Supporting Information

Visible-Light-Driven Copper-Catalyzed Aerobic Oxidative Cascade Cyclization of *N*-Tosylhydrazones and Terminal Alkynes: Regioselective Synthesis of 3-Arylcoumarins

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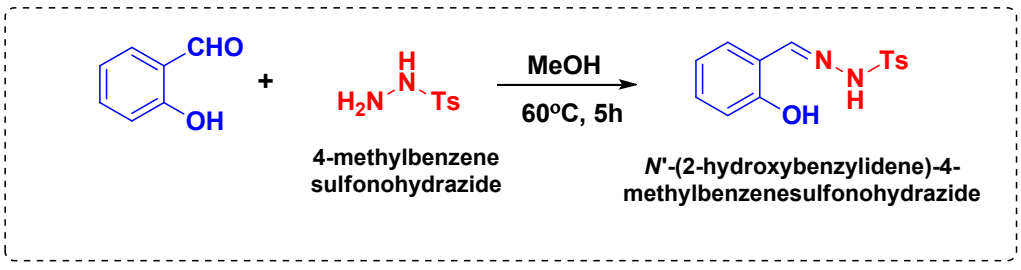
Experimental section

General: All reactions were conducted in oven-dried glasswares. All reactions were conducted using A blue light-emitting diode (LED) array (30 lamps, power density: 40 mW/cm^2 at 460 nm) was used as the visible-light source under oxygen (O_2) atmosphere in all reactions. All solvents were dried according to known methods and distilled prior to use. Starting materials were commercially available (Sigma-Aldrich or Alfa-Aesar or TCI-chemicals) and used as received. ^{1}H NMR and ^{13}C NMR spectra were recorded at 400 and 600 MHz using deuterated $CDCl_3$ or $CDCl_3$-DMSO-d_6 mixture. Chemical shifts (δ) were reported as parts per million (ppm) and the following abbreviations were used to identify the multiplicities: s= singlet, d= doublet, t= triplet, q= quartet, m= multiplet, b= broad and all combinations thereof can be explained by their integral parts. Unless otherwise specified, the proton/carbon signal of 2 residual solvent (at δ 7.24 or 2.50 and δ 77.00 or 39.51 ppm, respectively) was used as the internal reference. EPR spectra were recorded by a Bruker ESP-300E instrument.

General procedure for the synthesis of (E)-N'-(2-hydroxybenzylidene)-4-methylbenzenesulfonohydrazide (Starting material): [s1]

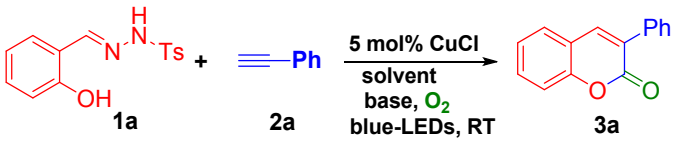
In a 100 mL round bottom flask, 2-hydroxybenzaldehyde (1 g) and 4-methylbenzenesulfonohydrazide (1.52 g, 1.0 equiv.) was dissolved in methanol and stirred at 60 °C until completion of reaction (monitored by TLC). After completion of reaction, reaction mixture was work up with acidic water and ethyl acetate. The organic layer was washed with water three times and then to the organic part sodium sulphate was added. The resulting mixture was filtered through Whatmann filter paper. The filtrated was then evaporated to get the desired product. The product (E)-N'-(2-hydroxybenzylidene)-4-methylbenzenesulfonohydrazide was obtained in 97% yield (2.3 g).

Scheme S1: Synthesis of (E)-N'-(2-hydroxybenzylidene)-4-methylbenzenesulfonohydrazide



General procedure: To a dry test tube (20 mL) containing 5 mol% CuCl, was added 8 mL of dry CH_3CN, KO^{t}Bu (1.2 equiv., 0.6 mmol), 1a (0.5 mmol) and terminal acetylene (0.55 mmol) via syringe. The reaction mixture was then irradiated with blue LEDs (40 mW/cm^2 at 460 nm) under an oxygen atmosphere at room temperature (25-28 ^{o}C) until completion of the reaction (monitored by TLC). The reaction mixture was diluted with 40 % ethyl acetate in hexane and stirred for 10 min. The mixture was filtered through celite and silica gel pads, and washed with ethyl acetate. The filtrate was concentrated and the residue was purified by column chromatography on silica gel to collect the aryl/alkyl product.

Table S1. Optimization of reaction conditions [a]



entry	[Cu] Catalyst	Base (1.2eq)	Solvent	Yield [%] [b]
1 [c]	CuCl	-	CH_3CN	0
2	CuCl	K_2CO_3	CH_3CN	74
3	CuCl	Cs_2CO_3	CH_3CN	76
4	**CuCl**	**KO^{t}Bu**	**CH_3CN**	**89**
5	CuBr	KO^{t}Bu	CH_3CN	88
6	$CuCl_2$	KO^{t}Bu	CH_3CN	55
7 [d]	CuCl	KO^{t}Bu	CH_3CN-H_2O	78
8	CuCl	KO^{t}Bu	CH_3OH	0
9	CuCl	KO^{t}Bu	THF	trace
10	CuCl	KO^{t}Bu	DMF	24
11	CuCl	KO^{t}Bu	CH_3CN-CH_3OH	18
12 [e]	CuCl	KO^{t}Bu	CH_3CN	84
13 [f]	CuCl	KO^{t}Bu	CH_3CN	62
14 [g]	CuCl	KO^{t}Bu	CH_3CN	0
15 [h]	none	KO^{t}Bu	CH_3CN	n.r
16 [i]	CuCl	KO^{t}Bu	CH_3CN	0

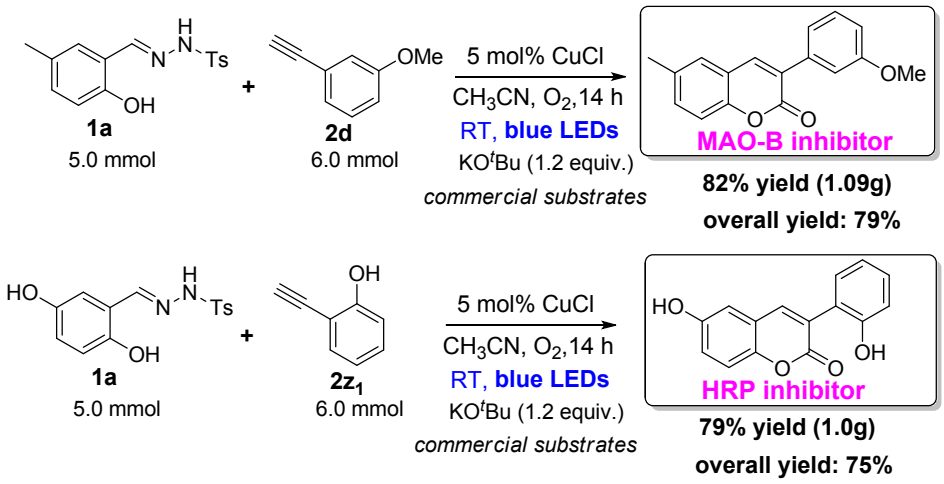
[a] Unless otherwise noted, reaction conditions are as follows: 1a (0.5 mmol), 2a (0.55 mmol), [Cu] catalyst (5 mol%), Solvent (8 mL). The reaction mixture was irradiated with blue LEDs (power density: 40 mW/cm^2 at 460 nm) for 12 h under O_2 (1 atm.). [b] Yield of the isolated product. [c] The reaction was carried without base. [d] 0.5 mL of water was added. [e] In the presence of air (1 atm). [f] Reaction irradiated with an ambient white light bulb for 16 h (power density: 8 mW/cm^2 at 460 nm). [g] The reactions were carried at 80 ^{o}C. [h] In the absence of [Cu] catalyst. [i] In the absence of O_2. n.r. = no reaction.

Experimental procedure for the synthesis of pharmaceutical drugs:

Preparation of 3-(3-methoxyphenyl)-6-methyl-2H-chromen-2-one (3d): To a dry flask (100 mL) containing 5 mol% CuCl was added 25 mL of dry CH_3CN, (E)-N'-(2-hydroxy-5-methylbenzylidene)-4-methylbenzenesulfonohydrazide 1.52 g (5.0 mmol), 0.67 g of potassium tert butoxide (1.2 equiv.) and 1-ethynyl-3-methoxybenzene 0.8g (6.0 mmol) via syringe. The reaction mixture was then irradiated with blue LEDs (40 mW/cm^2 at 460 nm) under an oxygen atmosphere/balloon at room temperature (25-28 ^{o}C) for 15 h. The reaction mixture was diluted with 40 % ethyl acetate in hexane and stirred for 10 min. The mixture was filtered through celite/silica gel pads, and washed with ethyl acetate. The filtrate was concentrated; and the residue was purified by column chromatography on silica gel to collect the 3-(3-methoxyphenyl)-6-methyl-2H-chromen-2-one (**3d**) as a white solid (4.1 mmol, 1.09 g, 82%)**.**

Preparation of 6-hydroxy-3-(2-hydroxyphenyl)-2H-chromen-2-one ($3z_1$): To a dry flask (100 mL) containing 5 mol% CuCl was added 25 mL of dry CH_3CN, (E)-N'-(2,5-dihydroxybenzylidene)-4-methylbenzenesulfonohydrazide (1.53g, 5.0 mmol), 0.67g of potassium tert butoxide (1.2 equiv.) and 2-ethynylphenol (0.7g, 6.0 mmol) via syringe. The reaction mixture was then irradiated with blue LEDs (40 mW/cm^2 at 460 nm) under an oxygen atmosphere/ balloon at room temperature (25-28 ^{o}C) for 20 h. The reaction mixture was diluted with 40 % ethyl acetate in hexane and stirred for 10 min. The mixture was filtered through celite and silica gel pads, and washed with ethyl acetate. The filtrate was concentrated and the residue was purified by column chromatography on silica gel to collect 6-hydroxy-3-(2-hydroxyphenyl)-2H-chromen-2-one **(3w)** as an off-white solid (3.95 mmol, 1.0 g, 79%).

Scheme S2. Application to the synthesis of 3-arylcoumarin bioactive molecules.



Evaluation of Green Chemistry metrics for 3d

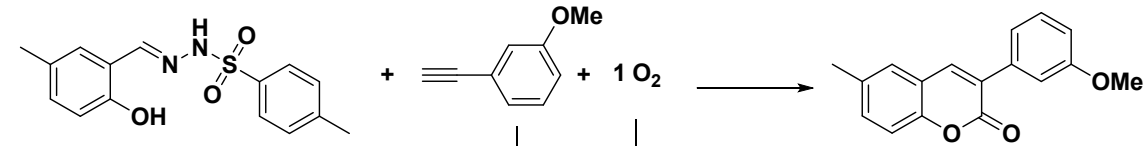
Atom economy defined as "how much of the reactants remain in the final desired product"

$$\text{Atom economy (AE)} = \frac{\text{Molecular mass of desired product}}{\text{Molecular mass of all reactants}} \times 100$$

Reaction mass efficiency (RME) defined as "the percentage of the mass of the reactants that remain in the product"

$$\text{Reaction mass efficiency (RME)} = \frac{\text{mass of desired product}}{\text{mass of all reactants}} \times 100$$

Reaction scheme



Chemical Formula: $C_{15}H_{16}N_2O_3S$
Molecular Weight: 304.3641
1.52g (5.0 mmol)

Chemical Formula: C_9H_8O
Molecular Weight: 132.1592
0.8g (6.0 mmol)

1x 32
= 32

Chemical Formula: $C_{17}H_{14}O_3$
Molecular Weight: 266.2913
1.09g (82%)

Total= 304+132+32 = 468

Reactant 1	(E)-N'-(2-hydroxy-5-methylbenzylidene)-4-methylbenzenesulfonohydrazide	1.52g	5.0 mmol	FW 304.36
Reactant 2	1-ethynyl-3-methoxybenzene	0.8g	6.0 mmol	FW 132.16
Base	*t*BuOK (1.2equiv.)	0.67g	6.0 mmol	FW 112.21
Solvent	ACN	19.65g	---	---
Auxiliary	---	---	---	---
Product	3-(3-methoxyphenyl)-6-methyl-2H-chromen-2-one	1.09g	4.10 mmol	FW 266.29

Product yield= 82%

E-factor $= \frac{1.52g + 0.8g + 0.67g + 19.65g - 1.09g}{1.09\ g}$ = **19.77 kg waste/ 1 kg product**

Atom economy $= \frac{266}{468} \times 100$ = 57%

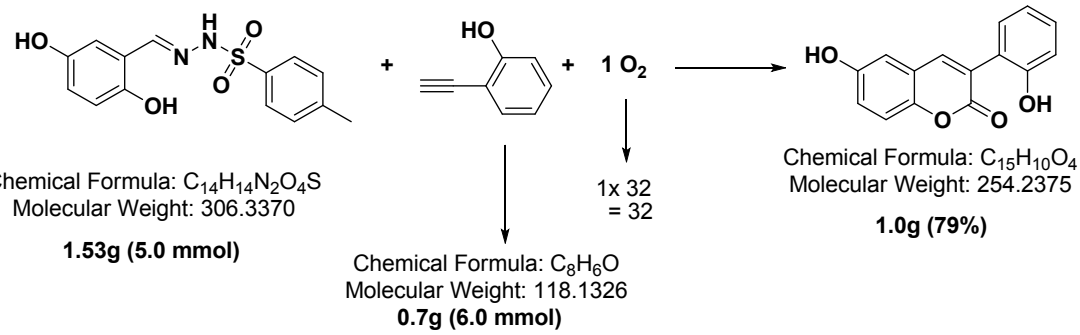
Atom efficiency = 82 % X 57% / 100 = 46.74%

Carbon efficiency $= \frac{17}{15 + 9} \times 100$ = 70.8%

Reaction mass efficiency $= \frac{1.09\ g}{1.52g + 0.8g} \times 100$ = 47%

Evaluation of Green Chemistry metrics for $3z_1$

Reaction scheme



Chemical Formula: $C_{14}H_{14}N_2O_4S$
Molecular Weight: 306.3370
1.53g (5.0 mmol)

Chemical Formula: C_8H_6O
Molecular Weight: 118.1326
0.7g (6.0 mmol)

1x 32
= 32

Chemical Formula: $C_{15}H_{10}O_4$
Molecular Weight: 254.2375
1.0g (79%)

Total= 306+118+32 = 456

Reactant 1	(E)-N'-(2,5-dihydroxybenzylidene)-4-methylbenzenesulfonohydrazide	1.53g	5.0 mmol	FW 306.33
Reactant 2	2-ethynylphenol	0.7g	6.0 mmol	FW 118.13
Base	*t*BuOK (1.2equiv.)	0.67g	6.0 mmol	FW 112.21
Solvent	ACN	19.65g	---	---
Auxiliary	---	---	---	---
Product	6-hydroxy-3-(2-hydroxyphenyl)-2H-chromen-2-one	1.0g	3.95 mmol	FW 254.23

Product yield= 79%

$$\text{E-factor} = \frac{1.53g + 0.7g + 0.67g + 19.65g - 1.0g}{1.0\ g} = \textbf{21.55 kg waste/ 1 kg product}$$

$$\text{Atom economy} = \frac{254}{456} \times 100 = 55.7\%$$

$$\text{Atom efficiency} = 79\ \% \times 55.7\% / 100 = 44\%$$

$$\text{Carbon efficiency} = \frac{15}{14 + 8} \times 100 = 68.18\%$$

$$\text{Reaction mass efficiency} = \frac{1.0g}{1.53g + 0.7g} \times 100 = 44.84\%$$

Preparation of copper(I) phenylacetylide:[s2] CuI (1.0 g, 5.0 mmol) was dissolved in ammonium hydroxide to form a blue solution. While stirring, phenylacetylene (0.5 g, 5.1 mmol in 50 mL ethanol) was added drop wise to the solution. The system was allowed to stand for 15 min to form a yellow precipitate suspension. The precipitate was filtered out and washed with water, ethanol, and diethyl ether, three times each. The solid was vacuum-dried, and 0.65 g (yield 75%) of a bright yellow solid was obtained. The spectroscopic data for the yellow solid are shown below: IR (KBr, cm^{-1}) [s3]: 1929 (C≡C), 1596, 1568; UV-Vis λ_{abs} = 471 nm.

EPR measurements: EPR spectra were recorded at room temperature on a Bruker ESP-300E(X band, 9.8 GHz) with parameters setting as shown below: receiver gain= 30 n; receiver phase= 0 deg; receiver harmonic= 1; field modulation frequency= 100000 Hz; microwave frequency [Hz]= 9.660469 e+09; field modulation amplitude [T]= 0.00016; receiver time constant [S] = 0.32768; microwave power= 0.015 W; receiver offset [%FS]= 0; DMPO (5-,5-dimethyl-1-pyrroline N-oxide) was employed as a radical trap for trapping of the superoxide radical anion.

The reaction under a standard condition (**1a**, **2a,** CuCl, 1 atm. O_2) in CH_3CN was irradiated with blue LEDs for 15 min in the presence of DMPO in an EPR chamber while recording the EPR spectra. The EPR signals shown in Figure **S1** is corresponding to DMPO-OO(H) which shows that superoxide anion radical was formed in the reaction solution. No superoxide EPR signal was observed from the reaction solution under the standard condition in the absence of CuCl or O_2 (Figures S2). These results indicate that copper(I) phenylacetylide undergoes single electron transfer to O_2, and generate superoxide free radical upon blue LEDs irradiation.

EPR spectra of the reaction mixture after blue LEDs irradiation

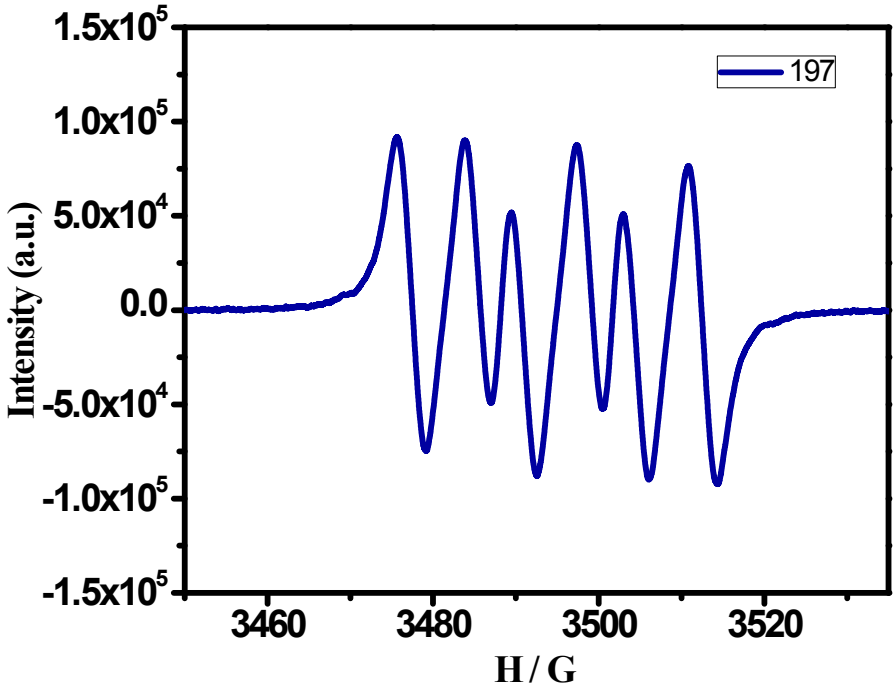


Figure S1: EPR spectra of the reaction mixture: **1a** (0.1 mmol), phenylacetylene (**2a)** (0.11 mmol) and 5 mol% of CuCl in CH_3CN, 0.5 mL of this reaction solution was taken out into a small vial,

followed by the addition of 0.01 mL of DMPO (5 x 10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere (1 atm) for 15 minutes. The reaction mixture was then analysed by EPR spectra. There are classical 6 peaks, the signals corresponding to (DMPO-OO(H)).

EPR spectra of the reaction mixture without CuCl

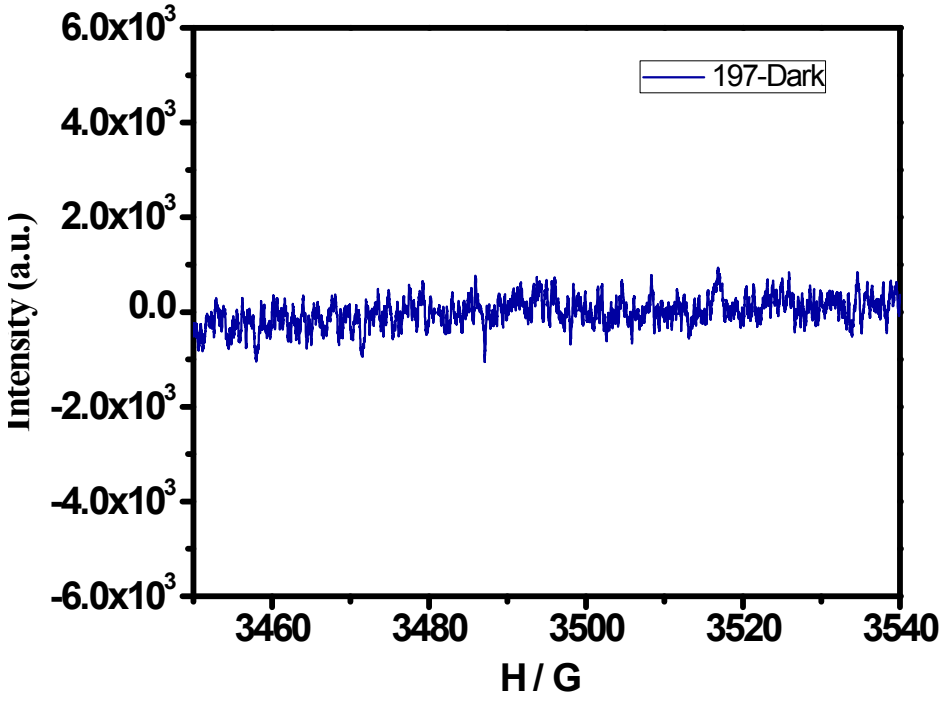


Figure S2: EPR spectra of the reaction mixture: **1a** (0.1 mmol), phenylacetylene (**2a)** (0.11 mmol) and 5 mol% of CuCl in CH_3CN, 0.5 mL of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5 x 10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere (1 atm.) for 15 minutes (in the absence of CuCl). The reaction mixtures was analysed by EPR spectra. No signals were detected.

UV-Visible spectra of Cu(I)-phenylacetylide

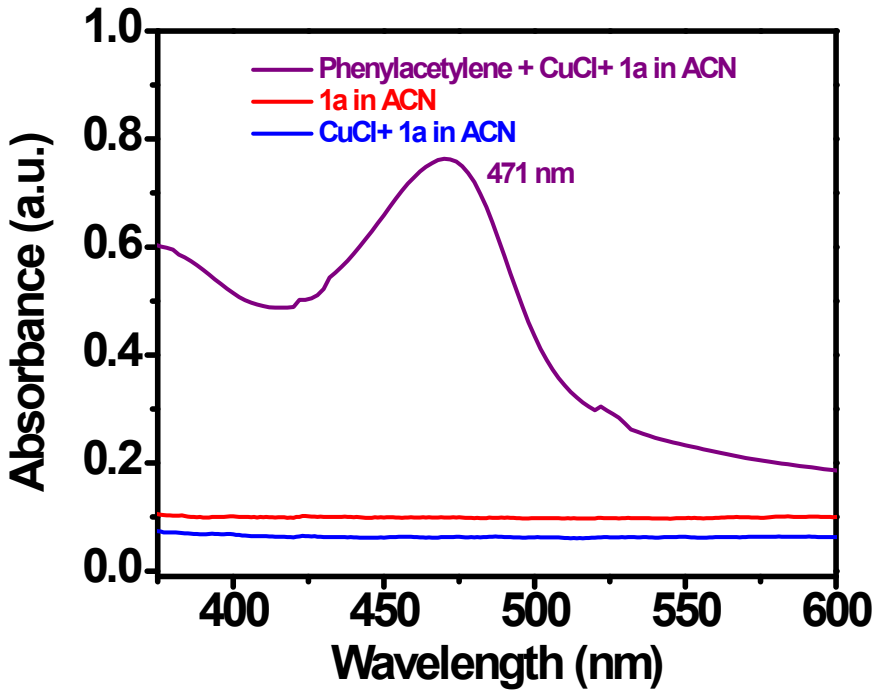
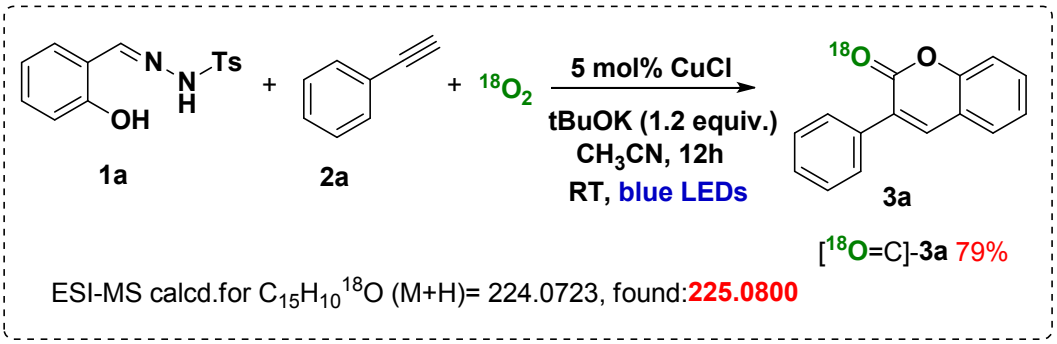


Figure S3: UV-visible spectra of reaction mixture in CH_3CN.

$^{18}O_2$ Labeling experiments:

We have performed an $^{18}O_2$ experiment under the standard condition (98% purity of $^{18}O_2$ gas, instead of $^{16}O_2$ air, was filled in the reaction system). From the ESI mass, the final product was determined to contain an ^{18}O was obtained exclusively, indicating that the oxygen atom in the product is originated from O_2.

Scheme S3. $^{18}O_2$ Labeling experiment for the product 3a**.**



Mass Data

Display Report

Analysis Info

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Method	Small molecule.m	Operator	NCTU
Sample Name	197-3	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

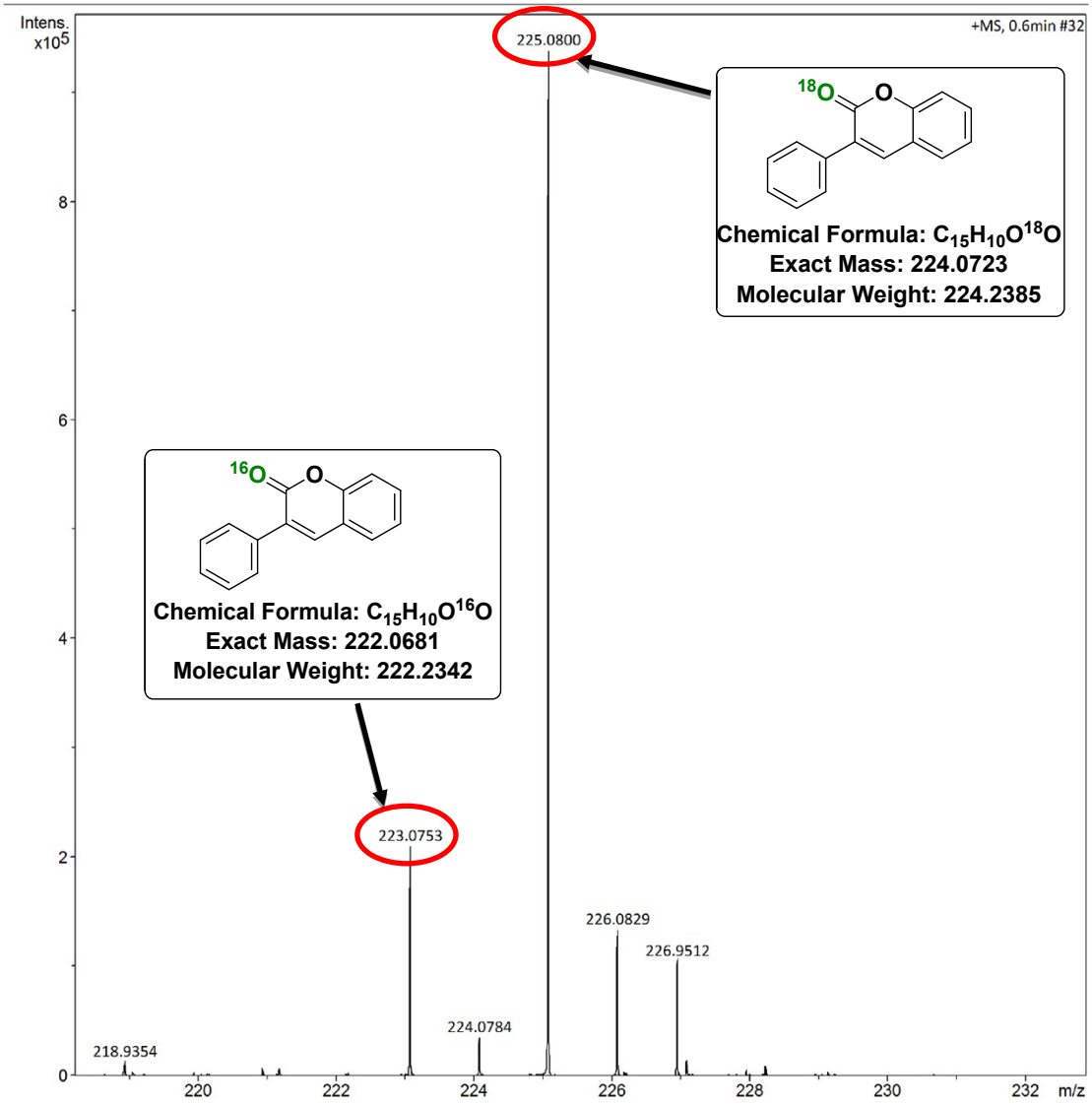


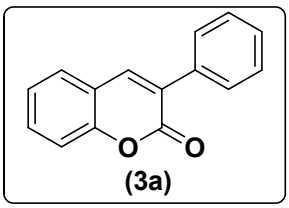
Figure S4: Mass spectrum of product **3a** ($^{18}O_2$ labeling experiment).

References:

[S1] Y. Xia, Y.Xia, F. Ye, Y.Zhang and J. Wang, *Org. Biomol. Chem.,* 2014, **12**, 9333.
[S2] W. Shi, Y. Luo, X. Luo, L. Chao, H. Zhang, J. Wang and A. Lei, *J. Am. Chem. Soc.* 2008, **130**, 14713.
[S3] Y. Okamoto and S. K. Kundu, *J. Phys. Chem.* 1973, **77**, 2677.

Spectroscopic Data:

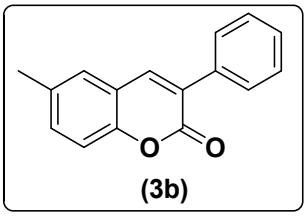
3-phenyl-2H-chromen-2-one (3a)



(3a)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.80 (s, 1H), 7.69 (d, *J*= 6.0 Hz, 2 H), 7.52 (t, *J*= 6.0 Hz, 2 H), 7.45-7.55 (m, 4 H), 7.28 (t, *J*= 6.0 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.5, 153.5, 139.8, 134.7, 131.3, 128.8, 128.5, 128.4, 128.3, 127.8, 124.4, 119.6 and 116.4; **ESI-MS** calcd for $C_{15}H_{10}O_2$ (M+H): 222.0681, found: 223.0749.

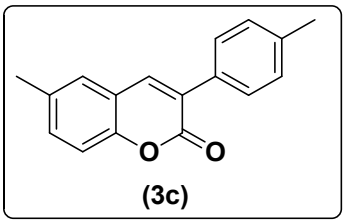
6-methyl-3-phenyl-2H-chromen-2-one (3b)



(3b)

Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.73 (s, 1H), 7.68 (d, *J*= 6.0 Hz, 2 H), 7.44-7.38 (m, 5 H), 7.31 (s, 1 H), 2.40 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.7, 151.6, 139.8, 134.8, 134.1, 132.2, 128.7, 128.5, 128.4, 128.2, 127.6, 119.4, 116.1 and 20.7; **ESI-MS** calcd for $C_{16}H_{12}O_2$ (M+H): 236.0837, found: 237.0914

6-methyl-3-p-tolyl-2H-chromen-2-one (3c)

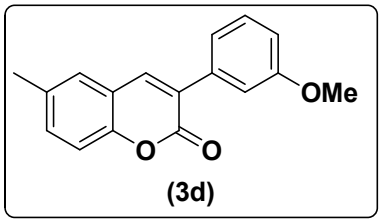


(3c)

Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.70 (s, 1H), 7.58 (d, *J*= 6.0 Hz, 2 H), 7.29-7.22 (m, 5 H), 2.39 (s, 3 H), 2.38 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.8, 157.5, 139.1, 138.7,

134.0, 132.2, 131.9, 129.1, 128.3, 128.1, 127.5, 119.5, 116.1, 21.2 and 20.7; **ESI-MS** calcd for $C_{17}H_{14}O_2$: 250.0994, found: 251.1081.

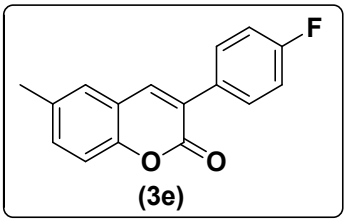
3-(3-methoxyphenyl)-6-methyl-2H-chromen-2-one (3d)



(3d)

Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.74 (s, 1H), 7.35-7.25 (m, 6 H), 6.92 (d, *J*= 6.0 Hz, 1 H), 3.83 (s, 3 H), 2.40 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.6, 159.5, 139.9, 136.1, 134.1, 132.4, 129.4, 128.0, 127.6, 120.9, 119.3, 116.1, 114.4, 114.2, 55.3 and 20.7; **ESI-MS** calcd for $C_{17}H_{14}O_3$: 266.0943, found: 267.1023

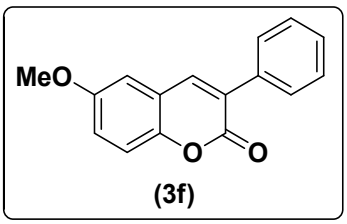
3-(4-fluorophenyl)-6-methyl-2H-chromen-2-one (3e)



(3e)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.71 (s, 1H), 7.66 (d, *J*= 6.0 Hz, 2 H), 7.30 (d, *J*= 6.0 Hz, 2 H), 7.23 (s, 1 H), 7.11 (t, *J*= 6.0 Hz, 2 H), 2.40 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 163.8, 162.1, 160.7, 151.6, 139.7, 134.2, 132.5, 130.4, 130.3, 127.6, 127.1, 119.2, 116.1, 115.5, 115.3 and 20.7; **ESI-MS** calcd for $C_{16}H_{11}FO_2$ (M+H): 254.0743, found: 255.0832

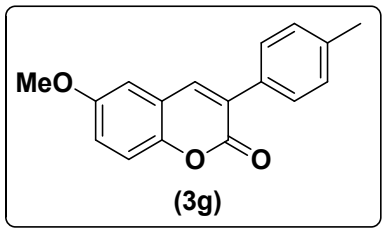
6-methoxy-3-phenyl-2H-chromen-2-one (3f)



(3f)

Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.74 (s, 1H), 7.68 (d, *J*= 6.0 Hz, 2 H), 7.44-738 (m, 3 H), 7.28 (d, *J*= 6.0 Hz, 1 H), 7.09 (d, *J*= 6.0 Hz, 1 H), 6.95 (s, 1 H), 3.84 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.7, 156.1, 148.0, 139.6, 134.7, 128.8, 128.6, 128.5, 128.4, 120.0, 119.1, 117.4, 109.9 and 55.8; **ESI-MS** calcd for $C_{16}H_{12}O_3$ (M+H): 252.0786, found: 253.0875

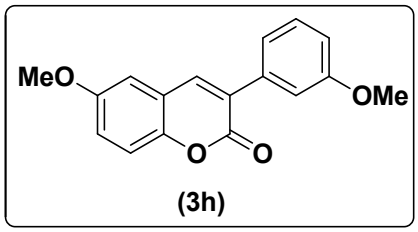
6-methoxy-3-p-tolyl-2H-chromen-2-one (3g)



(3g)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.71 (s, 1H), 7.59 (d, *J*= 6.0 Hz, 2 H), 7.27-7.23 (m, 3 H), 7.08 (d, *J*= 6.0 Hz, 1 H), 6.94 (s, 1 H), 3.84 (s, 3 H), 2.38 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.8, 156.1, 147.9, 139.0, 138.9, 131.8, 129.1, 128.6, 128.4, 120.1, 118.9, 117.4, 109.8, 55.8 and 21.2; **ESI-MS** calcd for $C_{17}H_{14}O_3$ (M+H): 266.0943, found: 267.1027.

