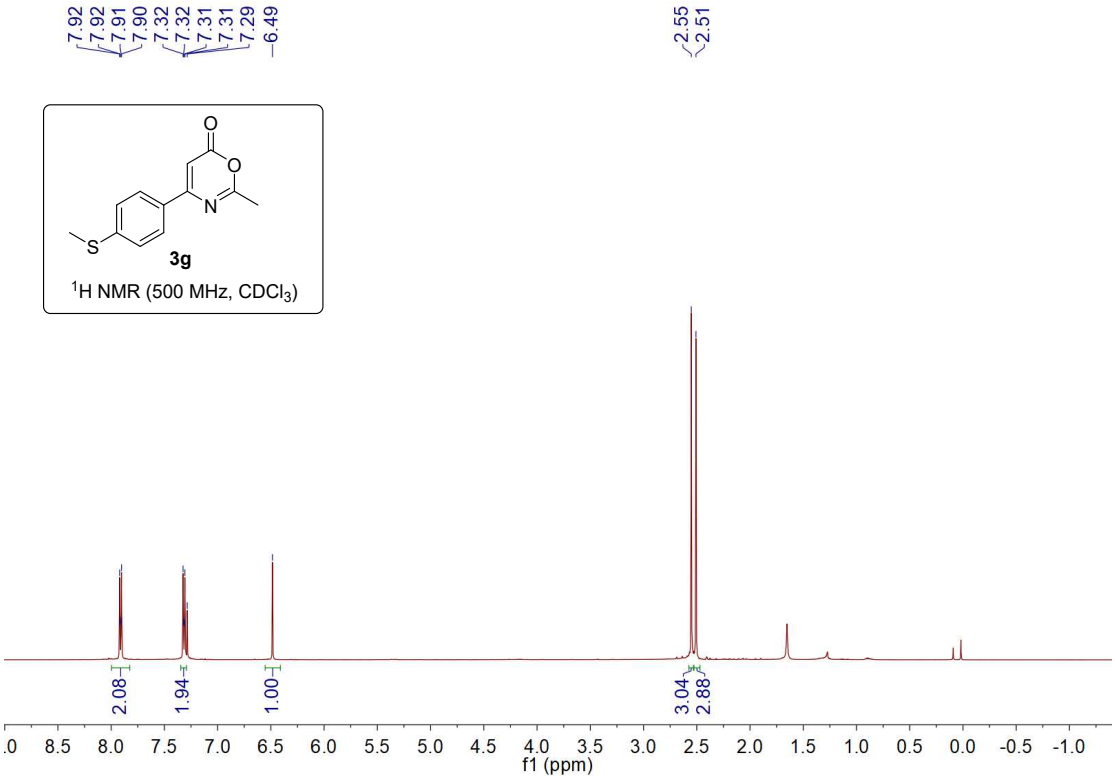


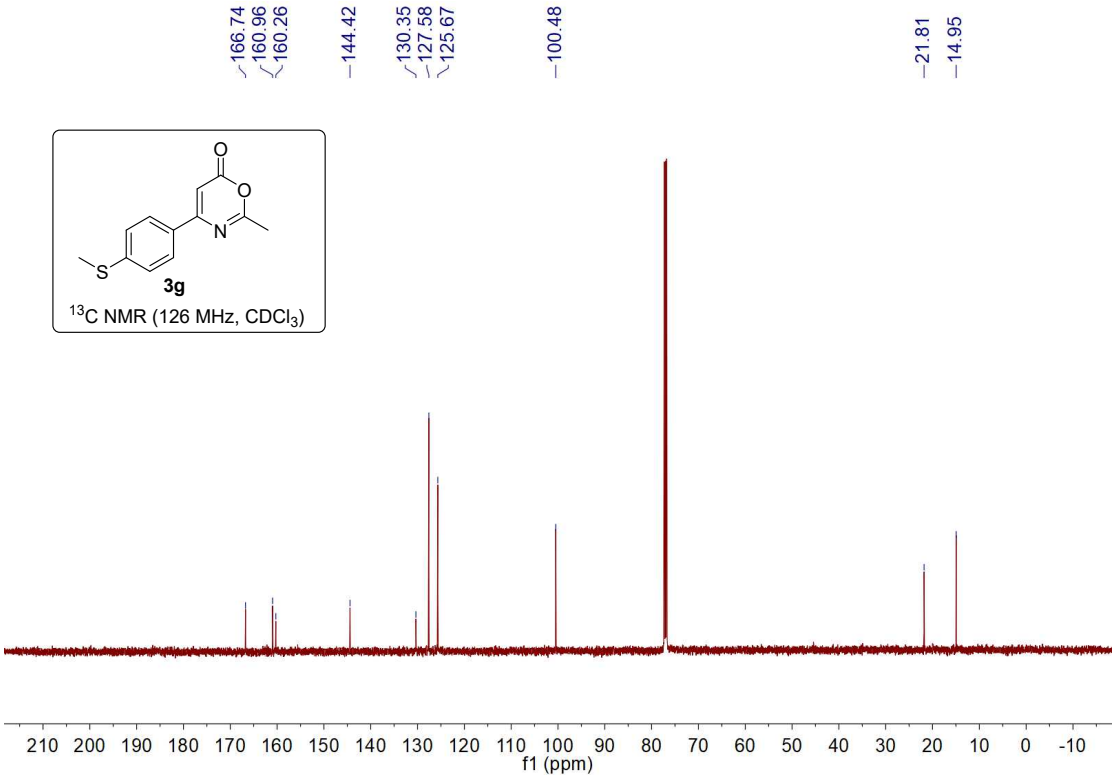


4-(3-methoxyphenyl)-2-methyl-6H-1,3-oxazin-6-one (3f)

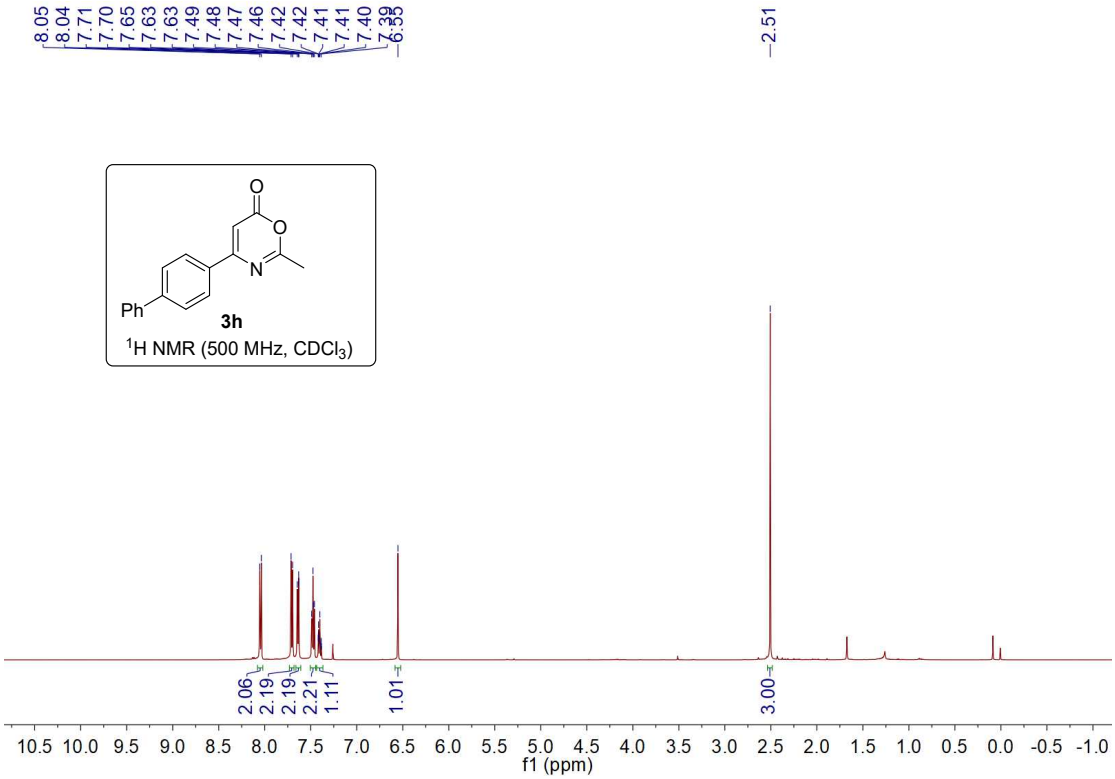


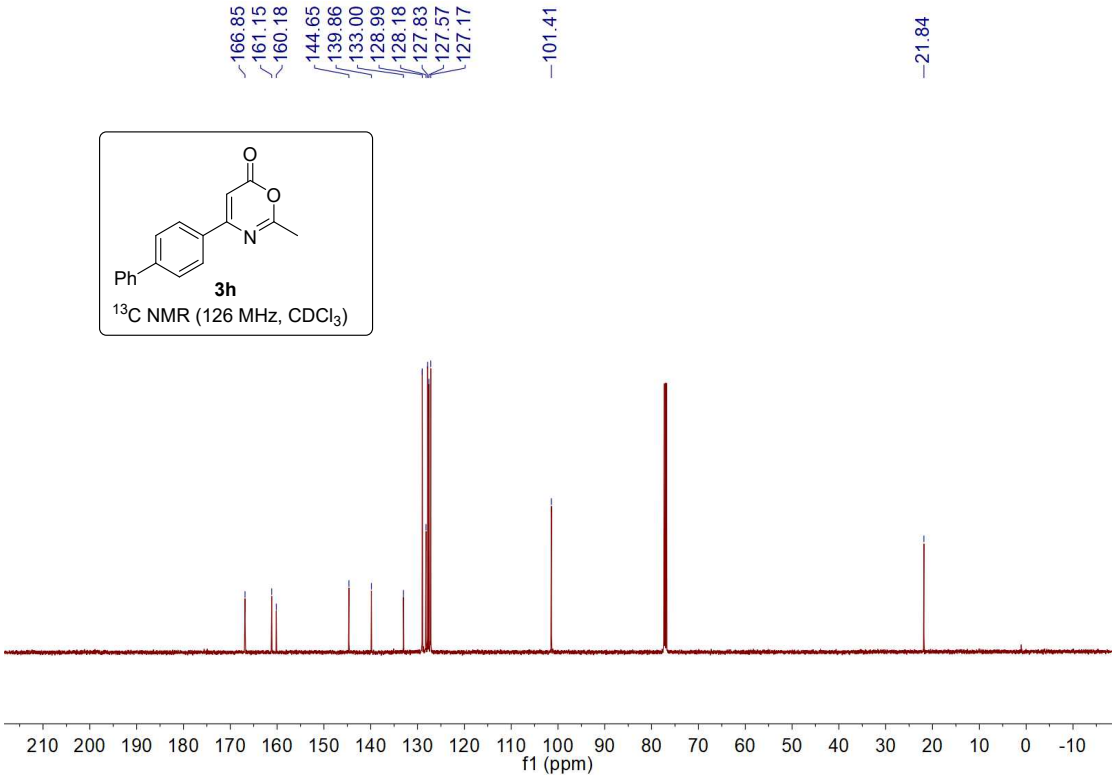
2-methyl-4-(4-(methylthio)phenyl)-6H-1,3-oxazin-6-one (3g)



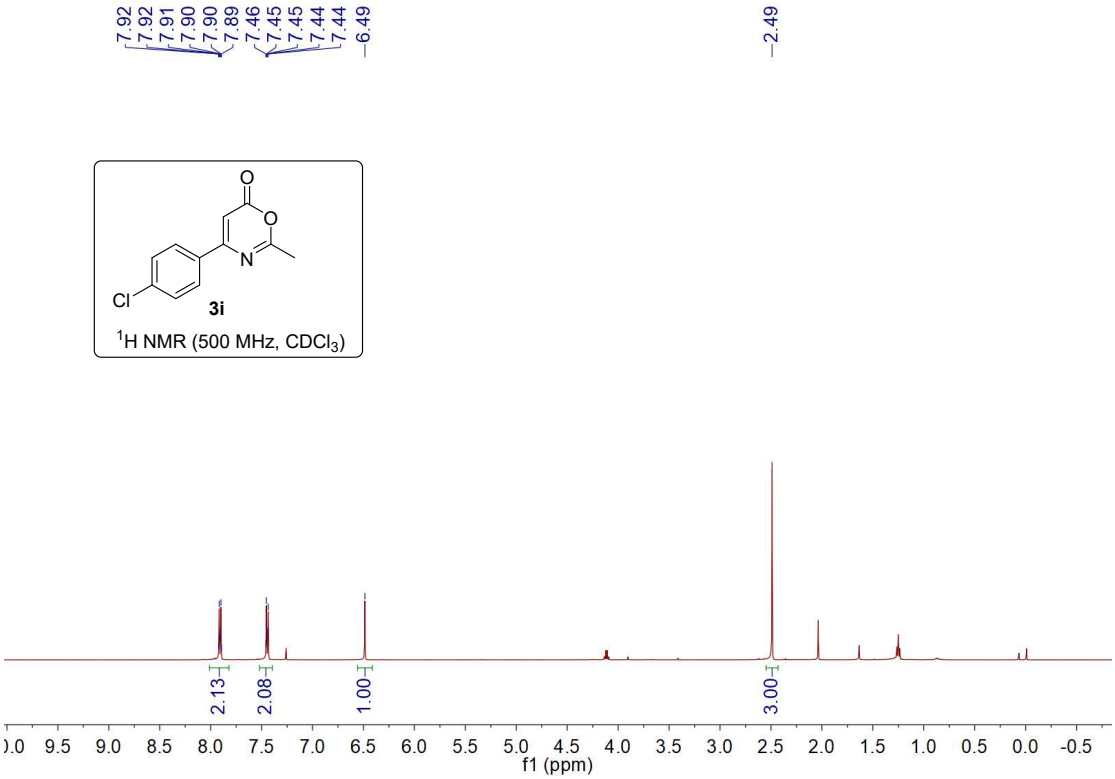


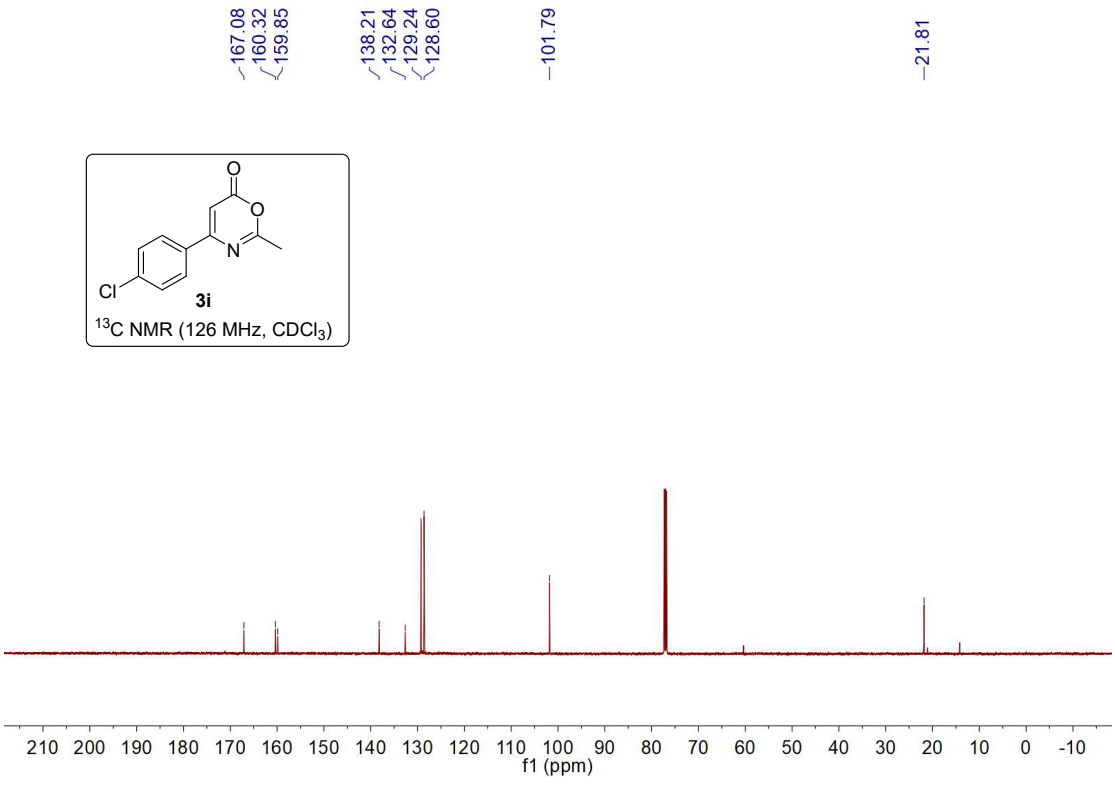
4-([1,1'-biphenyl]-4-yl)-2-methyl-6H-1,3-oxazin-6-one (3h)



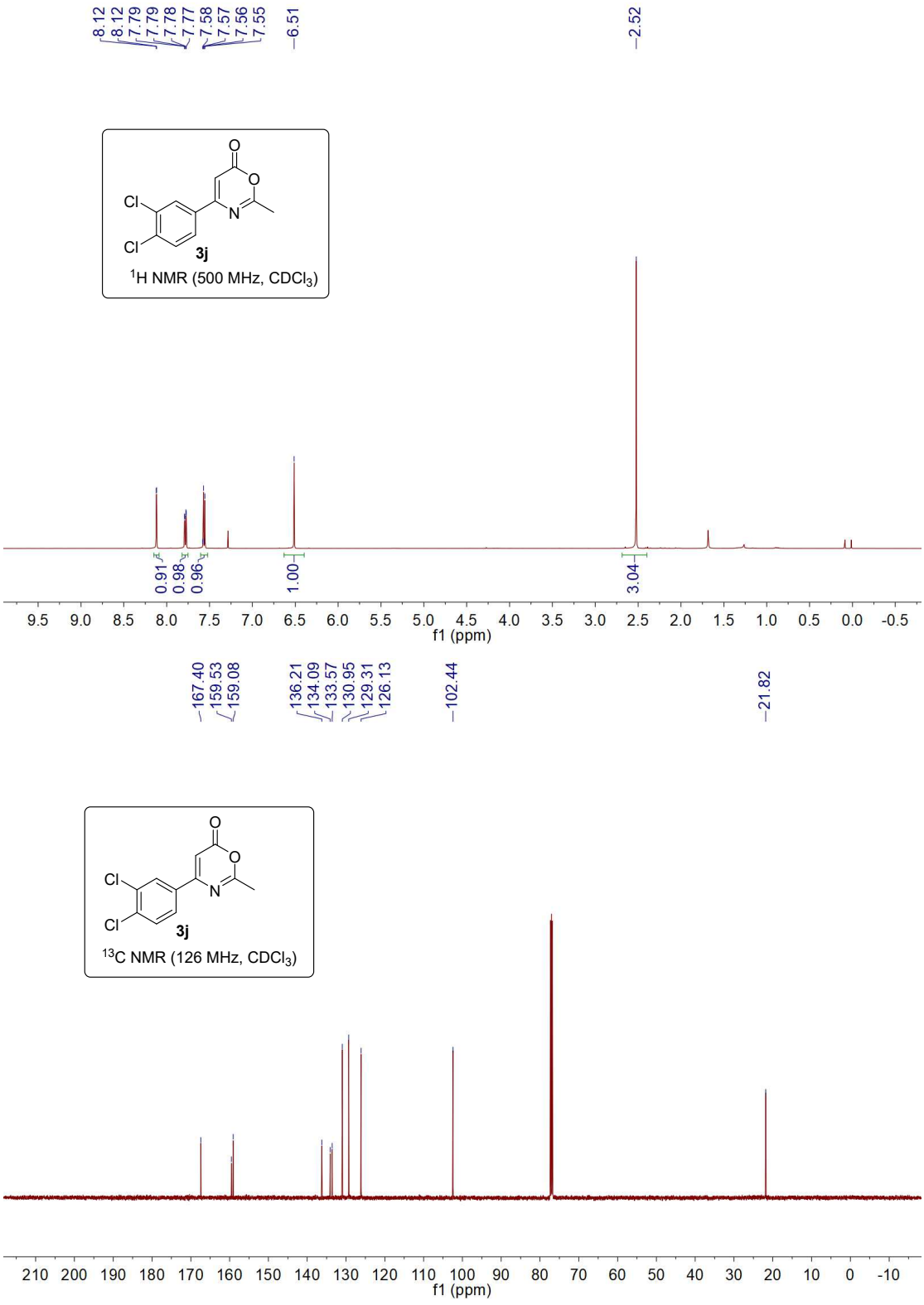


4-(4-chlorophenyl)-2-methyl-6H-1,3-oxazin-6-one (3i)

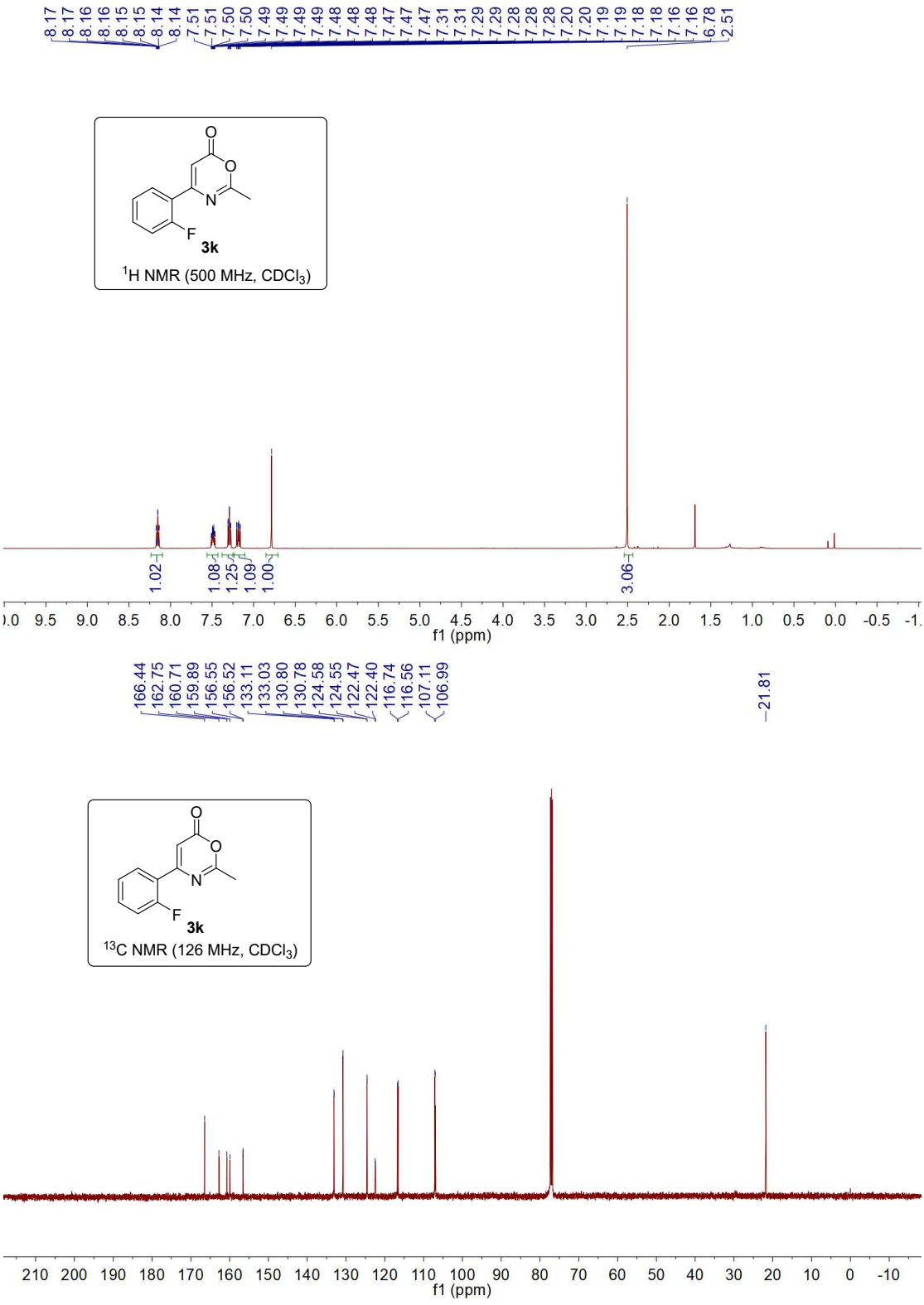




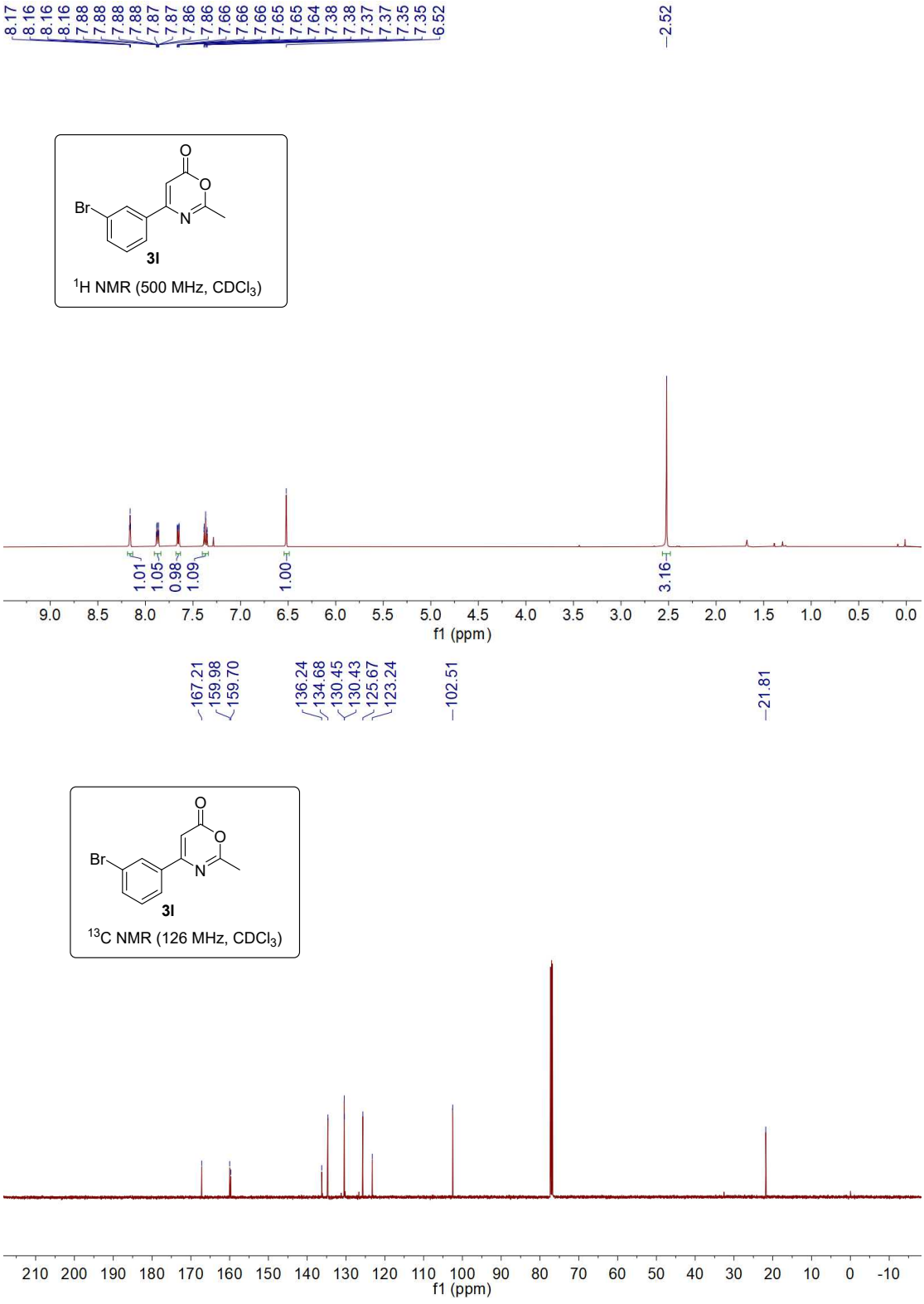
4-(3,4-dichlorophenyl)-2-methyl-6H-1,3-oxazin-6-one (3j)



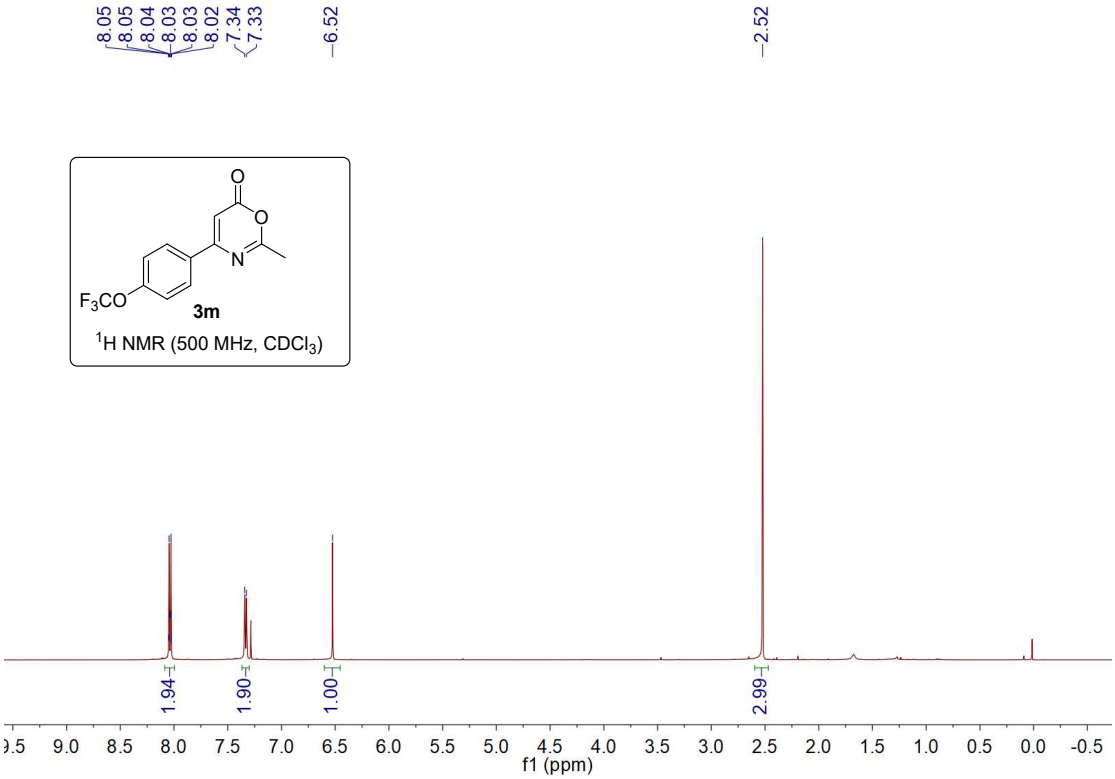
4-(2-fluorophenyl)-2-methyl-6H-1,3-oxazin-6-one (3k)