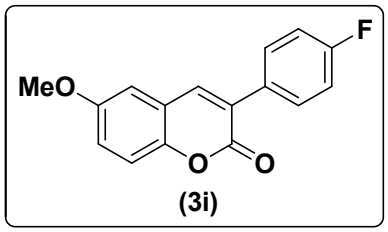
6-methoxy-3-(3-methoxyphenyl)-2H-chromen-2-one (3h)



(3h)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.74 (s, 1H), 7.32 (t, *J*= 12.0 Hz, 1 H), 7.27-7.23 (m, 3 H), 7.08 (d, *J*= 6.0 Hz, 1 H), 6.93 (t, *J*= 6.0 Hz, 2 H), 3.83 (s, 3 H), 3.82 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.5, 159.4, 156.0, 147.9, 139.8, 136.0, 129.4, 128.3, 120.8, 119.8, 119.1, 117.4, 114.4, 114.1, 109.8, 55.7 and 55.3; **ESI-MS** calcd for $C_{17}H_{14}O_4$ (M+H): 282.0892, found: 283.0968

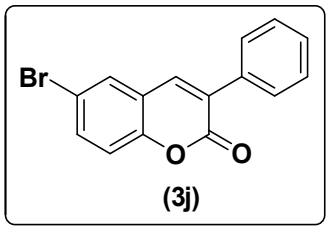
3-(4-fluorophenyl)-6-methoxy-2H-chromen-2-one (3i)



(3i)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.71 (s, 1H), 7.67 (d, *J*= 6.0 Hz, 2 H), 7.27 (d, *J*= 12.0 Hz, 1 H), 7.10 (t, *J*= 6.0 Hz, 3 H), 6.93 (d, *J*= 12.0 Hz, 1 H), 3.84 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 163.9, 162.2, 160.6, 156.2, 147.9, 139.4, 130.7, 130.4, 130.3, 127.6, 119.9, 119.2, 117.4, 115.5, 115.3, 109.9 and 55.8; **ESI-MS** calcd for $C_{16}H_{11}FO_3$ (M+H): 270.0692, found: 271.0812

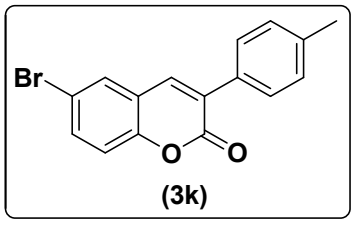
6-bromo-3-phenyl-2H-chromen-2-one (3j)



(3j)

Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.70 (s, 1H), 7.66 (d, *J*= 12.0 Hz, 3 H), 7.59 (d, *J*= 6.0 Hz, 1 H), 7.45-7.40 (m, 3 H), 7.23 (s, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 159.8, 152.2, 138.2, 134.1, 134.0, 130.0, 129.4, 129.1, 128.5, 128.5, 121.1, 118.1 and 116.9; **ESI-MS** calcd for $C_{15}H_9BrO_2$ (M+Na): 299.9786, found: 322.9665

6-bromo-3-p-tolyl-2H-chromen-2-one (3k)

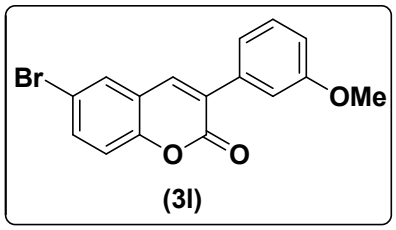


(3k)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.67 (s, 1H), 7.64 (s, 1H), 7.58 (t, *J*= 6.0 Hz, 3 H), 7.25-7.22 (m, 3 H), 7.22 (m, 3 H), 2.39 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 159.9, 152.1,

139.3, 137.5, 133.8, 131.2, 129.9, 129.4, 129.2, 128.3, 121.2, 1181, 116.9 and 21.2; **ESI-MS** calcd for $C_{16}H_{11}BrO_2$ (M+Na): 313.9942, found: 336.9849

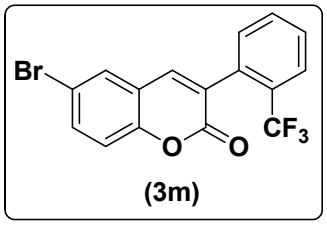
6-bromo-3-(3-methoxyphenyl)-2H-chromen-2-one (3l)



(3l)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.72 (s, 1H), 7.67 (s, 1 H), 7.60 (d, *J*= 12.0 Hz, 1 H), 7.36 (t, *J*= 6.0 Hz, 1 H), 7.25-7.23 (m, 3 H), 6.96 (d, *J*= 6.0 Hz, 1 H), 3.85 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 159.5, 152.3, 138.4, 135.5, 134.1, 130.1, 129.5, 129.3, 128.5, 121.1, 120.8, 118.1, 117.0, 114.8, 114.2 and 55.3; **ESI-MS** calcd for $C_{16}H_{11}BrO_3$ (M+Na): 329.9892, found: 352.9800

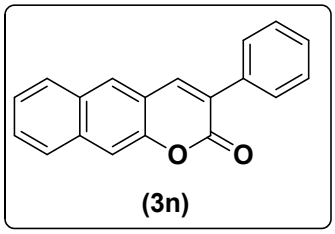
6-bromo-3-(2-(trifluoromethyl)phenyl)-2H-chromen-2-one (3m)



(3m)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.77 (s, 1H), 7.65-7.53 (m, 5 H), 7.39 (d, *J*= 12.0 Hz, 1 H), 7.27 (d, *J*= 12.0 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 159.7, 152.7, 140.5, 134.6, 132.6, 131.8, 131.5, 130.3, 129.3, 129.1, 128.1, 126.6, 126.5, 124.7, 122.9, 120.2, 118.4 and 117.1; **ESI-MS** calcd for $C_{16}H_8BrF_3O_2$ (M+Na): 367.9660, found: 390.9564

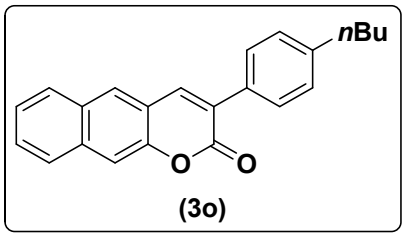
3-phenyl-2H-benzo[g]chromen-2-one (3n)



(3n)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.55 (s, 1H), 8.27 (d, *J*= 12.0 Hz, 1 H), 7.96 (d, *J*= 6.0 Hz, 1 H), 7.90 (d, *J*= 6.0 Hz, 1 H), 7.78 (d, *J*= 6.0 Hz, 2 H), 7.67 (t, *J*= 6.0 Hz, 1 H), 7.54 (t, *J*= 6.0 Hz, 1 H), 7.47 (t, *J*= 6.0 Hz, 3 H), 7.42 (d, *J*= 6.0 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.6, 153.1, 135.6, 135.0, 132.6, 130.3, 129.0, 128.8, 128.6, 128.5, 128.1, 127.2, 126.0, 121.3, 116.6 and 113.7; **ESI-MS** calcd for $C_{19}H_{12}O_2$ (M+H): 272.0837, found: 273.0915.

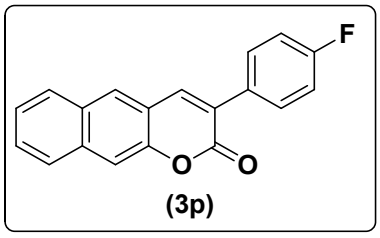
3-(4-butylphenyl)-2H-benzo[g]chromen-2-one (3o)



(3o)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.55 (s, 1H), 8.27 (d, *J*= 12.0 Hz, 1 H), 7.95 (d, *J*= 12.0 Hz, 1 H), 7.90 (d, *J*= 12.0 Hz, 1 H), 7.70 (d, *J*= 6.0 Hz, 2 H), 7.68 (t, *J*= 6.0 Hz, 1 H), 7.56 (d, *J*= 6.0 Hz, 1 H), 7.48 (d, *J*= 6.0 Hz, 1 H), 7.29 (d, *J*= 6.0 Hz, 2 H), 2.66 (t, *J*= 6.0 Hz, 2 H), 1.65-1.61 (m, 2 H), 1.40-1.36 (m, 2 H), 0.93 (t, *J*= 12.0 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.7, 152.9, 143.9, 135.1, 132.4, 132.3, 130.3, 129.0, 128.6, 128.4, 128.1, 127.2, 125.9, 121.4, 116.6, 113.8, 35.4, 33.5, 22.3 and 13.9; **ESI-MS** calcd for $C_{23}H_{20}O_2$ (M+Na): 328.1463, found: 351.1368

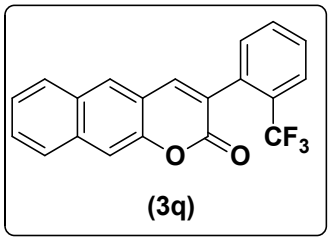
3-(4-fluorophenyl)-2H-benzo[g]chromen-2-one (3p)



(3p)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.32 (d, *J*= 12.0 Hz, 1 H), 8.01 (d, *J*= 12.0 Hz, 1 H), 7.95 (d, *J*= 6.0 Hz, 1 H), 7.82-7.80 (m, 2 H), 7.72 (t, *J*= 6.0 Hz, 1 H), 7.60 (t, *J*= 6.0 Hz, 1 H), 7.52 (d, *J*= 12.0 Hz, 1 H), 7.19 (t, *J*= 12.0 Hz, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 163.9, 162.2, 160.6, 153.1, 135.5, 132.8, 131.0, 130.4, 129.1, 129.0, 128.2, 126.2, 126.1, 121.3, 116.7, 115.6, 115.5 and 113.6; **ESI-MS** calcd for $C_{19}H_{11}FO_2$ (M+Na): 290.0743, found: 313.0622.

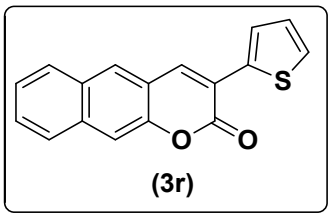
3-(2-(trifluoromethyl)phenyl)-2H-benzo[g]chromen-2-one (3q)



(3q)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.44 (s, 1H), 8.18 (d, *J*= 6.0 Hz, 1 H), 8.01 (d, *J*= 6.0 Hz, 1 H), 7.92 (d, *J*= 6.0 Hz, 1 H), 7.80 (d, *J*= 12.0 Hz, 1 H), 7.64 (t, *J*= 6.0 Hz, 2 H), 7.57-7.49 (m, 4 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.4, 153.7, 137.9, 133.5, 133.3, 131.9, 131.8, 130.3, 129.1, 129.0, 128.9, 128.3, 126.6, 126.5, 126.1, 125.8, 121.3, 116.8 and 112.9; **ESI-MS** calcd for $C_{20}H_{11}F_3O_2$ (M+Na): 340.0711, found: 360.0614

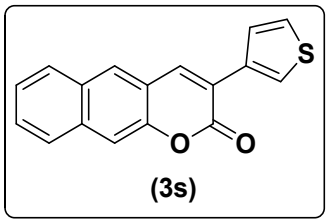
3-(thiophen-2-yl)-2H-benzo[g]chromen-2-one (3r)



(3r)

Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.72 (s, 1H), 8.29 (d, *J*= 12.0 Hz, 1 H), 7.93 (d, *J*= 12.0 Hz, 1 H), 7.89-7.88 (m, 2 H), 7.69 (t, *J*= 6.0 Hz, 1 H), 7.57-7.54 (m, 1 H), 7.46-7.43 (m, 2 H), 7.15 (d, *J*= 6.0 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 159.4, 152.2, 136.4, 132.5, 131.3, 130.4, 129.1, 128.9, 128.1, 127.6, 127.0, 126.1, 121.4, 120.8, 116.6 and 113.5.

3-(thiophen-3-yl)-2H-benzo[g]chromen-2-one (3s)

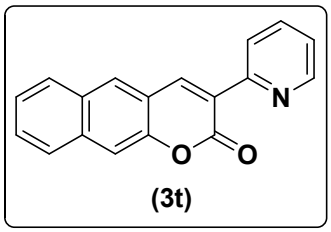


(3s)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.67 (s, 1H), 7.93 (d, *J*= 6.0 Hz, 1 H), 7.90 (s, 1 H), 7.89 (d, *J*= 6.0 Hz, 1 H), 7.68 (d, *J*= 6.0 Hz, 1 H), 7.62 (t, *J*= 6.0 Hz, 1 H), 7.56 (t, *J*= 6.0 Hz, 1

H), 7.46 (d, *J*= 12.0 Hz, 1 H), 7.43-7.41 (m, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.1, 152.4, 134.7, 132.9, 132.4, 130.3, 129.1, 128.9, 128.1, 126.2, 126.0, 125.8, 123.6, 121.7, 121.3, 116.6 and 113.5; **ESI-MS** calcd for $C_{17}H_{10}O_2S$ (M+Na): 278.0402, found: 301.0306.

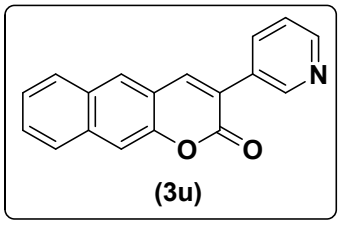
3-(pyridin-2-yl)-2H-benzo[g]chromen-2-one (3t)



(3t)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 9.58 (s, 1H), 8.72 (s, 1 H), 8.50 (d, *J*= 6.0 Hz, 1 H), 8.45 (d, *J*= 6.0 Hz, 1 H), 7.98 (d, *J*= 12.0 Hz, 1 H), 7.88 (d, *J*= 6.0 Hz, 1 H), 7.77 (t, *J*= 6.0 Hz, 1 H), 7.68 (d, *J*= 6.0 Hz, 1 H), 7.55 (t, *J*= 6.0 Hz, 1 H), 7.47 (d, *J*= 12.0 Hz, 1 H), 7.29 (d, *J*= 6.0 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.3, 153.7, 151.4, 149.3, 138.2, 136.6, 133.5, 130.3, 129.5, 128.9, 128.3, 126.1, 123.9, 123.3, 122.0, 116.5 and113.8.

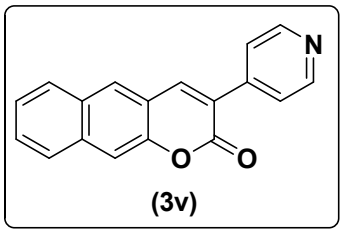
3-(pyridin-3-yl)-2H-benzo[g]chromen-2-one (3u)



(3u)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.64 (s, 1H), 8.28 (d, *J*= 6.0 Hz, 1 H), 8.22 (d, *J*= 12.0 Hz, 1 H), 8.00 (d, *J*= 6.0 Hz, 2 H), 7.92 (d, *J*= 6.0 Hz, 1 H), 7.72-7.60 (m, 2 H), 7.58 (t, *J*= 6.0 Hz, 1 H), 7.50 (d, *J*= 12.0 Hz, 1 H), 7.44 (s, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.3, 153.6, 149.6, 148.8, 136.3, 136.2, 133.4, 130.3, 129.1, 129.0, 128.5, 126.2, 124.0, 121.3, 116.6, and 113.5; **ESI-MS** calcd for $C_{18}H_{11}NO_2$ (M+H): 273.0790, found: 274.0860.

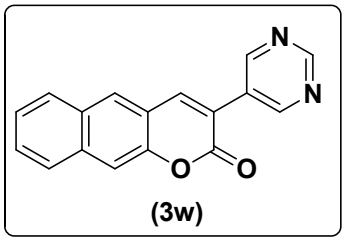
3-(pyridin-4-yl)-2H-benzo[g]chromen-2-one (3v)



(3v)

Pale yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.86 (s, 1H), 8.71 (s, 2H), 8.34 (d, *J*= 6.0 Hz, 1 H), 8.05-8.01 (m, 3 H), 7.90 (d, *J*= 12.0 Hz, 1 H), 7.69 (t, *J*= 12.0 Hz, 1 H), 7.57 (t, *J*= 6.0 Hz, 1 H), 7.46 (d, *J*= 12.0 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 159.2, 154.2, 146.6, 138.7, 134.9, 130.2, 129.2, 129.0, 128.8, 127.9, 126.5, 123.6, 122.5, 121.3, 116.4, 113.1.

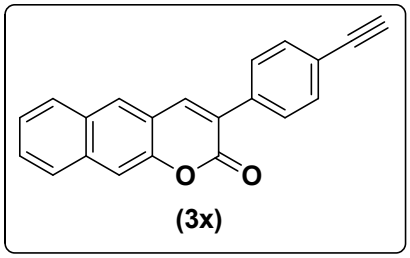
3-(pyrimidin-5-yl)-2H-benzo[g]chromen-2-one (3w)



(3w)

Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 9.12 (s, 2H), 8.67 (s, 1 H), 8.26 (d, *J*= 6.0 Hz, 1 H), 7.95 (d, *J*= 12.0 Hz, 1 H), 7.52 (s, 1 H), 7.61 (s, 1 H), 7.49 (s, 2 H), 7.40 (s, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 157.9, 155.8, 137.0, 133.9, 130.1, 128.9, 128.7, 128.4, 126.2, 121.2 and 116.2.

3-(4-ethynylphenyl)-2H-benzo[g]chromen-2-one (3x)

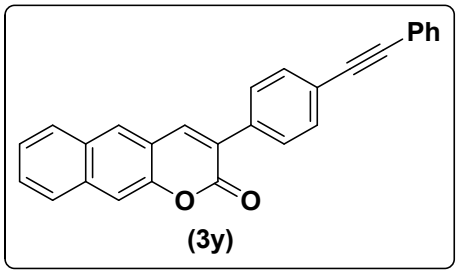


(3x)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.29 (d, *J*= 12.0 Hz, 1 H), 7.98 (d, *J*= 12.0 Hz, 1 H), 7.91 (d, *J*= 6.0 Hz, 1 H), 7.78 (d, *J*= 6.0 Hz, 2 H), 7.69 (t, *J*= 6.0 Hz, 1 H), 7.58 (t, *J*= 6.0 Hz, 2 H), 7.48 (d, *J*= 12.0 Hz, 1 H), 7.44 (d, *J*= 6.0 Hz, 1 H), 3.15 (s, 1 H); **^{13}C NMR** (150

MHz, $CDCl_3$): δ 160.3, 153.3, 135.9, 135.4, 133.1, 132.2, 130.3, 129.1, 128.4, 128.3, 126.1, 122.5, 121.3, 116.6, 113.6, 83.2 and 78.4; **ESI-MS** calcd for $C_{21}H_{12}O_2$ (M+H): 296.0837, found: 297.0916.

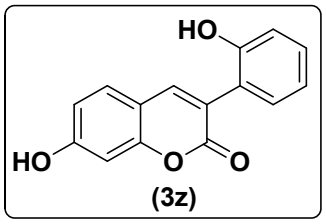
3-(4-(phenylethynyl)phenyl)-2H-benzo[g]chromen-2-one (3y)



(3y)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.65 (s, 1H), 8.34 (d, *J*= 6.0 Hz, 1 H), 8.02 (d, *J*= 12.0 Hz, 1 H), 7.96 (d, *J*= 6.0 Hz, 2 H), 7.85 (d, *J*= 6.0 Hz, 1 H), 7.74-7.52 (m, 6 H), 7.37 (t, *J*= 6.0 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.4, 153.2, 135.7, 134.8, 133.0, 131.7, 131.6, 130.3, 129.2, 129.1, 128.5, 128.5, 128.4, 128.3, 126.4, 126.1, 123.8, 123.0, 121.4, 116.7, 113.7, 90.7 and 89.1; **ESI-MS** calcd for $C_{27}H_{16}O_2$ (M+Na): 372.1150, found: 395.1041.

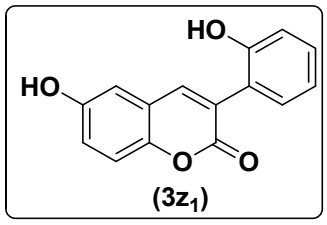
7-hydroxy-3-(2-hydroxyphenyl)-2H-chromen-2-one (3z)



(3z)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 9.83 (s, 1H), 8.40 (s, 1 H), 7.71 (s, 1 H), 7.27 (d, *J*= 12.0 Hz, 1 H), 7.20 (d, *J*= 6.0 Hz, 1 H), 7.15 (d, *J*= 6.0 Hz, 1 H), 6.88 (d, *J*= 12.0 Hz, 1 H), 6.84 (d, *J*= 12.0 Hz, 1 H), 6.75 (d, *J*= 6.0 Hz, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 162.2, 161.0, 154.8, 154.4, 143.4, 130.4, 129.5, 128.9, 122.6, 121.4, 119.9, 117.2, 113.7, 112.0 and 102.2; **ESI-MS** calcd for $C_{15}H_{10}O_4$ (M+H): 254.0579, found: 255.0664.

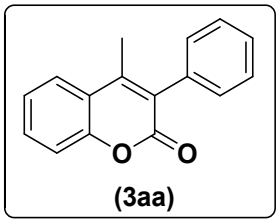
6-hydroxy-3-(2-hydroxyphenyl)-2H-chromen-2-one ($3z_1$)



($3z_1$)

White solid; **^{1}H NMR** (600 MHz, DMSO-d_6): δ 7.81 (s, 1 H), 7.28-7.16 (m, 3 H), 7.03 (d, *J*= 6.0 Hz, 2 H), 6.97-6.93 (m, 1 H), 6.88 (d, *J*= 6.0 Hz, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 163.0, 156.3, 155.4, 148.3, 145.5, 143.8, 131.9, 130.9, 127.6, 123.7, 121.5, 121.1, 120.6, 120.5, 118.3, 118.0, 117.1, 116.9, 113.4, and 113.3; **ESI-MS** calcd for $C_{15}H_{10}O_4$ (M+Na): 254.0579, found: 277.0475.

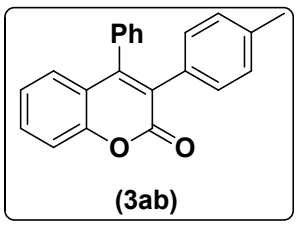
4-methyl-3-phenyl-2H-chromen-2-one (3aa)



(3aa)

Pale white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.66 (d, *J*= 6.0 Hz, 1 H), 7.52 (t, *J*= 6.0 Hz, 1 H), 7.44 (t, *J*= 6.0 Hz, 2 H), 7.39-7.35 (m, 2 H), 7.32-7.28 (m, 3 H), 2.30 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.9, 152.6, 147.5, 134.4, 131.2, 129.9, 128.3, 128.1, 127.3, 125.0, 124.2, 120.5, 116.8 and 16.5; **ESI-MS** calcd for $C_{16}H_{12}O_2$ (M+H): 236.0837, found: 237.0932.

3,4-diphenyl-2H-chromen-2-one (3ab)

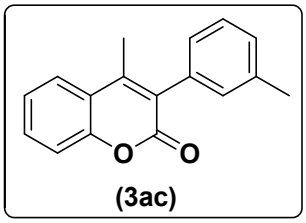


(3ab)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 9.51 (s, 1H), 8.70 (d, *J*= 6.0 Hz, 2 H), 8.57 (d, *J*= 12.0 Hz, 1 H), 8.29 (d, *J*= 12.0 Hz, 1 H), 7.81 (t, *J*= 6.0 Hz, 1 H), 7.66-7.49 (m, 4 H),7.35 (t, *J*=

6.0 Hz, 2 H), 2.621 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.2, 151.6, 138.6, 138.2, 134.3, 132.0, 130.2, 129.9, 129.6, 128.9, 128.7, 128.3, 126.3, 123.6, 123.5, 122.4, 118.5, 117.2, 115.8 and 22.6; **ESI-MS** calcd for $C_{22}H_{16}O_2$ (M+H): 312.1150, found: 313.1239.

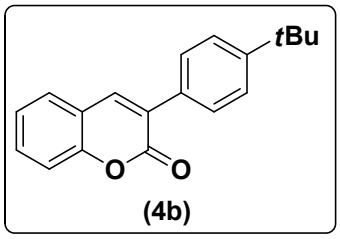
4-methyl-3-m-tolyl-2H-chromen-2-one (3ac)



(3ac)

Semi-white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.65 (d, *J*= 6.0 Hz, 1 H), 7.52 (d, *J*= 6.0 Hz, 1 H), 7.37-7.30 (m, 3 H), 7.19 (d, *J*= 6.0 Hz, 1 H), 7.10-7.06 (m, 2 H), 2.38 (m, 3 H), 2.39 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ161.0, 152.6, 147.5, 138.0, 134.3, 131.2, 130.5, 128.9, 128.3, 127.5, 126.9, 125.0, 124.1, 120.5, 116.8, 21.4 and 16.5; **ESI-MS** calcd for $C_{17}H_{14}O_2$ (M+H): 250.0994, found: 251.1093.

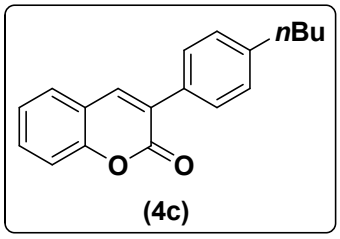
3-(4-tert-butylphenyl)-2H-chromen-2-one (4b)



(4b)

Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.78 (s, 1 H), 7.64 (d, *J*= 6.0 Hz, 2 H), 7.52-7.45 (m, 4 H), 7.34 (t, *J*= 6.0 Hz, 1 H), 7.27 (t, *J*= 6.0 Hz, 1 H), 1.33 (s, 9 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.7, 153.4, 152.0, 139.2, 131.7, 131.1, 128.2, 128.1, 127.7, 125.4, 124.4, 119.7, 116.4, 34.6 and 31.2; **ESI-MS** calcd for $C_{19}H_{18}O_2$ (M+H): 278.1307, found: 279.1383

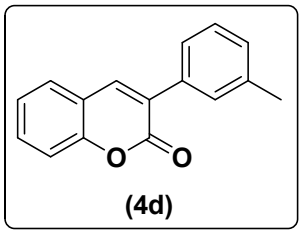
3-(4-butylphenyl)-2H-chromen-2-one (4c)



(4c)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.77 (s, 1 H), 7.60 (d, *J*= 6.0 Hz, 2 H), 7.52-7.48 (m, 2 H), 7.30-7.25 (m, 3 H), 6.94-6.90 (m, 1 H), 2.64 (t, *J*= 6.0 Hz, 2 H), 1.63-1.58 (m, 2 H), 1.38-1.34 (m, 2 H), 0.92 (t, *J*= 6.0 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.7, 153.4, 143.9, 139.2, 135.5, 131.1, 128.5, 128.3, 127.7, 124.4, 122.5, 119.0, 116.4, 109.1, 35.4, 33.4, 22.3 and 13.9; **ESI-MS** calcd for $C_{19}H_{18}O_2$ (M+H): 278.1307, found: 279.1381

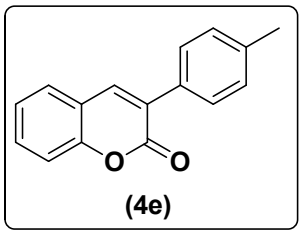
3-*m*-tolyl-2H-chromen-2-one (4d)



(4d)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.77 (s, 1 H), 7.52-7.47 (m, 4 H), 7.35-7.26 (m, 3 H), 7.20 (d, *J*= 6.0 Hz, 1 H), 2.40 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.5, 153.5, 139.7, 138.0, 134.6, 131.2, 129.6, 129.1, 128.5, 128.3, 127.8, 125.6, 124.4, 119.7, 116.4 and 21.4; **ESI-MS** calcd for $C_{16}H_{12}O_2$ (M+H): 236.0837, found: 237.0909.

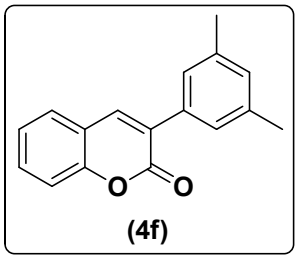
3-p-tolyl-2H-chromen-2-one (4e)



(4e)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.73 (s, 1 H), 7.59 (d, *J*= 6.0 Hz, 2 H), 7.52-7.48 (m, 3 H), 7.35 (d, *J*= 6.0 Hz, 1 H), 7.28-7.23 (m, 2 H), 2.38 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.6, 153.4, 129.1, 138.9, 131.8, 131.1, 129.1, 128.4, 127.7, 124.4, 119.7, 116.4 and 21.2.

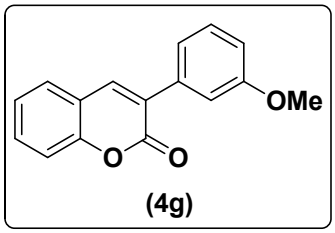
3-(3,5-dimethylphenyl)-2H-chromen-2-one (4f)



(4f)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.76 (s, 1 H), 7.51-7.48 (m, 2 H), 7.34 (d, *J*= 12.0 Hz, 1 H), 7.28-7.03 (m, 4 H), 2.36 (s, 3 H), 2.35 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.6, 153.4, 139.6, 137.9, 134.6, 131.2, 130.5, 128.6, 127.47, 126.2, 124.4, 119.7, 116.4 and 21.3; **ESI-MS** calcd for $C_{17}H_{14}O_2$ (M+H): 250.0994, found: 251.1070

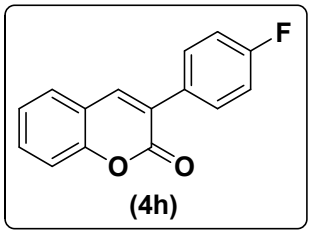
3-(3-methoxyphenyl)-2H-chromen-2-one (4g)



(4g)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.78 (s, 1 H), 7.52-7.49 (m, 2 H), 7.34 (t, *J*= 6.0 Hz, 2 H), 7.28-7.23 (m, 3 H), 6.93 (d, *J*= 6.0 Hz, 1 H), 3.83 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.4, 159.4, 153.4, 139.9, 135.9, 131.4, 129.4, 128.1, 127.8, 124.4, 120.8, 119.5, 116.3, 114.4, 114.1 and 55.3; **ESI-MS** calcd for $C_{16}H_{12}O_3$ (M+H): 252.0786, found: 253.0863

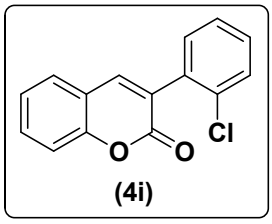
3-(4-fluorophenyl)-2H-chromen-2-one (4h)



(4h)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.76 (s, 1 H), 7.67 (d, *J*= 6.0 Hz, 2 H), 7.52-7.49 (m, 2 H), 7.33 (d, *J*= 12.0 Hz, 1 H), 7.29-7.26 (m, 1 H), 7.11-7.08 (m, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 163.8, 162.1, 160.4, 153.4, 139.6, 131.4, 130.6, 130.4, 130.3, 127.8, 127.2, 124.5, 119.5, 116.4, 115.5 and 115.3; **ESI-MS** calcd for $C_{15}H_9FO_2$ (M+H): 240.0587, found: 241.0662.

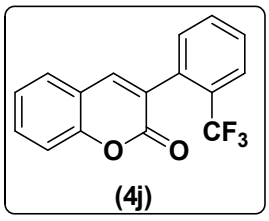
3-(2-chlorophenyl)-2H-chromen-2-one (4i)



(4i)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.72 (s, 1 H), 7.55-7.46 (m, 3 H), 7.40-7.27 (m, 5 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 159.7, 153.9, 142.6, 133.7, 133.6, 131.8, 131.3, 130.0, 129.8, 128.0, 127.0, 126.8, 124.5, 119.0 and 116.6; **ESI-MS** calcd for $C_{15}H_9ClO_2$ (M+H): 256.0291, found: 257.0370

3-(2-(trifluoromethyl)phenyl)-2H-chromen-2-one (4j)

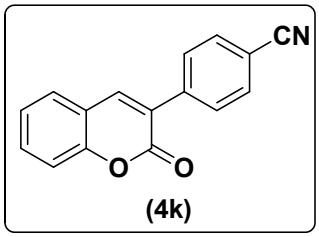


(4j)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.75 (d, *J*= 6.0 Hz, 1 H), 7.62 (d, *J*= 12.0 Hz, 1 H), 7.59-7.49 (m, 4 H), 7.40-7.36 (m, 2 H), 7.29 (t, *J*= 6.0 Hz, 1 H);**^{13}C NMR** (150 MHz, $CDCl_3$): δ

160.3, 153.9, 141.9, 133.2, 1319, 131.8, 131.7, 129.6, 129.4, 129.2, 128.1, 127.0, 126.4, 118.8, and 116.7; **ESI-MS** calcd for $C_{16}H_9F_3O_2$ (M+H): 290.0555, found: 291.0633

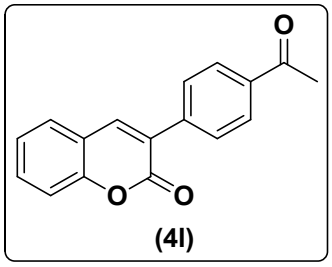
4-(2-oxo-2H-chromen-3-yl)benzonitrile (4k)



(4k)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.88 (s, 1 H), 7.82 (d, *J*= 6.0 Hz, 2 H), 7.70 (d, *J*= 6.0 Hz, 2 H), 7.61-7.55 (m, 2 H), 7.36 (d, *J*= 6.0 Hz, 1 H), 7.32 (t, *J*= 6.0 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 159.8, 153.7, 141.3, 139.1, 133.0, 132.3, 132.1, 129.1, 128.2, 126.4, 124.8, 119.1, 118.4, 116.6 and 112.3.

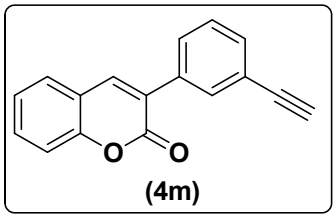
3-(4-acetylphenyl)-2H-chromen-2-one (4l)



(4l)

Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.00 (d, *J*=6.0 Hz, 2 H), 7.87 (s, 1 H), 7.79 (d, *J*= 6.0 Hz, 2 H), 7.55-7.52 (m, 2 H), 7.34 (d, *J*= 6.0 Hz, 1 H), 7.30 (t, *J*= 6.0 Hz, 1 H), 2.60 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 197.5, 160.1, 153.6, 140.8, 139.2, 136.9, 122.3, 132.0, 128.7, 128.4, 128.1, 124.6, 119.3, 116.5 and 26.6; **ESI-MS** calcd for $C_{17}H_{12}O_3$ (M+H): 264.0786, found: 265.0862

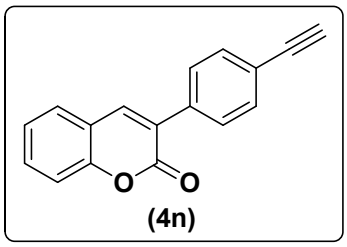
3-(3-ethynylphenyl)-2H-chromen-2-one (4m)



(4m)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.78 (d, *J*= 6.0 Hz, 2 H), 7.70 (d, *J*= 6.0 Hz, 1 H), 7.53-7.49 (m, 3 H), 7.39-7.26 (m, 3 H), 3.08 (s, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.2, 153.5, 140.2, 134.8, 132.3, 132.0, 131.6, 129.0, 128.4, 127.9, 127.3, 124.5, 122.4, 119.4, 116.4, 83.1 and 77.7; **ESI-MS** calcd for $C_{17}H_{10}O_2$ (M+H): 246.0681, found: 247.0754.

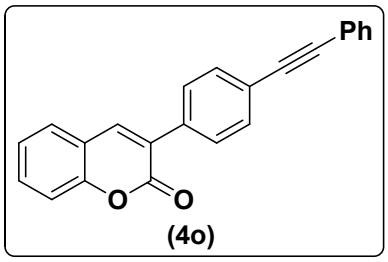
3-(4-ethynylphenyl)-2H-chromen-2-one (4n)



(4n)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.81 (s, 1 H), 7.67 (d, *J*= 6.0 Hz, 2 H), 7.55-7.51 (m, 4 H), 7.34 (d, *J*= 6.0 Hz, 1 H), 7.28 (t, *J*= 12.0 Hz, 1 H), 3.13 (s, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.2, 153.5, 140.1, 135.0, 132.1, 131.7, 1284, 128.0, 127.4, 124.6, 122.6, 119.4, 116.4 and 83.2; **ESI-MS** calcd for $C_{17}H_{10}O_2$ (M+Na): 246.0681, found: 269.0587.

3-(4-(phenylethynyl)phenyl)-2H-chromen-2-one (4o)

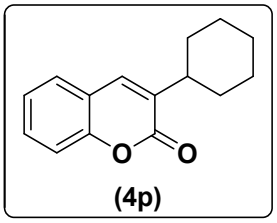


(4o)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.84 (s, 1 H), 7.71 (d, *J*= 6.0 Hz, 2 H), 7.59-7.53 (m, 6 H), 7.37-7.28 (m, 5 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.3, 153.5, 139.9, 134.4, 132.3, 131.7,

131.6, 129.0, 128.4, 128.3, 127.9, 127.5, 124.5, 123.8, 123.0, 119.5, 116.5, 90.7 and 89.0; **ESI-MS** calcd for $C_{23}H_{14}O_2$ (M+Na): 322.0994, found: 345.0897.

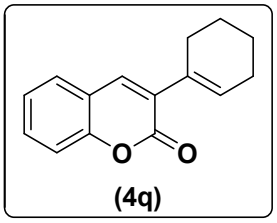
3-cyclohexyl-2H-chromen-2-one (4p)



(4p)

Semi-white oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.18 (s, 1H), 7.60 (d, *J*= 6.0 Hz, 1 H), 7.46 (s, 1 H), 7.34 (s, 2 H), 2.56-2.55 (m, 1 H), 2.02-1.86 (m, 4 H), 1.76-1.74 (m, 2 H), 1.47-1.37 (m, 4 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 173.2, 157.0, 135.6, 133.5, 130.0, 129.5, 125.6, 124.8, 118.0, 42.8, 30.5, 25.8 and 25.7; **ESI-MS** calcd for $C_{15}H_{16}O_2$ (M+H): 228.1150, found: 229.1233..

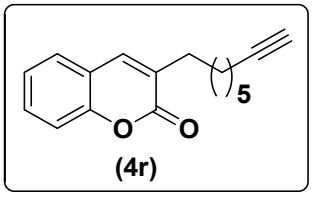
3-cyclohexenyl-2H-chromen-2-one (4q)



(4q)

Semi-white oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.15 (d, *J*= 6.0 Hz, 1 H), 7.62 (t, *J*= 6.0 Hz, 1 H), 7.42 (d, *J*= 6.0 Hz, 1 H), 7.33 (t, *J*= 12.0 Hz, 1 H), 6.97 (s, 1 H), 6.28 (s, 1 H), 2.30-2.28 (m, 4 H), 1.79-1.75 (m, 2 H), 1.68-1.66 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 178.9, 163.7, 156.0, 133.9, 133.5, 129.8, 129.6, 129.5, 125.5, 124.6, 123.7, 117.7, 106.1, 25.9, 24.1, 22.1 and 21.5; **ESI-MS** calcd for $C_{15}H_{14}O_2$ (M+H): 226.0994, found: 227.1079.

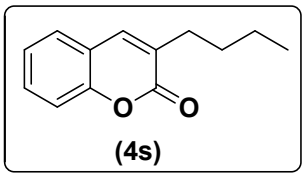
3-octyl-2H-chromen-2-one (4r)



(4r)

Semi-white oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.81 (d, *J*= 6.0 Hz, 1 H), 7.31 (d, *J*= 6.0 Hz, 1 H), 7.18 (t, *J*= 6.0 Hz, 1 H), 6.92 (t, *J*= 6.0 Hz, 1 H), 6.79 (t, *J*= 6.0 Hz, 1 H), 2.61 (t, *J*= 6.0 Hz, 2 H), 2.43 (s, 1 H), 2.19-2.16 (m, 2 H), 1.92-1.73 (m, 4 H), 1.57-1.39 (m, 4 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 150.6, 144.6, 134.9, 131.2, 129.7, 128.2, 125.6, 121.9, 117.8, 116.7, 83.0, 68.3, 34.2, 28.4, 28.1, 26.6, 21.6 and 18.3; **ESI-MS** calcd for $C_{17}H_{18}O_2$ (M+Na): 254.1307, found: 255.1385.

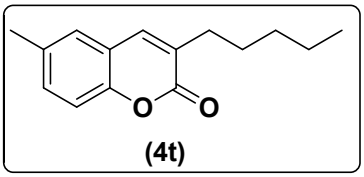
3-butyl-2H-chromen-2-one (4s)



(4s)

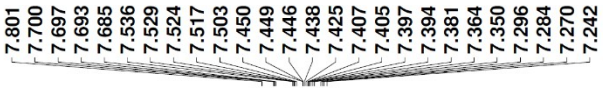
White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.16 (d, *J*= 6.0 Hz, 1 H), 7.62 (t, *J*= 6.0 Hz 1 H), 7.40 (d, *J*= 12.0 Hz, 1 H), 7.35 (t, *J*= 6.0 Hz, 1 H), 6.16 (s, 1 H), 2.60 (t, *J*= 6.0 Hz, 2 H), 1.73-1.68 (m, 2 H), 1.44-1.38 (m, 2 H), 0.94 (t, *J*= 6.0 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 178.4, 156.5, 133.4, 125.6, 124.8, 123.7, 117.8, 109.7, 34.0, 28.8, 22.1 and 13.7 ; **ESI-MS** calcd for $C_{13}H_{14}O_2$ (M+H): 202.0994, found: 203.1076.

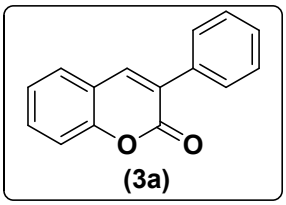
6-methyl-3-pentyl-2H-chromen-2-one (4t)



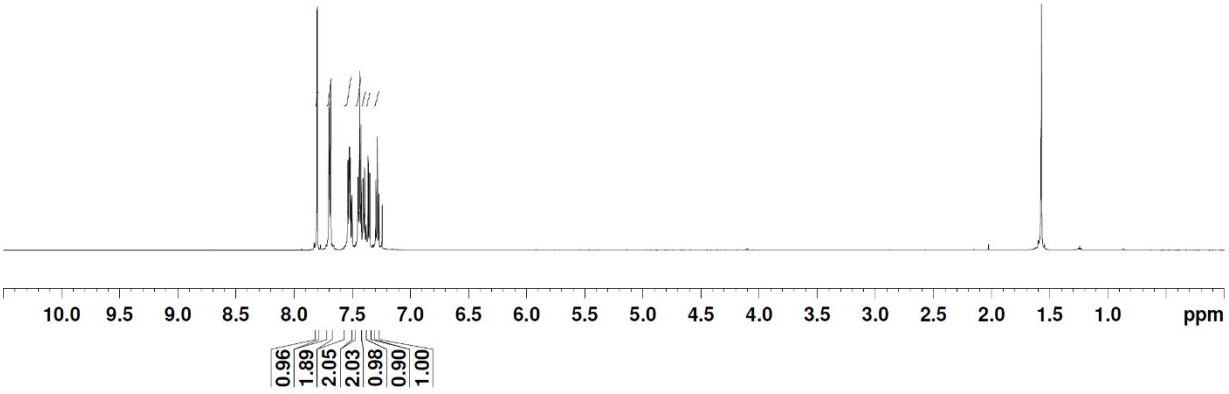
(4t)

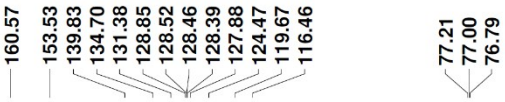
Semi-white oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.94 (s, 1H), 7.43 (d, *J*= 6.0 Hz, 1 H), 7.29 (d, *J*= 6.0 Hz, 1 H), 6.13 (s, 1 H), 2.59 (t, *J*= 6.0 Hz, 2 H), 2.42 (s, 3 H), 2.31-2.28 (m, 2 H), 1.73-1.67 (m, 2 H), 1.43-1.38 (m, 2 H), 0.94 (t, *J*= 6.0 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 178.5, 169.6, 154.8, 134.5, 129.2, 128.6, 125.0, 117.5, 109.6, 34.0, 28.8, 26.4, 22.1, 20.8 and 13.7; **ESI-MS** calcd for $C_{15}H_{18}O_2$ (M+H): 230.1307, found: 231.1388.