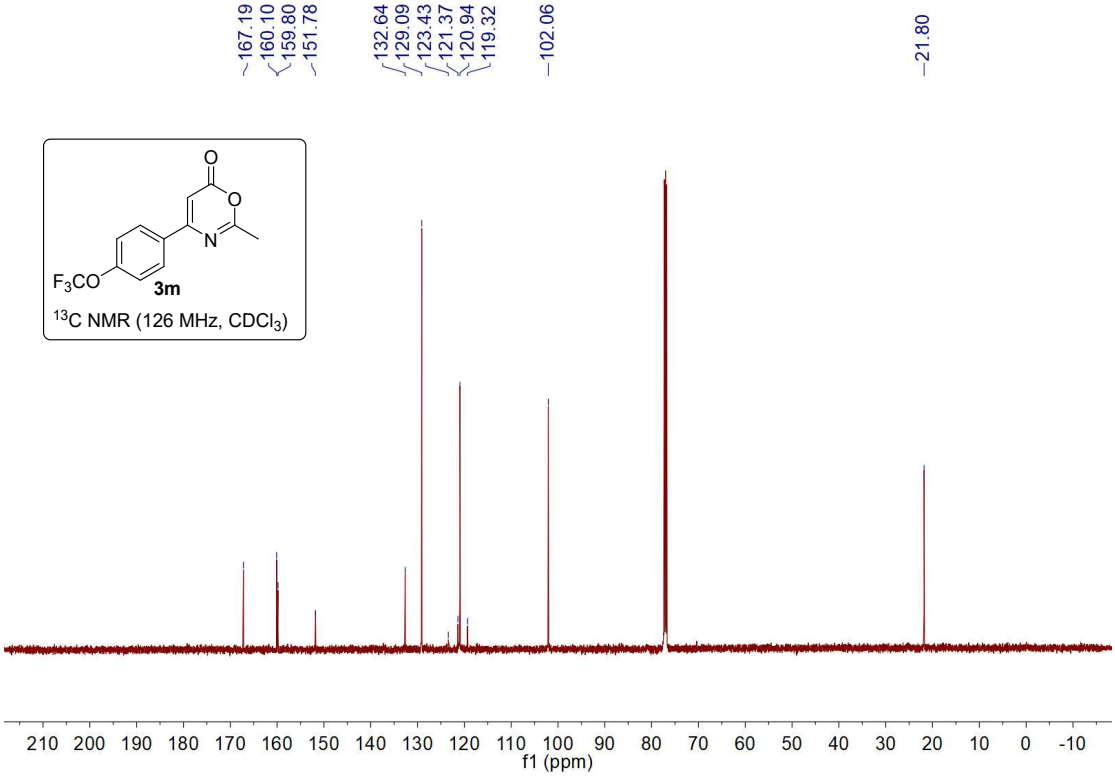


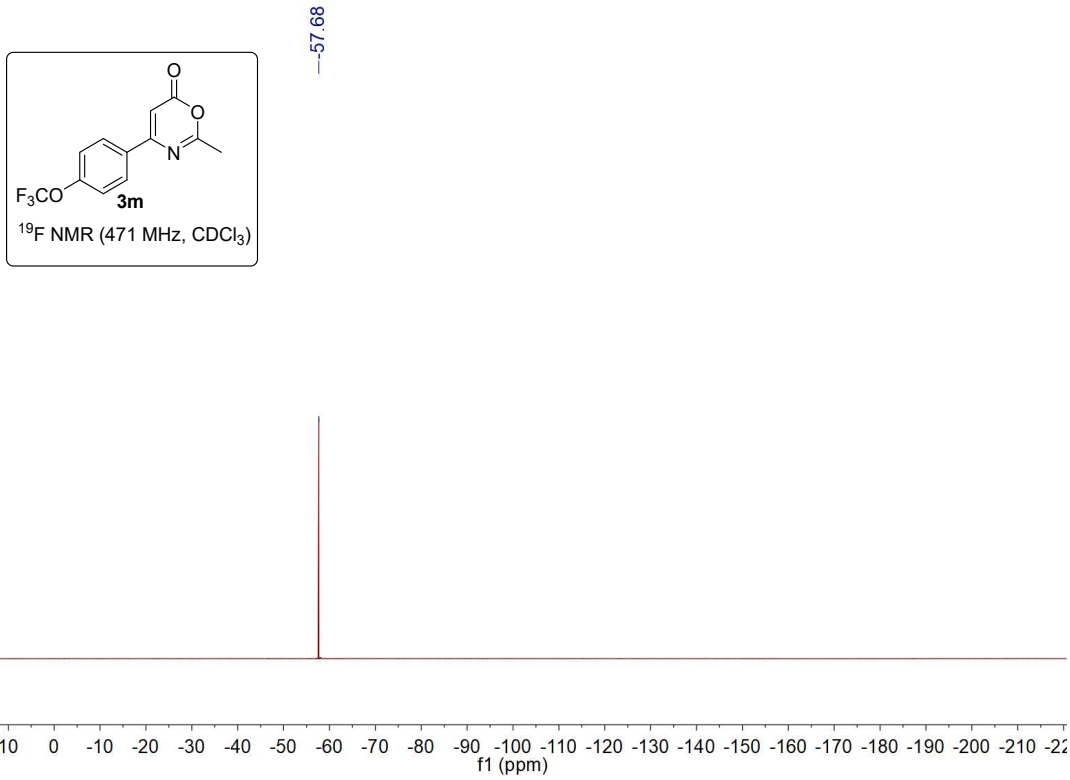
4-(3-bromophenyl)-2-methyl-6H-1,3-oxazin-6-one (3l)



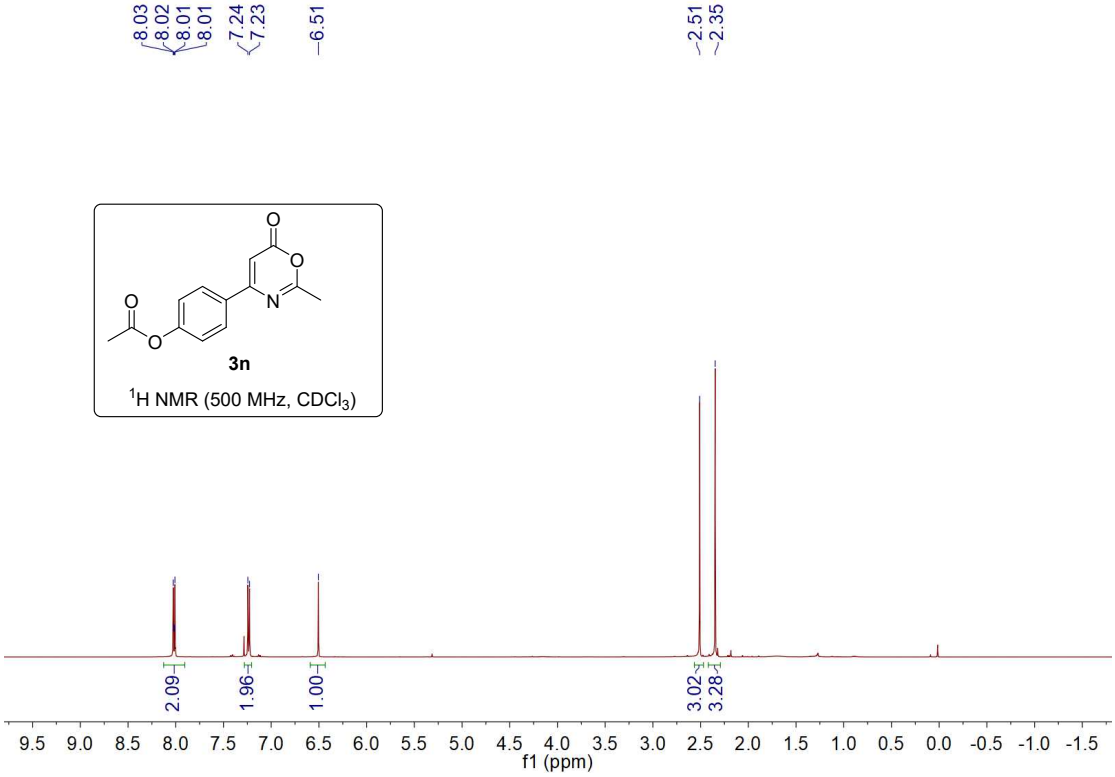
2-methyl-4-(4-(trifluoromethoxy)phenyl)-6H-1,3-oxazin-6-one (3m)

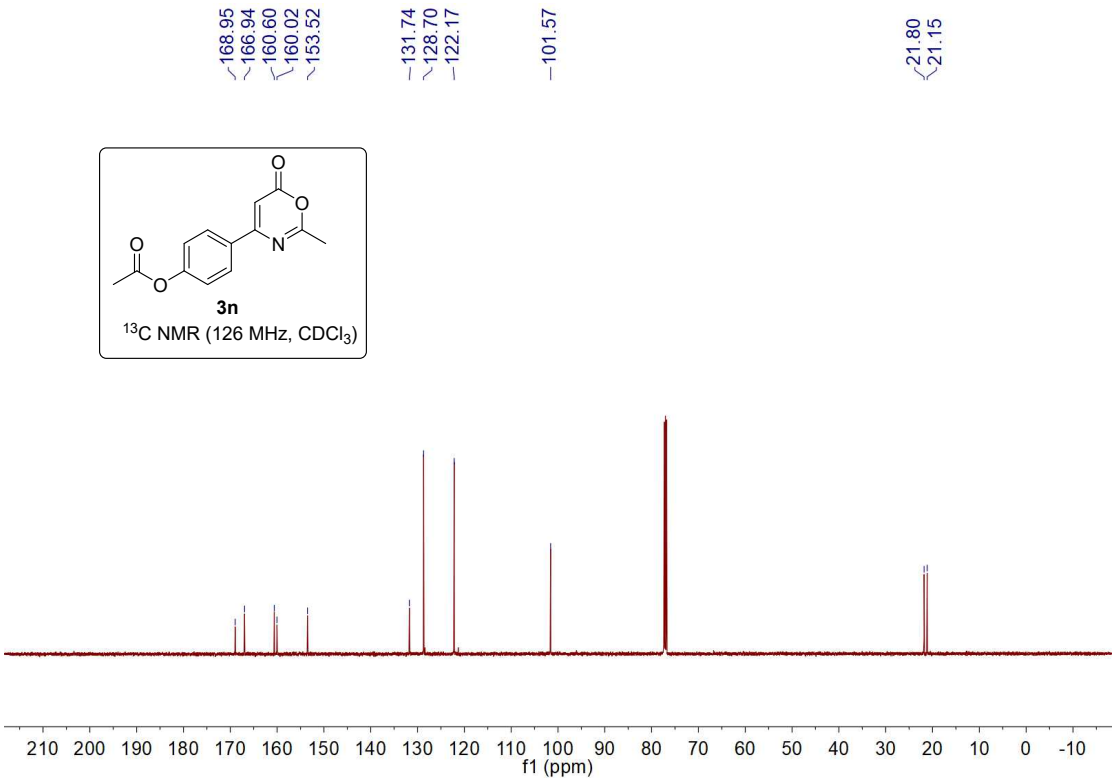

8.05
8.05
8.04
8.03
8.03
8.02
7.34
7.33
6.52
2.52
O
O
N
F3CO
3m
1H NMR (500 MHz, CDCl3)
1.94
1.90
1.00
2.99
f1 (ppm)


167.19
160.10
159.80
151.78
132.64
129.09
123.43
121.37
120.94
119.32
102.06
21.80
O
O
N
F3CO
3m
13C NMR (126 MHz, CDCl3)
f1 (ppm)

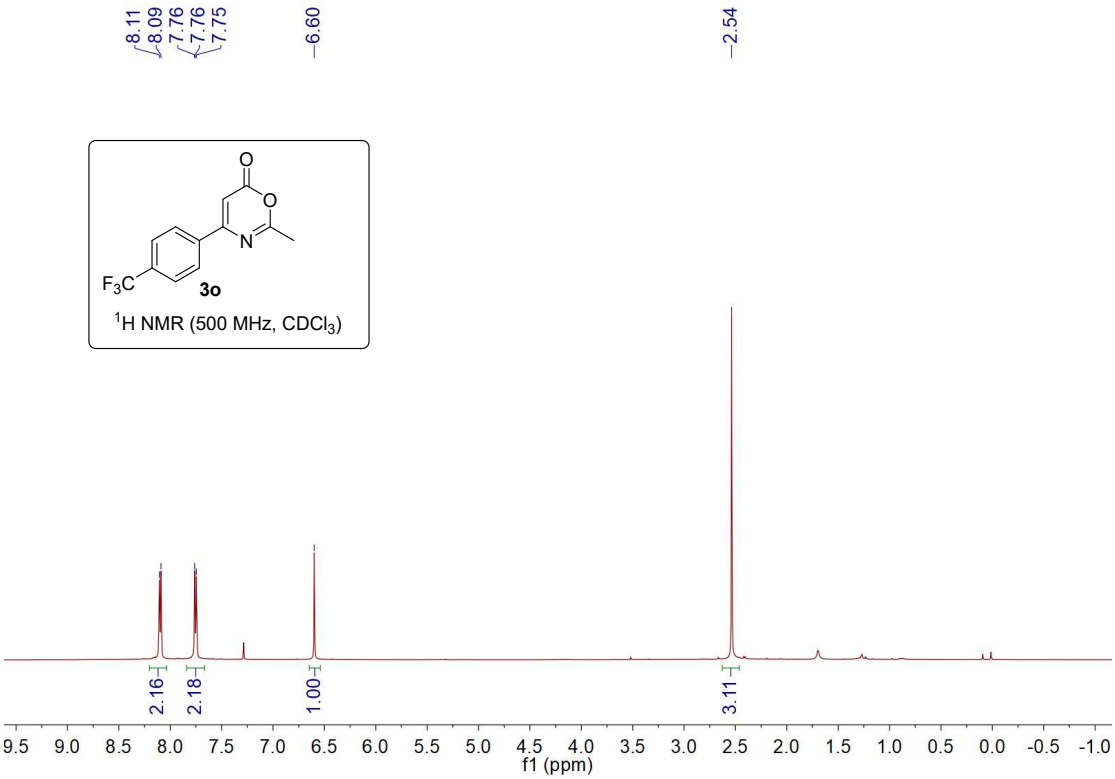


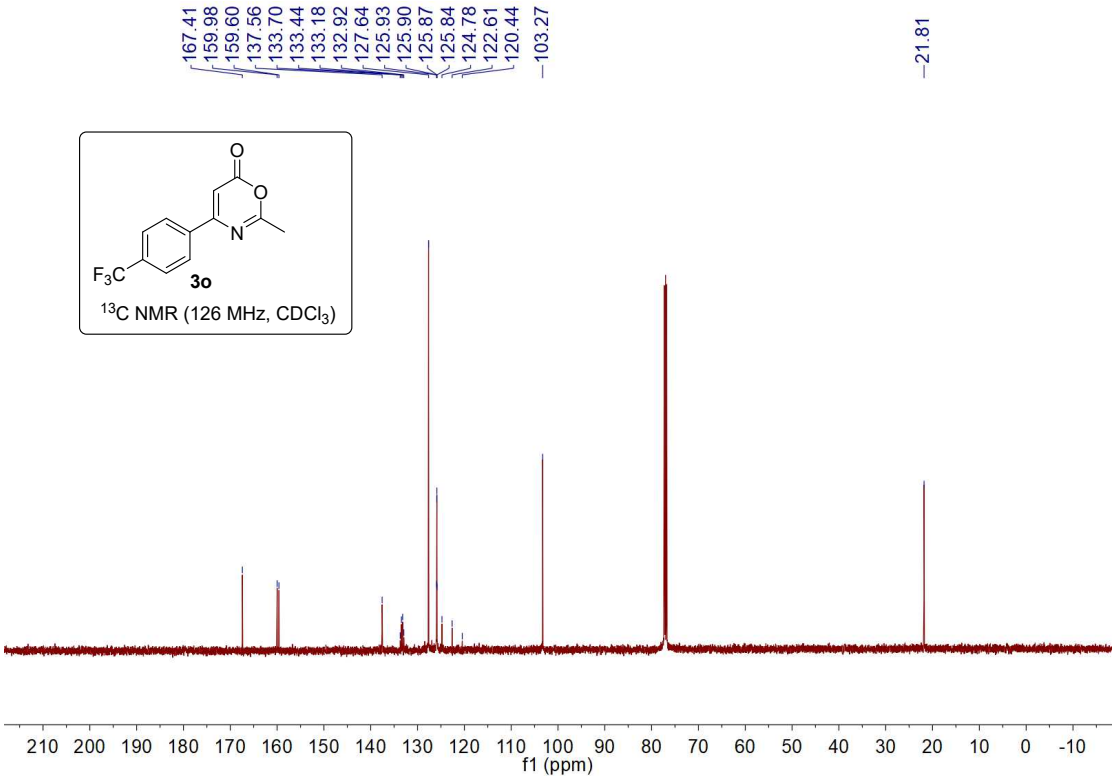
4-(2-methyl-6-oxo-6H-1,3-oxazin-4-yl)phenyl acetate (3n)

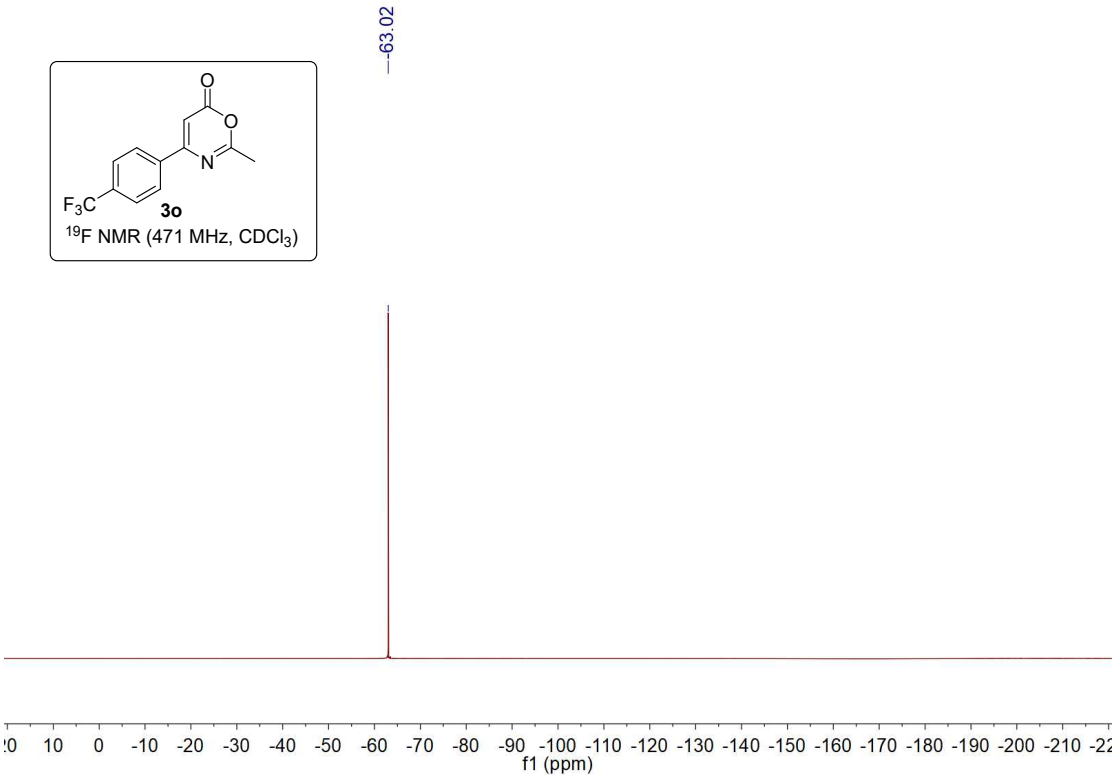




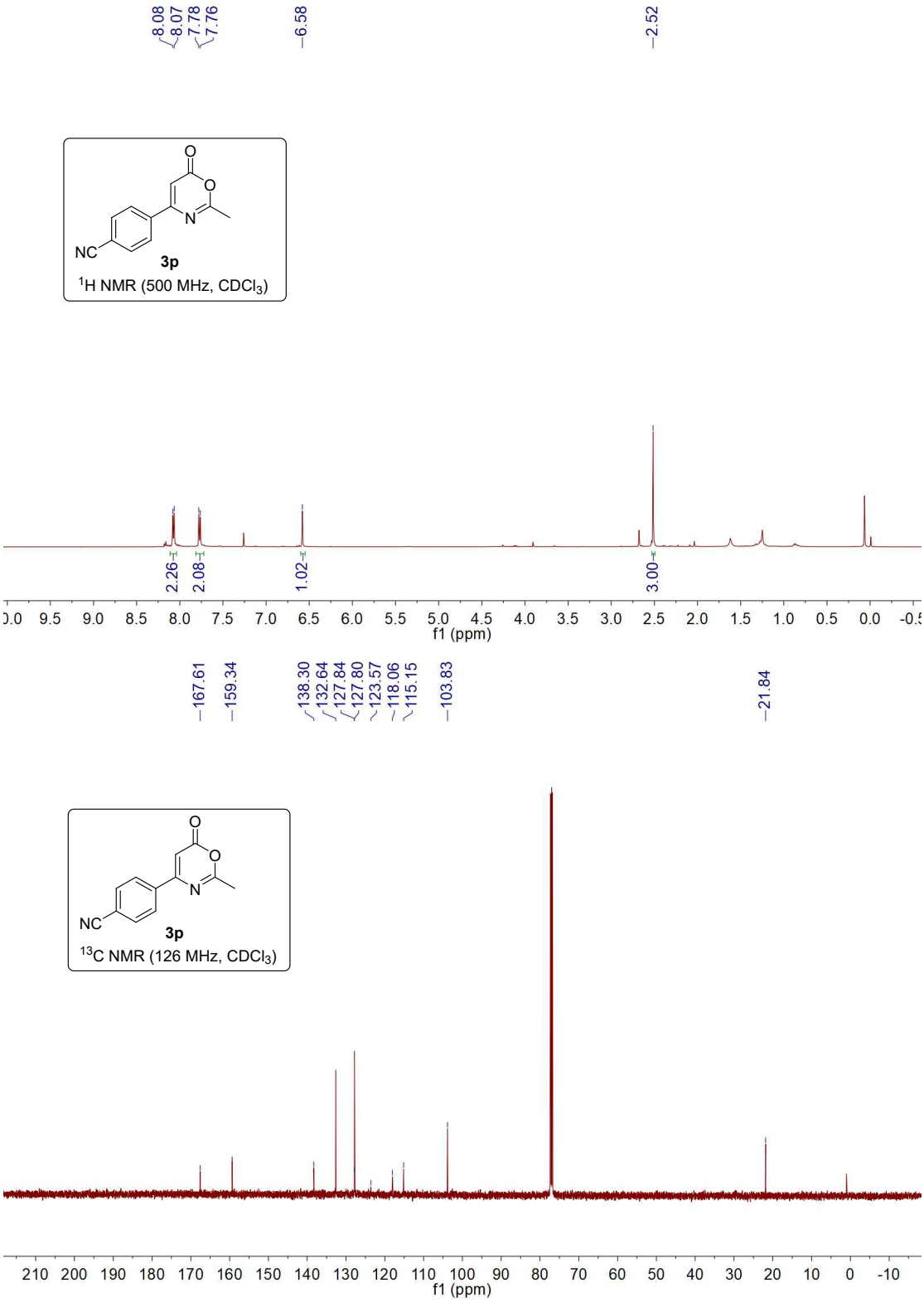
2-methyl-4-(4-(trifluoromethyl)phenyl)-6H-1,3-oxazin-6-one (3o)



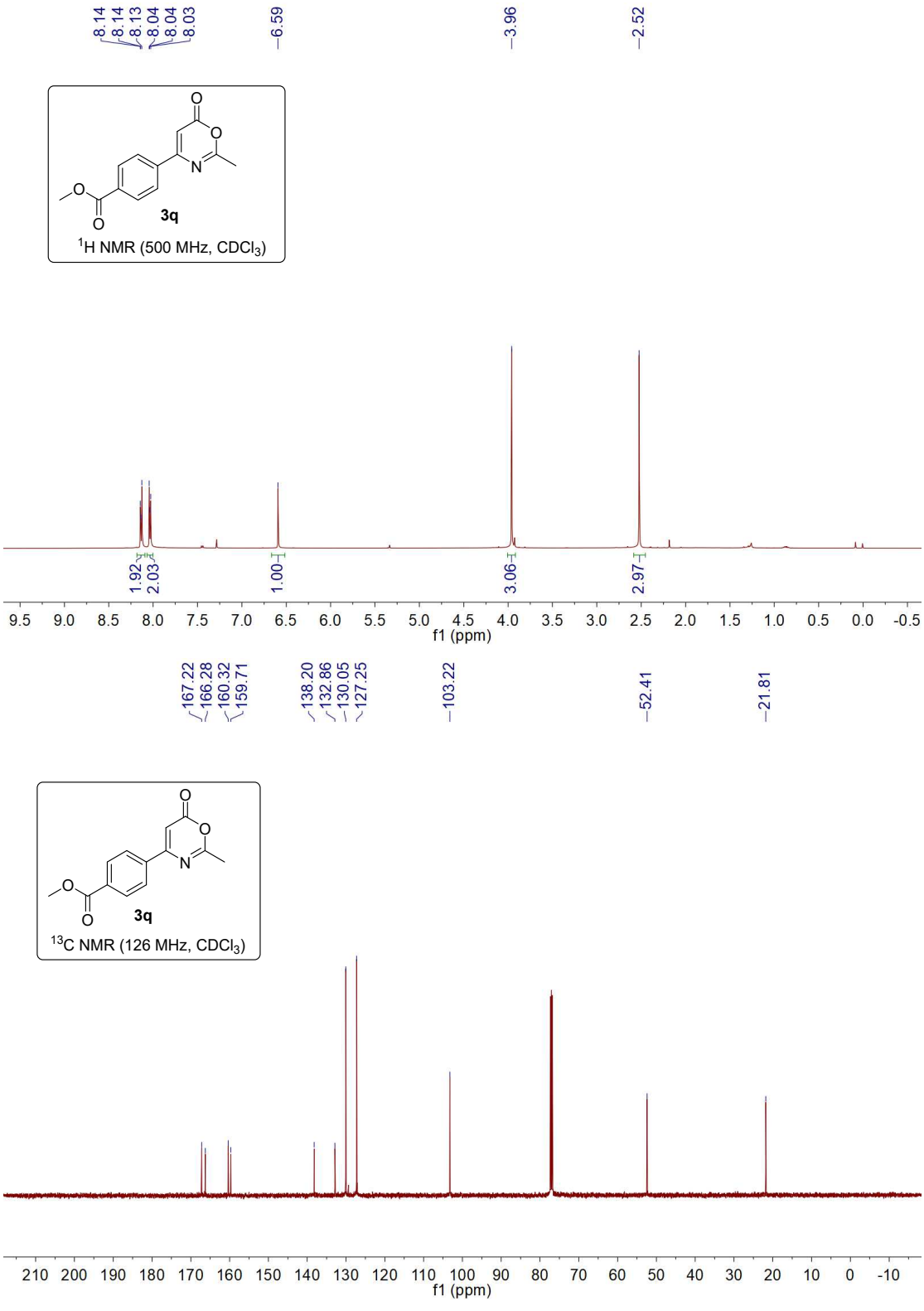




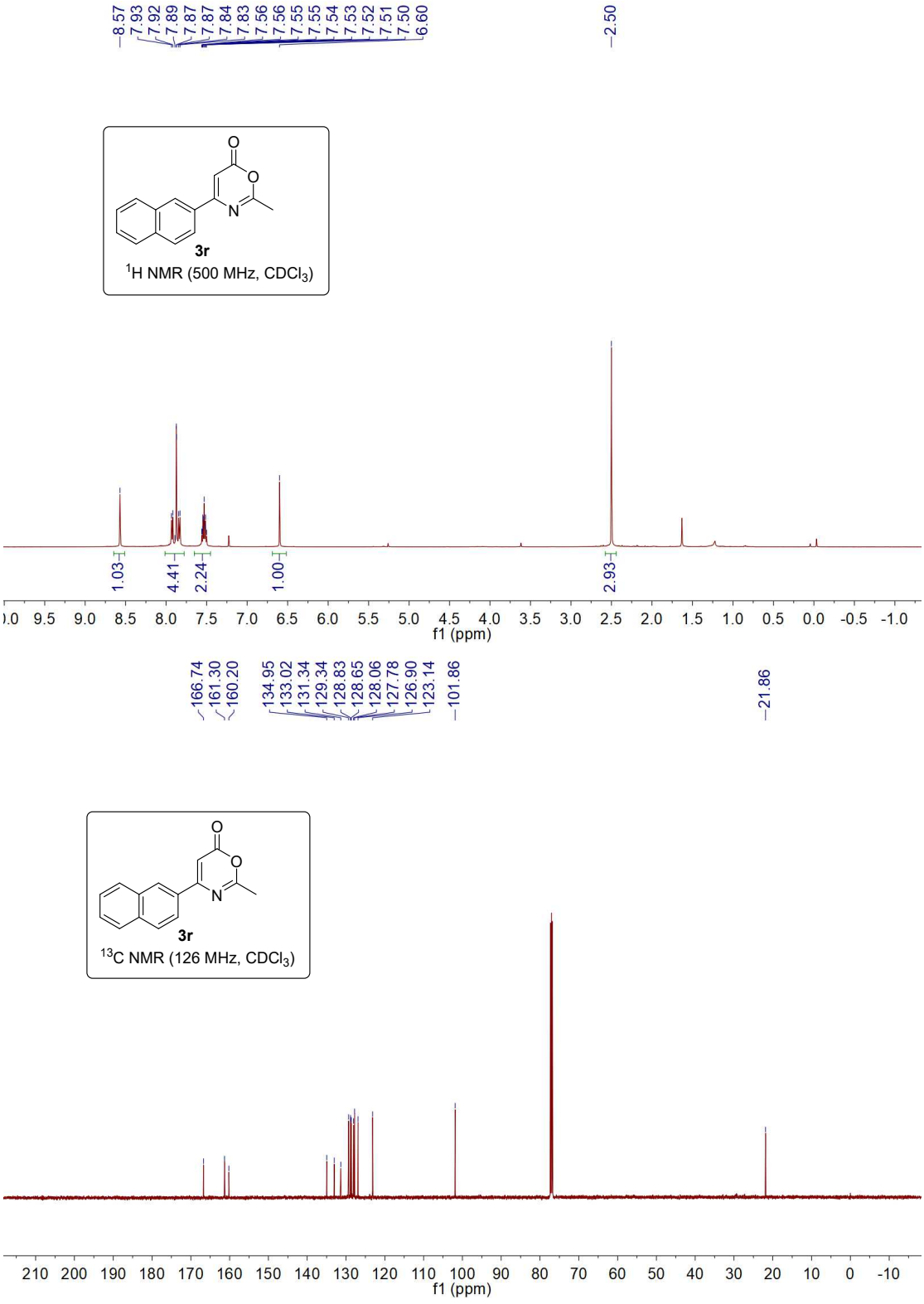
4-(2-methyl-6-oxo-6H-1,3-oxazin-4-yl)benzonitrile (3p)



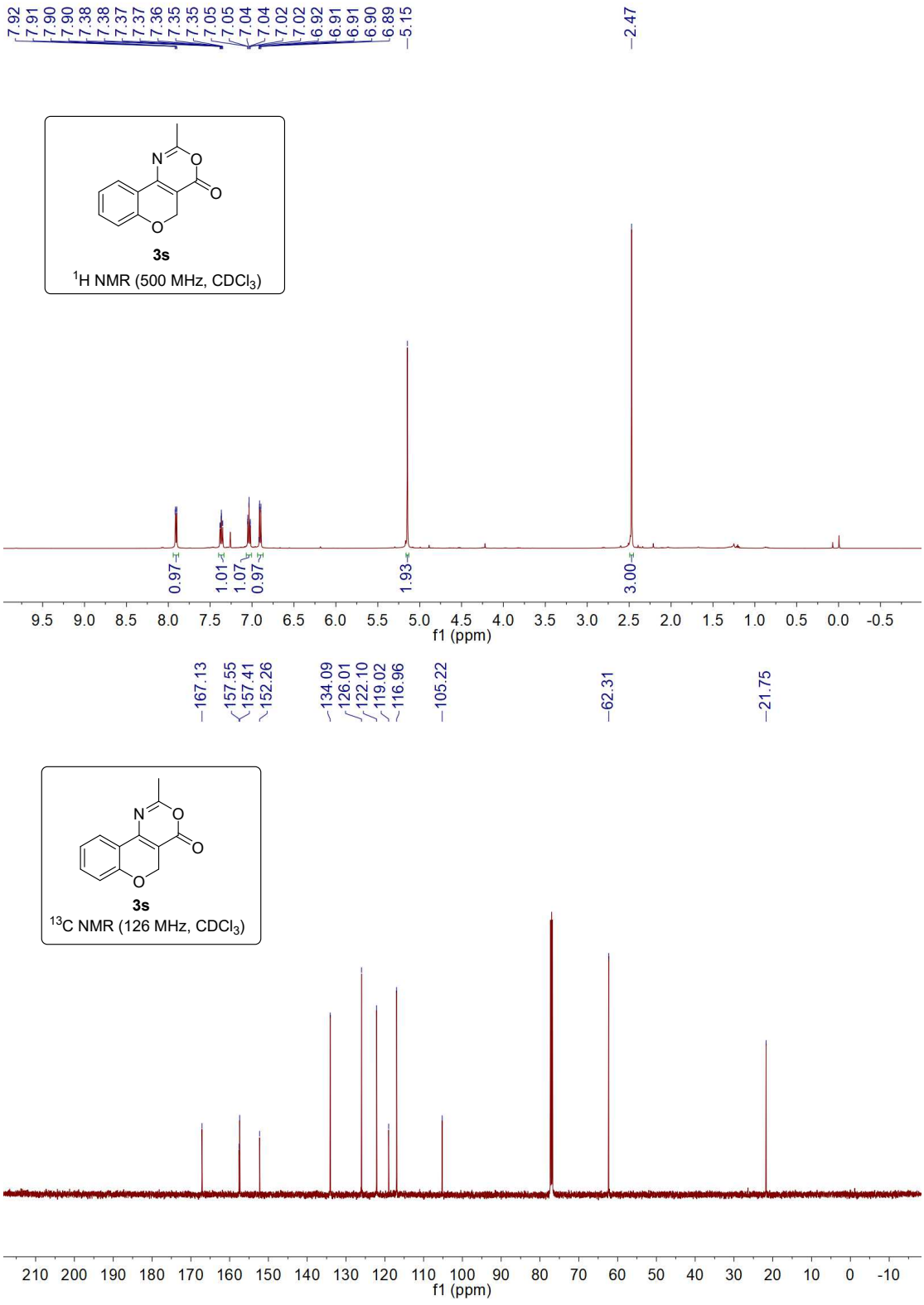
methyl 4-(2-methyl-6-oxo-6H-1,3-oxazin-4-yl)benzoate (3q)