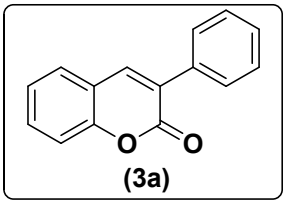

7.801
7.700
7.697
7.693
7.685
7.536
7.529
7.524
7.517
7.503
7.450
7.449
7.446
7.438
7.425
7.407
7.405
7.397
7.394
7.381
7.364
7.350
7.296
7.284
7.270
7.242


O
O

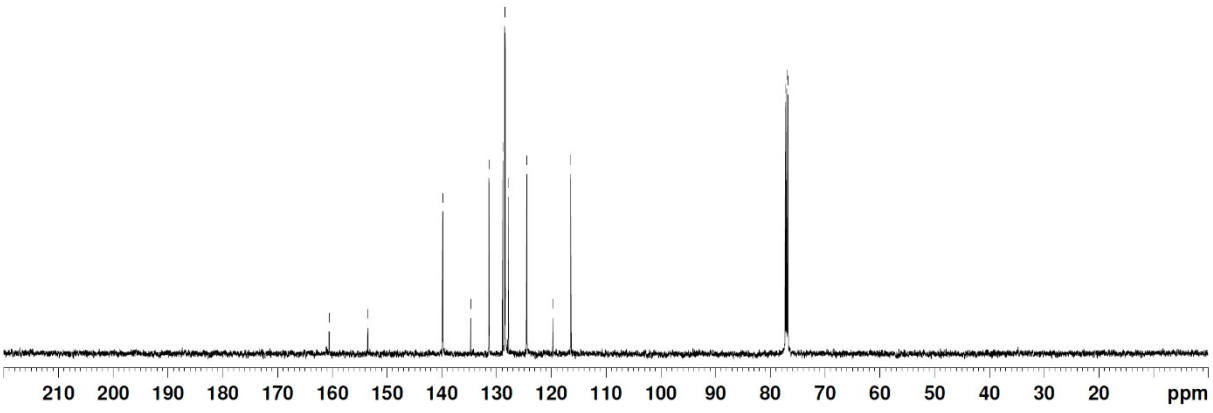
(3a)

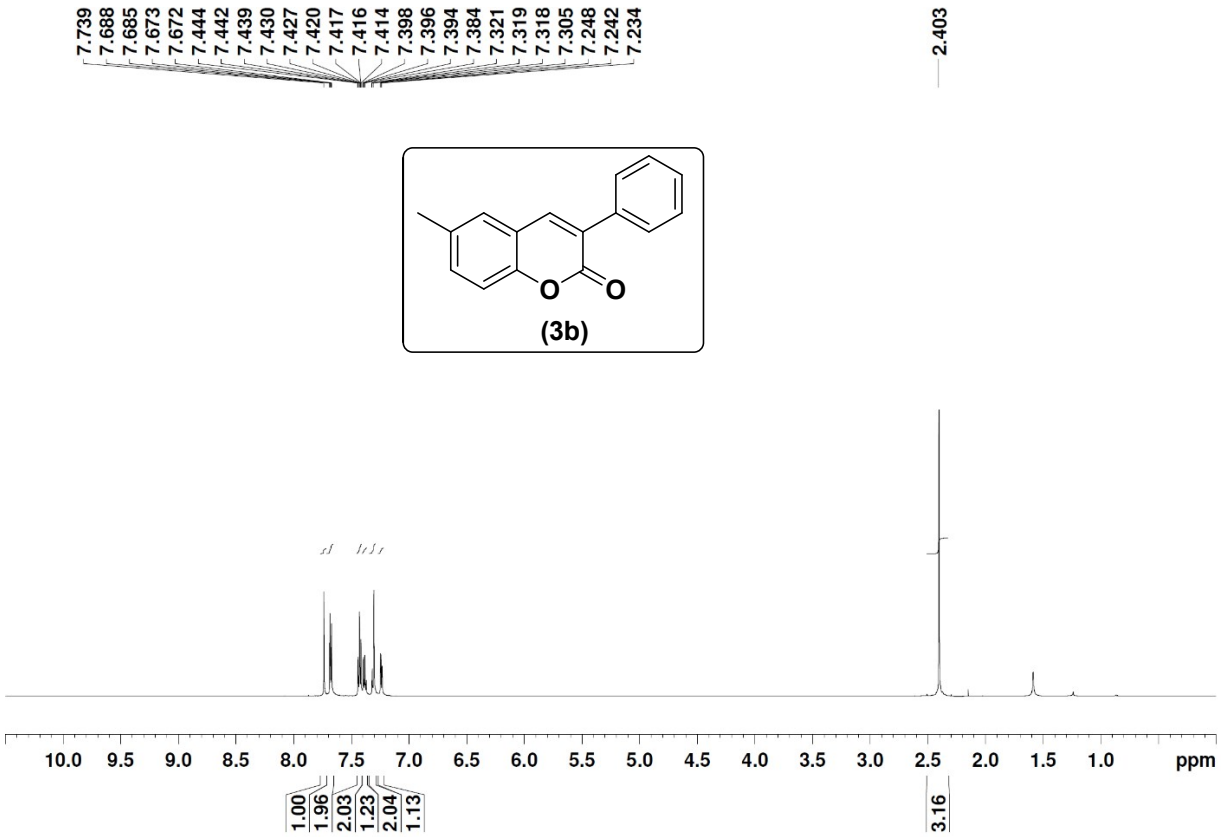

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.96
1.89
2.05
2.03
0.98
0.90
1.00

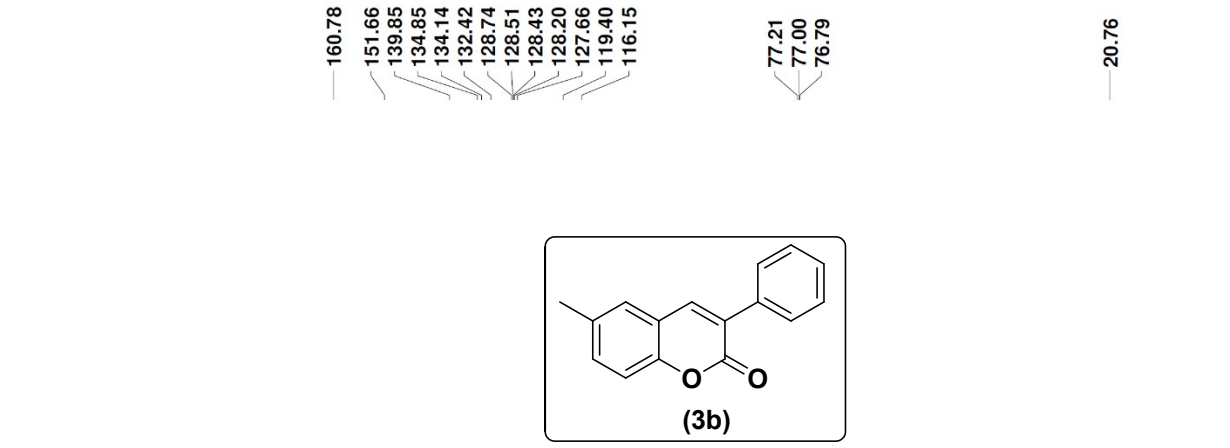

160.57
153.53
139.83
134.70
131.38
128.85
128.52
128.46
128.39
127.88
124.47
119.67
116.46
77.21
77.00
76.79

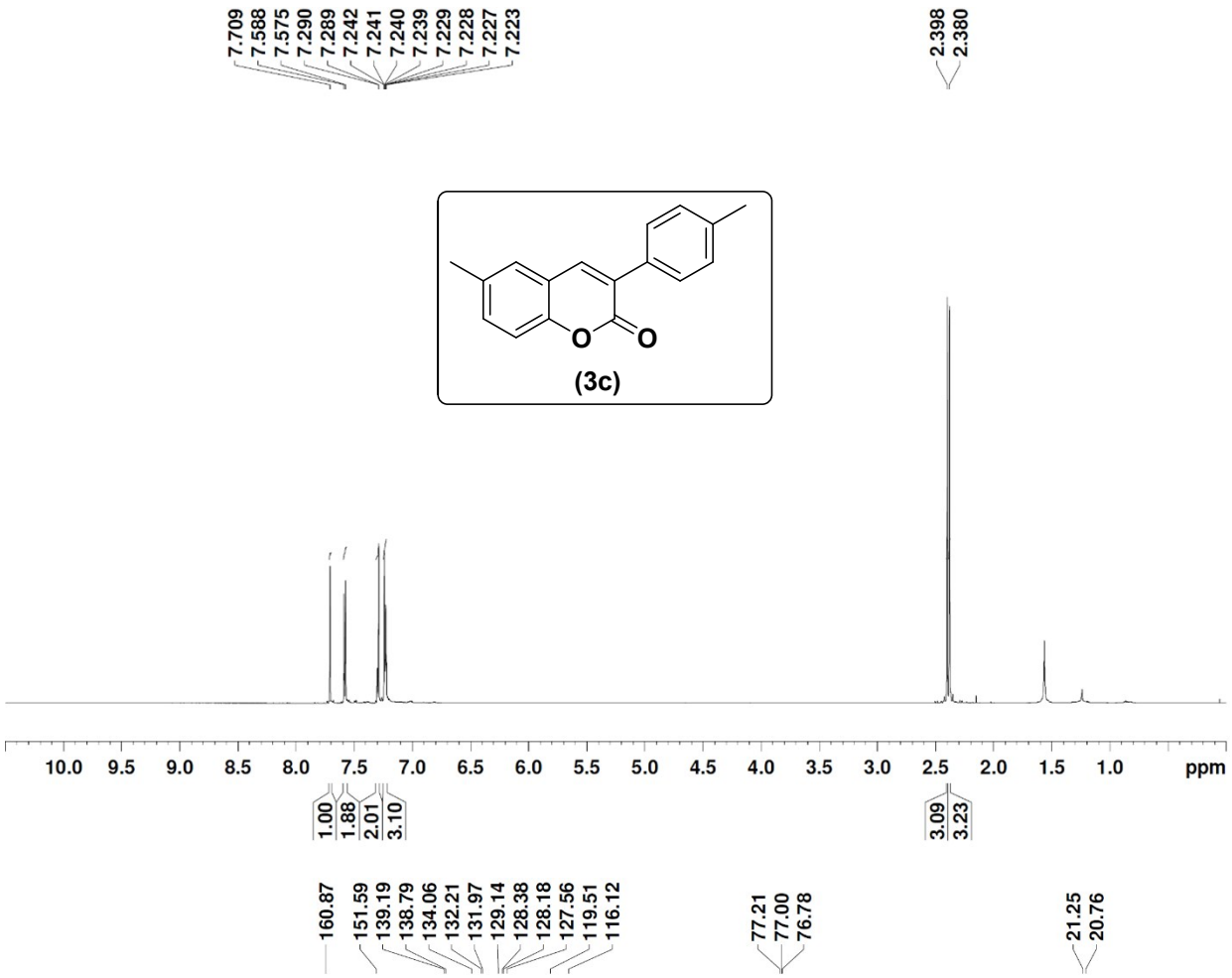

O
O

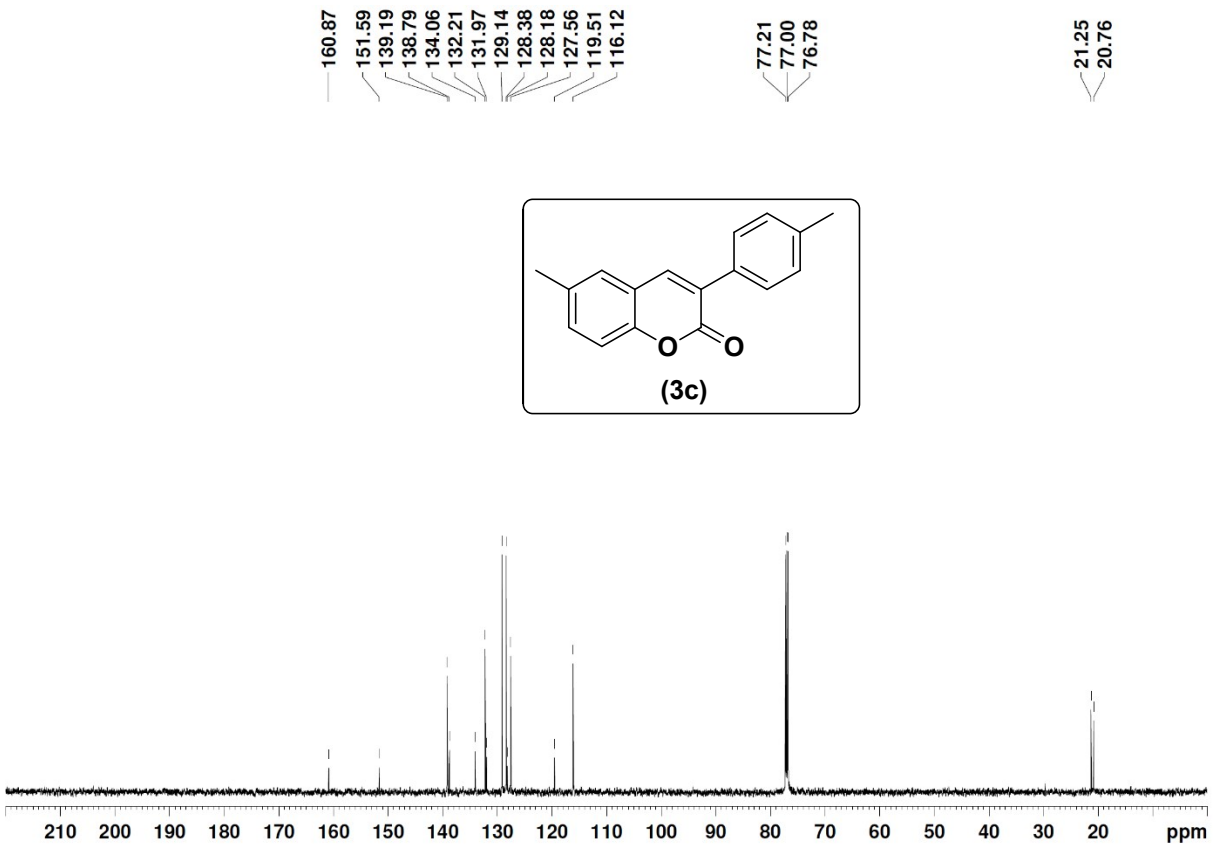
(3a)

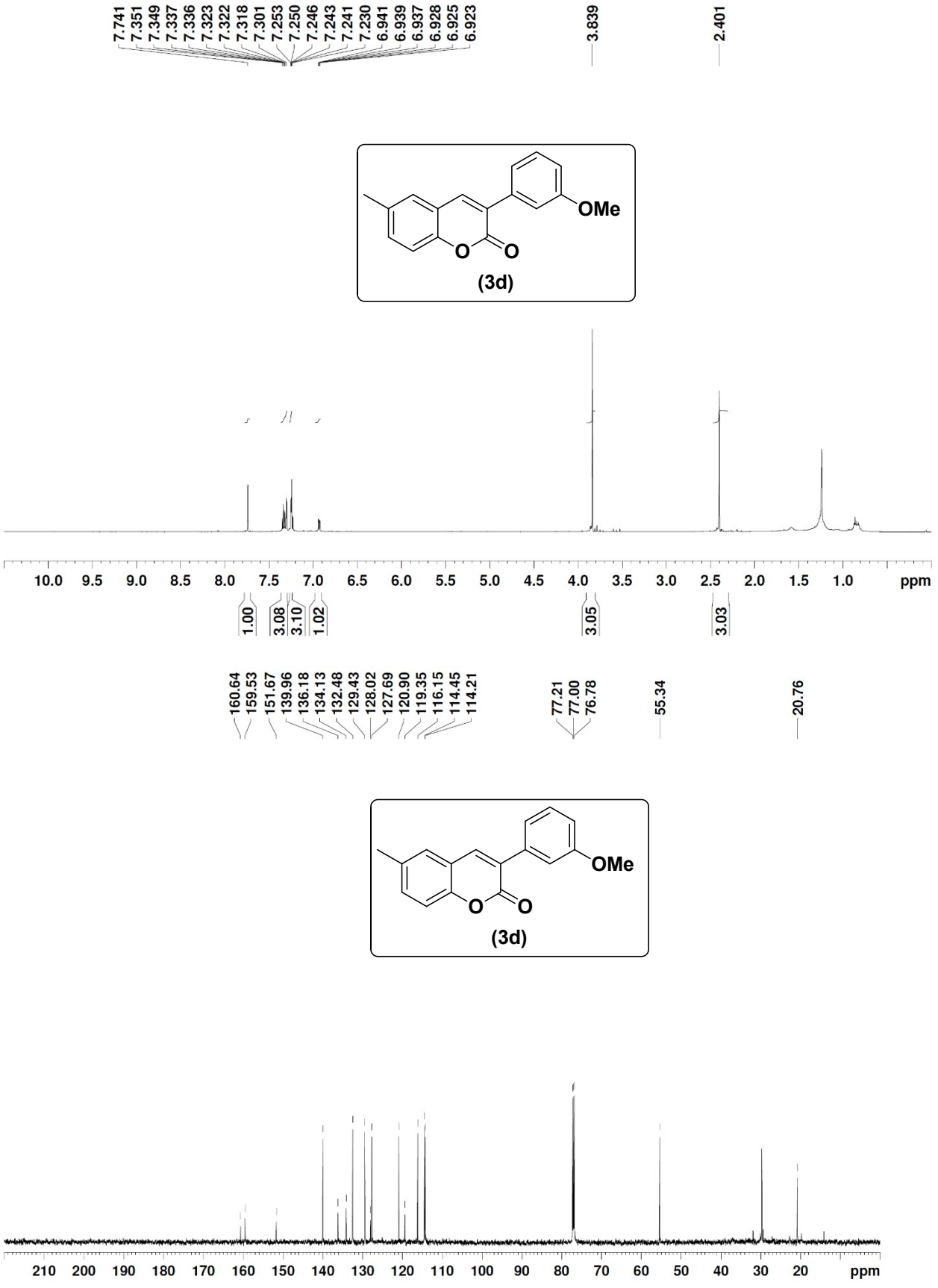

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

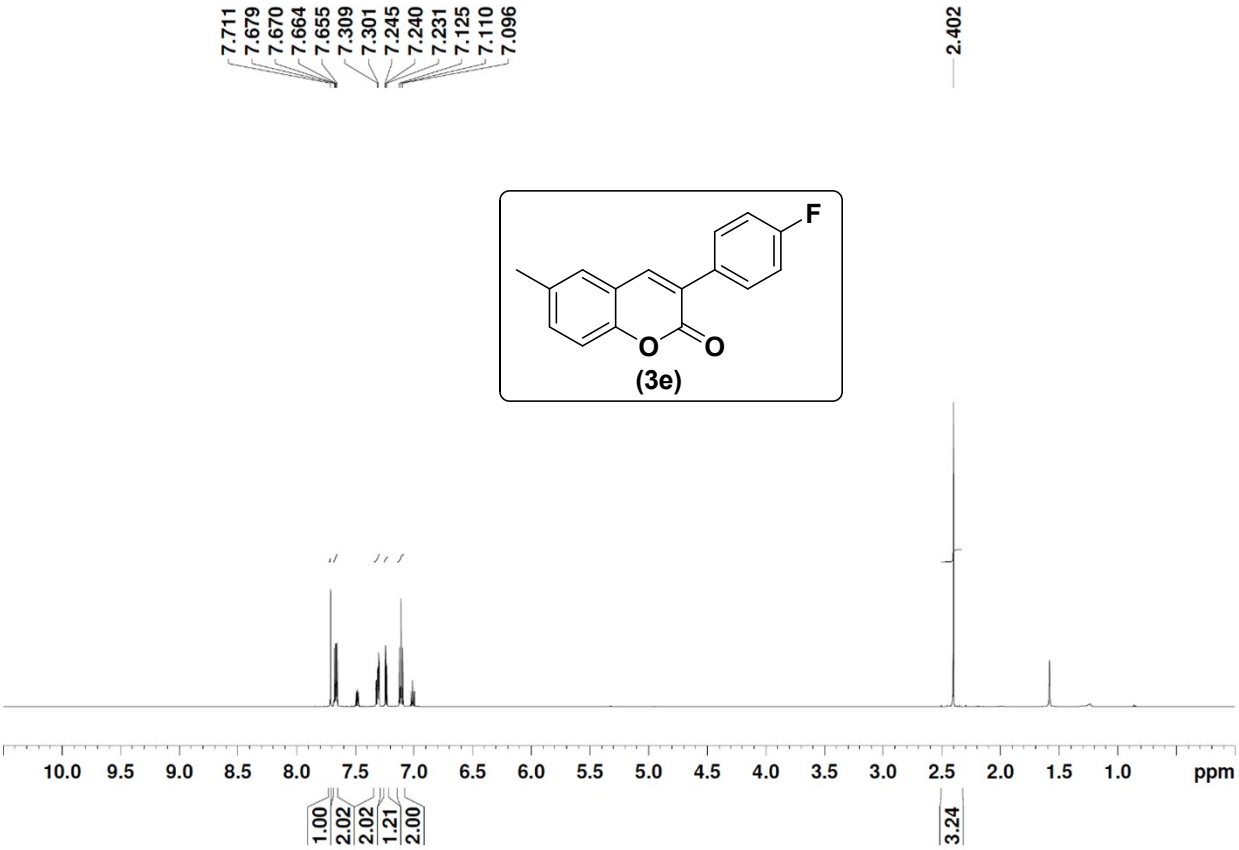

7.739
7.688
7.685
7.673
7.672
7.444
7.442
7.439
7.430
7.427
7.420
7.417
7.416
7.414
7.398
7.396
7.394
7.384
7.321
7.319
7.318
7.305
7.248
7.242
7.234
2.403
(3b)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.96
2.03
1.23
2.04
1.13
3.16

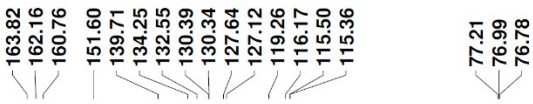

160.78
151.66
139.85
134.85
134.14
132.42
128.74
128.51
128.43
128.20
127.66
119.40
116.15
77.21
77.00
76.79
20.76
(3b)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

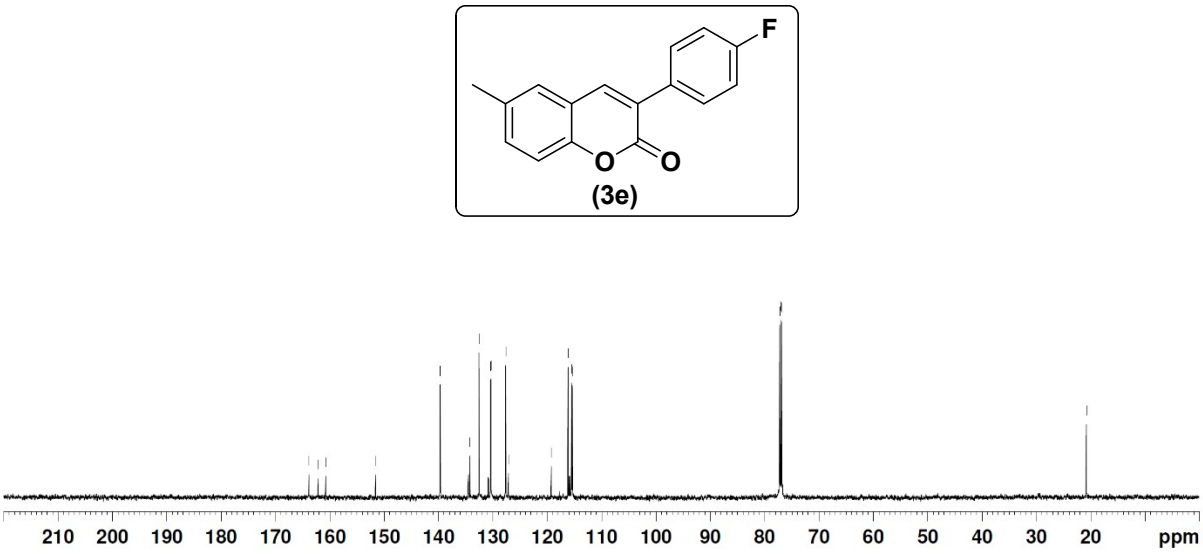

7.709
7.588
7.575
7.290
7.289
7.242
7.241
7.240
7.239
7.229
7.228
7.227
7.223
2.398
2.380
(3c)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.88
2.01
3.10
3.09
3.23

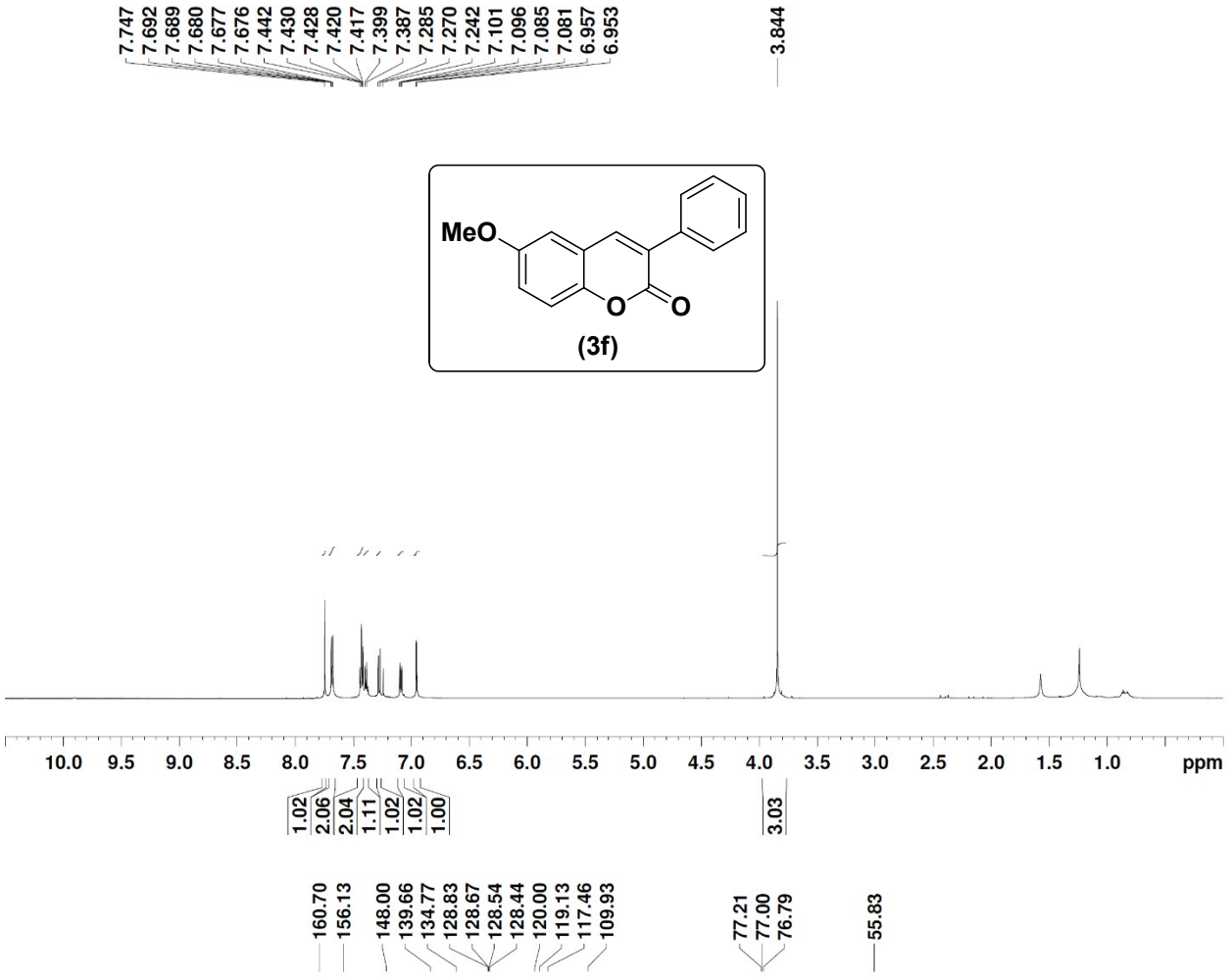

160.87
151.59
139.19
138.79
134.06
132.21
131.97
129.14
128.38
128.18
127.56
119.51
116.12
77.21
77.00
76.78
21.25
20.76
(3c)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

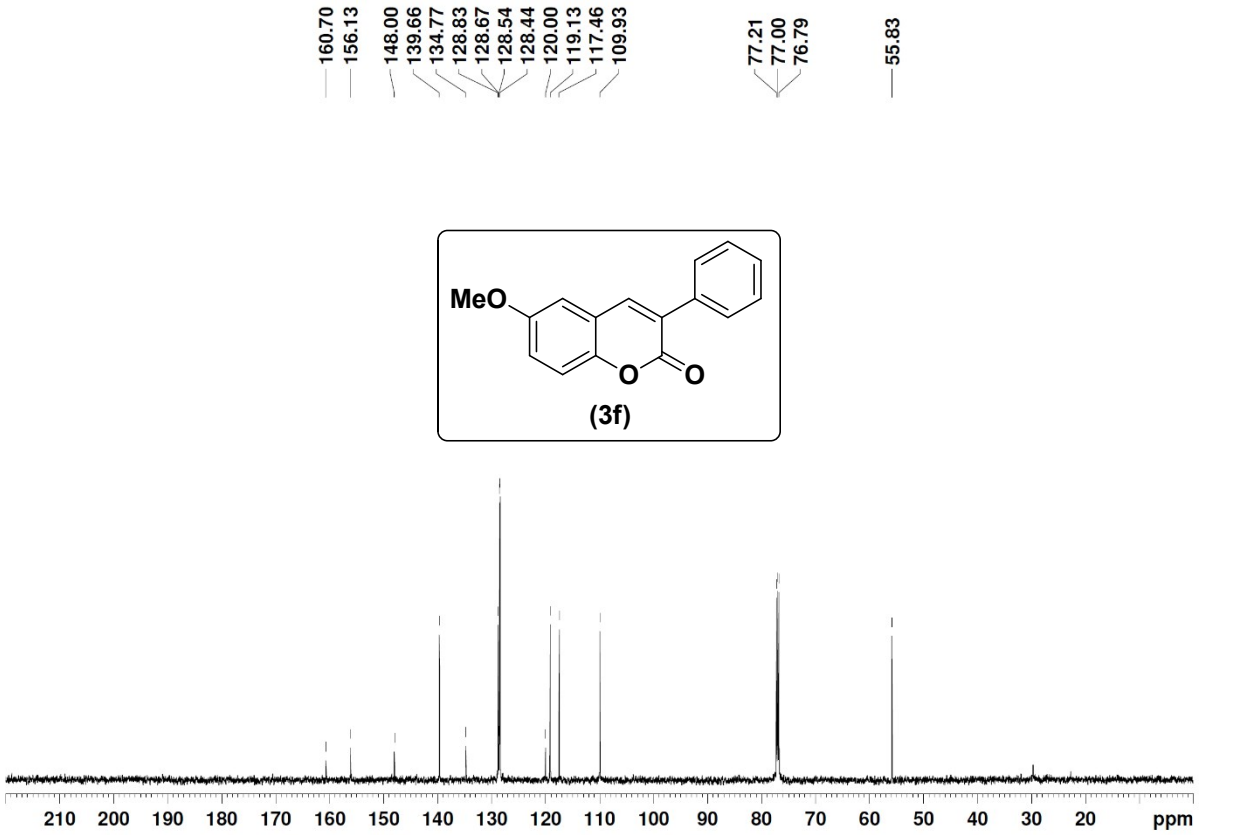

7.741
7.351
7.349
7.337
7.336
7.323
7.322
7.318
7.301
7.253
7.250
7.246
7.243
7.241
7.230
6.941
6.939
6.937
6.928
6.925
6.923
3.839
2.401
OMe
O
O
(3d)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
3.08
3.10
1.02
3.05
3.03
160.64
159.53
151.67
139.96
136.18
134.13
132.48
129.43
128.02
127.69
120.90
119.35
116.15
114.45
114.21
77.21
77.00
76.78
55.34
20.76
OMe
O
O
(3d)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

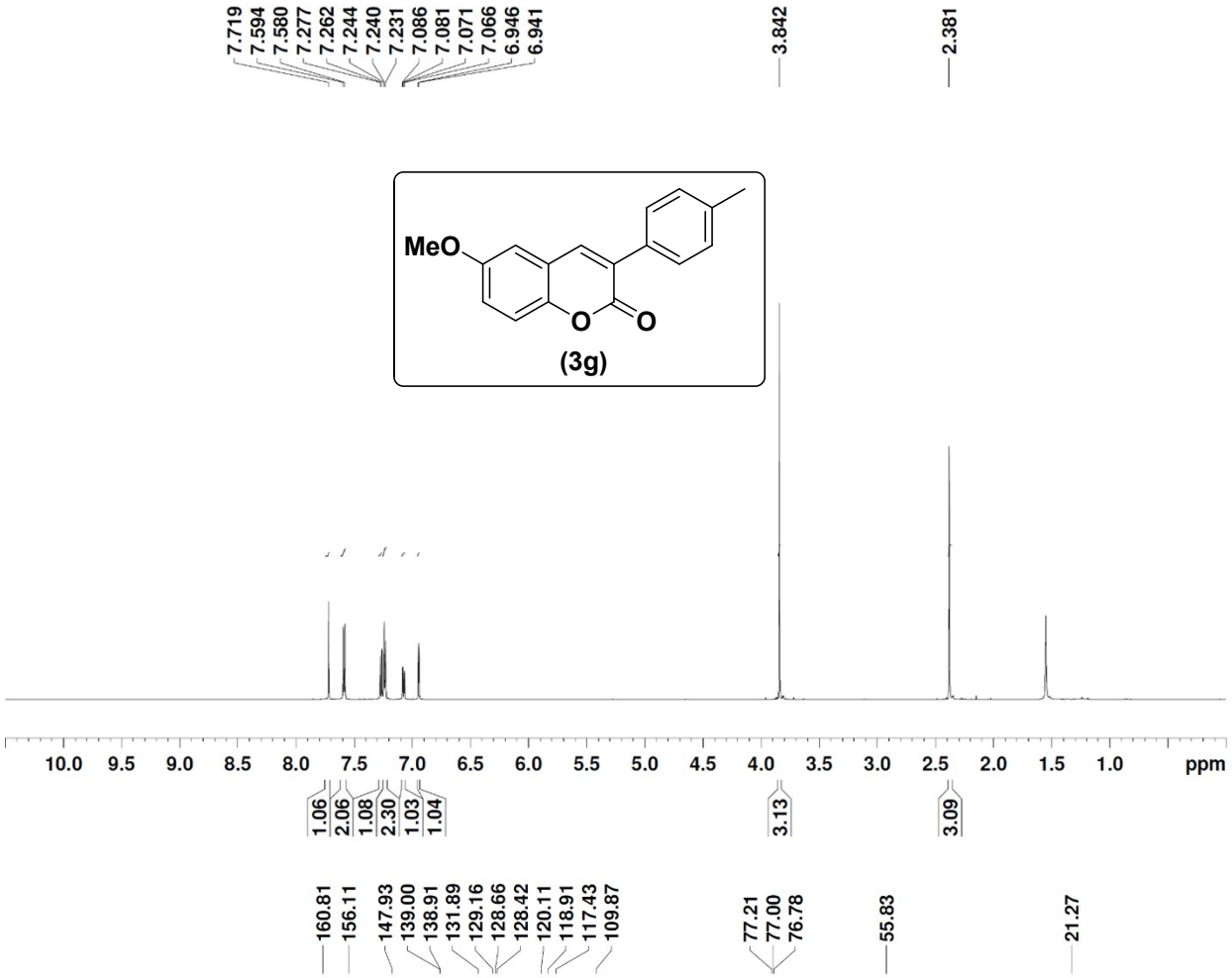

7.711
7.679
7.670
7.664
7.655
7.309
7.301
7.245
7.240
7.231
7.125
7.110
7.096
2.402
F
O
O
(3e)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.02
2.02
1.21
2.00
3.24

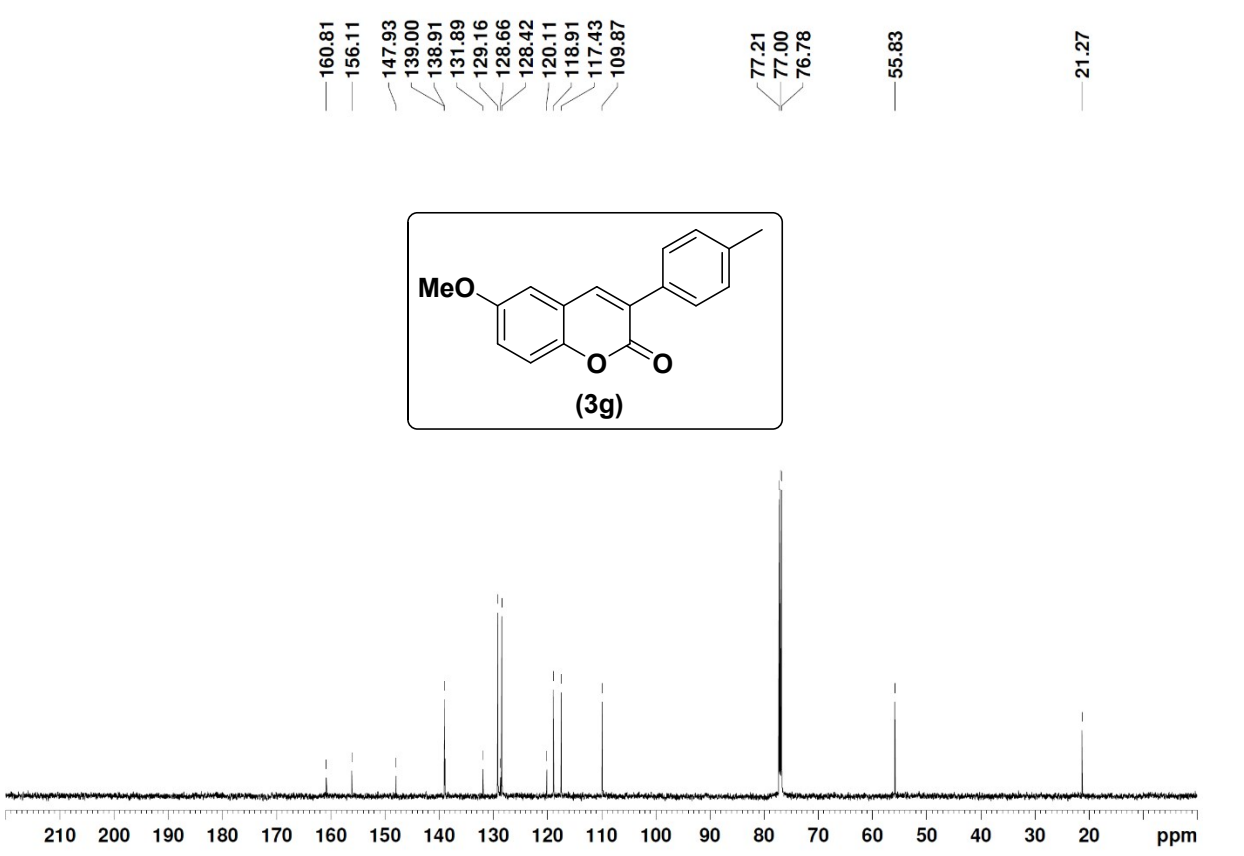

163.82
162.16
160.76
151.60
139.71
134.25
132.55
130.39
130.34
127.64
127.12
119.26
116.17
115.50
115.36
77.21
76.99
76.78
20.77