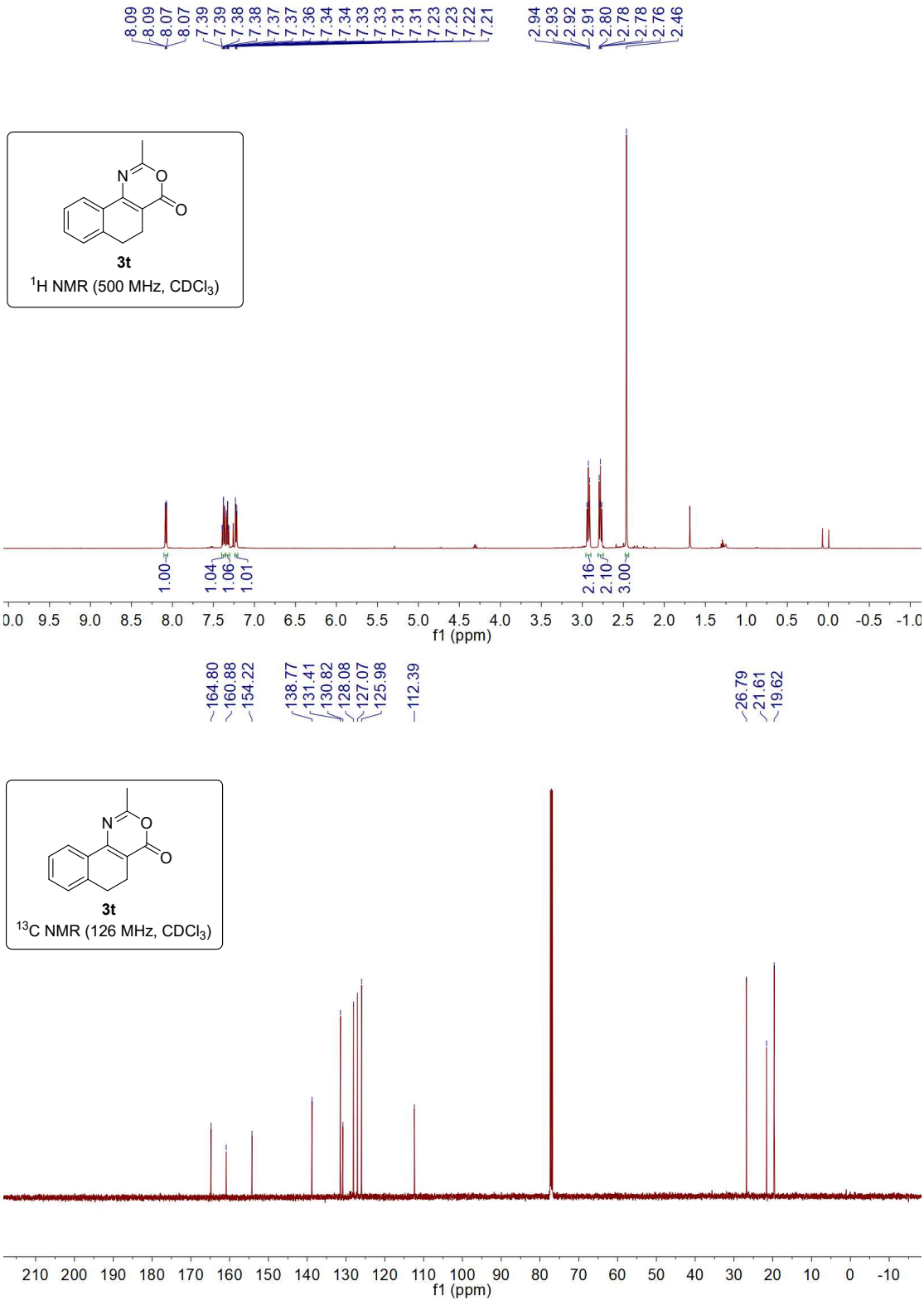
2-methyl-4-(naphthalen-2-yl)-6H-1,3-oxazin-6-one (3r)



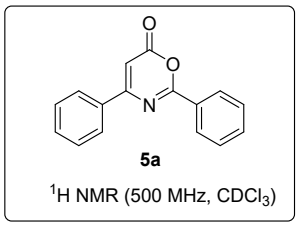
2-methyl-4H,5H-chromeno[4,3-d][1,3]oxazin-4-one (3s)

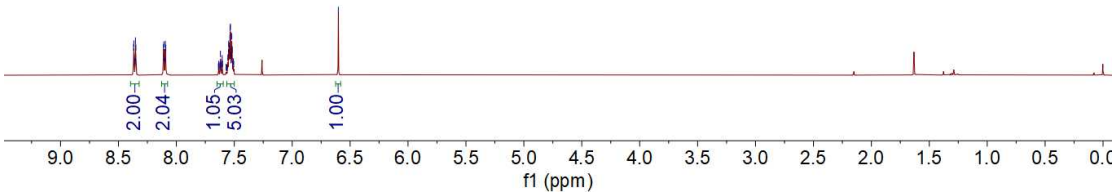


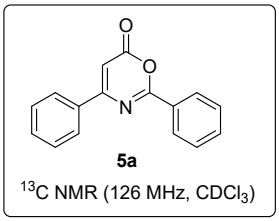
3-methyl-5,6-dihydro-1H-naphtho[2,1-d][1,3]oxazin-1-one (3t)

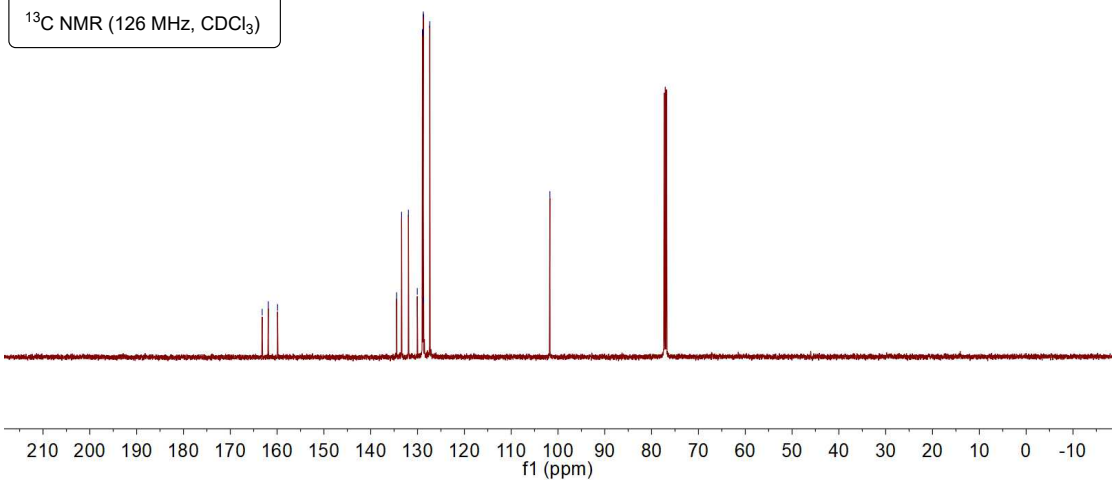


2,4-diphenyl-6H-1,3-oxazin-6-one (5a)

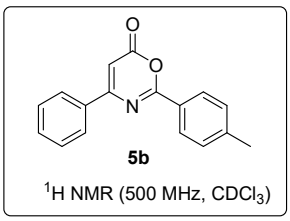


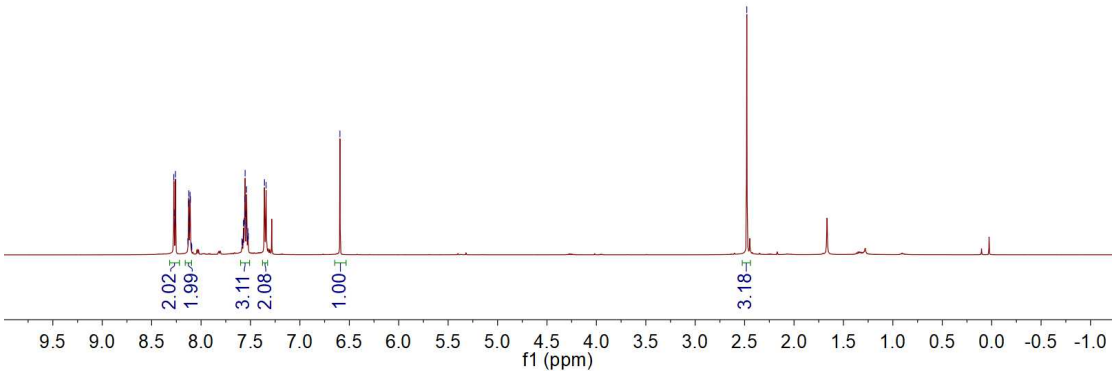


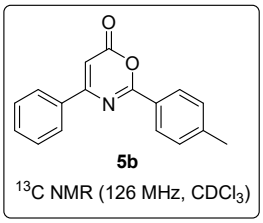


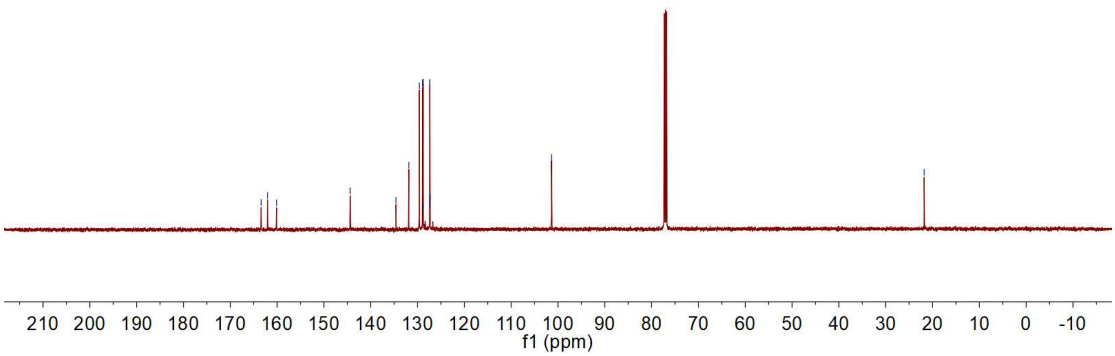


4-phenyl-2-(p-tolyl)-6H-1,3-oxazin-6-one (5b)

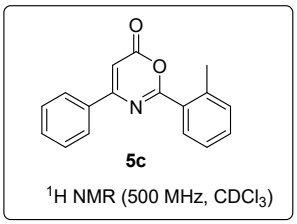


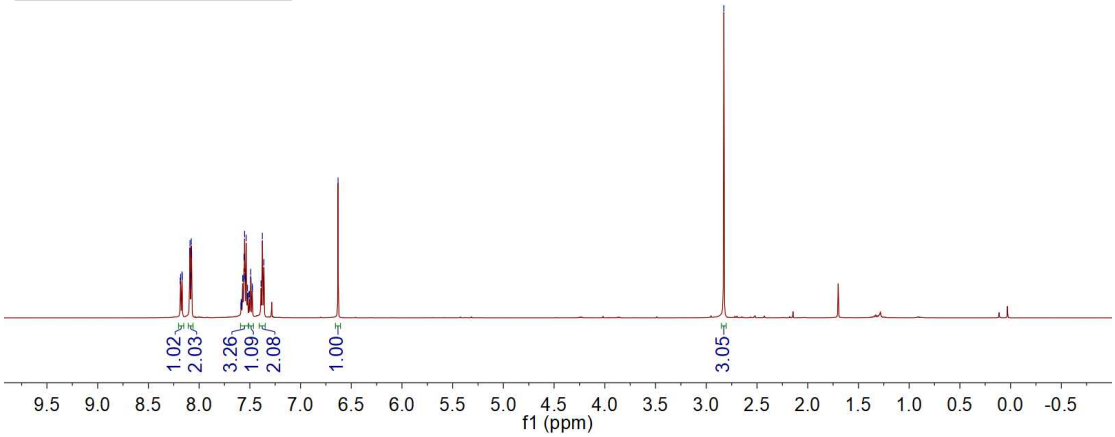


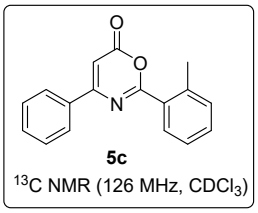


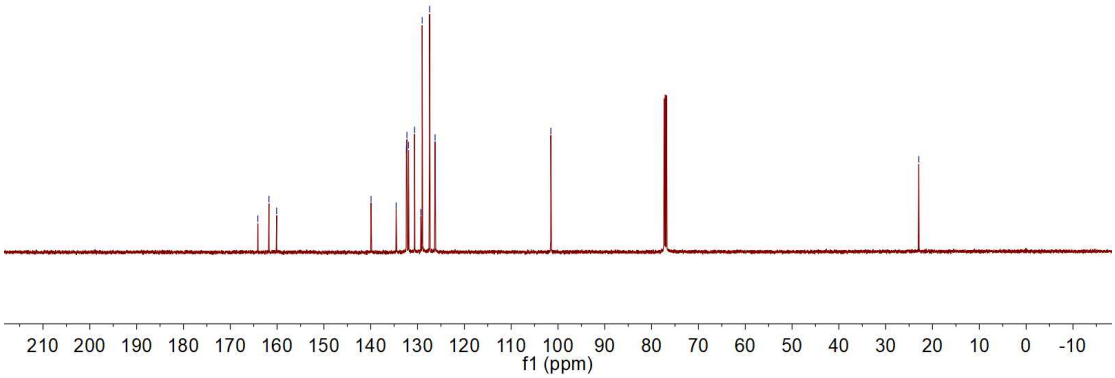


4-phenyl-2-(o-tolyl)-6H-1,3-oxazin-6-one (5c)

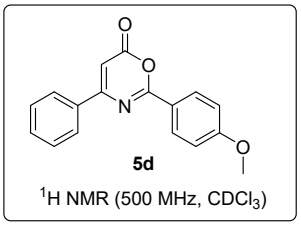


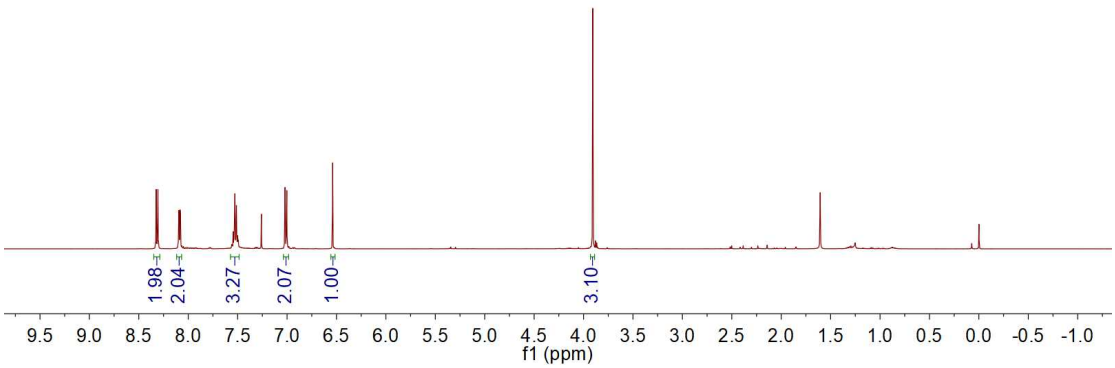


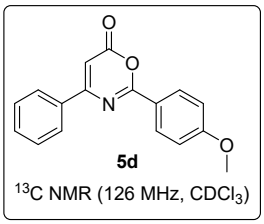


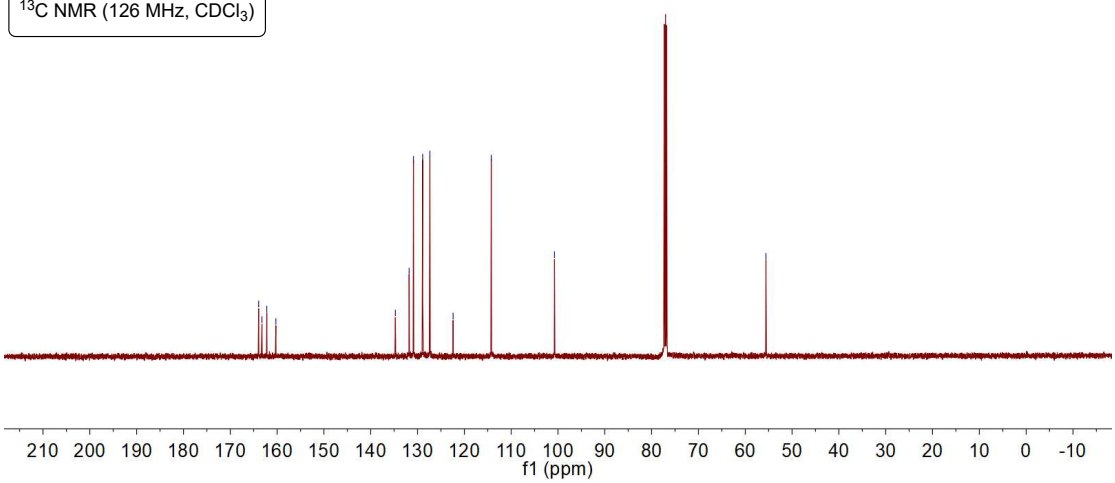


2-(4-methoxyphenyl)-4-phenyl-6H-1,3-oxazin-6-one (5d)

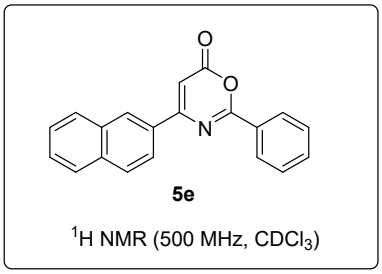






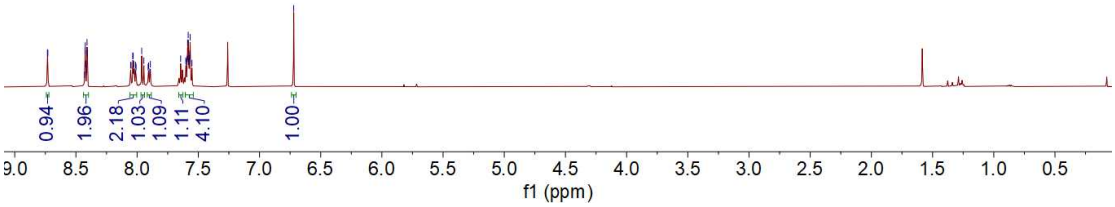


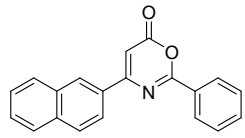
4-(naphthalen-2-yl)-2-phenyl-6H-1,3-oxazin-6-one (5e)



5e

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

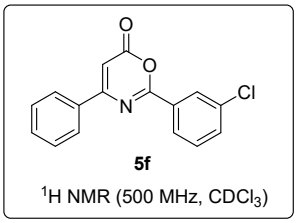




5e

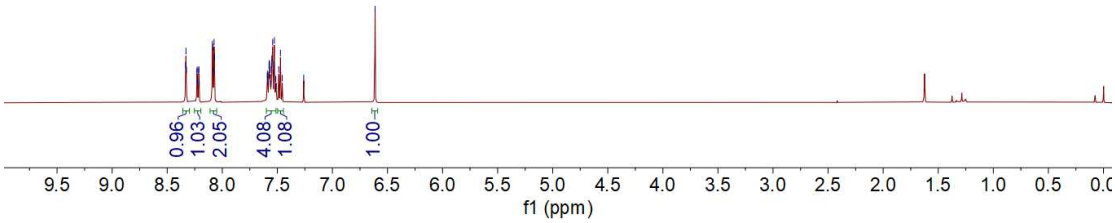
^{13}C NMR (126 MHz, $CDCl_3$)

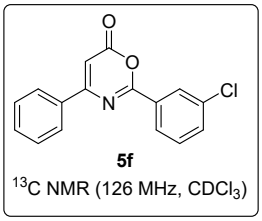
2-(3-chlorophenyl)-4-phenyl-6H-1,3-oxazin-6-one (5f)



5f

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

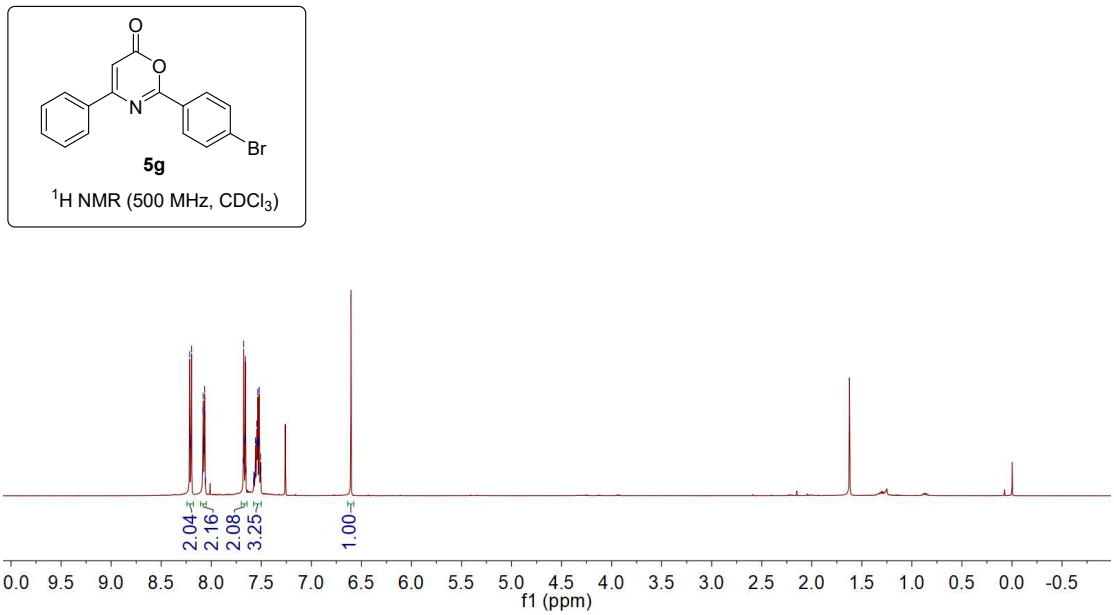


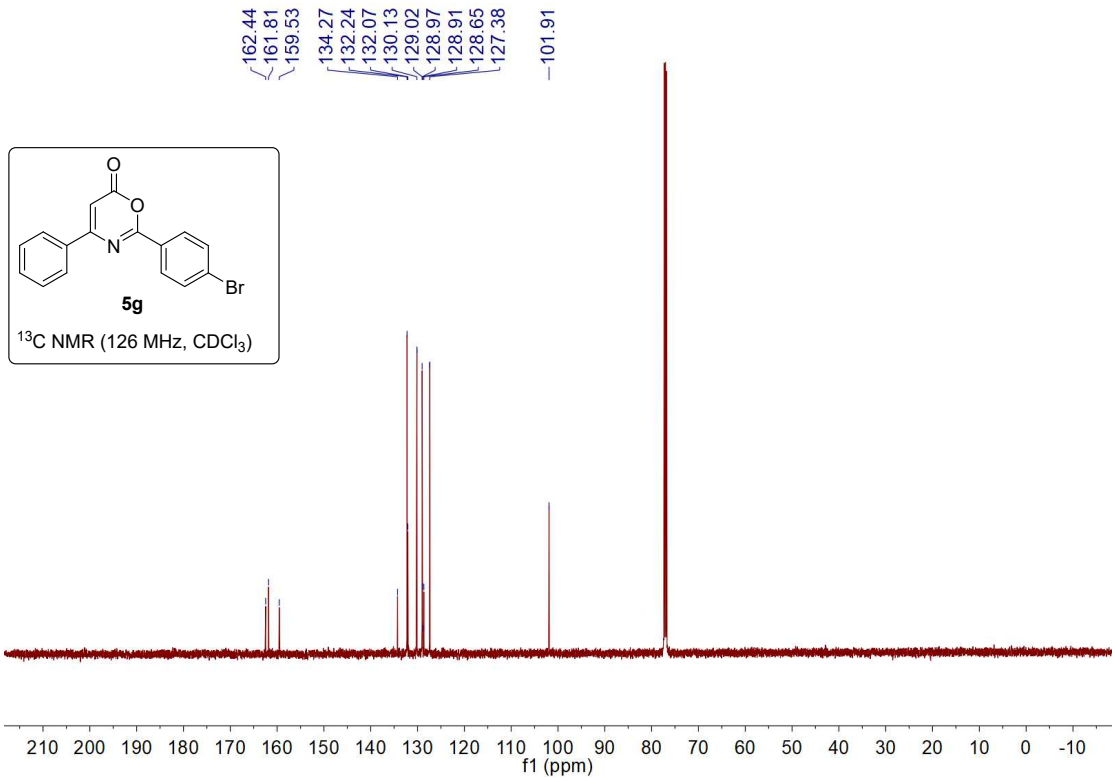


5f

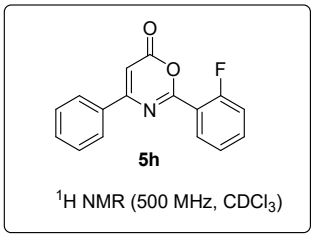
^{13}C NMR (126 MHz, $CDCl_3$)

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



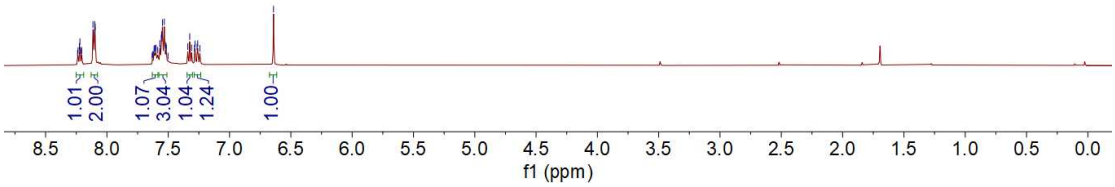


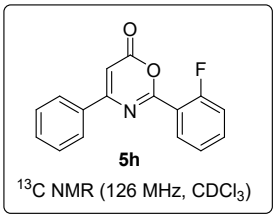
2-(2-fluorophenyl)-4-phenyl-6H-1,3-oxazin-6-one (5h)



5h

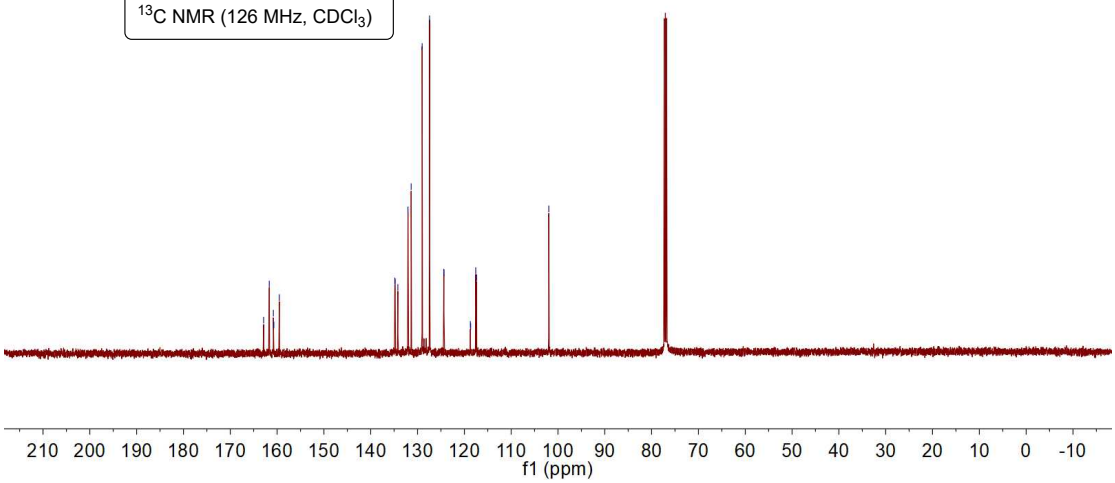
^{1}H NMR (500 MHz, $CDCl_3$)