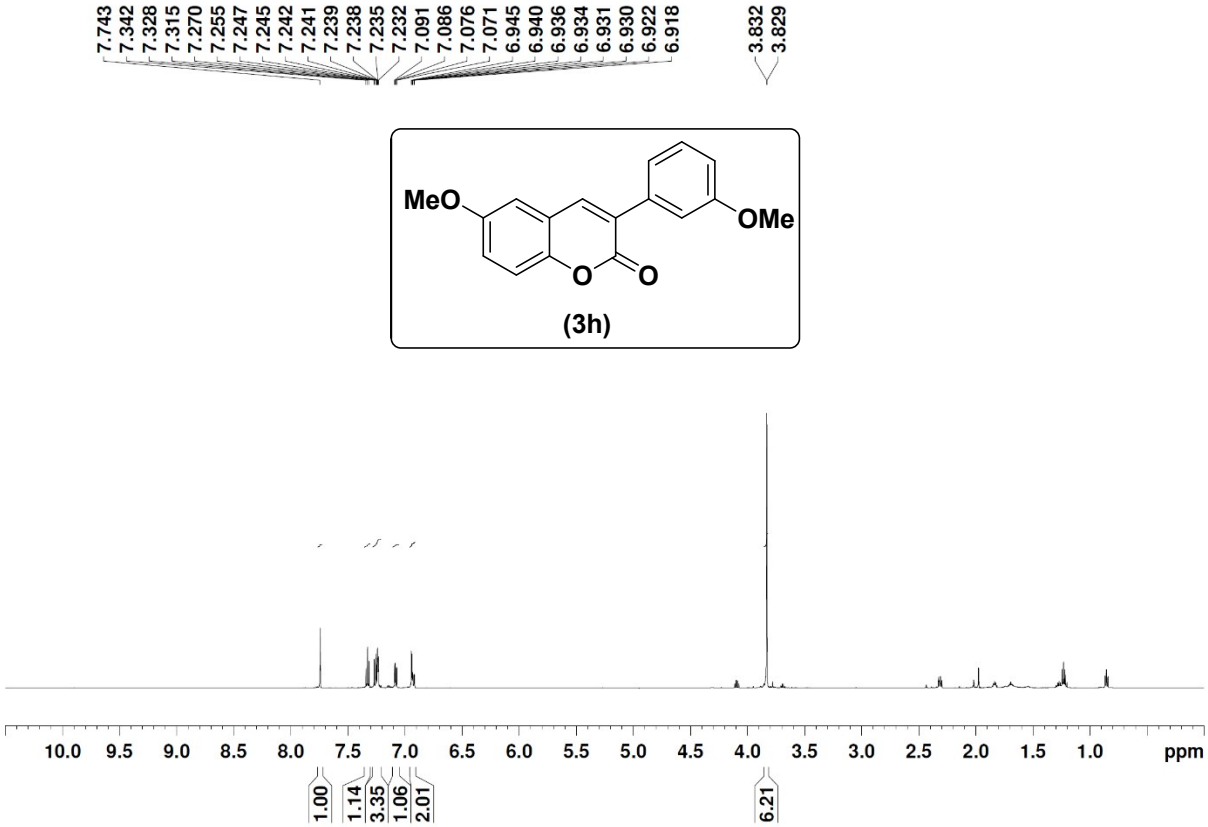

F
O
O
(3e)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

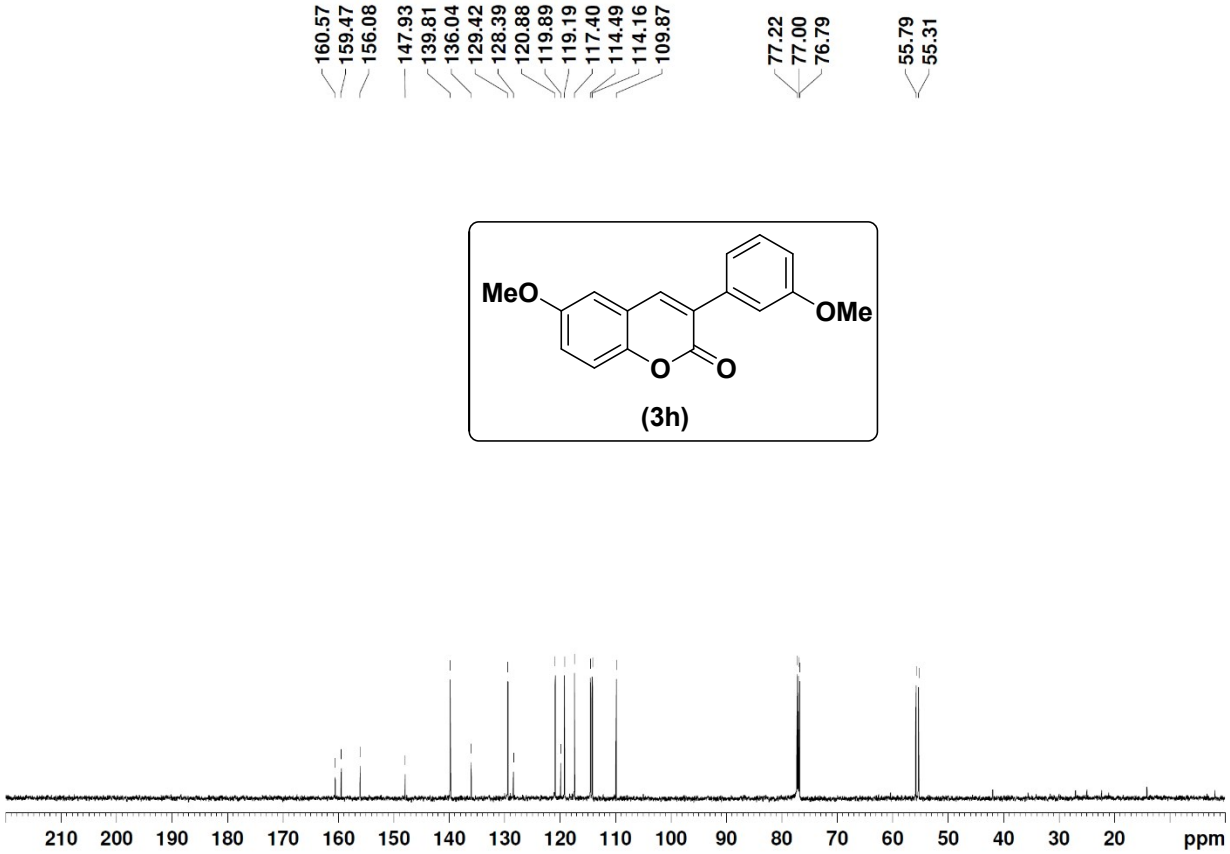

7.747
7.692
7.689
7.680
7.677
7.676
7.442
7.430
7.428
7.420
7.417
7.399
7.387
7.285
7.270
7.242
7.101
7.096
7.085
7.081
6.957
6.953
3.844
MeO
O
O
(3f)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.02
2.06
2.04
1.11
1.02
1.02
1.00
3.03

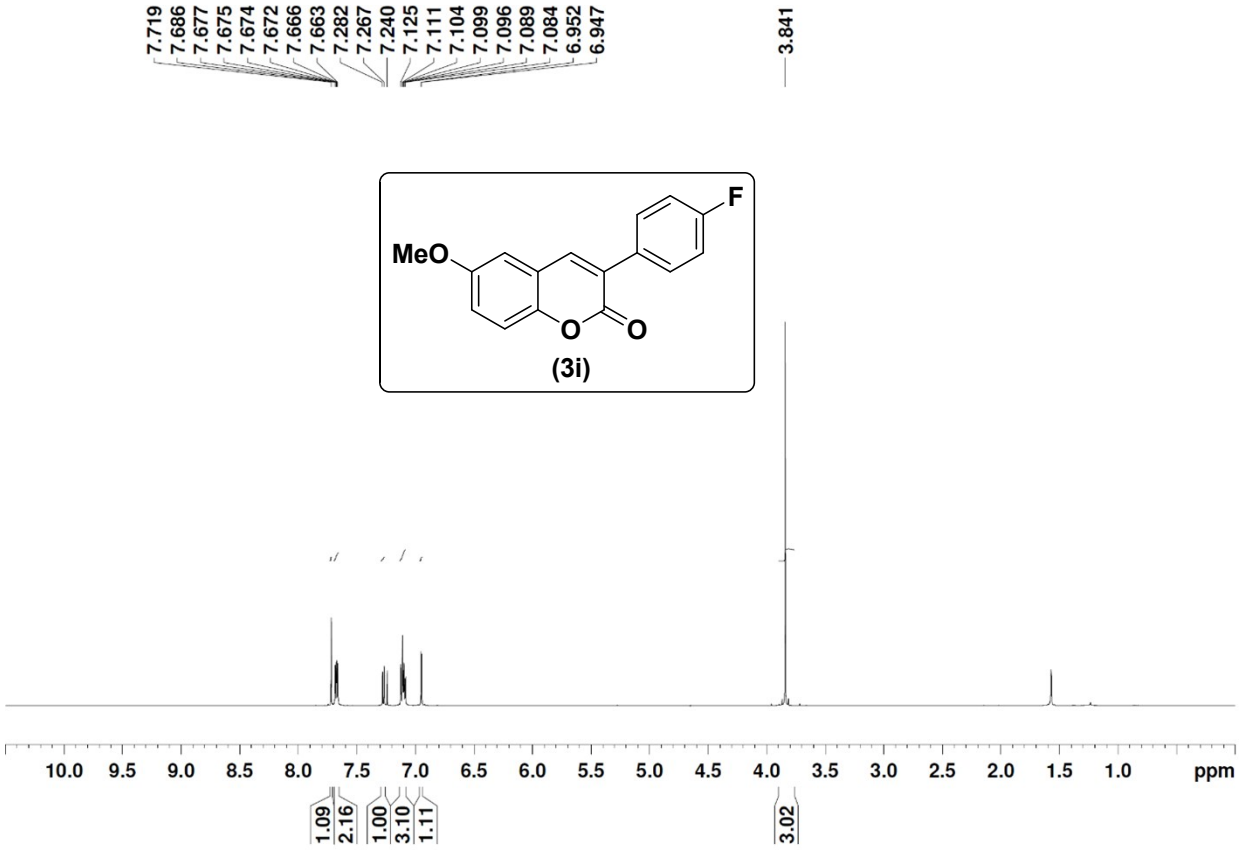

160.70
156.13
148.00
139.66
134.77
128.83
128.67
128.54
128.44
120.00
119.13
117.46
109.93
77.21
77.00
76.79
55.83
MeO
O
O
(3f)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

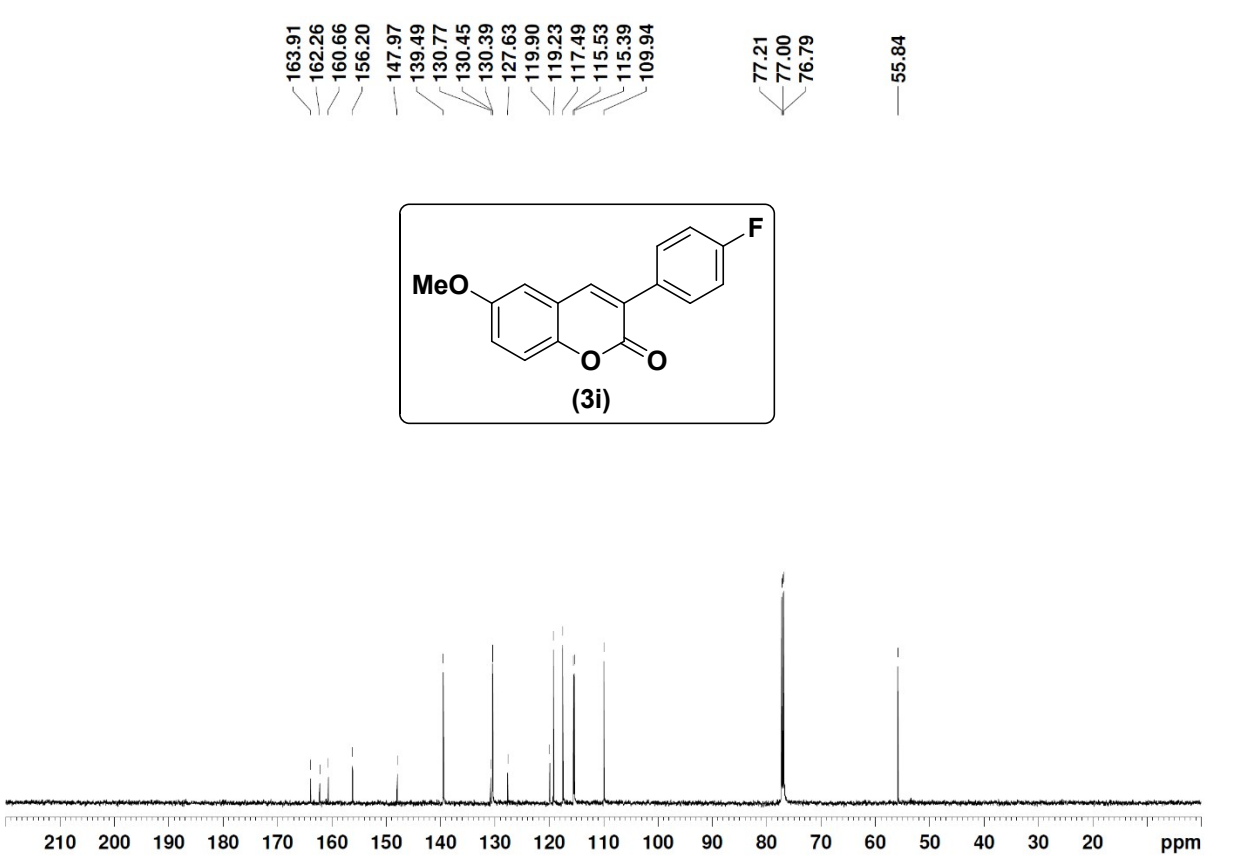

7.719
7.594
7.580
7.277
7.262
7.244
7.240
7.231
7.086
7.081
7.071
7.066
6.946
6.941
3.842
2.381
MeO
O
O
(3g)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.06
2.06
1.08
2.30
1.03
1.04
3.13
3.09


160.81
156.11
147.93
139.00
138.91
131.89
129.16
128.66
128.42
120.11
118.91
117.43
109.87
77.21
77.00
76.78
55.83
21.27
MeO
O
O
(3g)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.743
7.342
7.328
7.315
7.270
7.255
7.247
7.245
7.242
7.241
7.239
7.238
7.235
7.232
7.091
7.086
7.076
7.071
6.945
6.940
6.936
6.934
6.931
6.930
6.922
6.918
3.832
3.829
MeO
OMe
O
O
(3h)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.14
3.35
1.06
2.01
6.21


160.57
159.47
156.08
147.93
139.81
136.04
129.42
128.39
120.88
119.89
119.19
117.40
114.49
114.16
109.87
77.22
77.00
76.79
55.79
55.31
MeO
OMe
O
O
(3h)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.719
7.686
7.677
7.675
7.674
7.672
7.666
7.663
7.282
7.267
7.240
7.125
7.111
7.104
7.099
7.096
7.089
7.084
6.952
6.947
3.841
F
MeO
O
O
(3i)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.09
2.16
1.00
3.10
1.11
3.02


163.91
162.26
160.66
156.20
147.97
139.49
130.77
130.45
130.39
127.63
119.90
119.23
117.49
115.53
115.39
109.94
77.21
77.00
76.79
55.84
F
MeO
O
O
(3i)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.700
7.673
7.670
7.658
7.655
7.596
7.593
7.582
7.578
7.453
7.450
7.447
7.439
7.436
7.428
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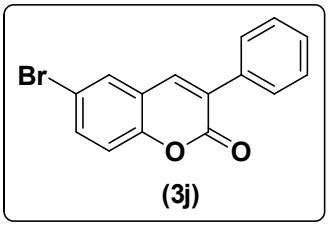
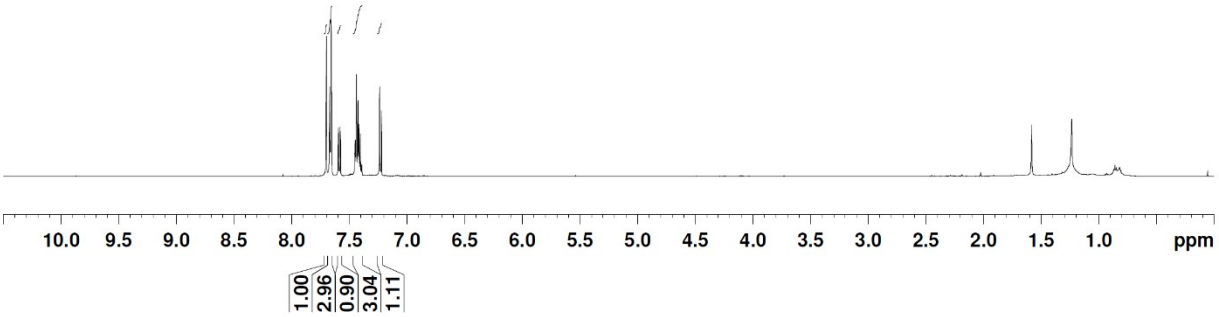
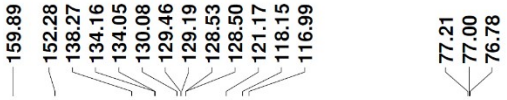
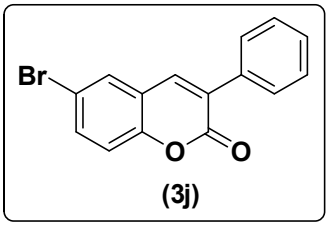
7.420
7.417
7.415
7.405
7.238
7.223


Br
O
O

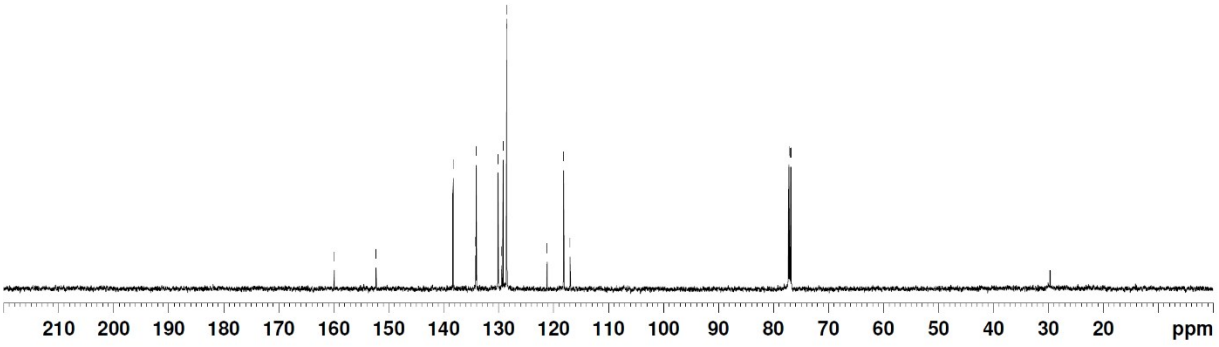
(3j)

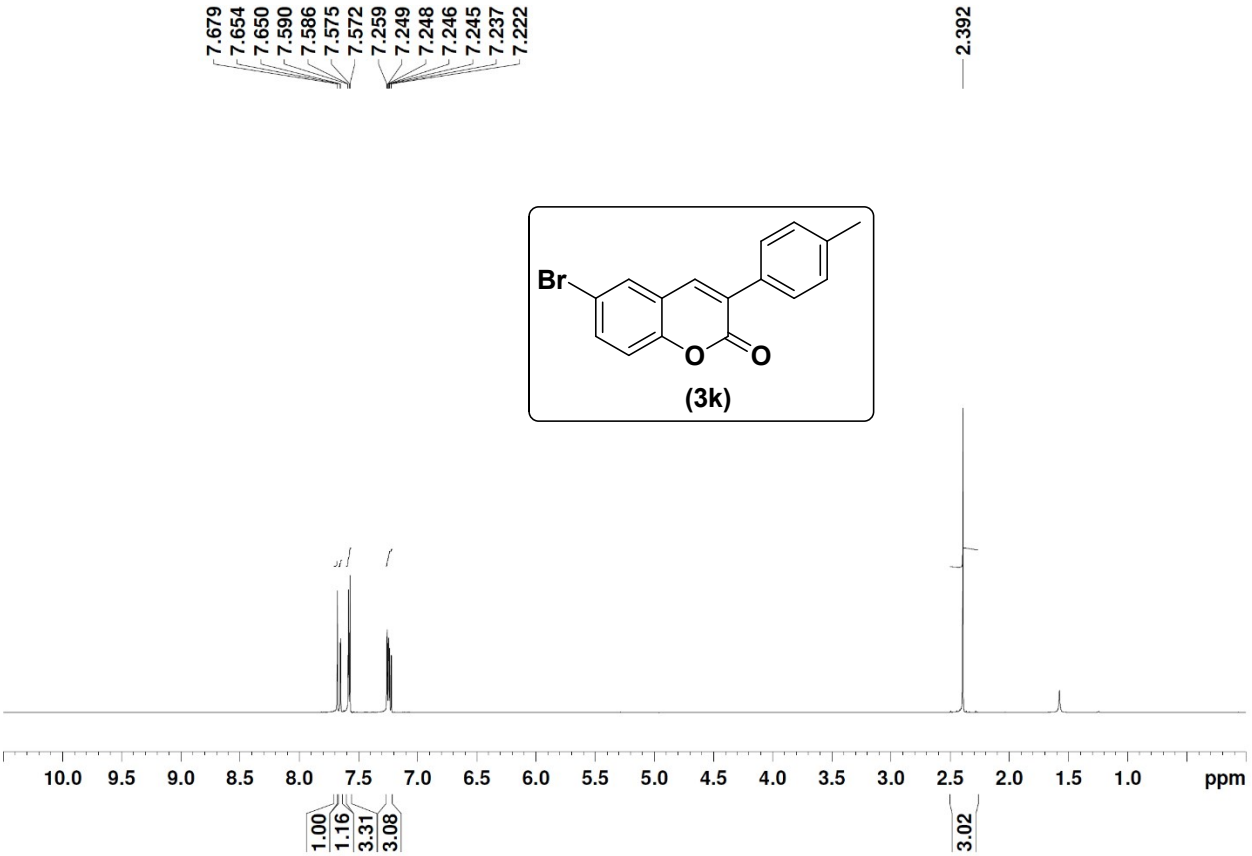

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.96
0.90
3.04
1.11

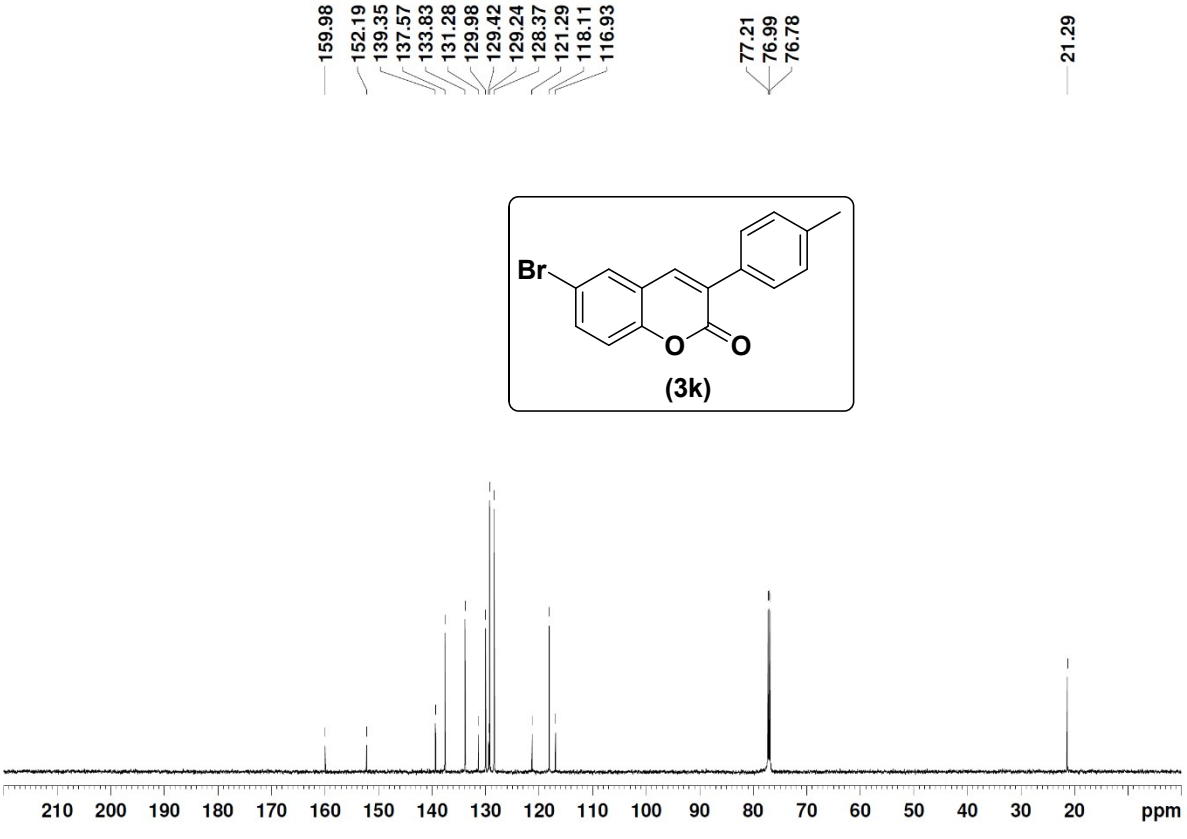

159.89
152.28
138.27
134.16
134.05
130.08
129.46
129.19
128.53
128.50
121.17
118.15
116.99
77.21
77.00
76.78

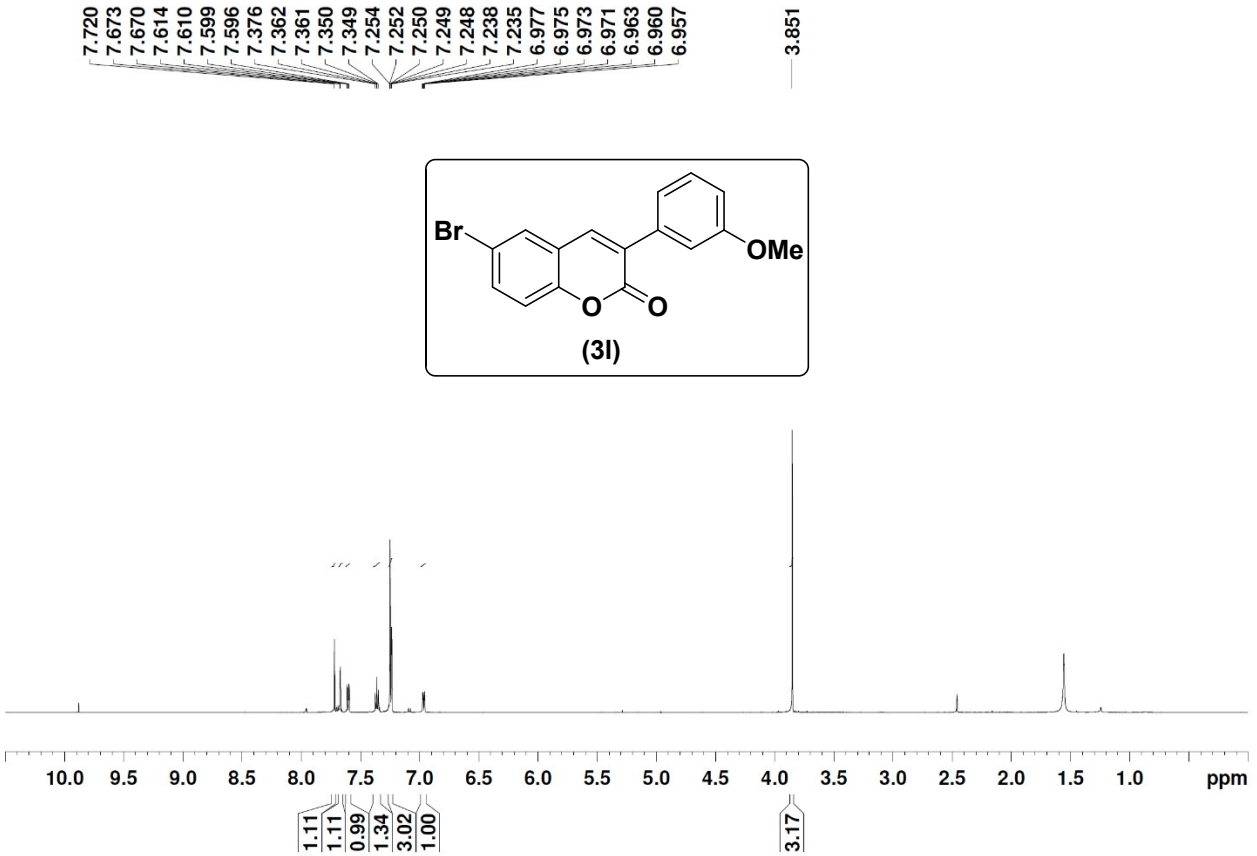

Br
O
O

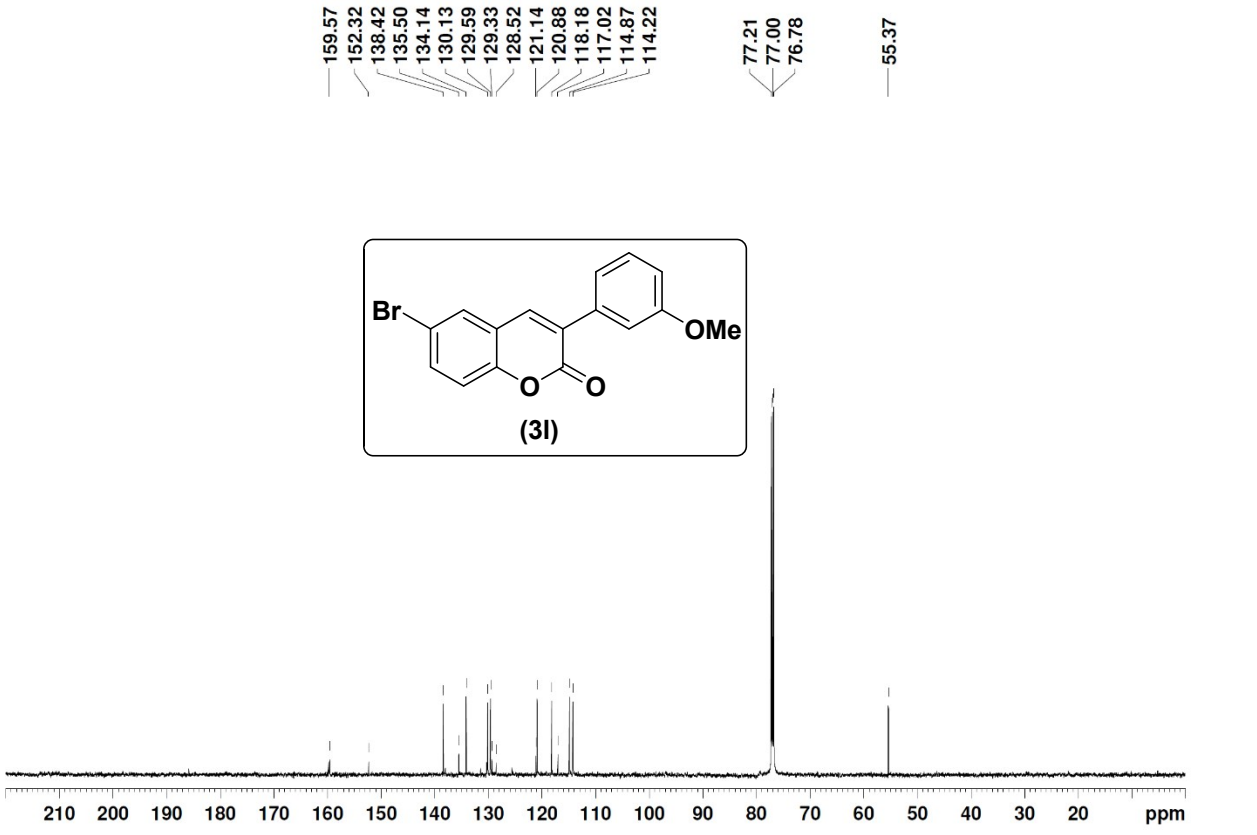
(3j)

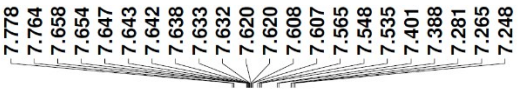

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

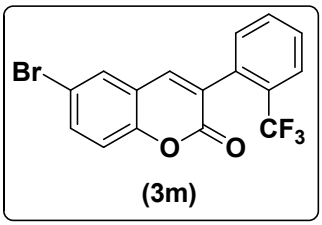

7.679
7.654
7.650
7.590
7.586
7.575
7.572
7.259
7.249
7.248
7.246
7.245
7.237
7.222
2.392
Br
O
O
(3k)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.16
3.31
3.08
3.02


159.98
152.19
139.35
137.57
133.83
131.28
129.98
129.42
129.24
128.37
121.29
118.11
116.93
77.21
76.99
76.78
21.29
Br
O
O
(3k)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

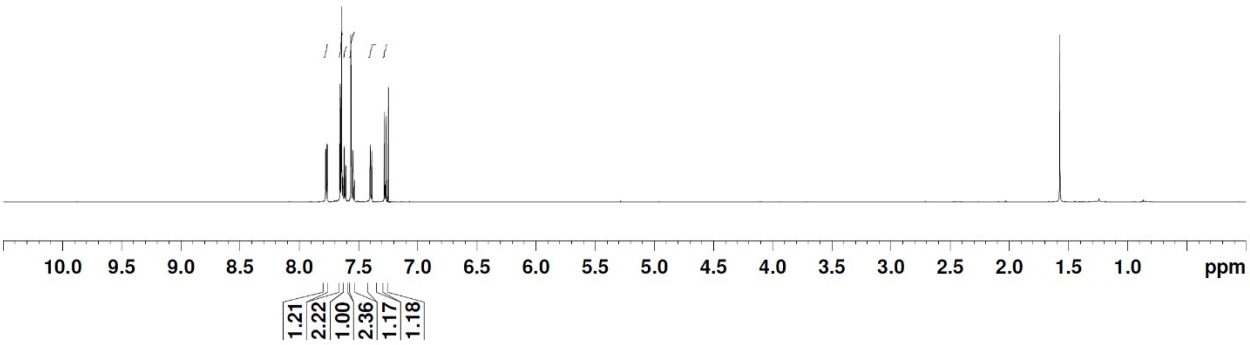

7.720
7.673
7.670
7.614
7.610
7.599
7.596
7.376
7.362
7.361
7.350
7.349
7.254
7.252
7.250
7.249
7.248
7.238
7.235
6.977
6.975
6.973
6.971
6.963
6.960
6.957
3.851
Br
OMe
O
O
(3l)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.11
1.11
0.99
1.34
3.02
1.00
3.17

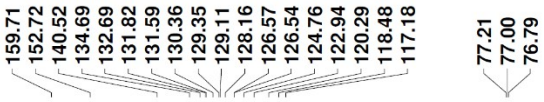

159.57
152.32
138.42
135.50
134.14
130.13
129.59
129.33
128.52
121.14
120.88
118.18
117.02
114.87
114.22
77.21
77.00
76.78
55.37
Br
OMe
O
O
(3l)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

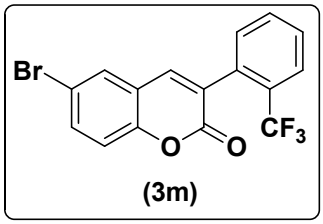

7.778
7.764
7.658
7.654
7.647
7.643
7.642
7.638
7.633
7.632
7.620
7.620
7.608
7.607
7.565
7.548
7.535
7.401
7.388
7.281
7.265
7.248


Br
O
O
CF3

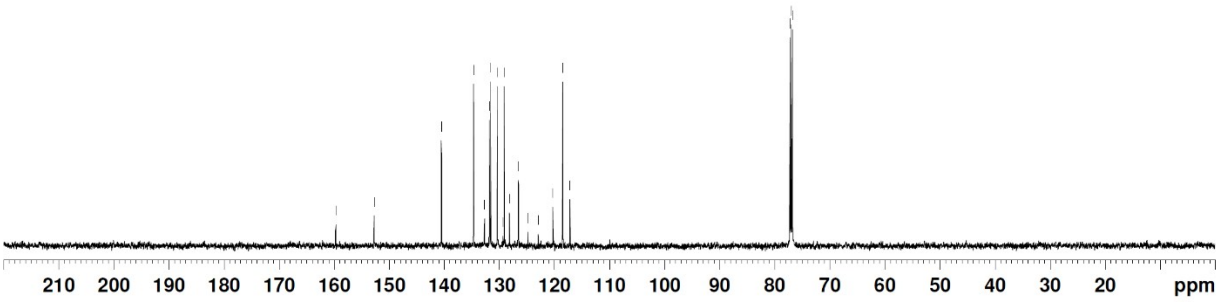
(3m)

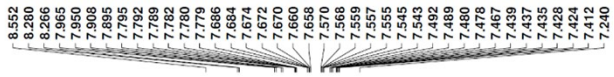

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
ppm
1.21
2.22
1.00
2.36
1.17
1.18

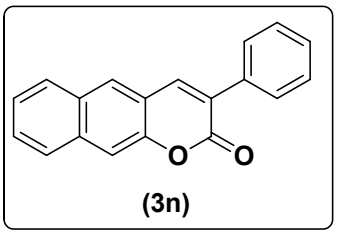

159.71
152.72
140.52
134.69
132.69
131.82
131.59
130.36
129.35
129.11
128.16
126.57
126.54
124.76
122.94
120.29
118.48
117.18
77.21
77.00
76.79


Br
O
O
CF3

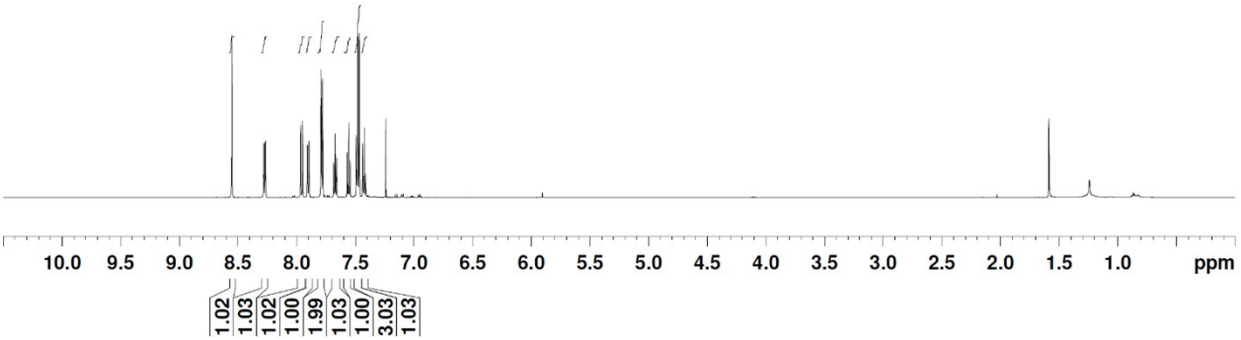
(3m)

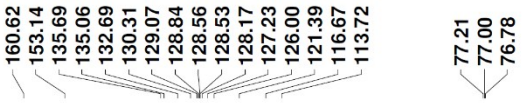

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
ppm

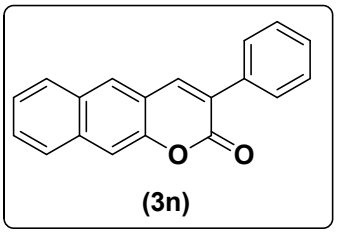

8.552
8.280
8.266
7.965
7.950
7.908
7.895
7.795
7.792
7.789
7.782
7.780
7.779
7.686
7.684
7.674
7.672
7.670
7.660
7.658
7.570
7.568
7.559
7.557
7.555
7.545
7.543
7.492
7.489
7.480
7.478
7.467
7.439
7.437
7.435
7.428
7.424
7.412
7.240


O
O

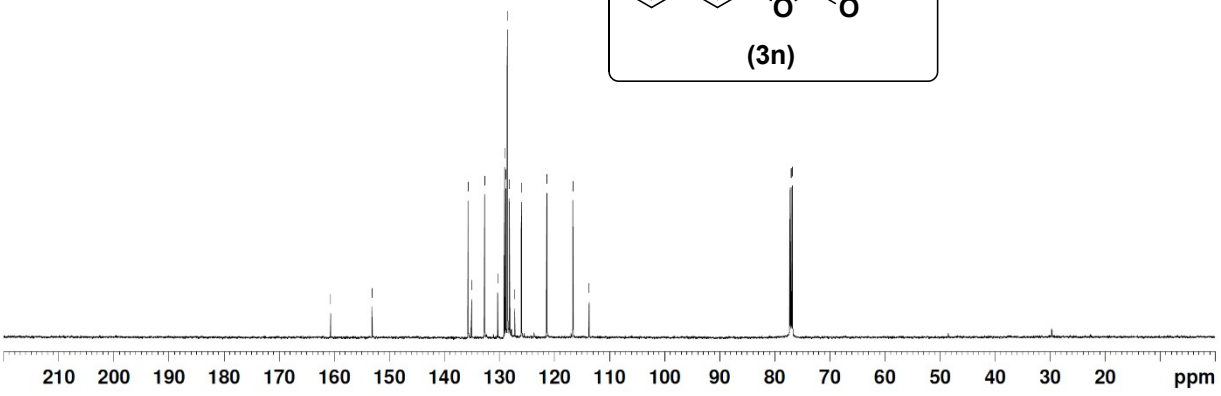
(3n)


10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.02
1.03
1.02
1.00
1.99
1.03
1.00
3.03
1.03

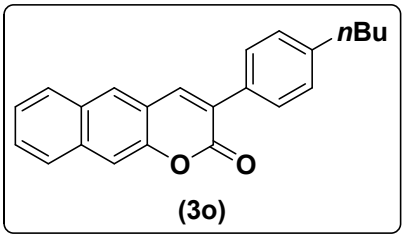

160.62
153.14
135.69
135.06
132.69
130.31
129.07
128.84
128.56
128.53
128.17
127.23
126.00
121.39
116.67
113.72
77.21
77.00
76.78

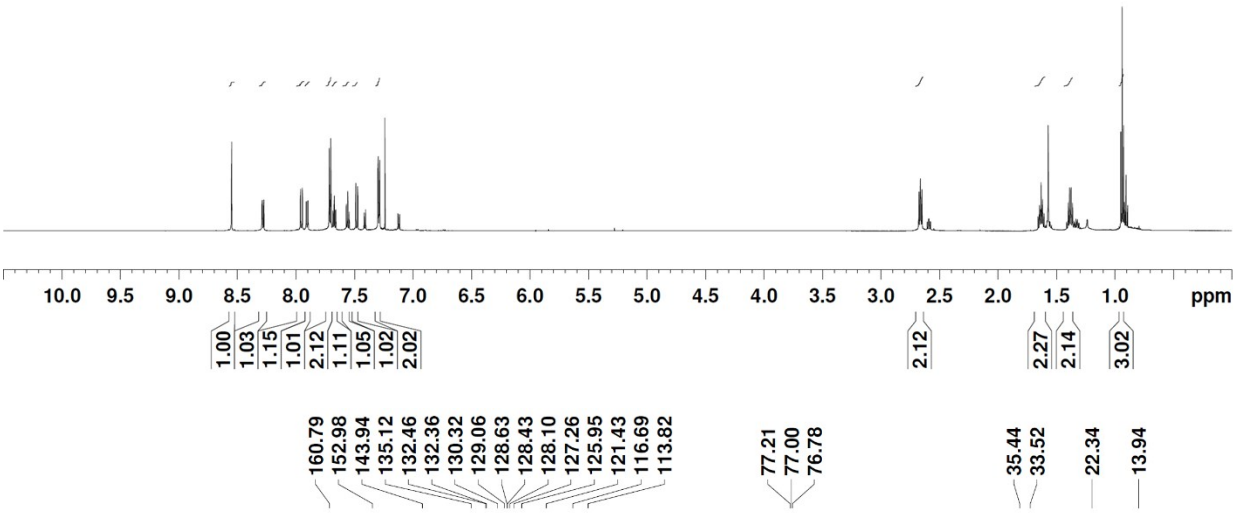

O
O

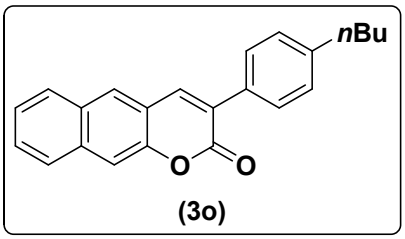
(3n)

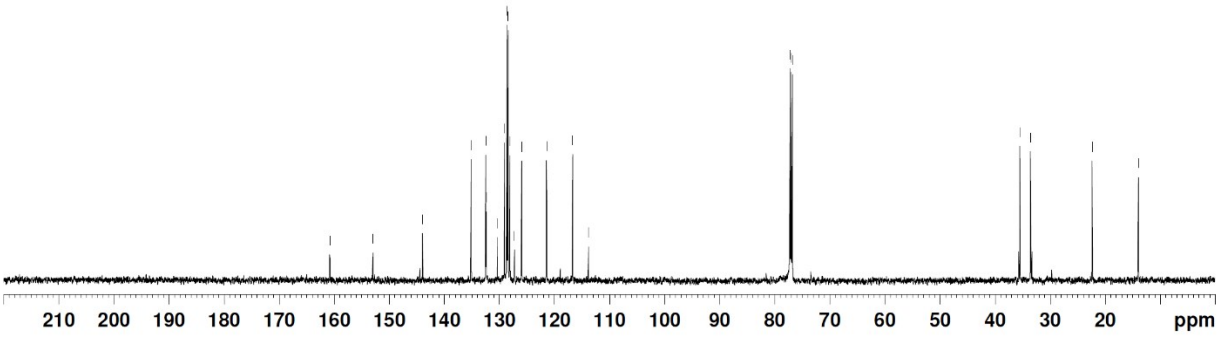

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

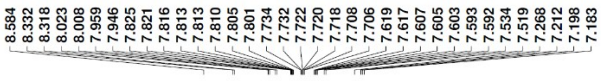

8.550
8.290
8.275
7.961
7.946
7.912
7.911
7.898
7.898
7.720
7.716
7.713
7.705
7.702
7.699
7.686
7.684
7.675
7.672
7.670
7.661
7.659
7.571
7.569
7.559
7.558
7.556
7.546
7.544
7.489
7.474
7.299
7.285
7.240
2.676
2.664
2.651
1.657
1.647
1.645
1.642
1.635
1.632
1.628
1.621
1.619
1.606
1.401
1.388
1.375
1.363
0.951
0.939
0.926

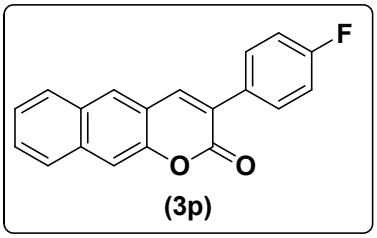

nBu
O
O
(3o)

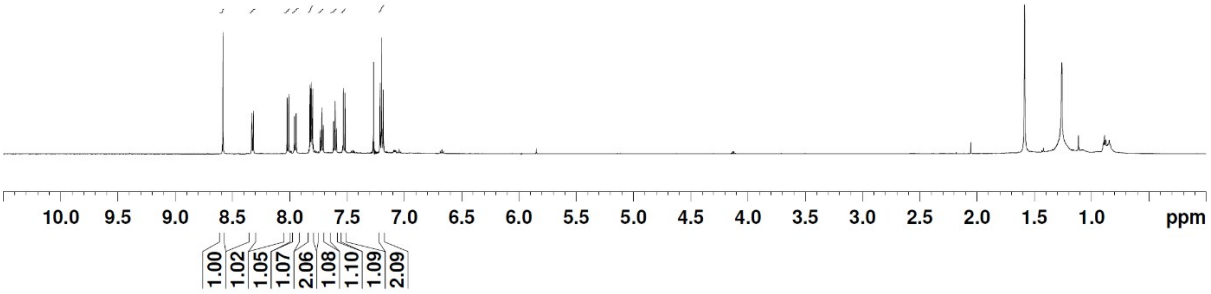

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.03
1.15
1.01
2.12
1.11
1.05
1.02
2.02
2.12
2.27
2.14
3.02
160.79
152.98
143.94
135.12
132.46
132.36
130.32
129.06
128.63
128.43
128.10
127.26
125.95
121.43
116.69
113.82
77.21
77.00
76.78
35.44
33.52
22.34
13.94

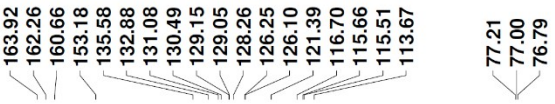

nBu
O
O
(3o)

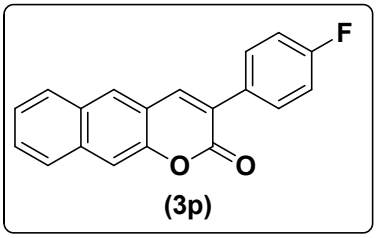

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.584
8.332
8.318
8.023
8.008
7.959
7.946
7.825
7.821
7.816
7.813
7.813
7.810
7.805
7.801
7.734
7.732
7.722
7.720
7.718
7.708
7.706
7.619
7.617
7.607
7.605
7.603
7.593
7.592
7.534
7.519
7.268
7.212
7.198
7.183


F
O
O
(3p)

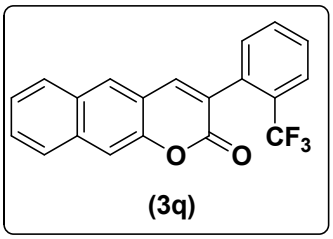

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.02
1.05
1.07
2.06
1.08
1.10
1.09
2.09


163.92
162.26
160.66
153.18
135.58
132.88
131.08
130.49
129.15
129.05
128.26
126.25
126.10
121.39
116.70
115.66
115.51
113.67
77.21
77.00
76.79

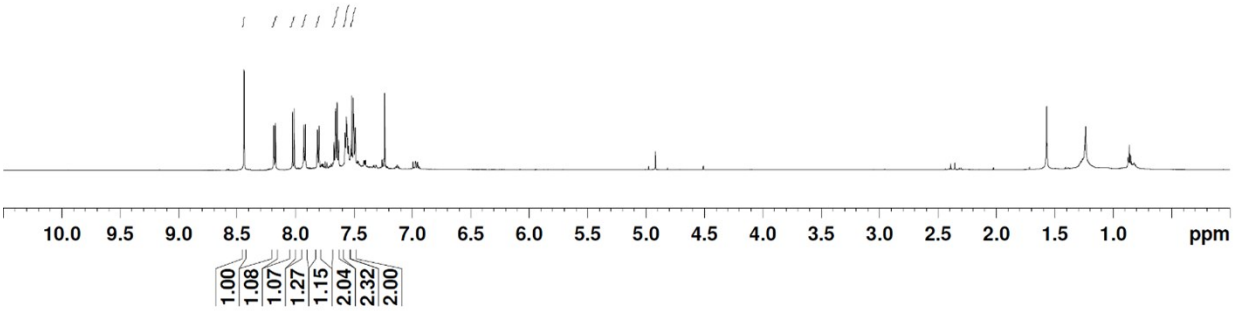

F
O
O
(3p)

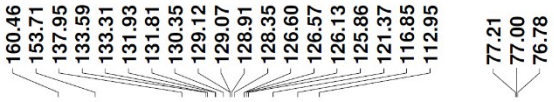
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

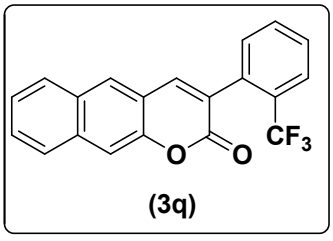

8.441
8.186
8.172
8.026
8.011
7.929
7.916
7.812
7.799
7.657
7.644
7.578
7.577
7.572
7.565
7.559
7.553
7.522
7.507
7.502
7.490
7.237


O
O
CF3

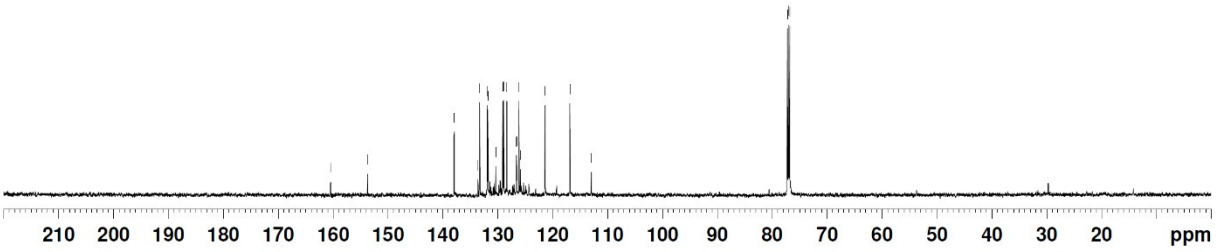
(3q)

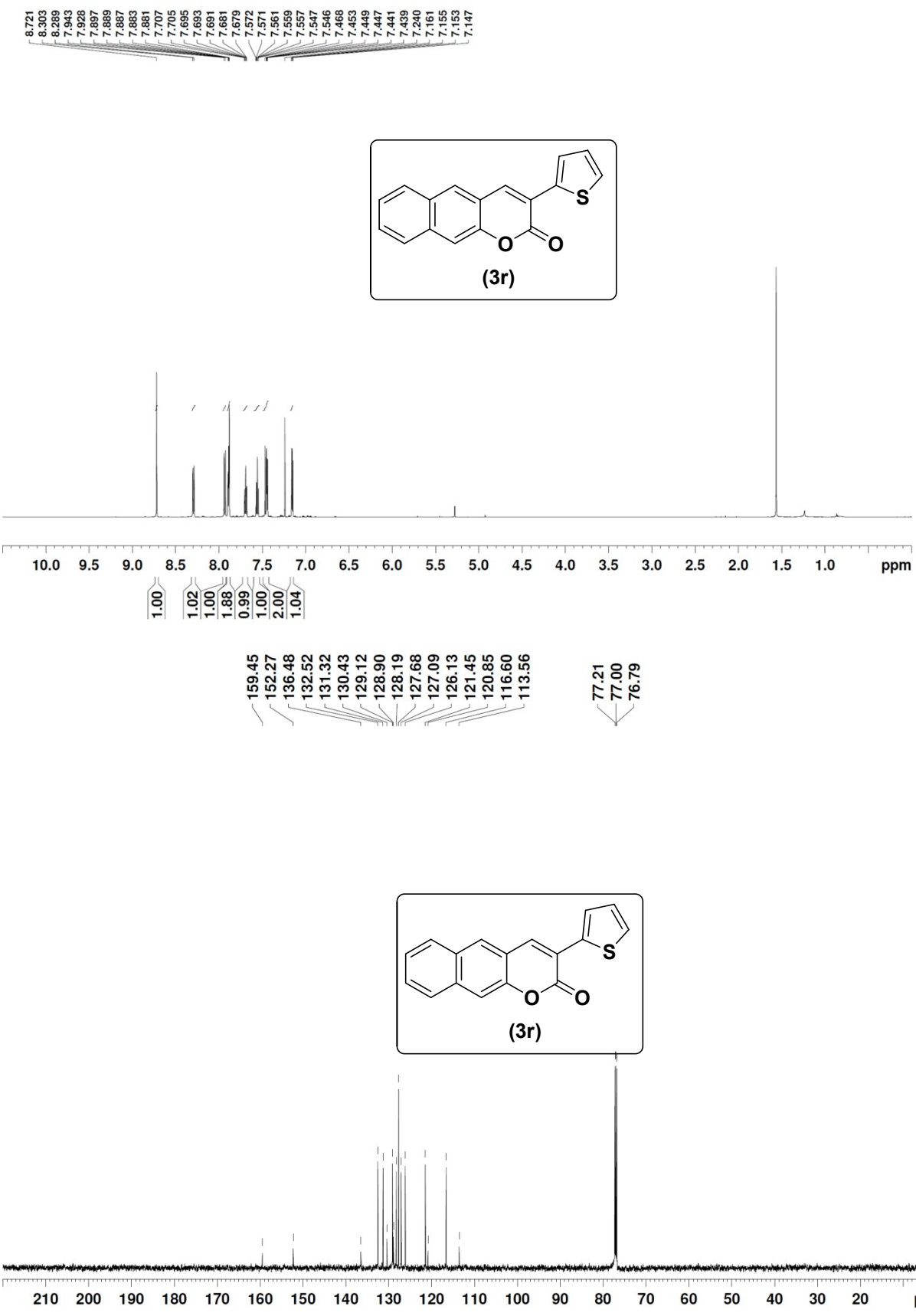

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.08
1.07
1.27
1.15
2.04
2.32
2.00

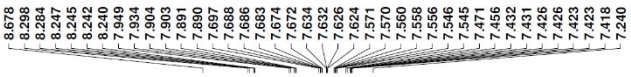

160.46
153.71
137.95
133.59
133.31
131.93
131.81
130.35
129.12
129.07
128.91
128.35
126.60
126.57
126.13
125.86
121.37
116.85
112.95
77.21
77.00
76.78

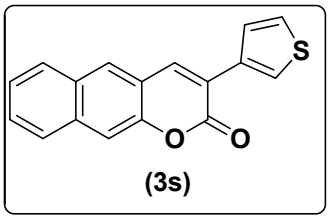

O
O
CF3

(3q)

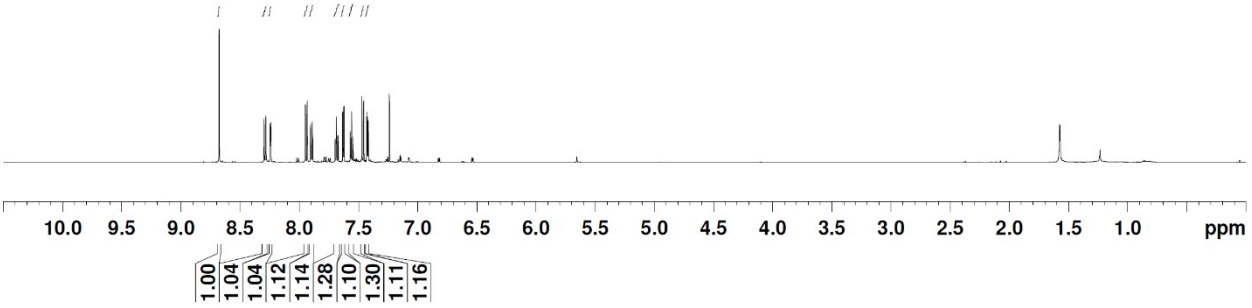

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

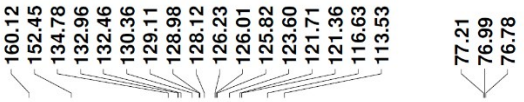

8.721
8.303
8.289
7.943
7.928
7.897
7.889
7.887
7.883
7.881
7.707
7.705
7.695
7.693
7.691
7.681
7.679
7.572
7.571
7.561
7.559
7.557
7.547
7.546
7.468
7.453
7.449
7.447
7.441
7.439
7.240
7.161
7.155
7.153
7.147
S
O
O
(3r)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.02
1.00
1.88
0.99
1.00
2.00
1.04
159.45
152.27
136.48
132.52
131.32
130.43
129.12
128.90
128.19
127.68
127.09
126.13
121.45
120.85
116.60
113.56
77.21
77.00
76.79
S
O
O
(3r)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

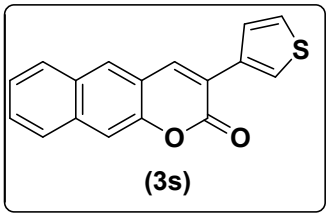

8.678
8.298
8.284
8.247
8.245
8.242
8.240
7.949
7.934
7.904
7.903
7.891
7.890
7.697
7.688
7.686
7.683
7.674
7.672
7.634
7.632
7.626
7.624
7.571
7.570
7.560
7.558
7.556
7.546
7.545
7.471
7.456
7.432
7.431
7.426
7.426
7.423
7.423
7.418
7.240


S
O
O

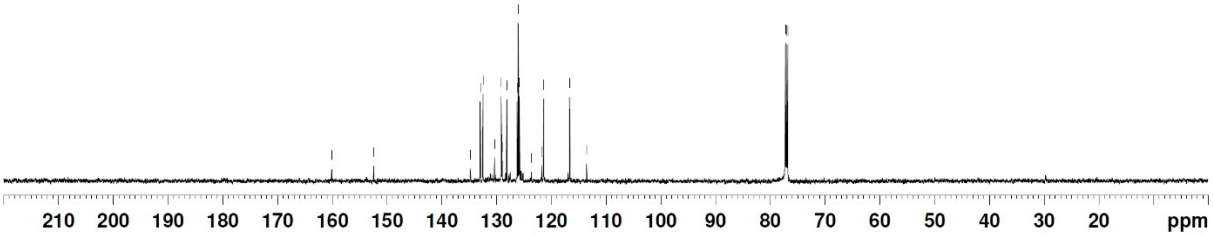
(3s)

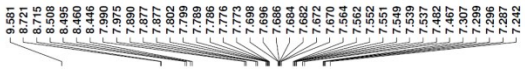

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.04
1.04
1.12
1.14
1.28
1.10
1.30
1.11
1.16

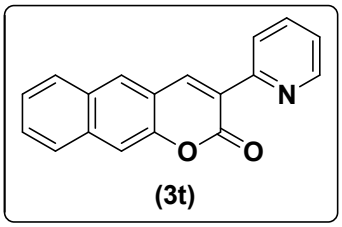

160.12
152.45
134.78
132.96
132.46
130.36
129.11
128.98
128.12
126.23
126.01
125.82
123.60
121.71
121.36
116.63
113.53
77.21
76.99
76.78


S
O
O

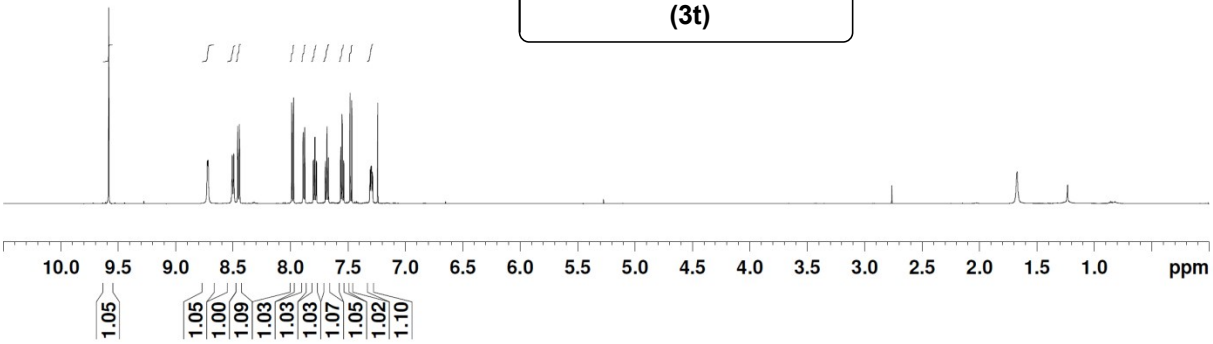
(3s)

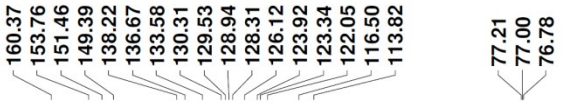

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

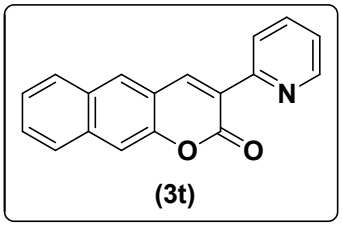

9.581
8.721
8.715
8.508
8.495
8.460
8.446
7.990
7.975
7.890
7.877
7.877
7.802
7.789
7.786
7.776
7.773
7.698
7.696
7.686
7.684
7.682
7.672
7.670
7.564
7.562
7.552
7.551
7.549
7.539
7.537
7.482
7.467
7.307
7.299
7.296
7.287
7.242


N
O
O

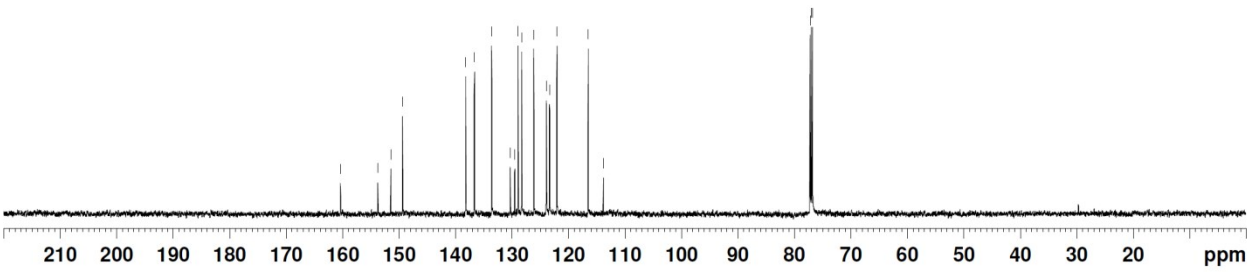
(3t)

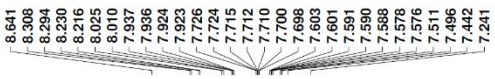

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.05
1.05
1.00
1.09
1.03
1.03
1.03
1.07
1.05
1.02
1.10

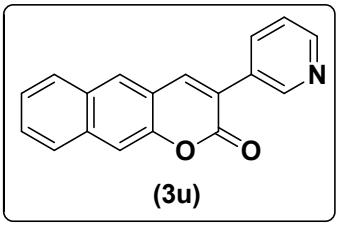

160.37
153.76
151.46
149.39
138.22
136.67
133.58
130.31
129.53
128.94
128.31
126.12
123.92
123.34
122.05
116.50
113.82
77.21
77.00
76.78


N
O
O

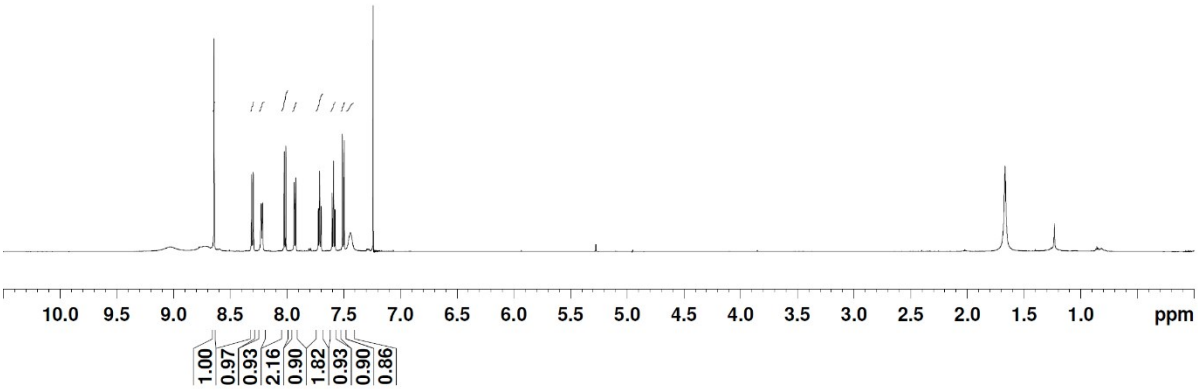
(3t)

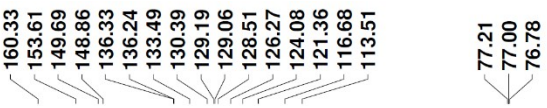

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

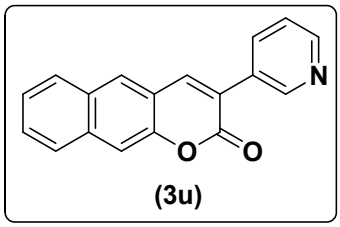

8.641
8.308
8.294
8.230
8.216
8.025
8.010
7.937
7.936
7.924
7.923
7.726
7.724
7.715
7.712
7.710
7.700
7.698
7.603
7.601
7.591
7.590
7.588
7.578
7.576
7.511
7.496
7.442
7.241


N
O
O

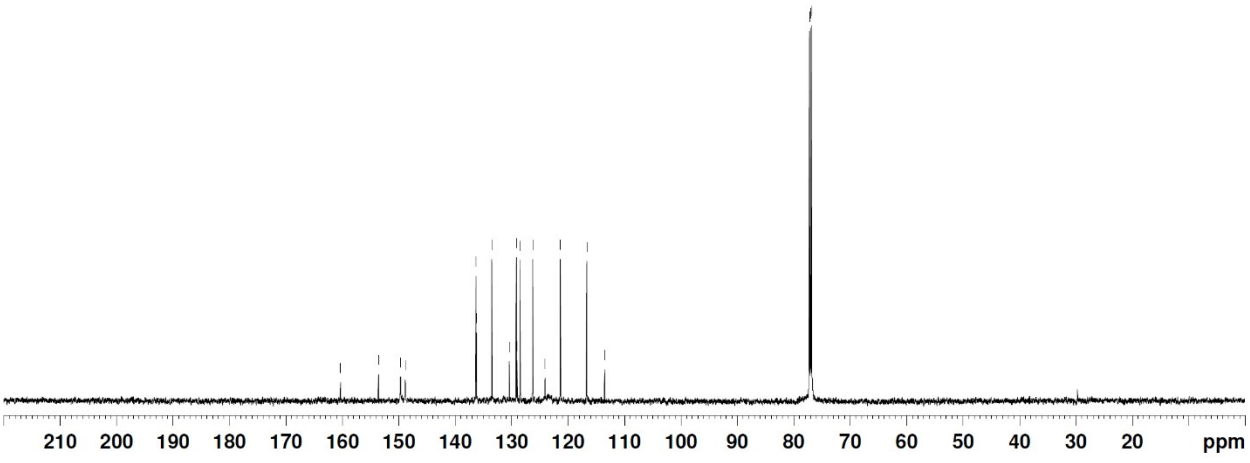
(3u)

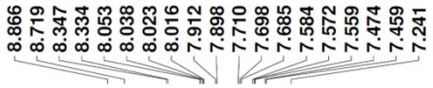

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
0.97
0.93
2.16
0.90
1.82
0.93
0.90
0.86

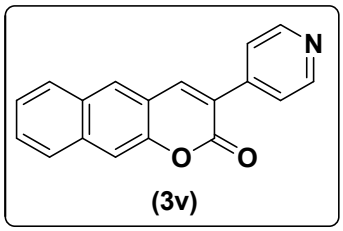

160.33
153.61
149.69
148.86
136.33
136.24
133.49
130.39
129.19
129.06
128.51
126.27
124.08
121.36
116.68
113.51
77.21
77.00
76.78


N
O
O

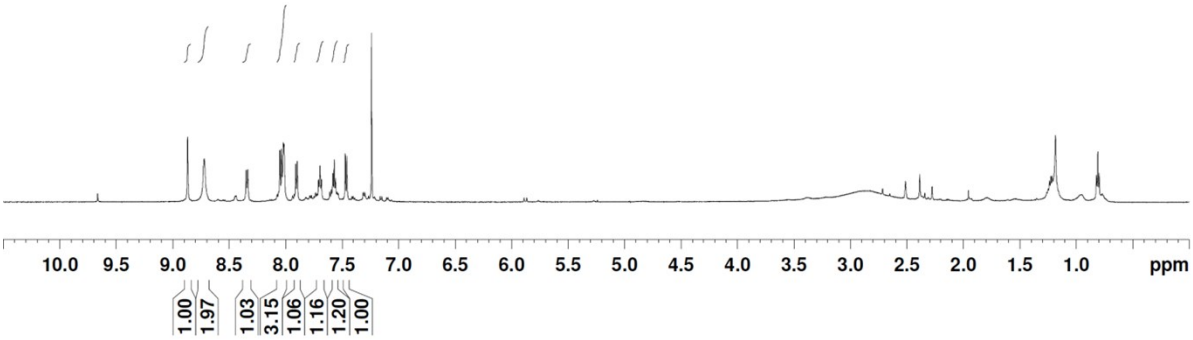
(3u)

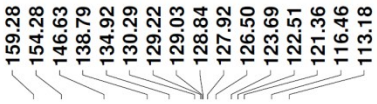

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

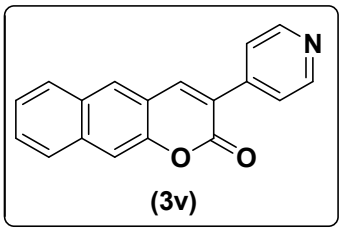

8.866
8.719
8.347
8.334
8.053
8.038
8.023
8.016
7.912
7.898
7.710
7.698
7.685
7.584
7.572
7.559
7.474
7.459
7.241


N
O
O

(3v)

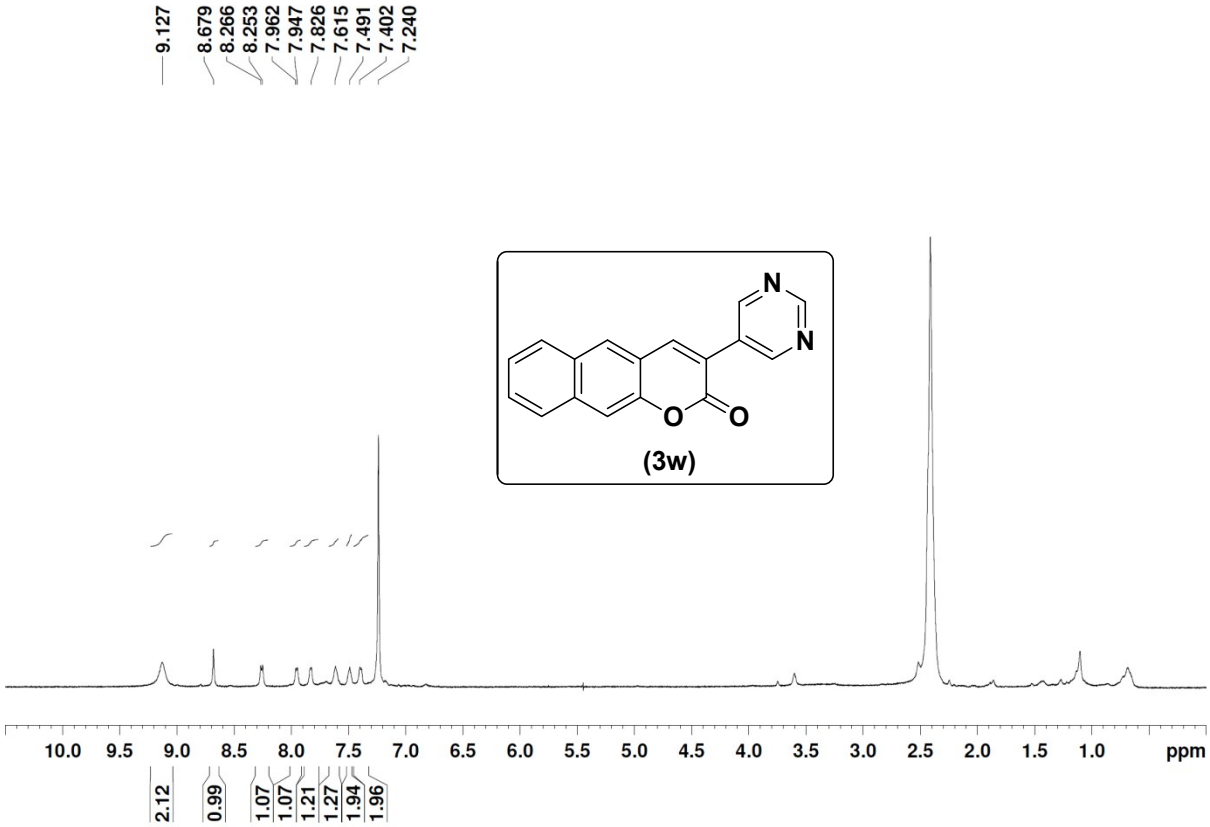

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.97
1.03
3.15
1.06
1.16
1.20
1.00

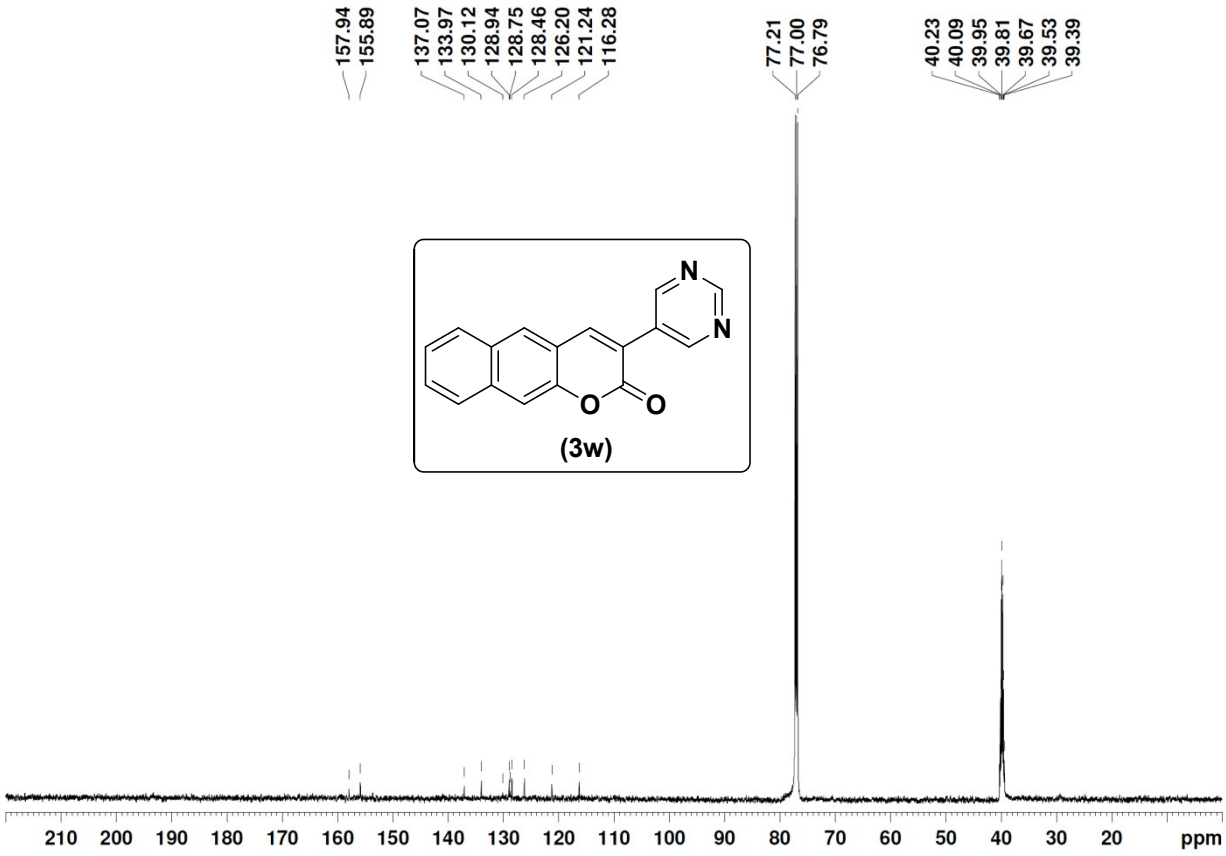

159.28
154.28
146.63
138.79
134.92
130.29
129.22
129.03
128.84
127.92
126.50
123.69
122.51
121.36
116.46
113.18
77.21
77.00
76.79

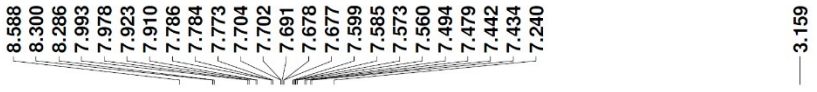

N
O
O

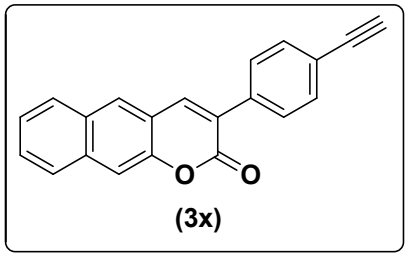
(3v)