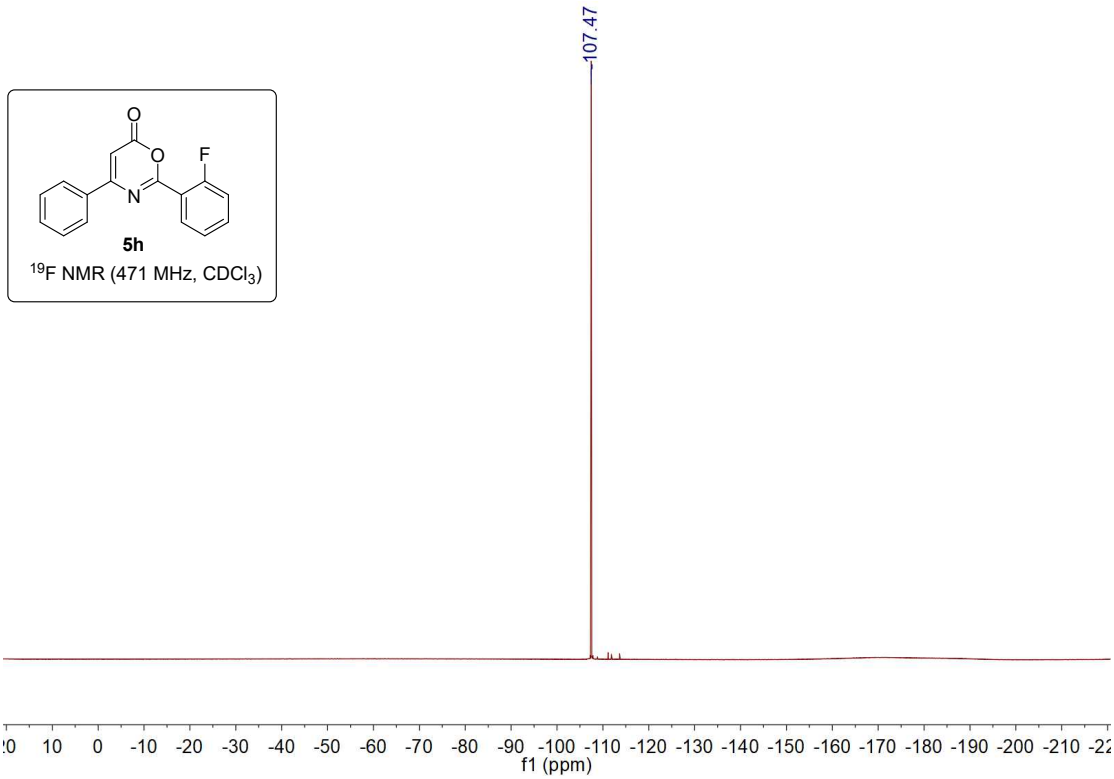




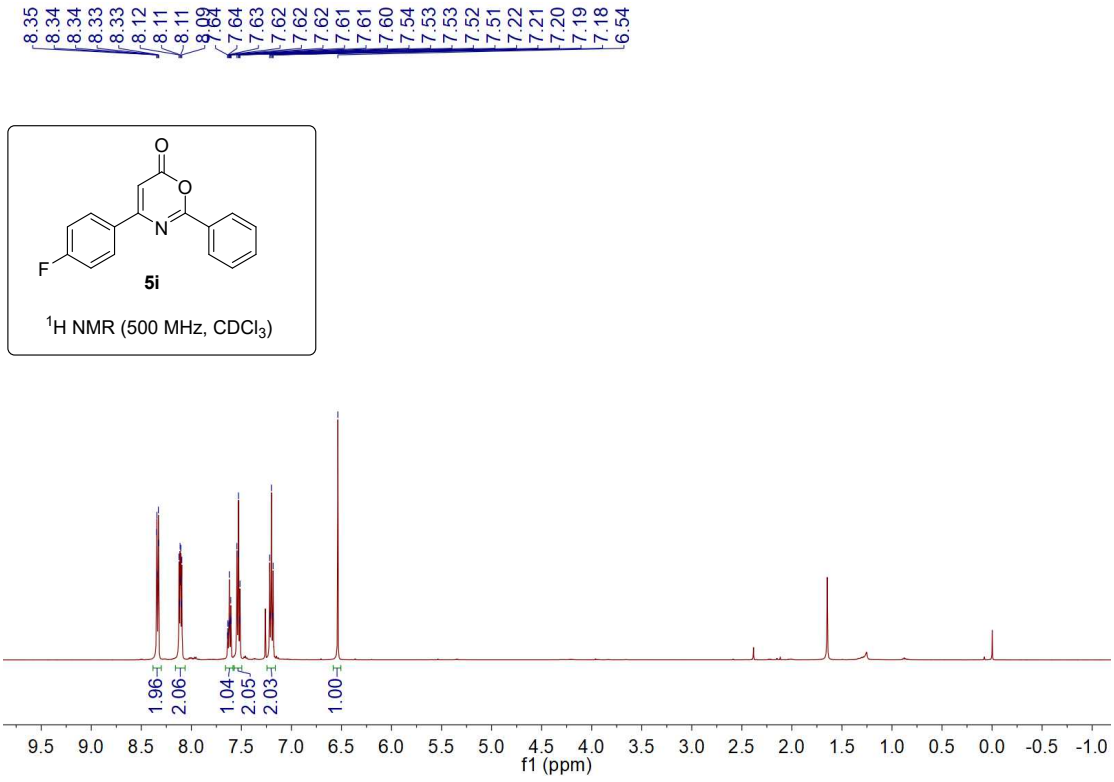
5h

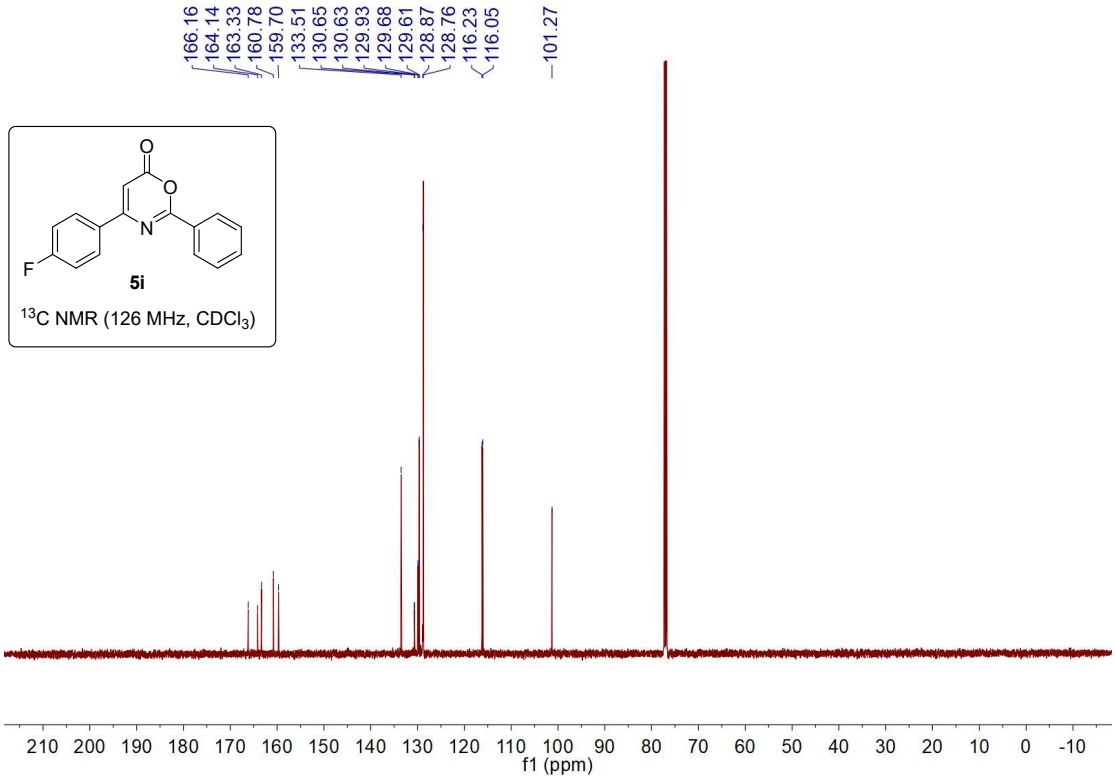
^{13}C NMR (126 MHz, $CDCl_3$)

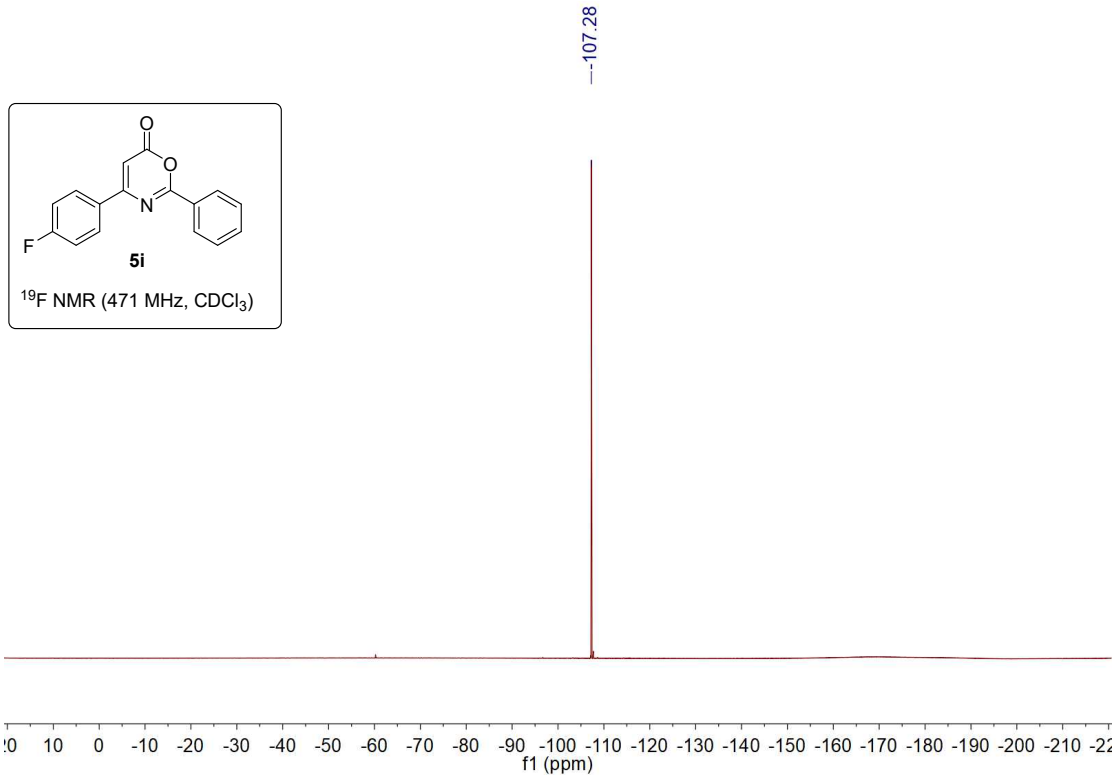




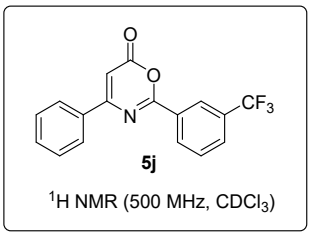
4-(4-fluorophenyl)-2-phenyl-6H-1,3-oxazin-6-one (5i)





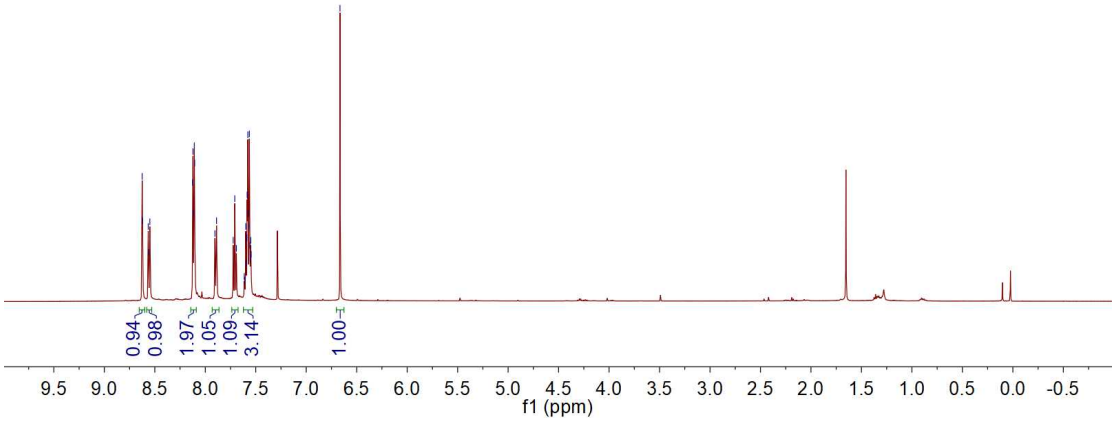


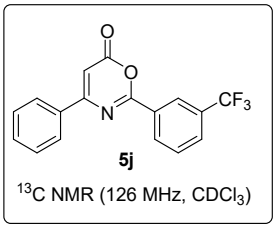
4-phenyl-2-(3-(trifluoromethyl)phenyl)-6H-1,3-oxazin-6-one (5j)



5j

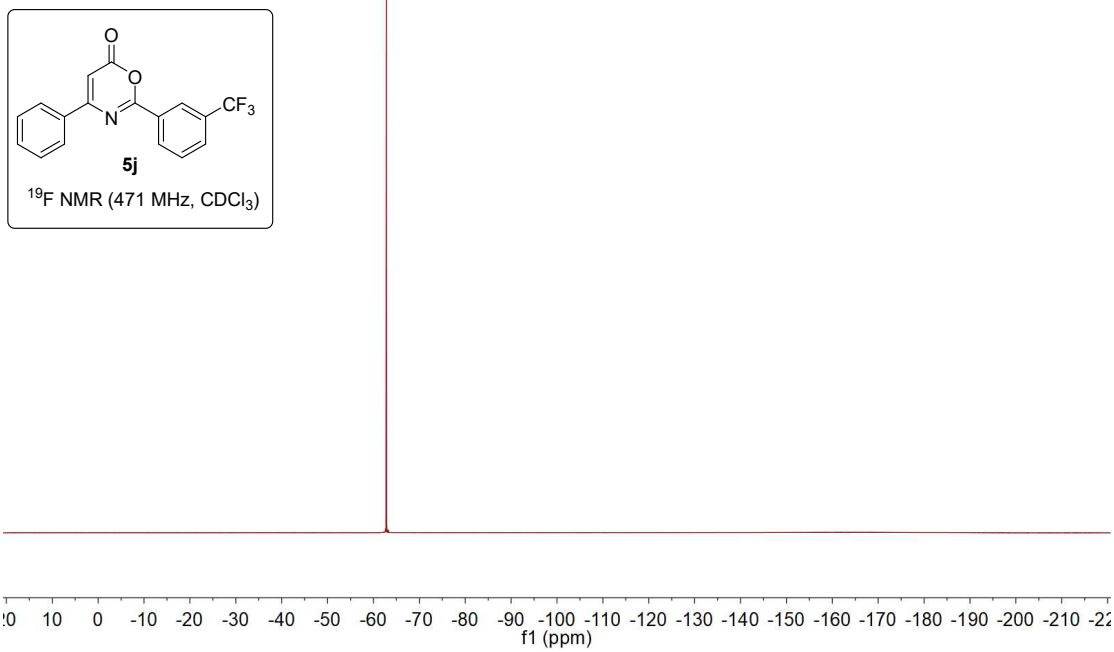
^{1}H NMR (500 MHz, $CDCl_3$)



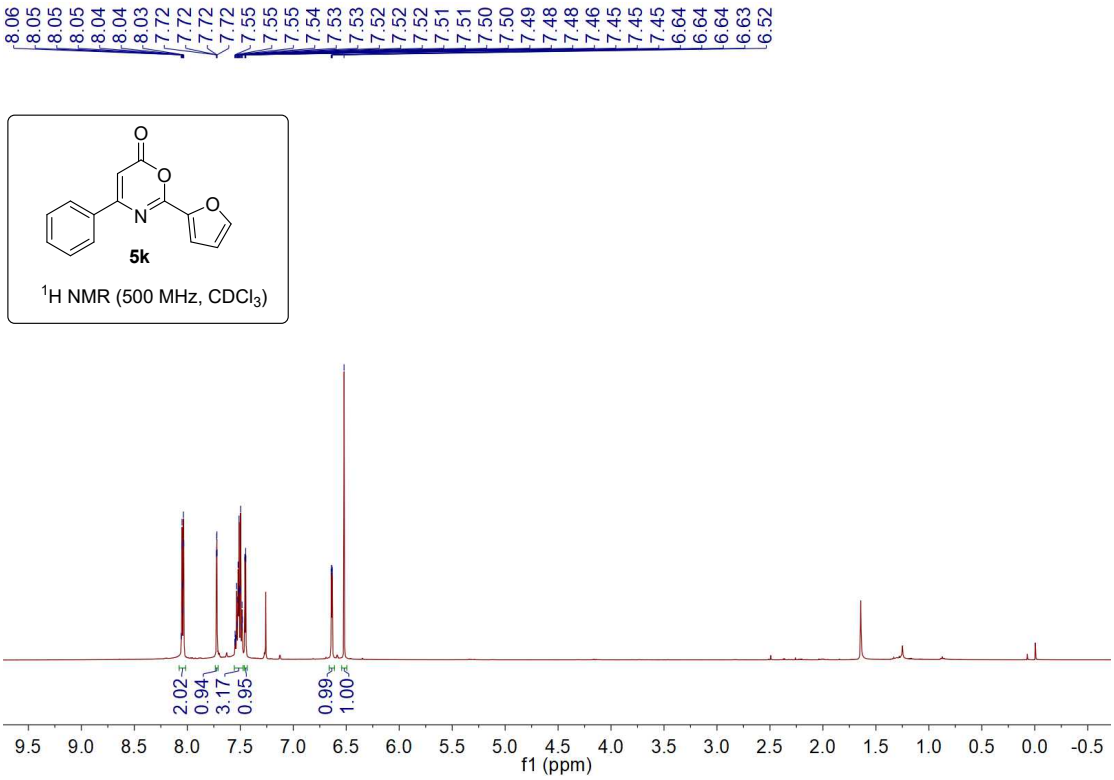


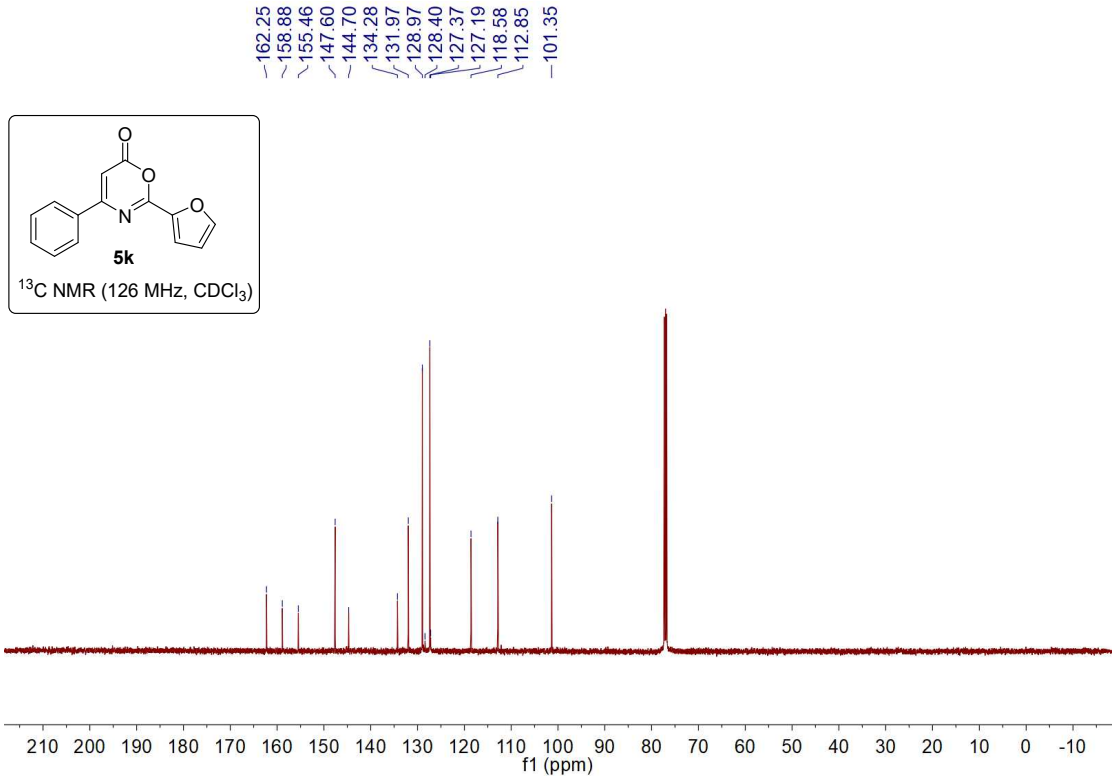
5j

^{13}C NMR (126 MHz, $CDCl_3$)