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

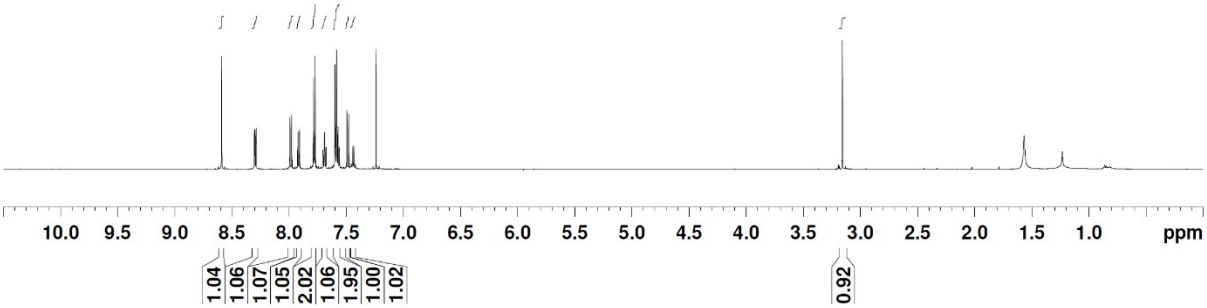

9.127
8.679
8.266
8.253
7.962
7.947
7.826
7.615
7.491
7.402
7.240
N
N
O
O
(3w)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.12
0.99
1.07
1.07
1.21
1.27
1.94
1.96

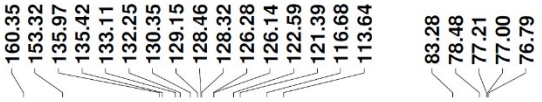

157.94
155.89
137.07
133.97
130.12
128.94
128.75
128.46
126.20
121.24
116.28
77.21
77.00
76.79
40.23
40.09
39.95
39.81
39.67
39.53
39.39
N
N
O
O
(3w)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

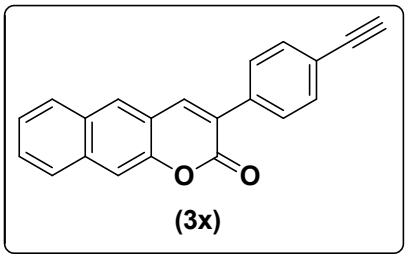

8.588
8.300
8.286
7.993
7.978
7.923
7.910
7.786
7.784
7.773
7.704
7.702
7.691
7.678
7.677
7.599
7.585
7.573
7.560
7.494
7.479
7.442
7.434
7.240
3.159


O
O

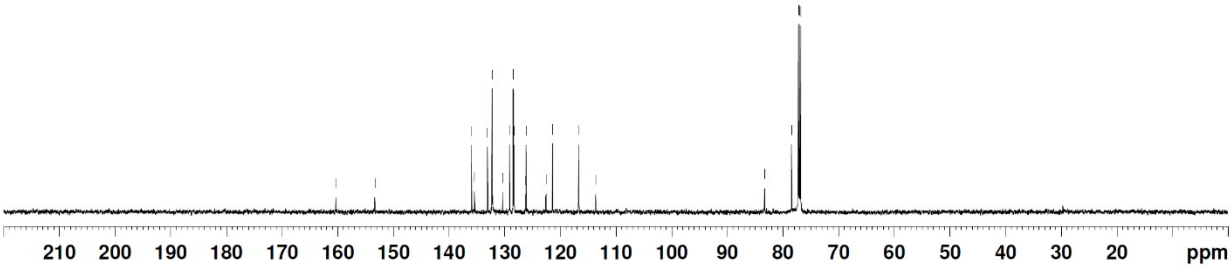
(3x)

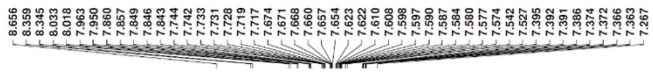

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.04
1.06
1.07
1.05
2.02
1.06
1.95
1.00
1.02
0.92

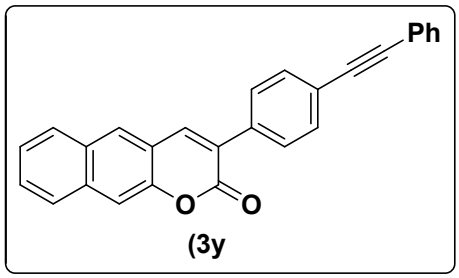

160.35
153.32
135.97
135.42
133.11
132.25
130.35
129.15
128.46
128.32
126.28
126.14
122.59
121.39
116.68
113.64
83.28
78.48
77.21
77.00
76.79


O
O

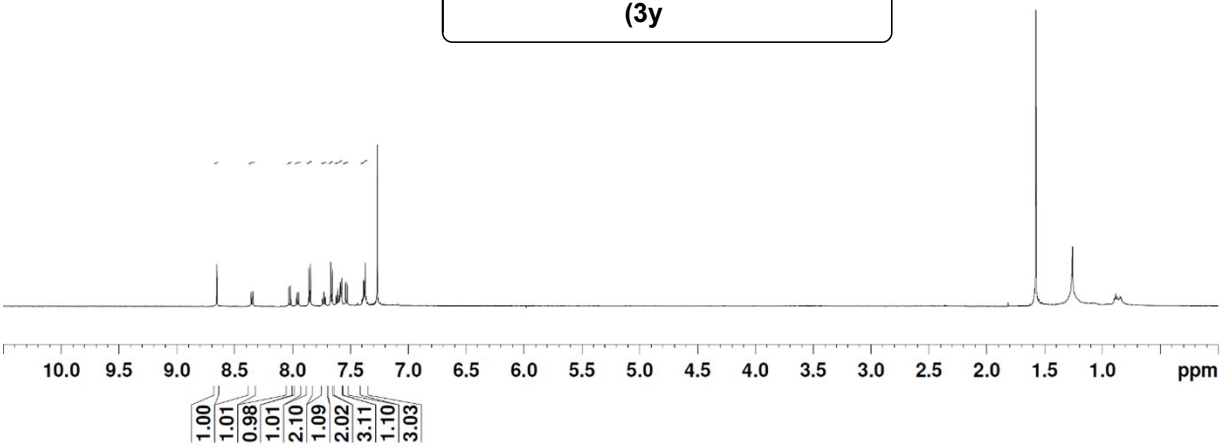
(3x)

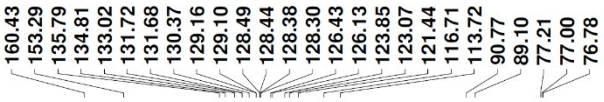

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

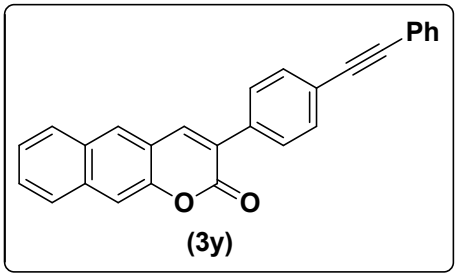

8.656
8.359
8.345
8.033
8.018
7.963
7.950
7.860
7.857
7.849
7.846
7.843
7.744
7.742
7.733
7.731
7.728
7.719
7.717
7.674
7.671
7.668
7.660
7.657
7.654
7.623
7.622
7.610
7.608
7.598
7.597
7.590
7.587
7.584
7.580
7.577
7.574
7.542
7.527
7.395
7.392
7.391
7.386
7.374
7.372
7.366
7.363
7.267


Ph
O
O

(3y

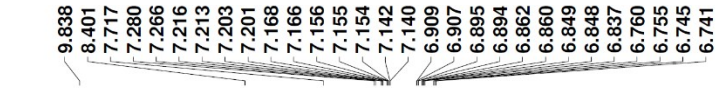

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.01
0.98
1.01
2.10
1.09
2.02
3.11
1.10
3.03

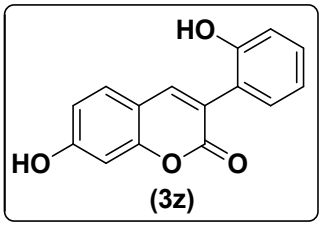

160.43
153.29
135.79
134.81
133.02
131.72
131.68
130.37
129.16
129.10
128.49
128.44
128.38
128.30
126.43
126.13
123.85
123.07
121.44
116.71
113.72
90.77
89.10
77.21
77.00
76.78

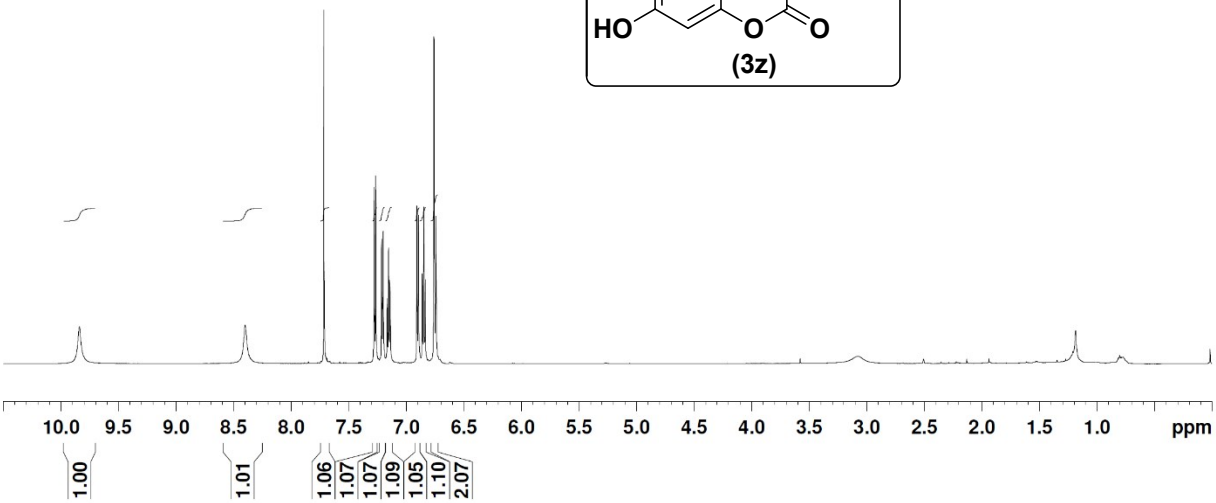

Ph
O
O

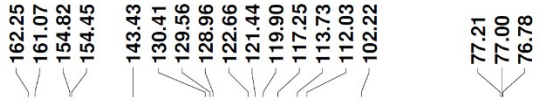
(3y)

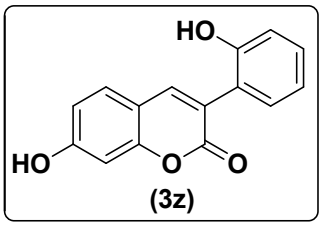
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

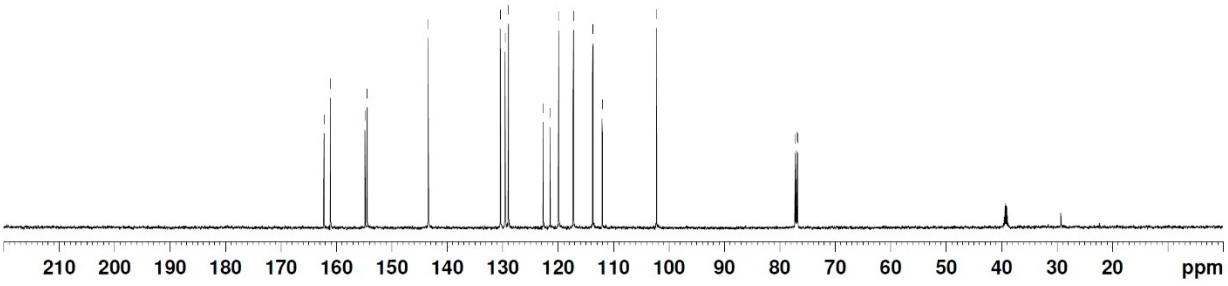

9.838
8.401
7.717
7.280
7.266
7.216
7.213
7.203
7.201
7.168
7.166
7.156
7.155
7.154
7.142
7.140
6.909
6.907
6.895
6.894
6.862
6.860
6.849
6.848
6.837
6.760
6.755
6.745
6.741


HO
HO
O
O
(3z)

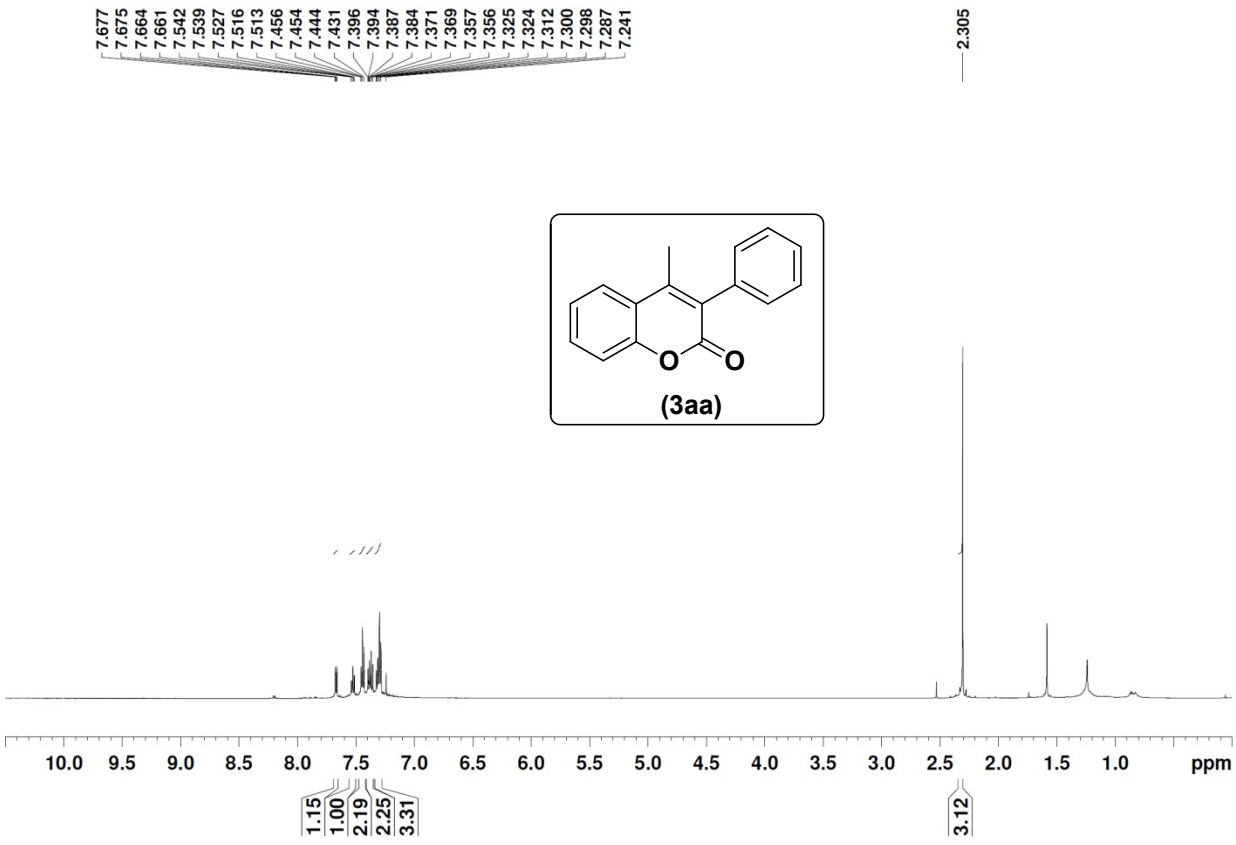

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.01
1.06
1.07
1.07
1.09
1.05
1.10
2.07

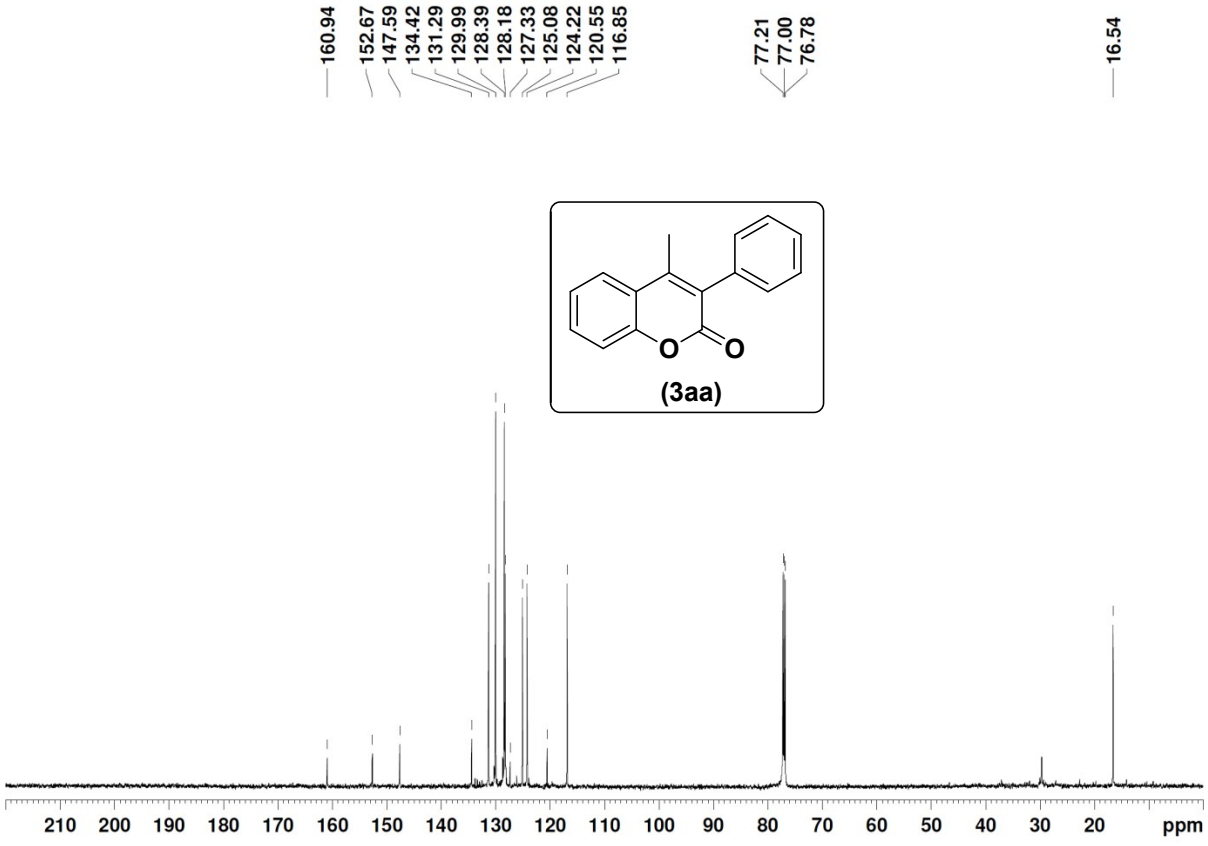

162.25
161.07
154.82
154.45
143.43
130.41
129.56
128.96
122.66
121.44
119.90
117.25
113.73
112.03
102.22
77.21
77.00
76.78

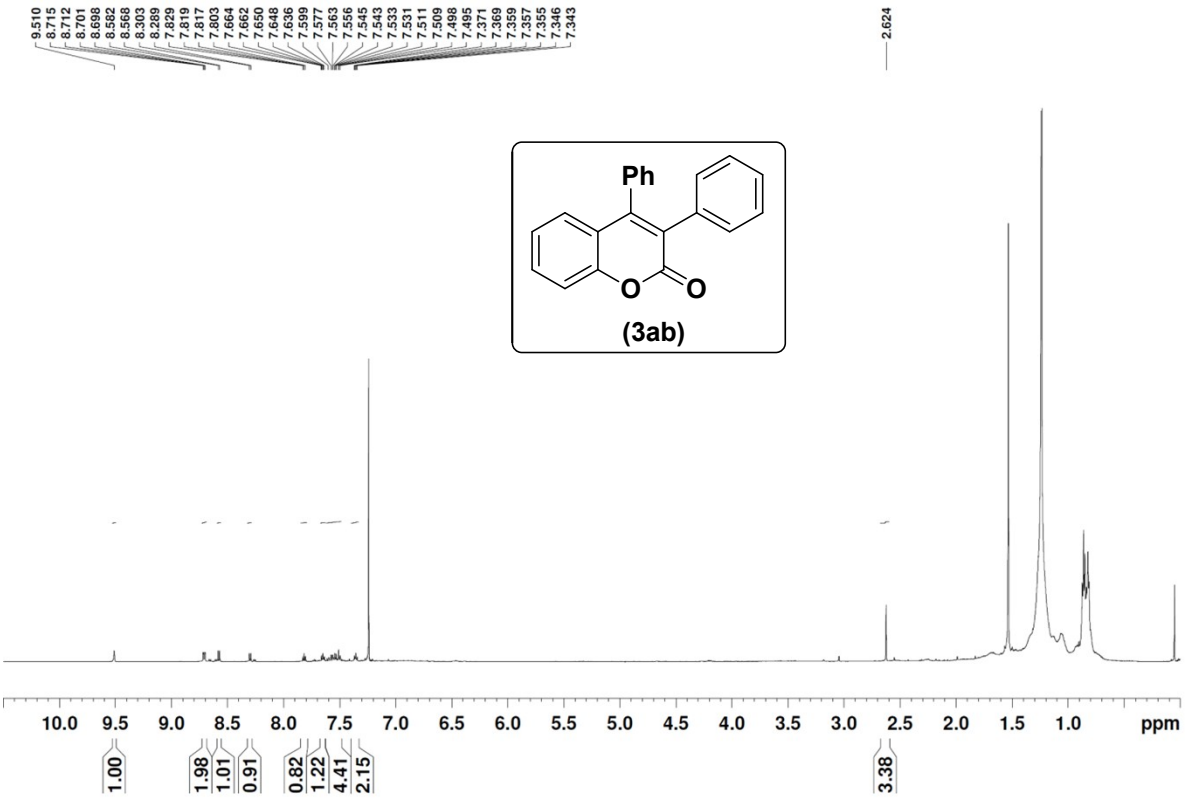

HO
HO
O
O
(3z)

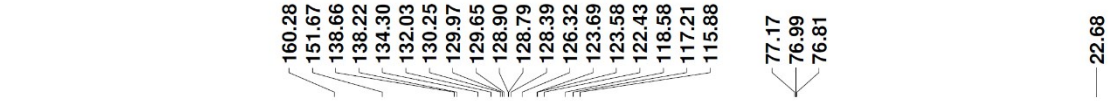

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

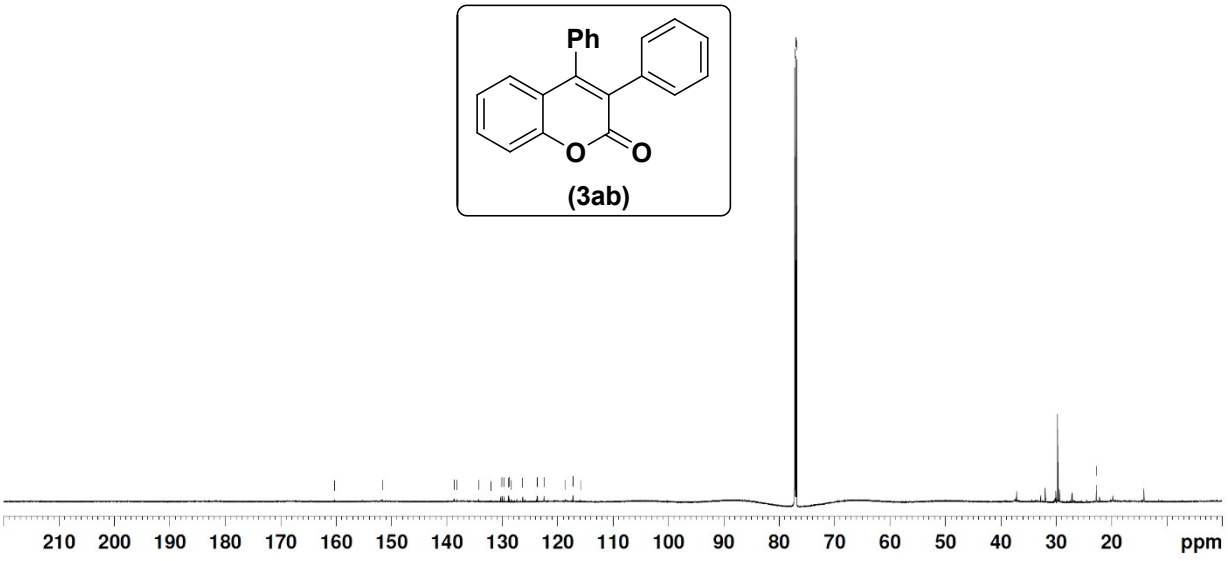

7.826
7.819
7.803
7.282
7.271
7.268
7.229
7.226
7.217
7.203
7.180
7.165
7.042
7.037
7.027
7.023
6.971
6.966
6.941
6.937
6.895
6.882
6.870
3.310
HO
HO
O
O
(3z1)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.01
1.16
1.99
1.82
1.02
2.02
163.02
156.30
155.45
148.37
145.59
143.85
131.96
130.97
127.65
123.71
121.52
121.16
120.69
120.50
118.39
118.02
117.10
116.90
113.47
113.34
49.42
49.28
49.14
49.00
48.85
48.71
48.57
HO
HO
O
O
(3z1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

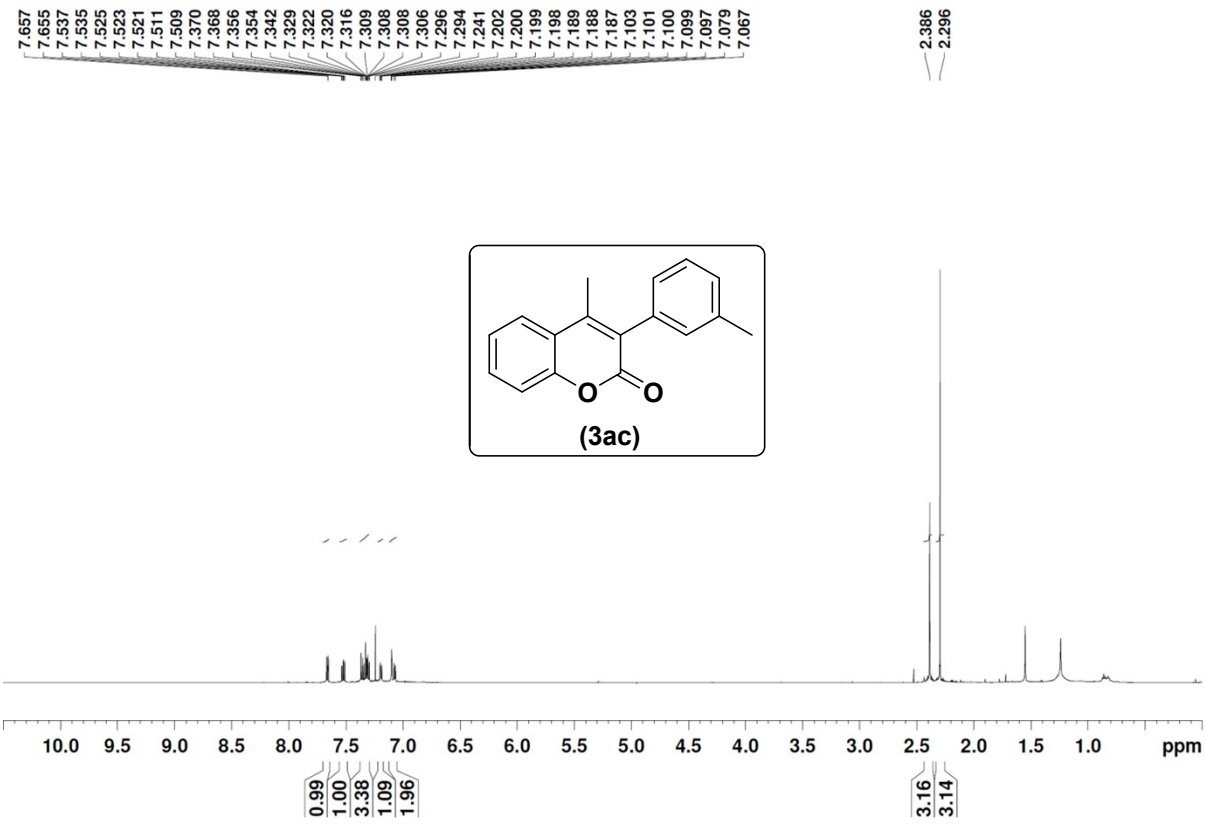

7.677
7.675
7.664
7.661
7.542
7.539
7.527
7.516
7.513
7.456
7.454
7.444
7.431
7.396
7.394
7.387
7.384
7.371
7.369
7.357
7.356
7.325
7.324
7.312
7.300
7.298
7.287
7.241
2.305
(3aa)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.15
1.00
2.19
2.25
3.31
3.12

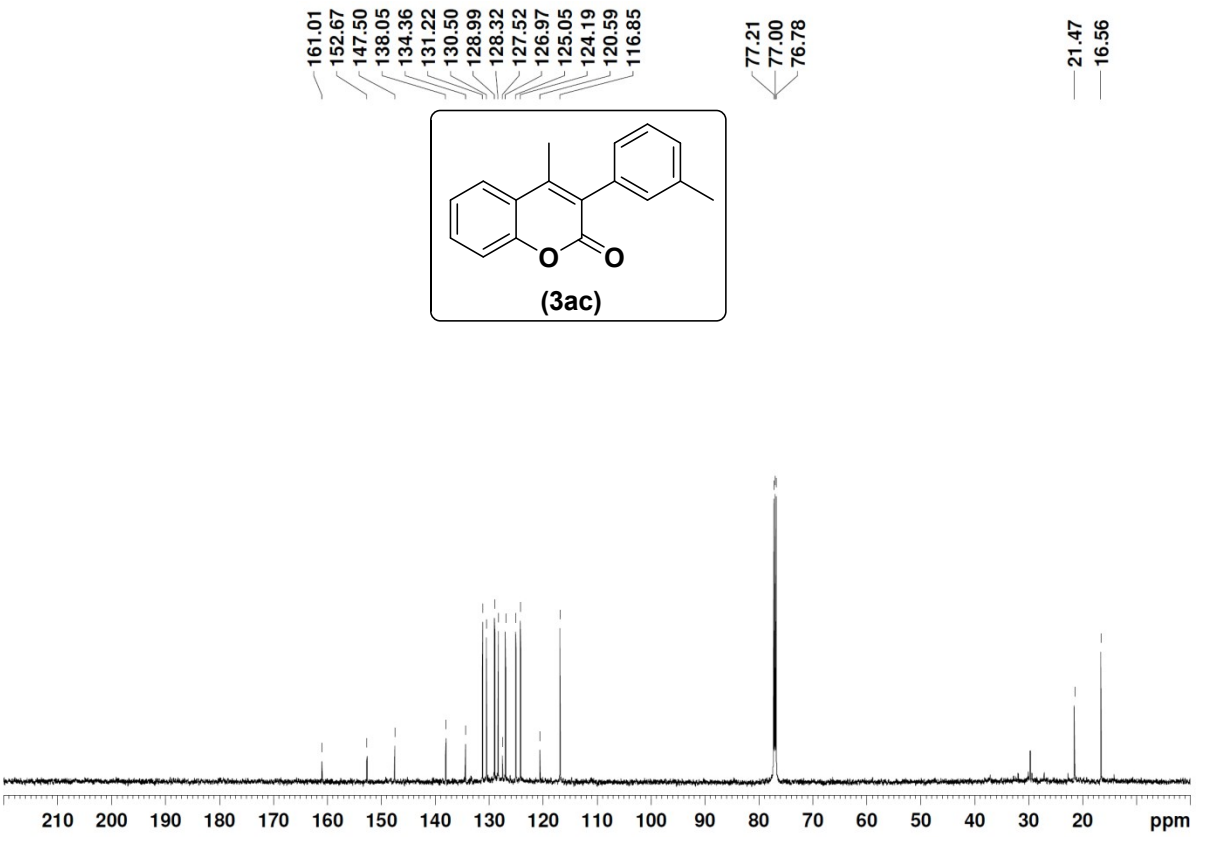

160.94
152.67
147.59
134.42
131.29
129.99
128.39
128.18
127.33
125.08
124.22
120.55
116.85
77.21
77.00
76.78
16.54
(3aa)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

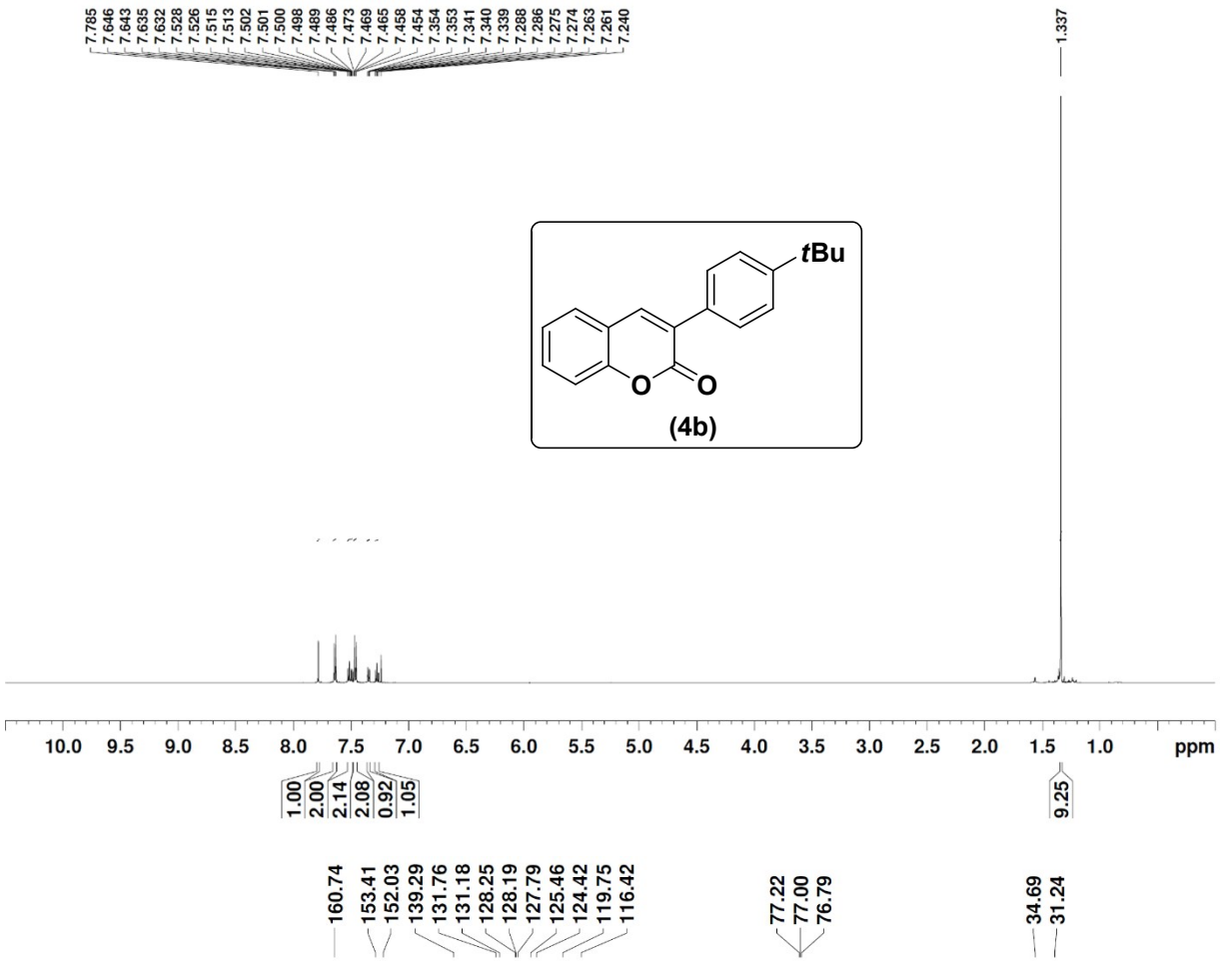

9.510
8.715
8.712
8.701
8.698
8.582
8.568
8.303
8.289
7.829
7.819
7.817
7.803
7.664
7.662
7.650
7.648
7.636
7.599
7.577
7.563
7.556
7.545
7.543
7.533
7.531
7.511
7.509
7.498
7.495
7.371
7.369
7.359
7.357
7.355
7.346
7.343
2.624
Ph
O
O
(3ab)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.98
1.01
0.91
0.82
1.22
4.41
2.15
3.38

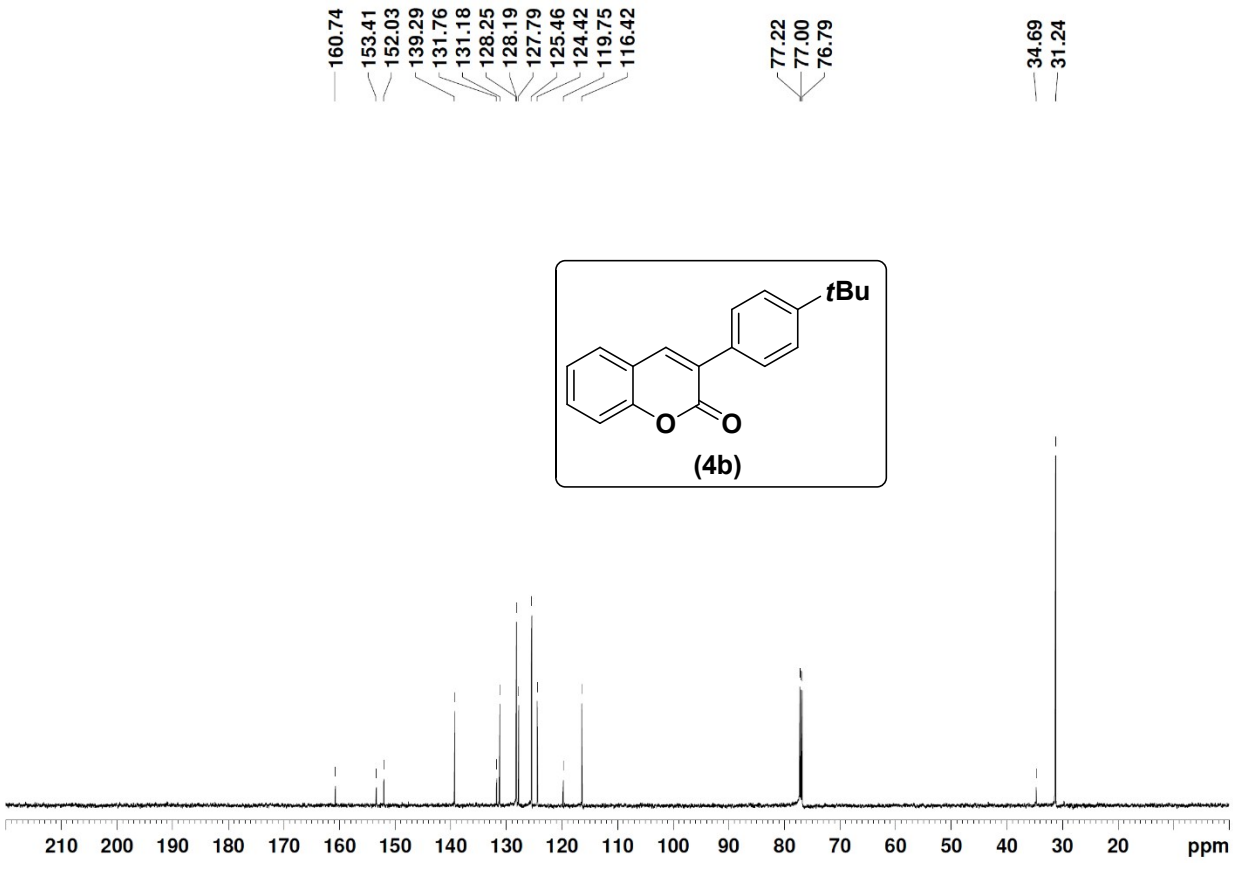

160.28
151.67
138.66
138.22
134.30
132.03
130.25
129.97
129.65
128.90
128.79
128.39
126.32
123.69
123.58
122.43
118.58
117.21
115.88
77.17
76.99
76.81
22.68


Ph
O
O
(3ab)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

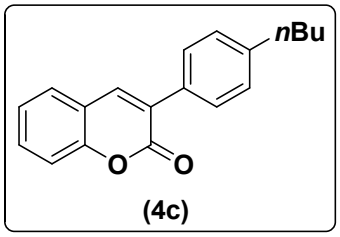

7.657
7.655
7.537
7.535
7.525
7.523
7.521
7.511
7.509
7.370
7.368
7.356
7.354
7.342
7.329
7.322
7.320
7.316
7.309
7.308
7.308
7.306
7.296
7.294
7.241
7.202
7.200
7.199
7.198
7.189
7.188
7.187
7.103
7.101
7.100
7.099
7.097
7.079
7.067
2.386
2.296
(3ac)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.99
1.00
3.38
1.09
1.96
3.16
3.14

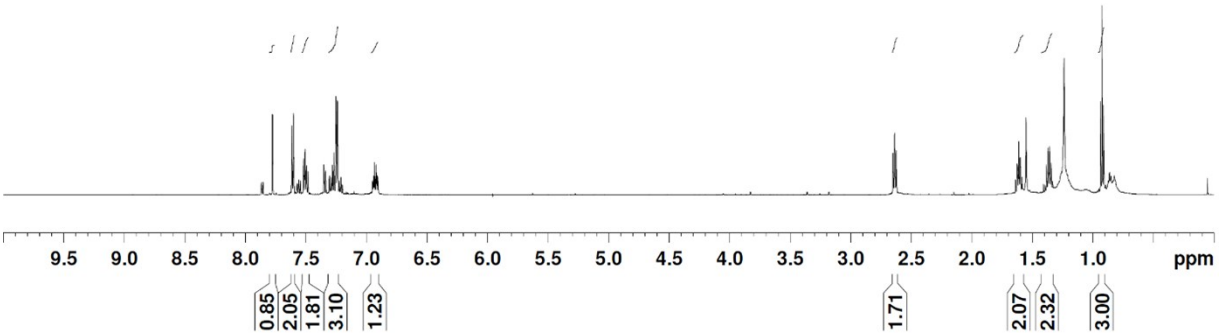

161.01
152.67
147.50
138.05
134.36
131.22
130.50
128.99
128.32
127.52
126.97
125.05
124.19
120.59
116.85
77.21
77.00
76.78
21.47
16.56
(3ac)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

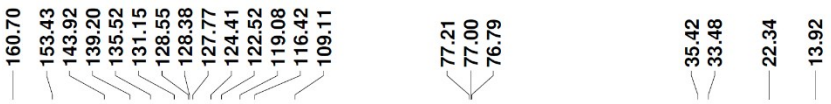

7.785
7.646
7.643
7.635
7.632
7.528
7.526
7.515
7.513
7.502
7.501
7.500
7.498
7.489
7.486
7.473
7.469
7.465
7.458
7.454
7.354
7.353
7.341
7.340
7.339
7.288
7.286
7.275
7.274
7.263
7.261
7.240
1.337
tBu
O
O
(4b)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.00
2.14
2.08
0.92
1.05
9.25

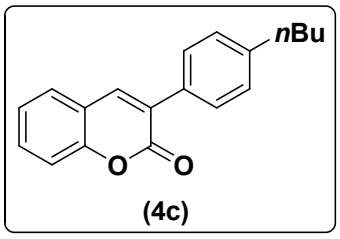

160.74
153.41
152.03
139.29
131.76
131.18
128.25
128.19
127.79
125.46
124.42
119.75
116.42
77.22
77.00
76.79
34.69
31.24
tBu
O
O
(4b)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

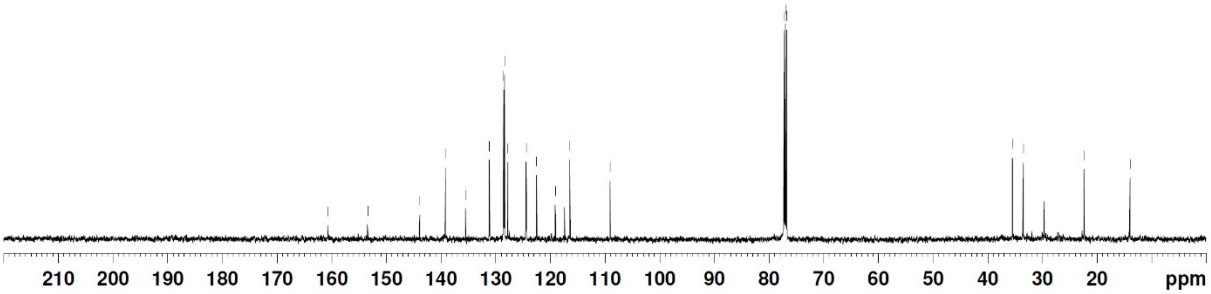

7.777
7.619
7.616
7.605
7.523
7.521
7.513
7.510
7.508
7.500
7.499
7.498
7.496
7.487
7.484
7.307
7.295
7.293
7.286
7.284
7.273
7.271
7.261
7.259
7.255
7.254
7.252
7.242
7.238
7.226
7.213
7.212
6.944
6.942
6.937
6.936
6.929
6.923
6.921
6.920
6.916
6.916
6.913
6.907
2.653
2.640
2.627
1.639
1.626
1.623
1.617
1.613
1.609
1.603
1.601
1.599
1.588
1.588
1.385
1.372
1.359
1.347
0.938
0.926
0.923
0.913

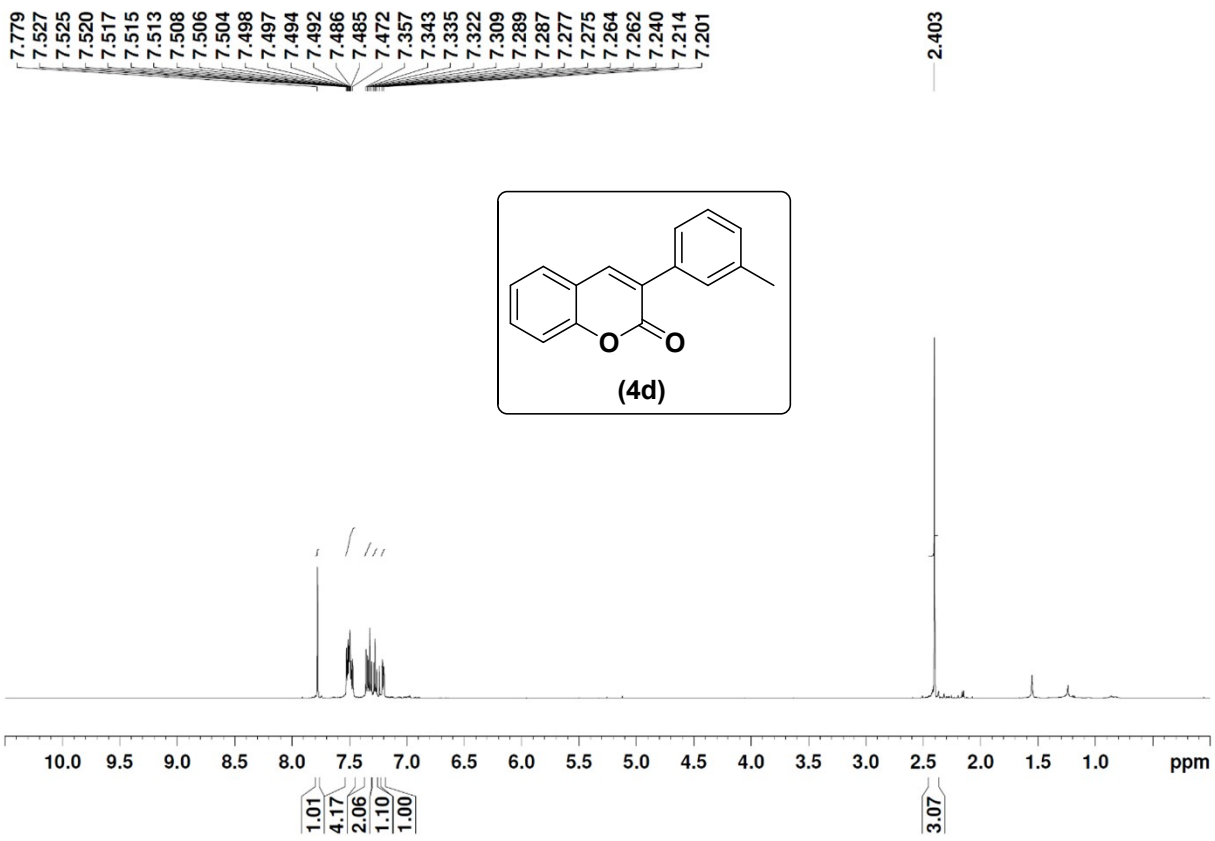

nBu
O
O
(4c)

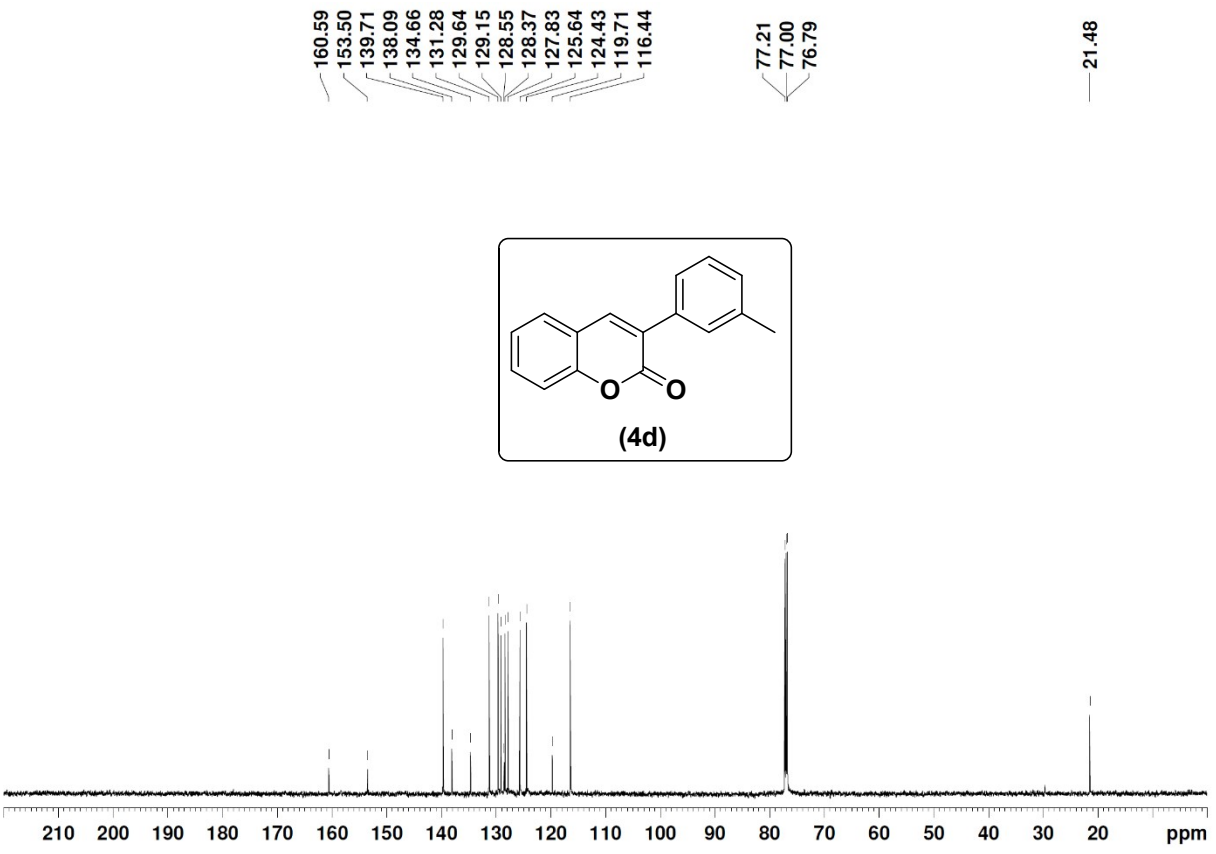

9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.85
2.05
1.81
3.10
1.23
1.71
2.07
2.32
3.00

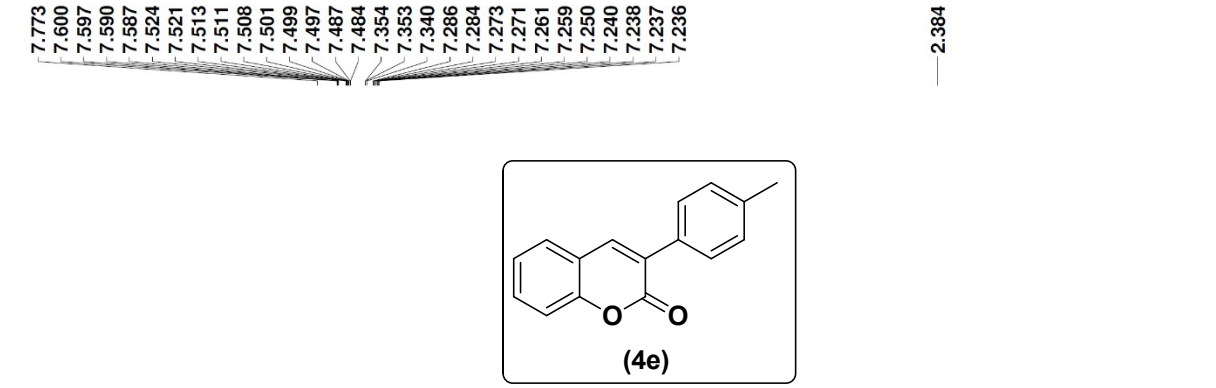

160.70
153.43
143.92
139.20
135.52
131.15
128.55
128.38
127.77
124.41
122.52
119.08
116.42
109.11
77.21
77.00
76.79
35.42
33.48
22.34
13.92

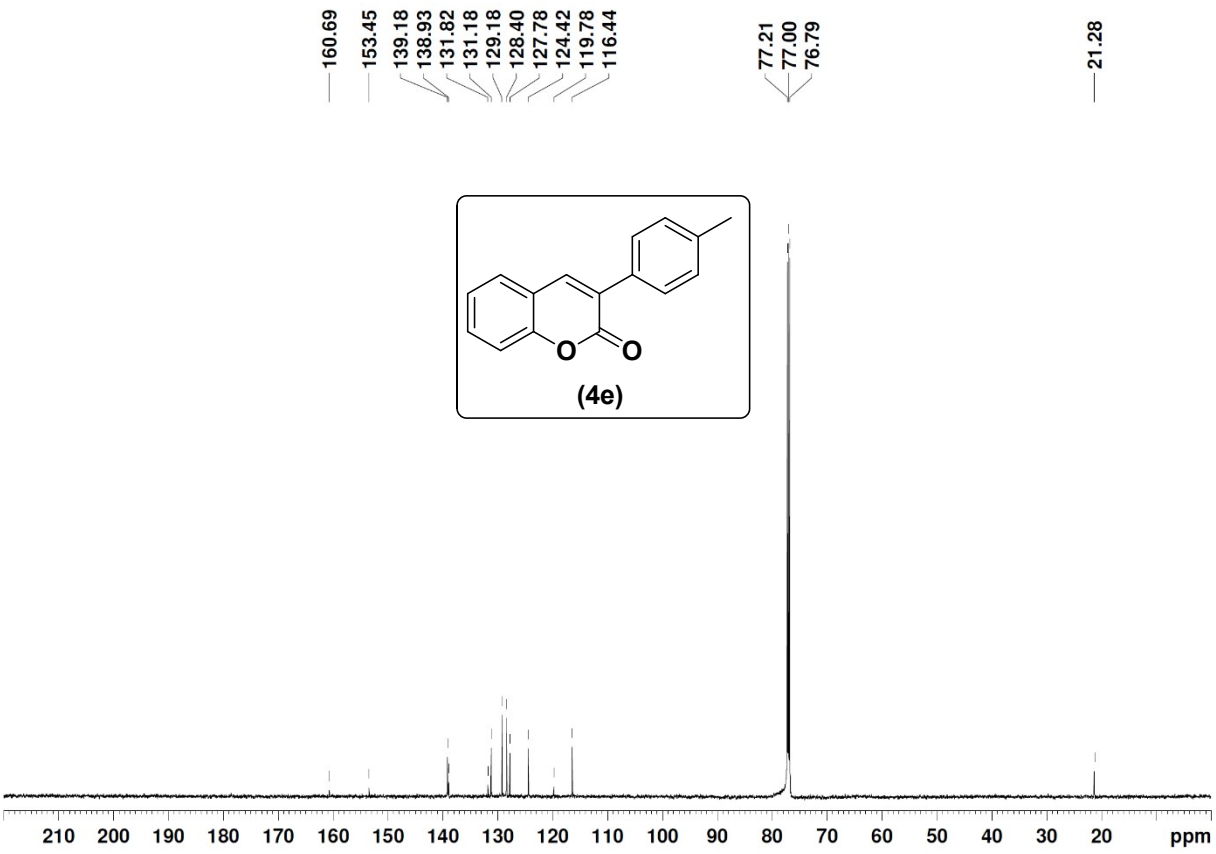

nBu
O
O
(4c)

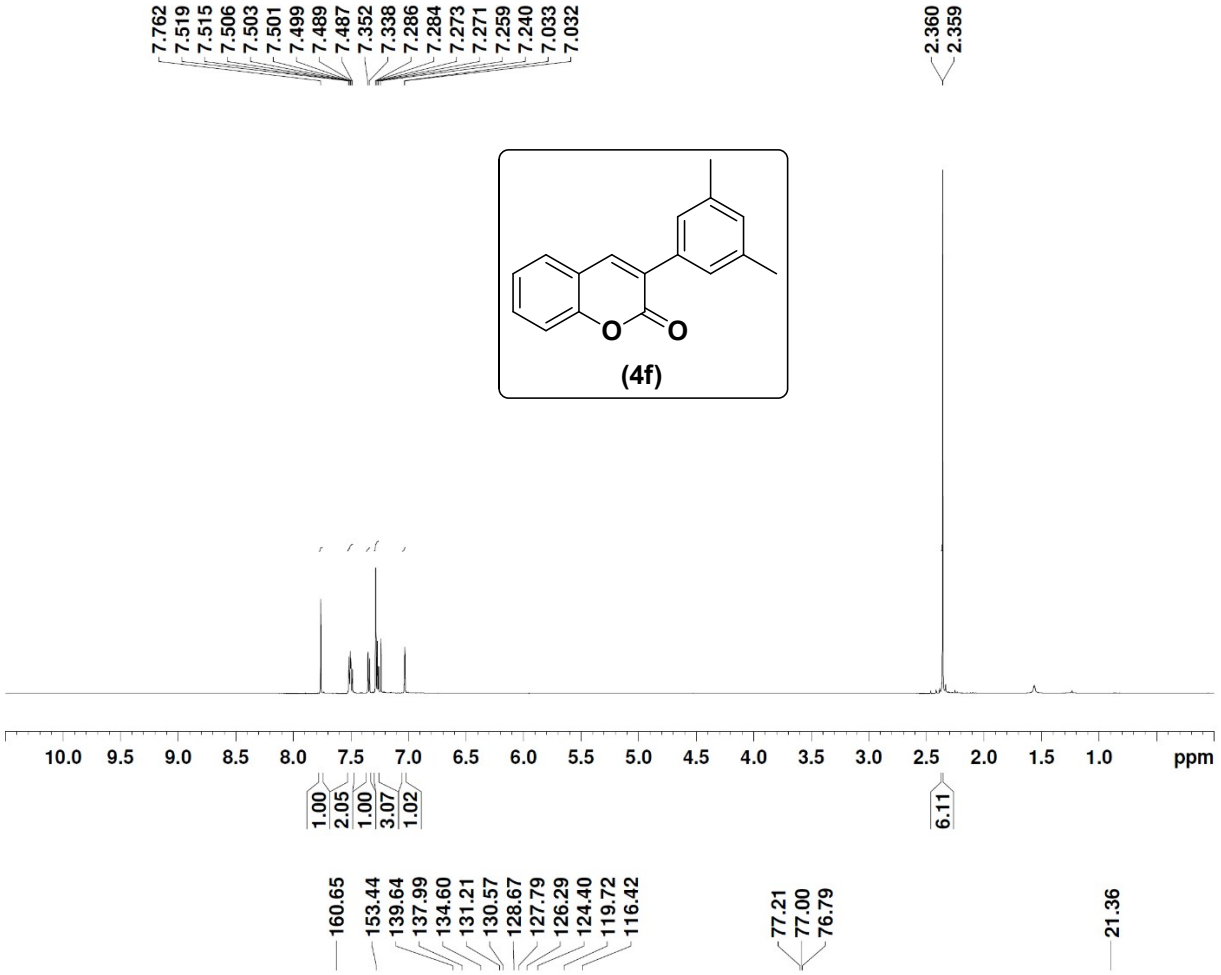

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

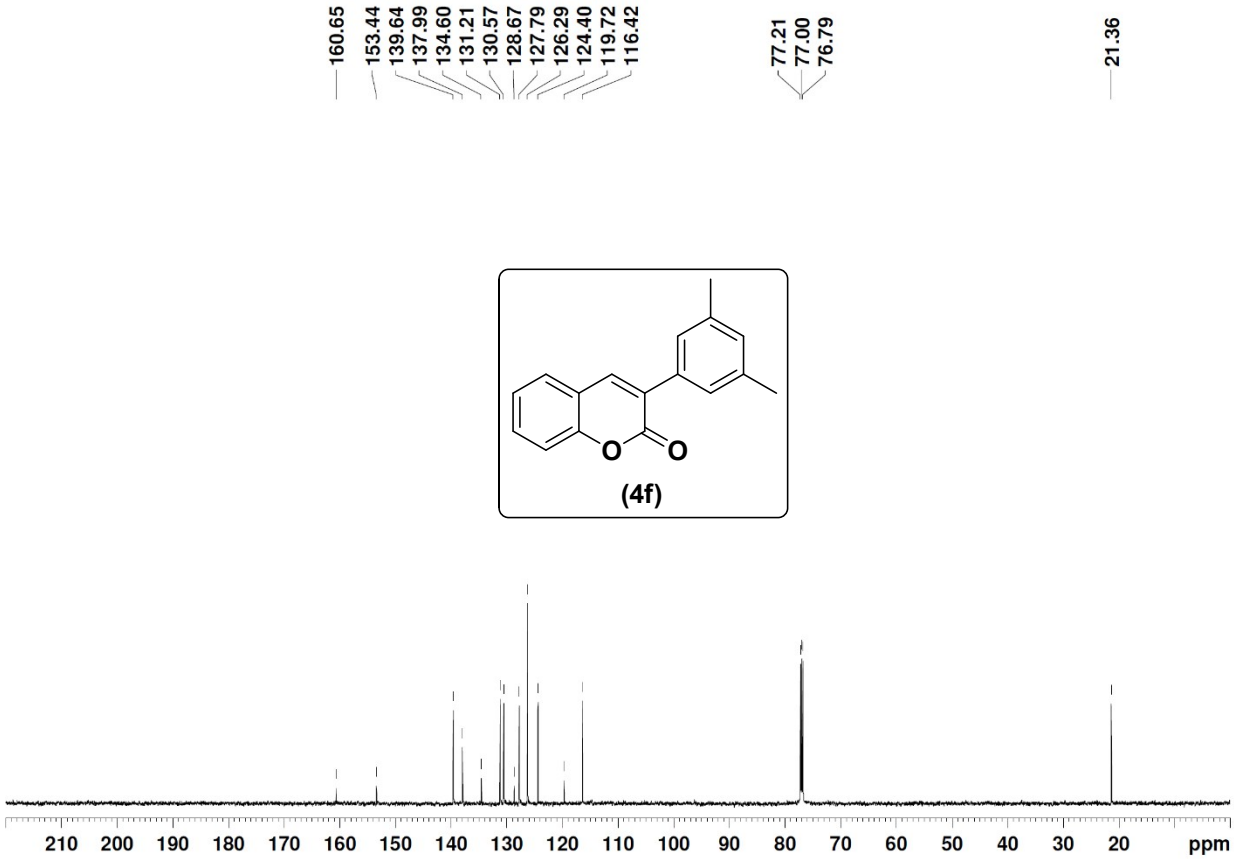

7.779
7.527
7.525
7.520
7.517
7.515
7.513
7.508
7.506
7.504
7.498
7.497
7.494
7.492
7.486
7.485
7.472
7.357
7.343
7.335
7.322
7.309
7.289
7.287
7.277
7.275
7.264
7.262
7.240
7.214
7.201
2.403
(4d)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.01
4.17
2.06
1.10
1.00
3.07

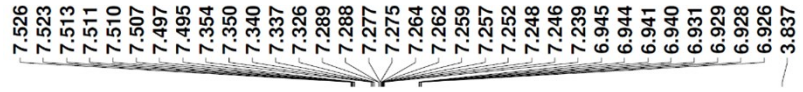

160.59
153.50
139.71
138.09
134.66
131.28
129.64
129.15
128.55
128.37
127.83
125.64
124.43
119.71
116.44
77.21
77.00
76.79
21.48
(4d)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

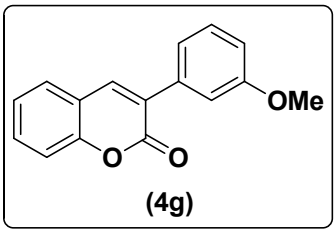

7.773
7.600
7.597
7.590
7.587
7.524
7.521
7.513
7.511
7.508
7.501
7.499
7.497
7.487
7.484
7.354
7.353
7.340
7.286
7.284
7.273
7.271
7.261
7.259
7.250
7.240
7.238
7.237
7.236
2.384
O
O
(4e)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
2.22
2.21
1.09
1.38
1.00
0.89
3.02

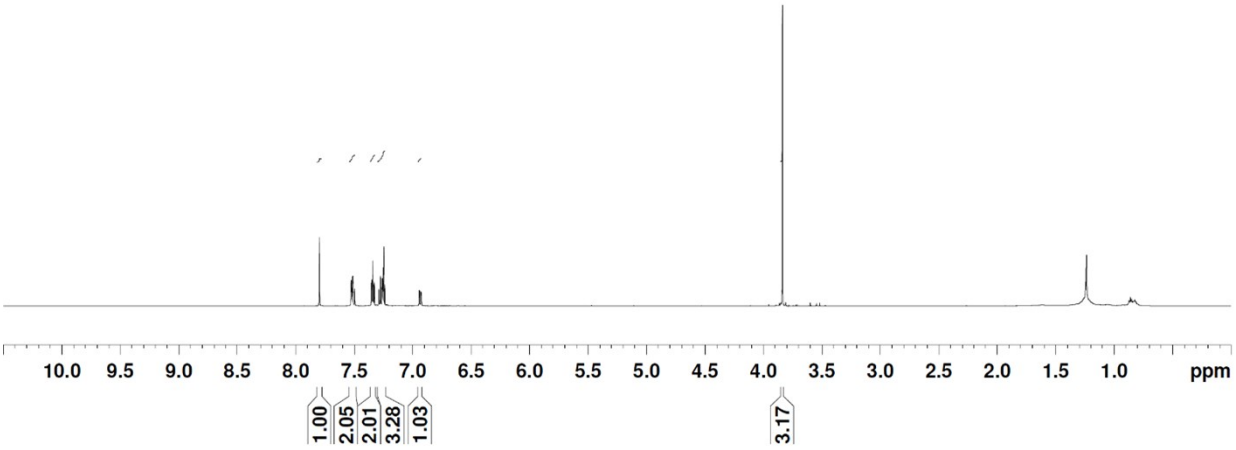

160.69
153.45
139.18
138.93
131.82
131.18
129.18
128.40
127.78
124.42
119.78
116.44
77.21
77.00
76.79
21.28
O
O
(4e)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

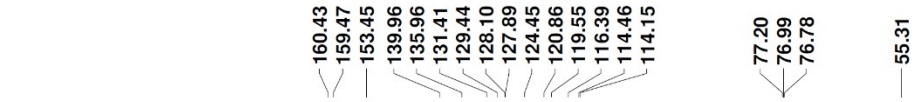

7.762
7.519
7.515
7.506
7.503
7.501
7.499
7.489
7.487
7.352
7.338
7.286
7.284
7.273
7.271
7.259
7.240
7.033
7.032
2.360
2.359
(4f)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.05
1.00
3.07
1.02
6.11

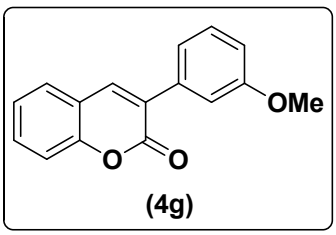

160.65
153.44
139.64
137.99
134.60
131.21
130.57
128.67
127.79
126.29
124.40
119.72
116.42
77.21
77.00
76.79
21.36
(4f)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

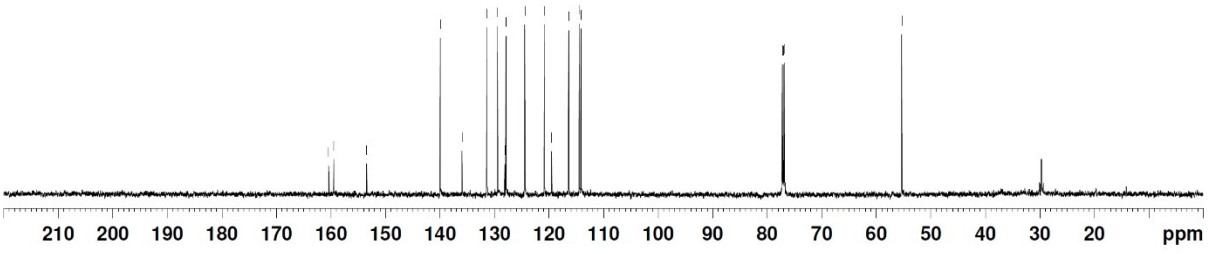

7.526
7.523
7.513
7.511
7.510
7.507
7.497
7.495
7.354
7.350
7.340
7.337
7.326
7.289
7.288
7.277
7.275
7.264
7.262
7.259
7.257
7.252
7.248
7.246
7.239
6.945
6.944
6.941
6.940
6.931
6.929
6.928
6.926
3.837

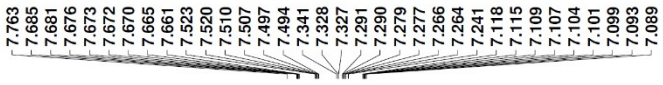

OMe
O
O
(4g)

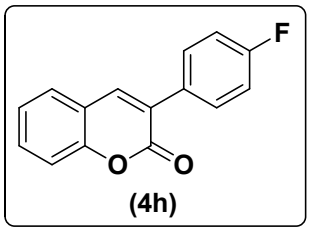

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.05
2.01
3.28
1.03
3.17


160.43
159.47
153.45
139.96
135.96
131.41
129.44
128.10
127.89
124.45
120.86
119.55
116.39
114.46
114.15
77.20
76.99
76.78
55.31

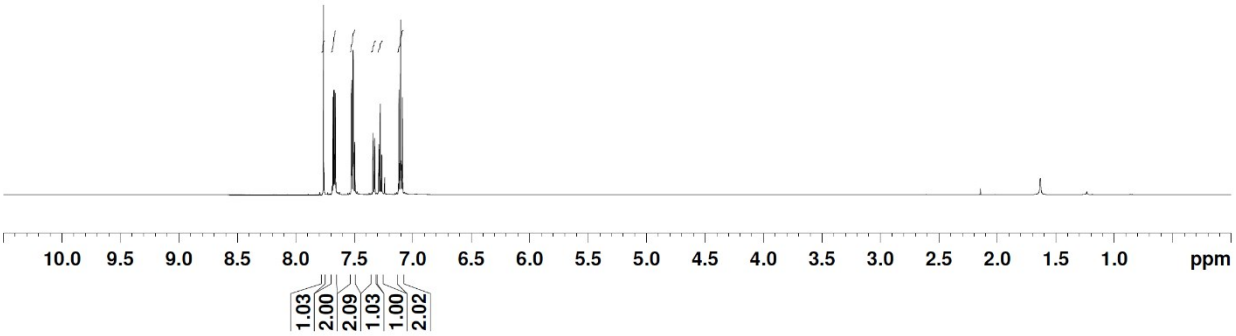

OMe
O
O
(4g)

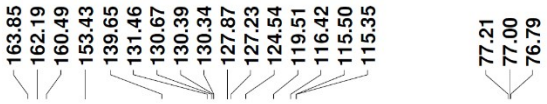

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

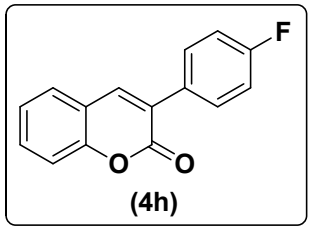

7.763
7.685
7.681
7.676
7.673
7.672
7.670
7.665
7.661
7.523
7.520
7.510
7.507
7.497
7.494
7.341
7.328
7.327
7.291
7.290
7.279
7.277
7.266
7.264
7.241
7.118
7.115
7.109
7.107
7.104
7.101
7.099
7.093
7.089


F
O
O

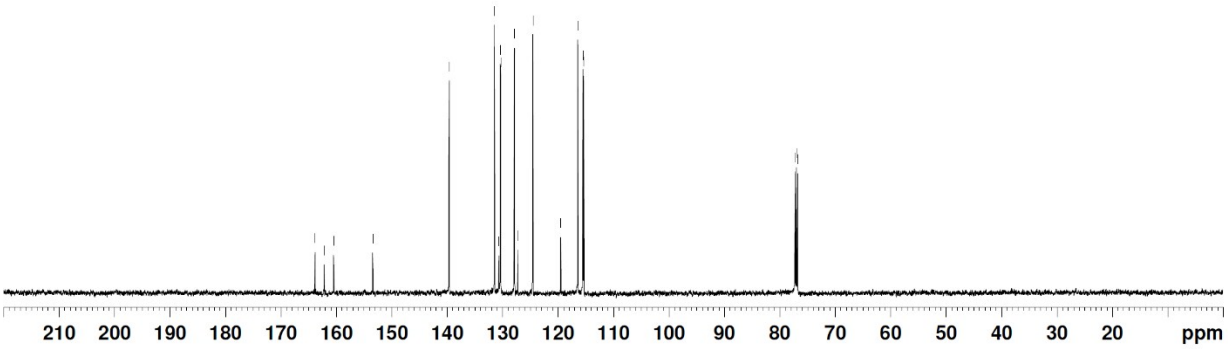
(4h)

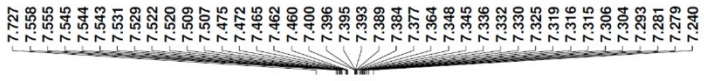

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.03
2.00
2.09
1.03
1.00
2.02

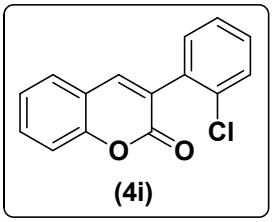

163.85
162.19
160.49
153.43
139.65
131.46
130.67
130.39
130.34
127.87
127.23
124.54
119.51
116.42
115.50
115.35
77.21
77.00
76.79


F
O
O

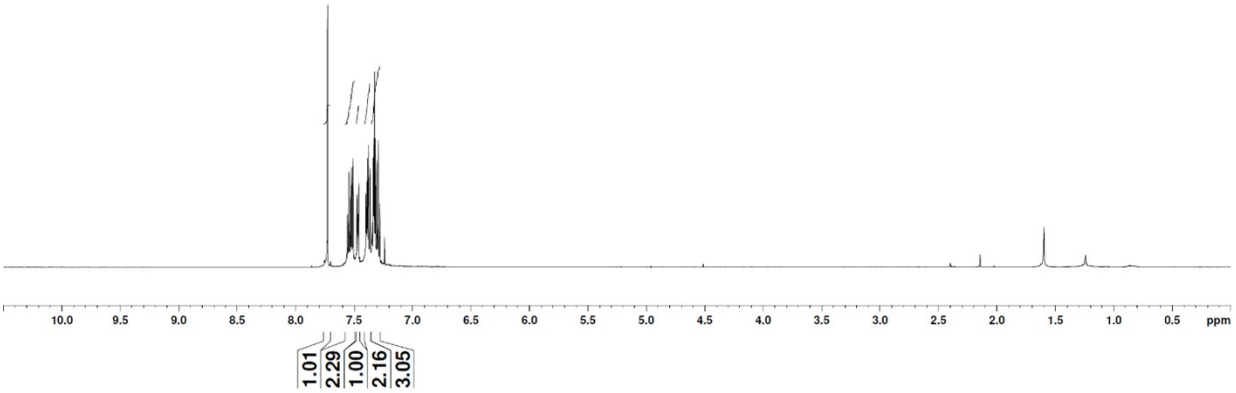
(4h)

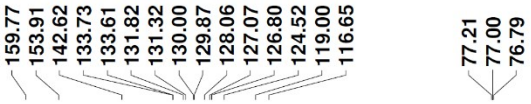

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

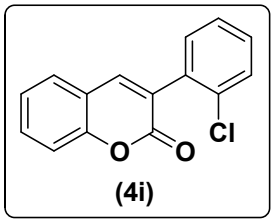

7.727
7.558
7.555
7.545
7.544
7.543
7.531
7.529
7.522
7.520
7.509
7.507
7.475
7.472
7.465
7.462
7.460
7.400
7.396
7.395
7.393
7.389
7.384
7.377
7.364
7.348
7.345
7.336
7.332
7.330
7.325
7.319
7.316
7.315
7.306
7.304
7.293
7.281
7.279
7.240


Cl
O
O

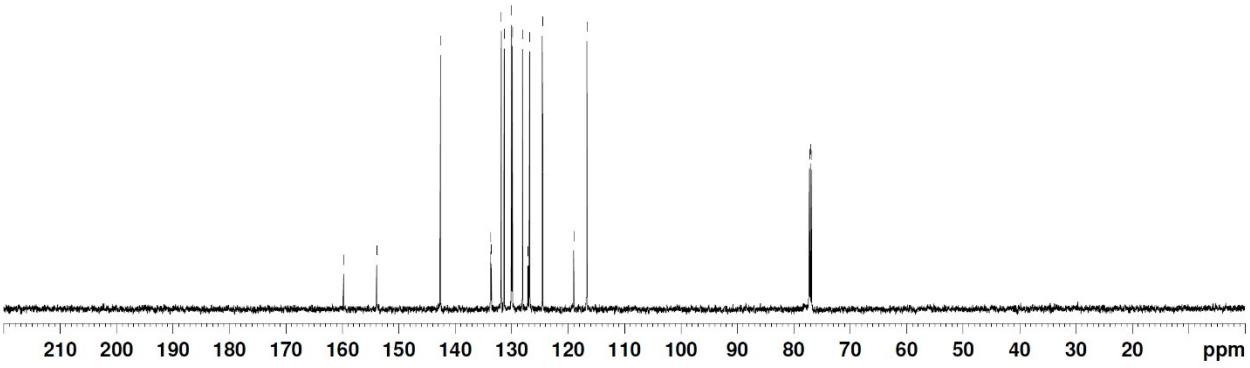
(4i)


10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.01
2.29
1.00
2.16
3.05

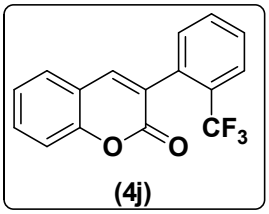

159.77
153.91
142.62
133.73
133.61
131.82
131.32
130.00
129.87
128.06
127.07
126.80
124.52
119.00
116.65
77.21
77.00
76.79


Cl
O
O

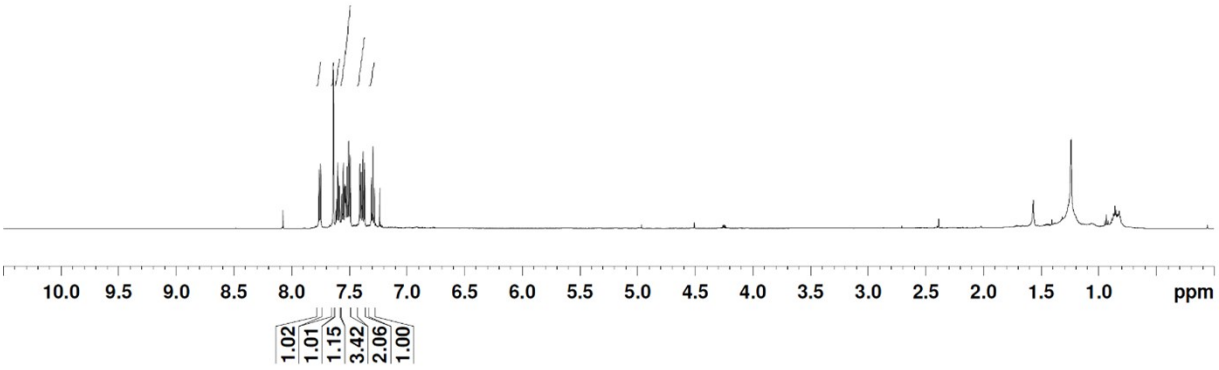
(4i)