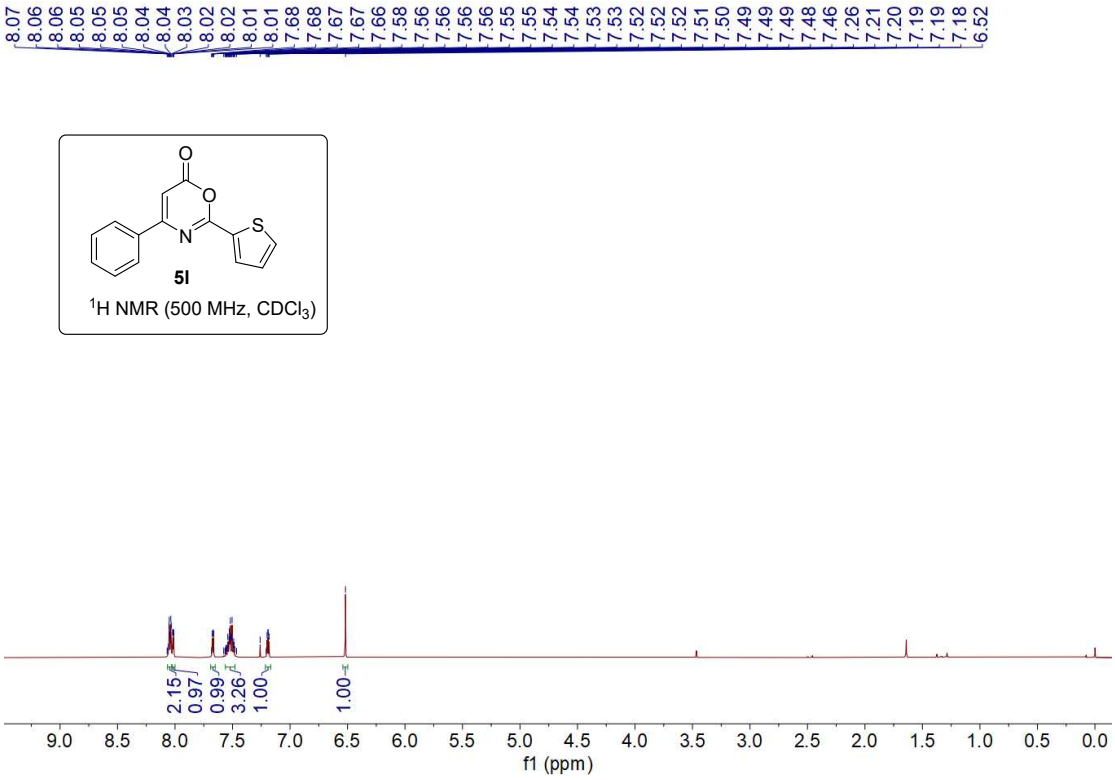


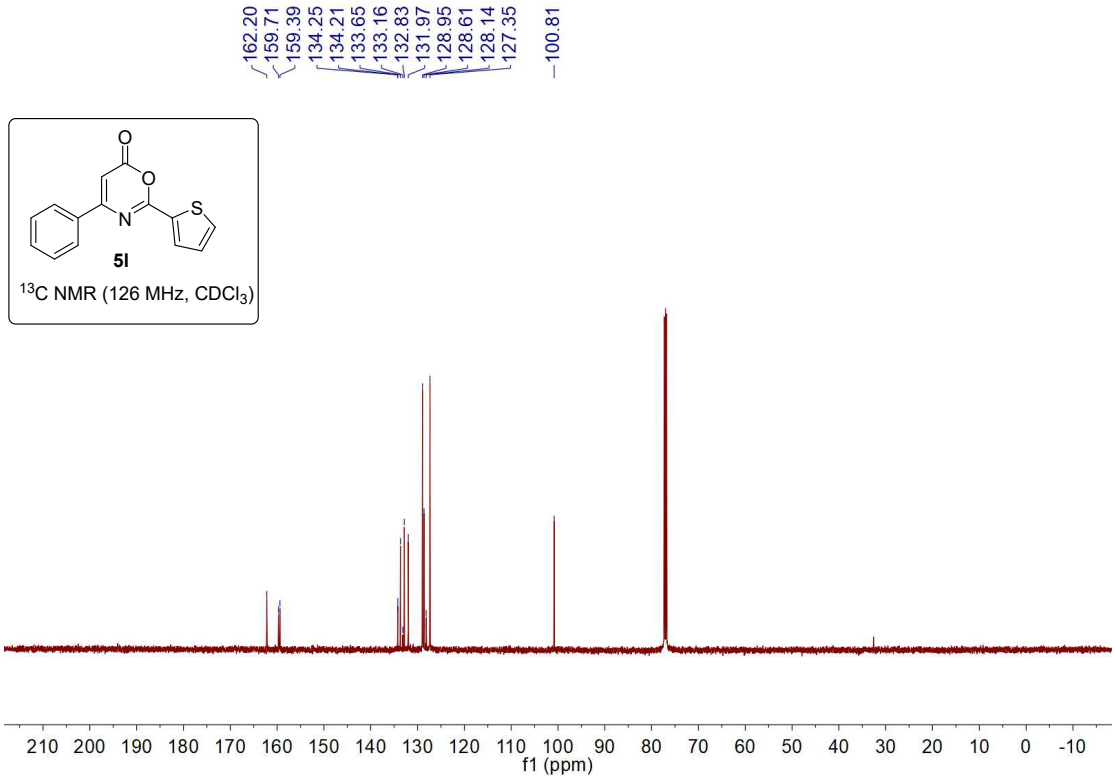
2-(furan-2-yl)-4-phenyl-6H-1,3-oxazin-6-one (5k)



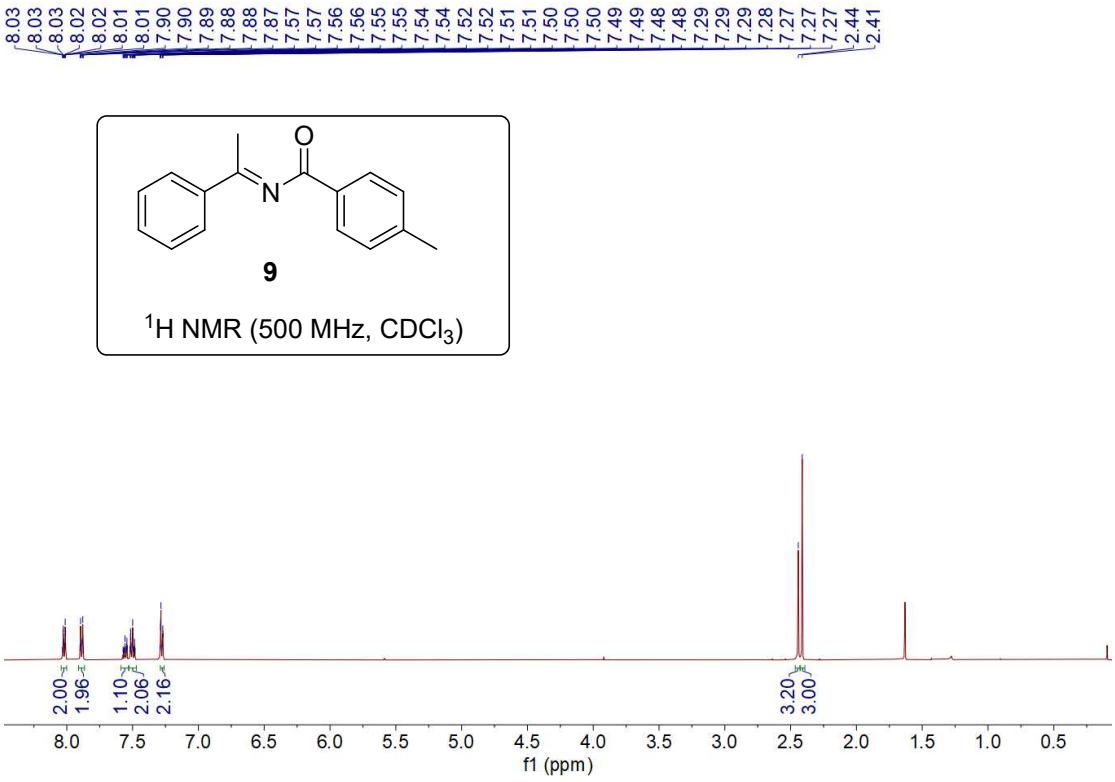


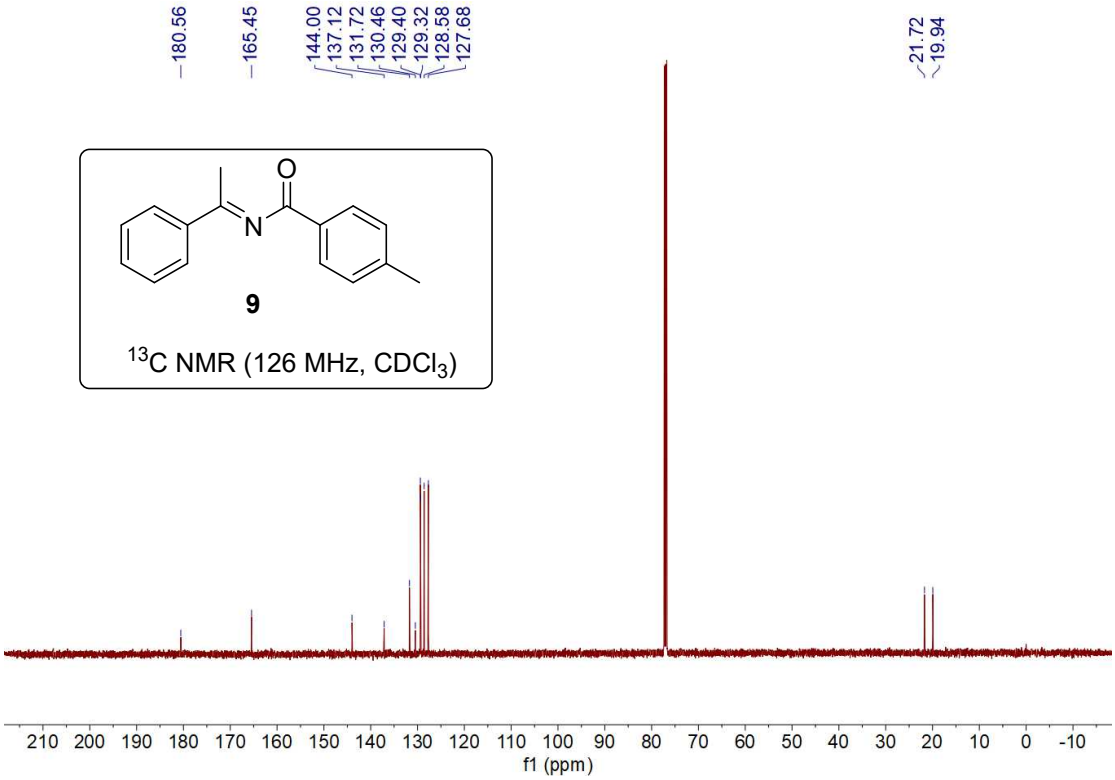
4-phenyl-2-(thiophen-2-yl)-6H-1,3-oxazin-6-one (5l)



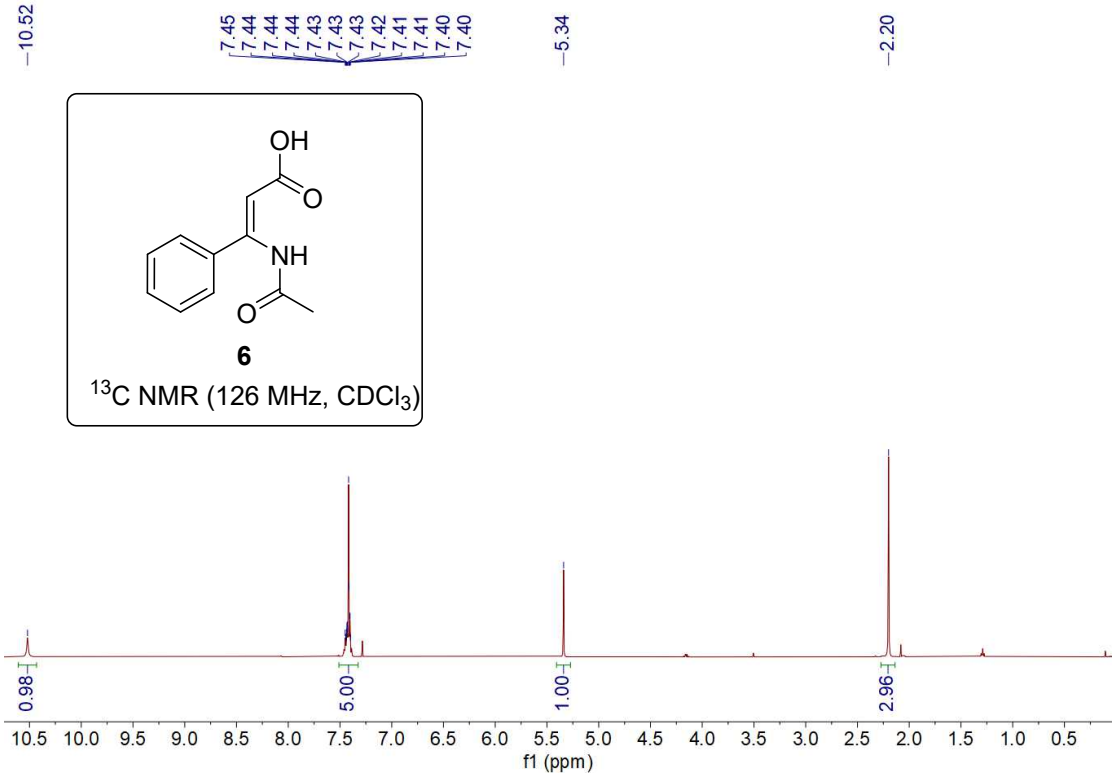


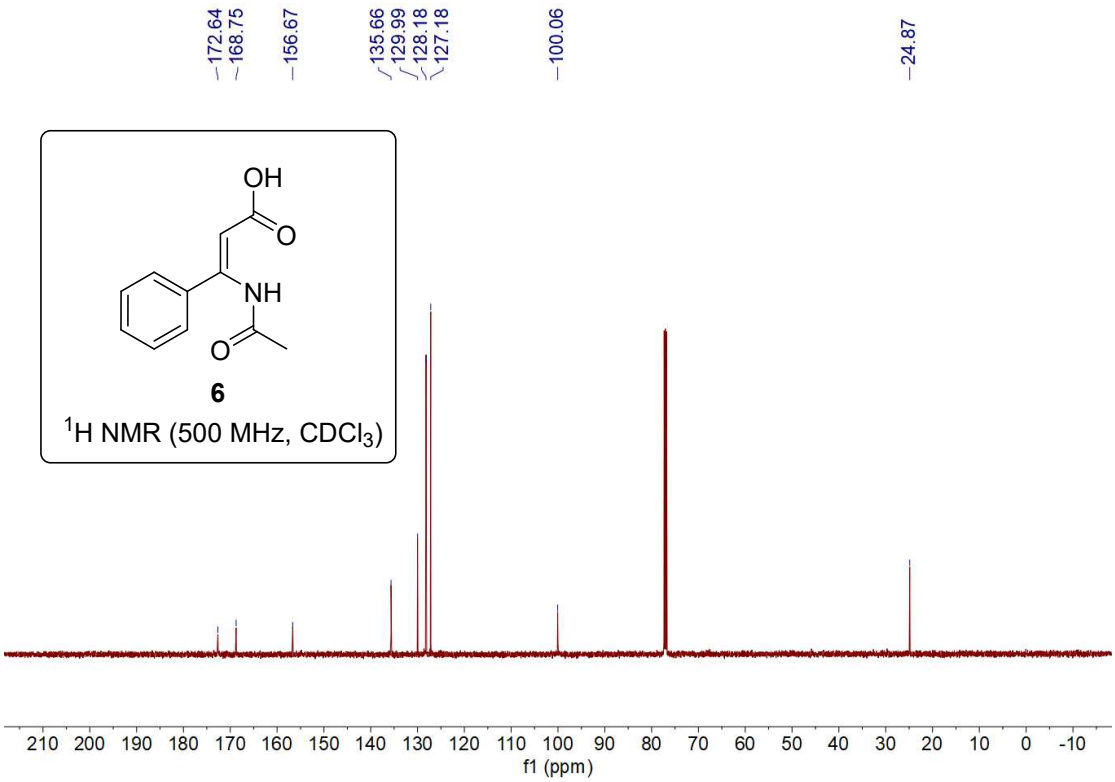
4-methyl-N-(1-phenylethylidene)benzamide (9)





(Z)-3-acetamido-3-phenylacrylic acid (6)




172.64
168.75
156.67
135.66
129.99
128.18
127.18
100.06
24.87
OH
O
NH
O
6
1H NMR (500 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)