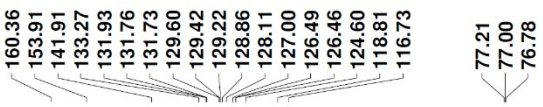

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

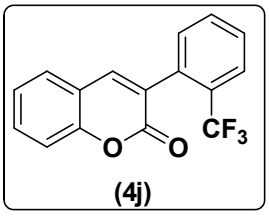

7.762
7.749
7.638
7.612
7.599
7.586
7.567
7.564
7.553
7.540
7.538
7.533
7.520
7.506
7.504
7.494
7.491
7.409
7.396
7.382
7.368
7.309
7.308
7.296
7.283
7.282
7.237


CF3
O
O

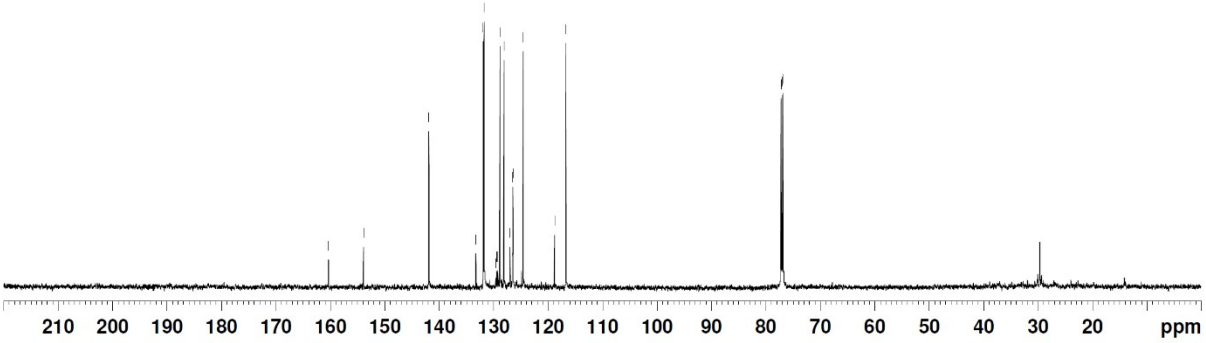
(4j)


10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.02
1.01
1.15
3.42
2.06
1.00

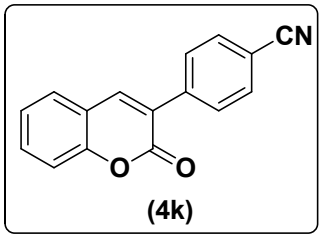

160.36
153.91
141.91
133.27
131.93
131.76
131.73
129.60
129.42
129.22
128.86
128.11
127.00
126.49
126.46
124.60
118.81
116.73
77.21
77.00
76.78


CF3
O
O

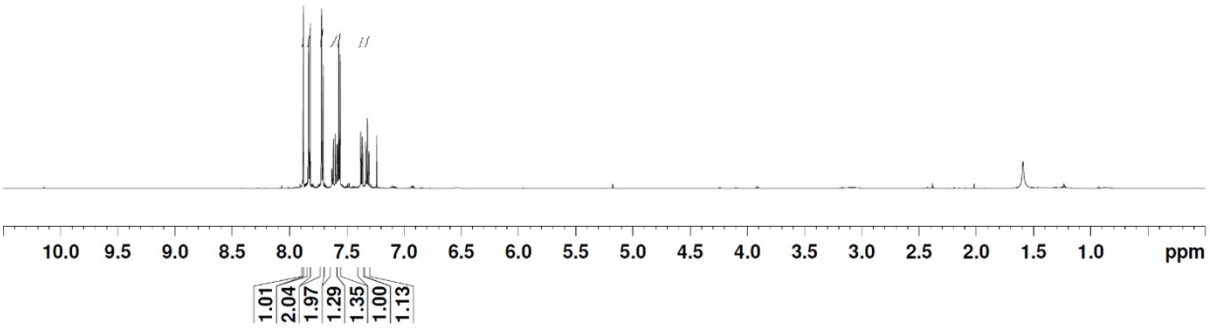
(4j)

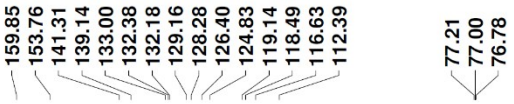

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

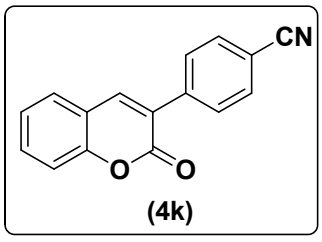

7.880
7.835
7.832
7.824
7.821
7.818
7.721
7.718
7.709
7.707
7.707
7.617
7.600
7.586
7.585
7.584
7.571
7.558
7.378
7.364
7.333
7.332
7.321
7.308
7.306
7.240


CN
O
O

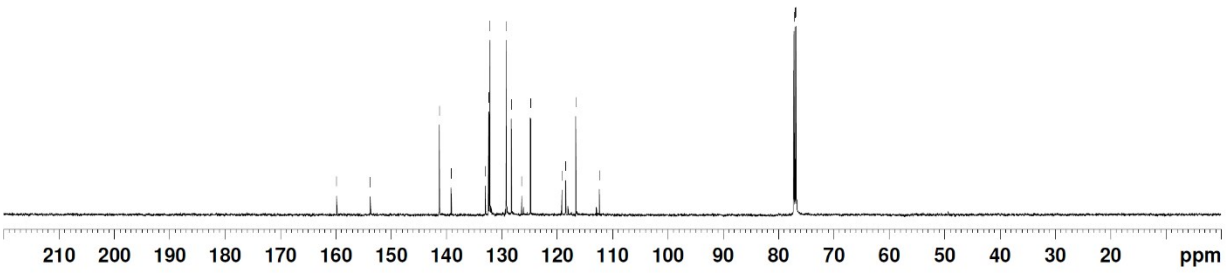
(4k)

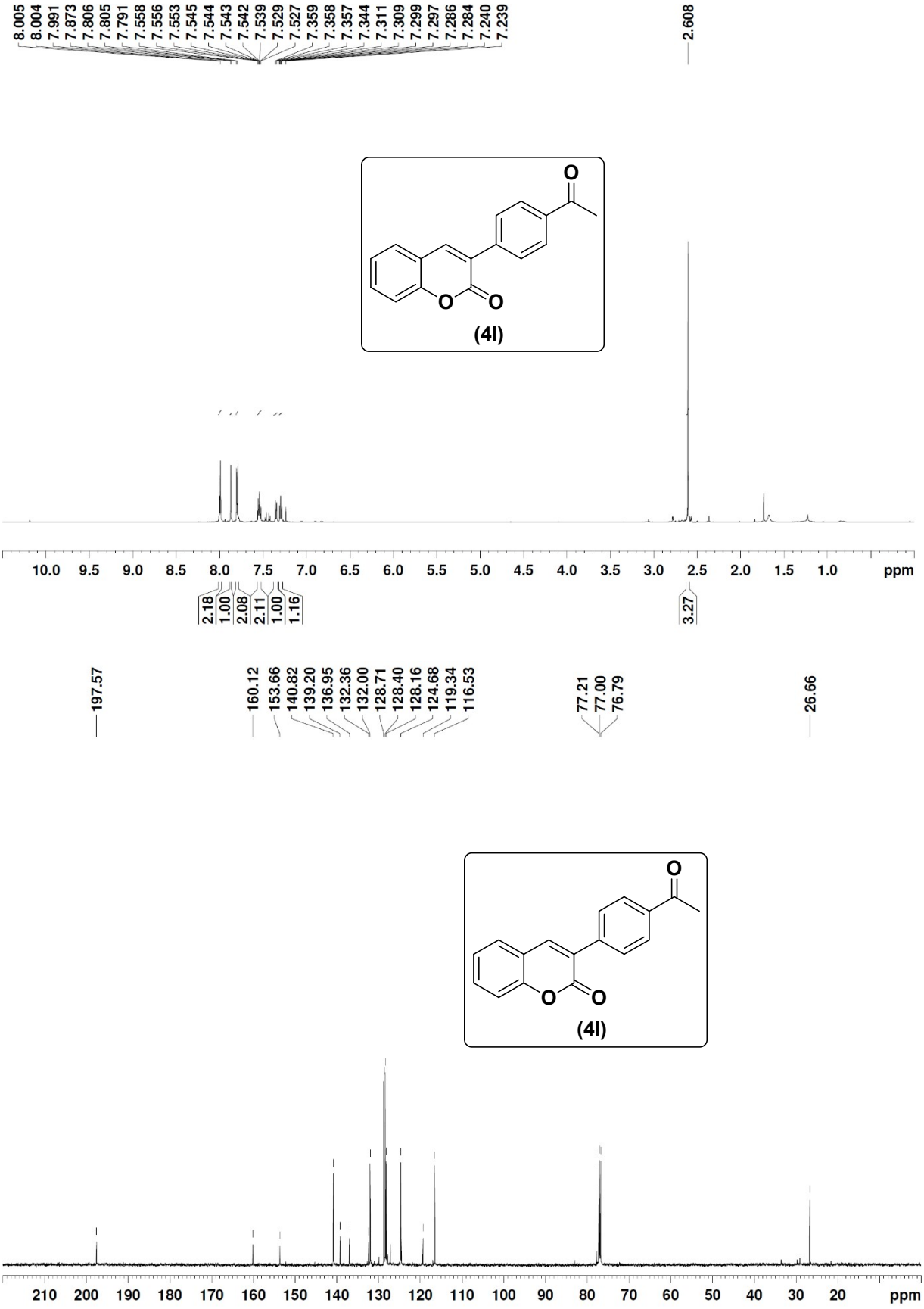

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.01
2.04
1.97
1.29
1.35
1.00
1.13

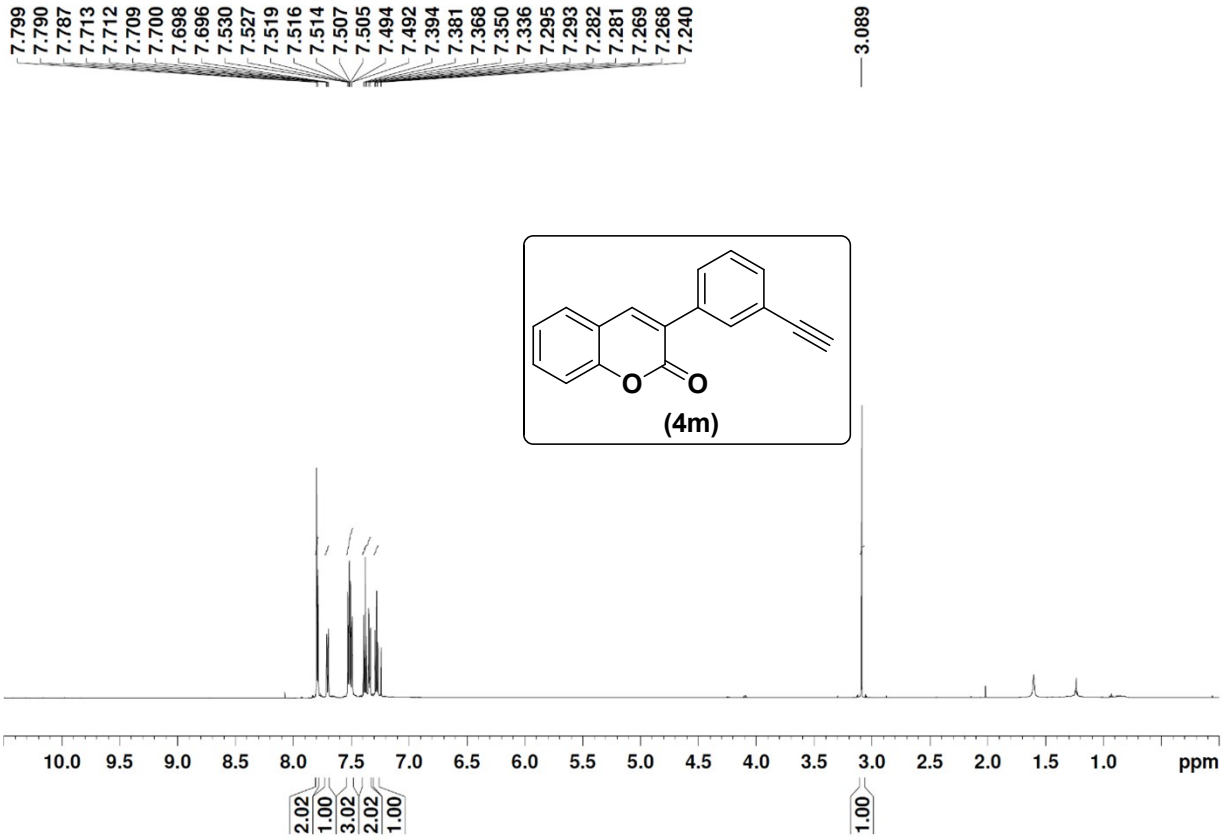

159.85
153.76
141.31
139.14
133.00
132.38
132.18
129.16
128.28
126.40
124.83
119.14
118.49
116.63
112.39
77.21
77.00
76.78

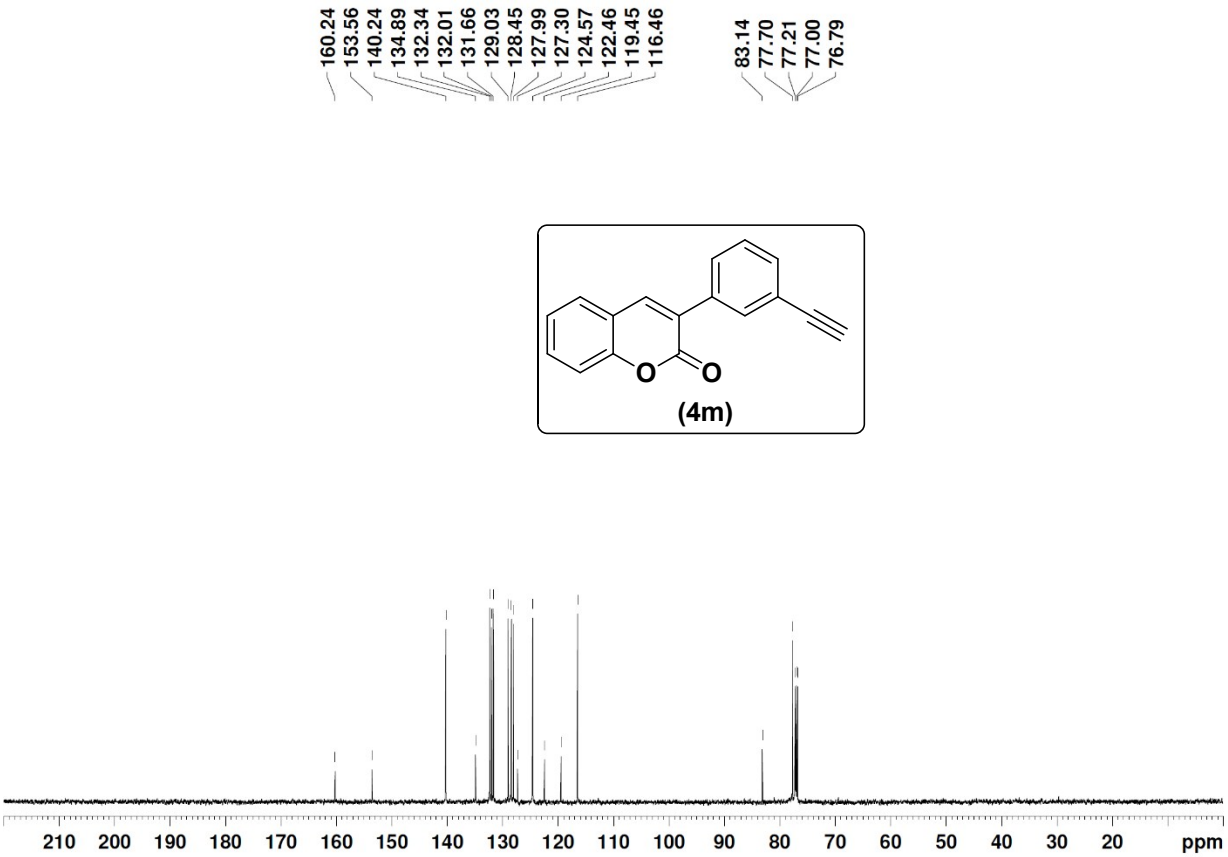

CN
O
O

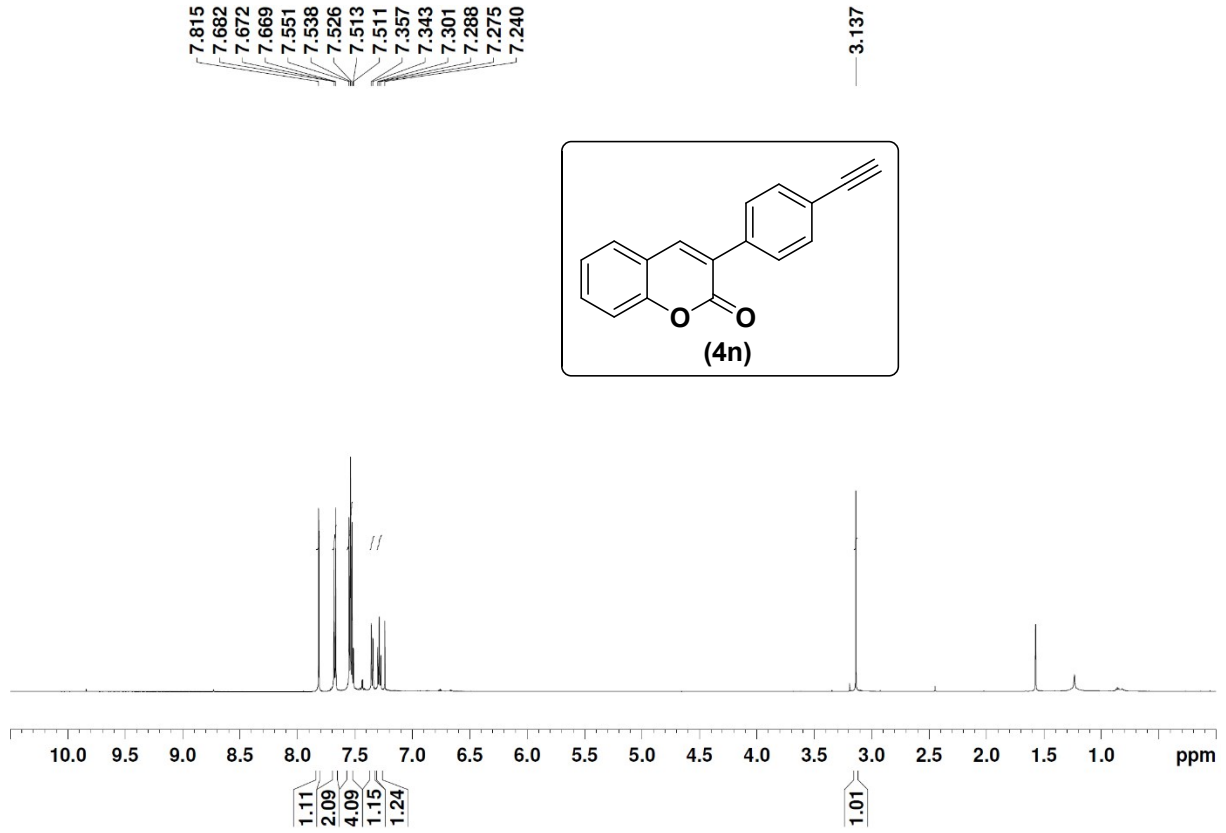
(4k)

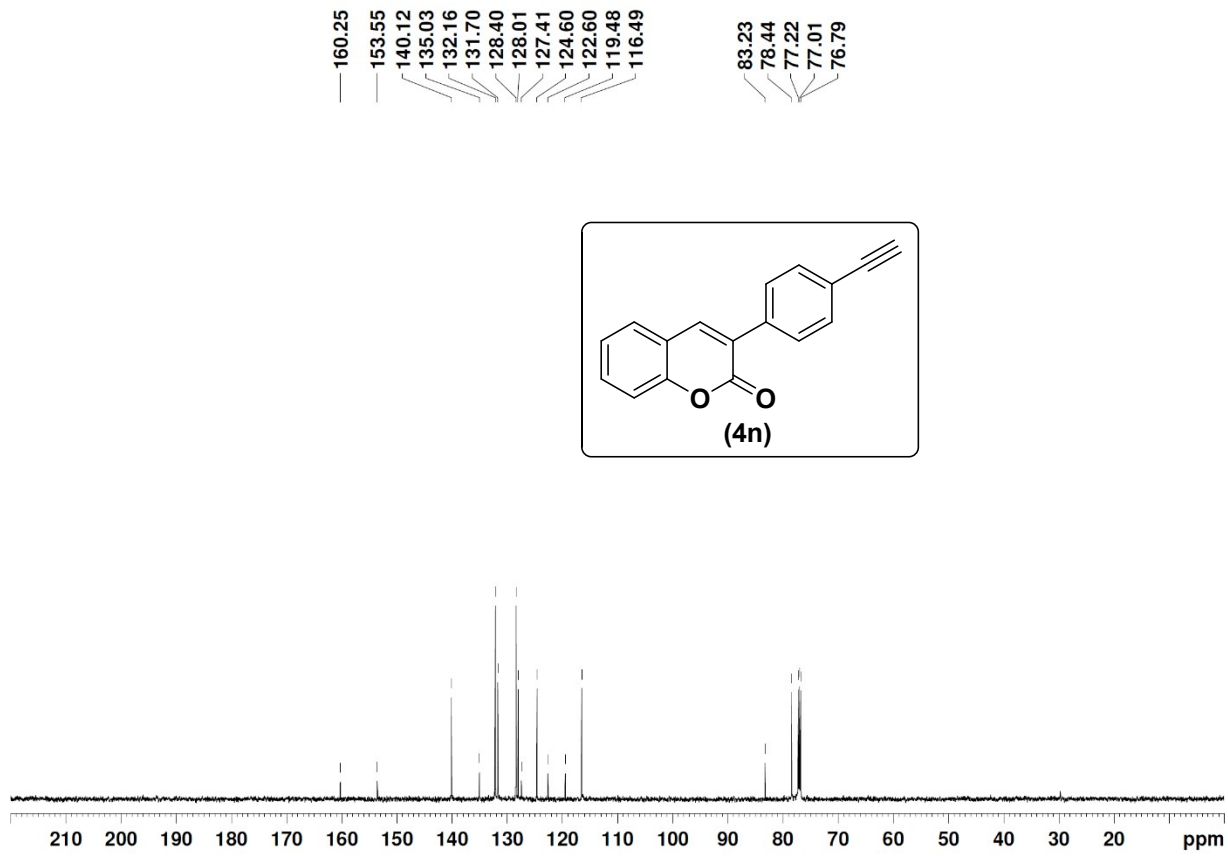

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

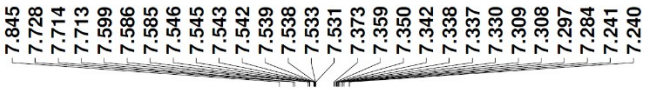

8.005
8.004
7.991
7.873
7.806
7.805
7.791
7.558
7.556
7.553
7.545
7.544
7.543
7.542
7.539
7.529
7.527
7.359
7.358
7.357
7.344
7.311
7.309
7.299
7.297
7.286
7.284
7.240
7.239
2.608
O
O
O
(4l)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.18
1.00
2.08
2.11
1.00
1.16
3.27
197.57
160.12
153.66
140.82
139.20
136.95
132.36
132.00
128.71
128.40
128.16
124.68
119.34
116.53
77.21
77.00
76.79
26.66
O
O
O
(4l)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.799
7.790
7.787
7.713
7.712
7.709
7.700
7.698
7.696
7.530
7.527
7.519
7.516
7.514
7.507
7.505
7.494
7.492
7.394
7.381
7.368
7.350
7.336
7.295
7.293
7.282
7.281
7.269
7.268
7.240
3.089
O
O
(4m)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.02
1.00
3.02
2.02
1.00
1.00


160.24
153.56
140.24
134.89
132.34
132.01
131.66
129.03
128.45
127.99
127.30
124.57
122.46
119.45
116.46
83.14
77.70
77.21
77.00
76.79
O
O
(4m)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.815
7.682
7.672
7.669
7.551
7.538
7.526
7.513
7.511
7.357
7.343
7.301
7.288
7.275
7.240
3.137
(4n)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.11
2.09
4.09
1.15
1.24
1.01


160.25
153.55
140.12
135.03
132.16
131.70
128.40
128.01
127.41
124.60
122.60
119.48
116.49
83.23
78.44
77.22
77.01
76.79
(4n)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.845
7.728
7.714
7.713
7.599
7.586
7.585
7.546
7.545
7.543
7.542
7.539
7.538
7.533
7.531
7.373
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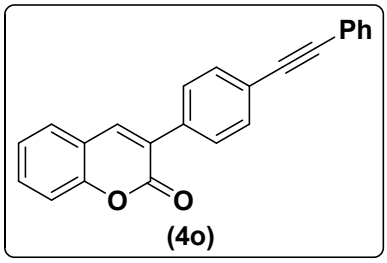
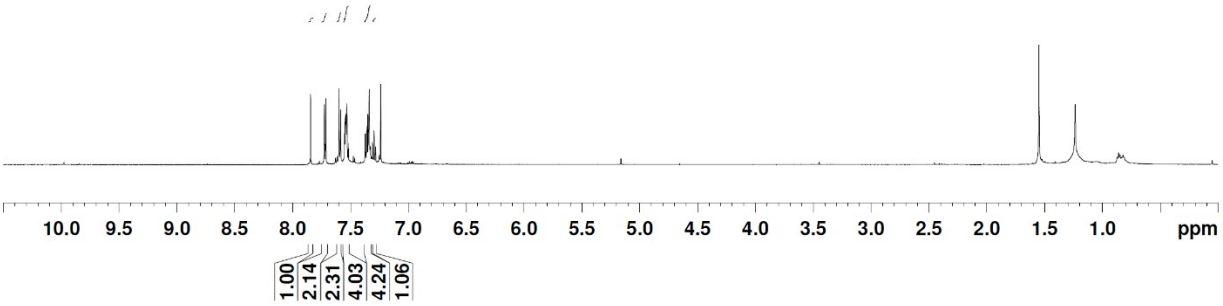
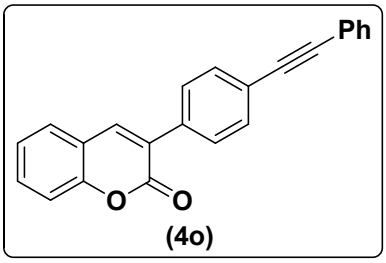
7.309
7.308
7.297
7.284
7.241
7.240


Ph
O
O

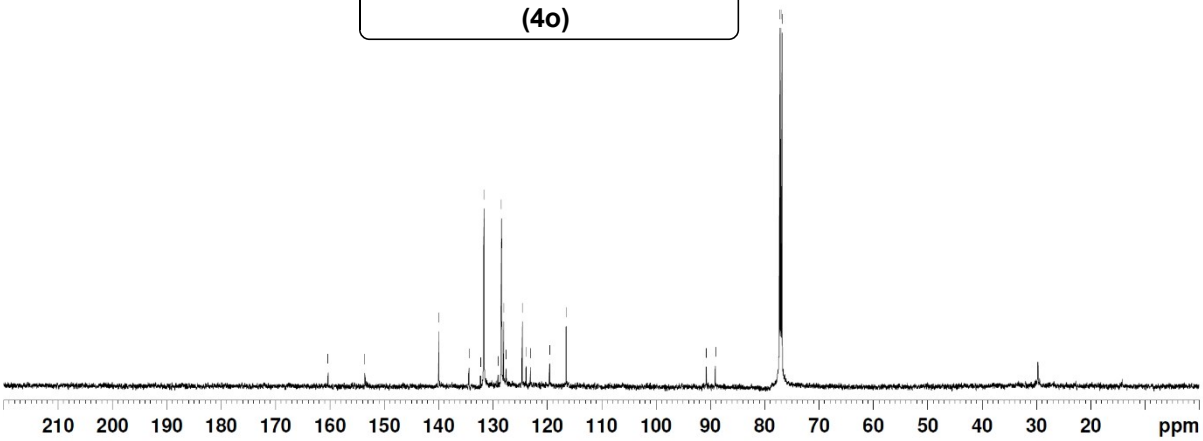
(4o)

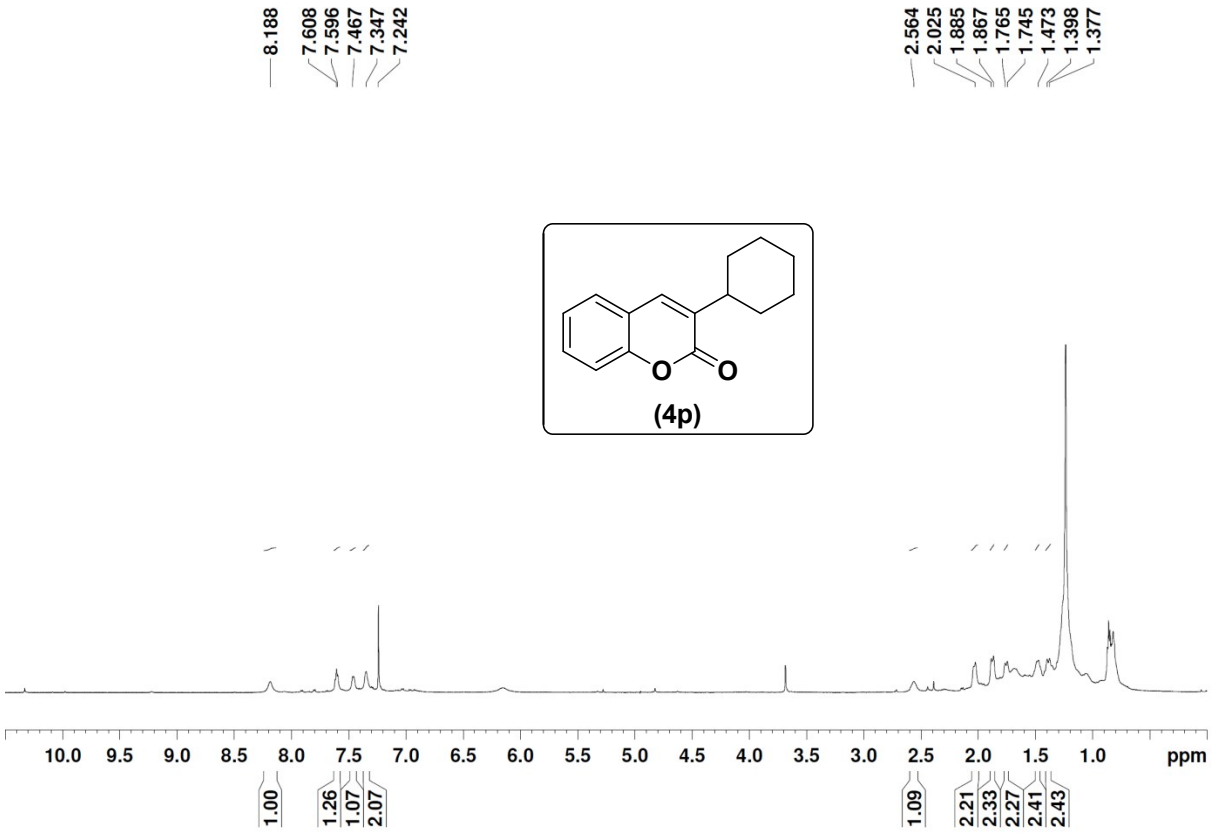

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
2.14
2.31
4.03
4.24
1.06

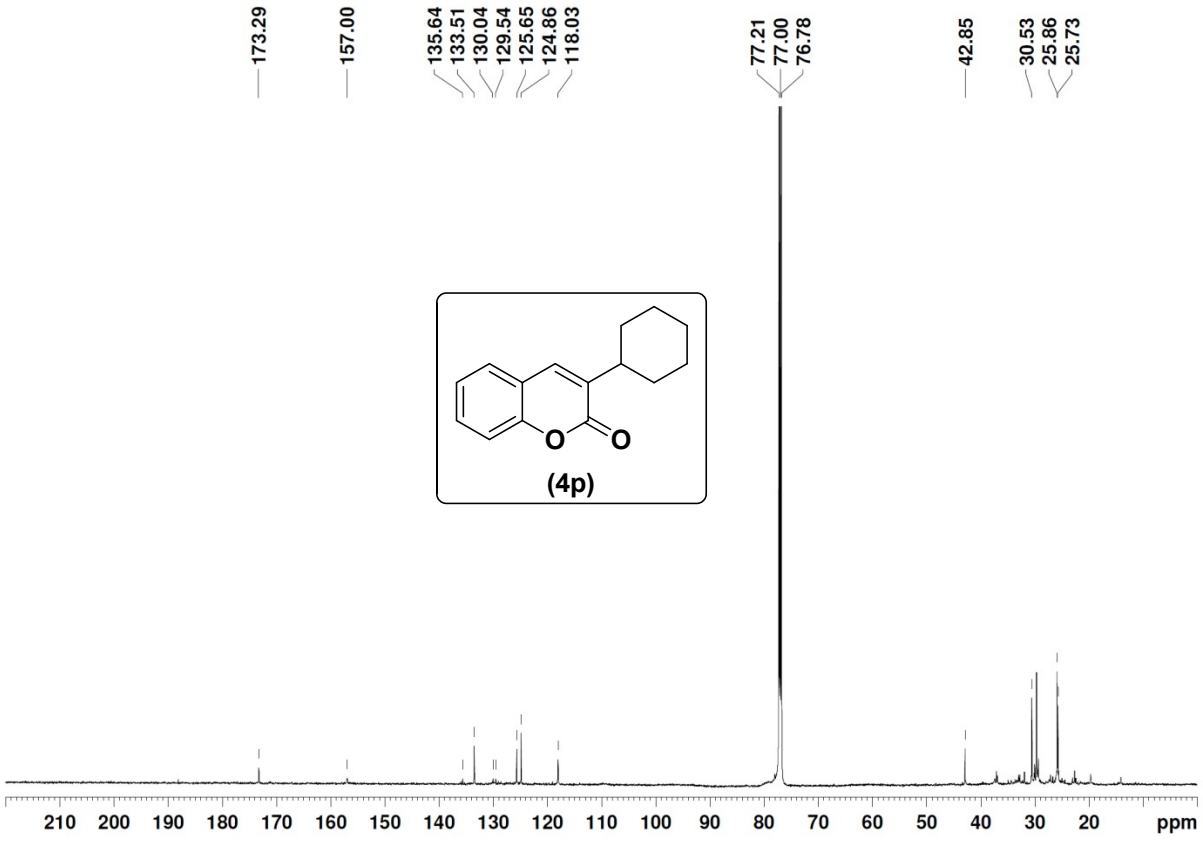

160.33
153.54
139.93
134.42
132.30
131.66
131.64
129.07
128.44
128.37
127.98
127.56
124.59
123.87
123.07
119.58
116.51
90.73
89.06
77.21
77.00
76.78

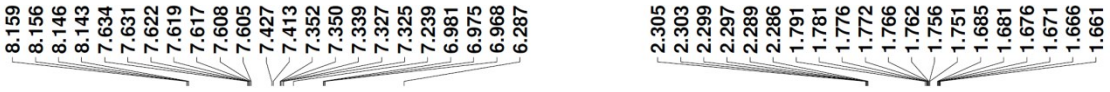

Ph
O
O

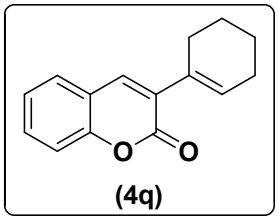
(4o)


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

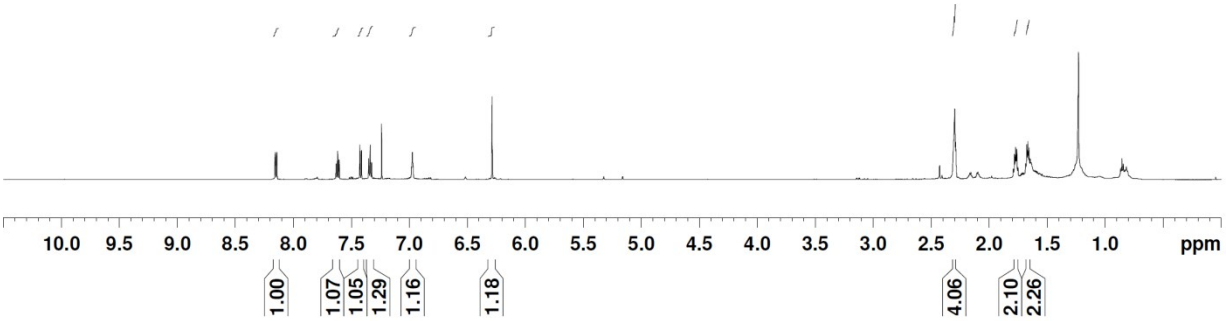

8.188
7.608
7.596
7.467
7.347
7.242
2.564
2.025
1.885
1.867
1.765
1.745
1.473
1.398
1.377
(4p)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.26
1.07
2.07
1.09
2.21
2.33
2.27
2.41
2.43


173.29
157.00
135.64
133.51
130.04
129.54
125.65
124.86
118.03
77.21
77.00
76.78
42.85
30.53
25.86
25.73
(4p)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

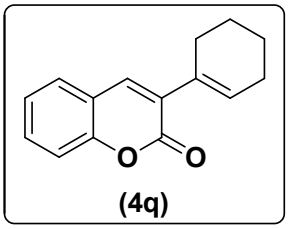

8.159
8.156
8.146
8.143
7.634
7.631
7.622
7.619
7.617
7.608
7.605
7.427
7.413
7.352
7.350
7.339
7.327
7.325
7.239
6.981
6.975
6.968
6.287
2.305
2.303
2.299
2.297
2.289
2.286
1.791
1.781
1.776
1.772
1.766
1.762
1.756
1.751
1.685
1.681
1.676
1.671
1.666
1.661


O
O

(4q)


10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.07
1.05
1.29
1.16
1.18
4.06
2.10
2.26


178.97
163.73
156.00
133.99
133.53
129.83
129.64
129.51
125.54
124.69
123.75
117.78
106.13
77.21
77.00
76.79
25.99
24.15
22.15
21.53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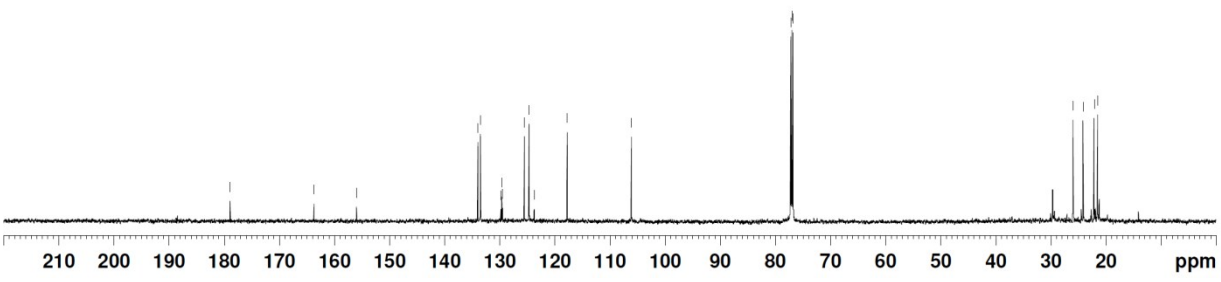
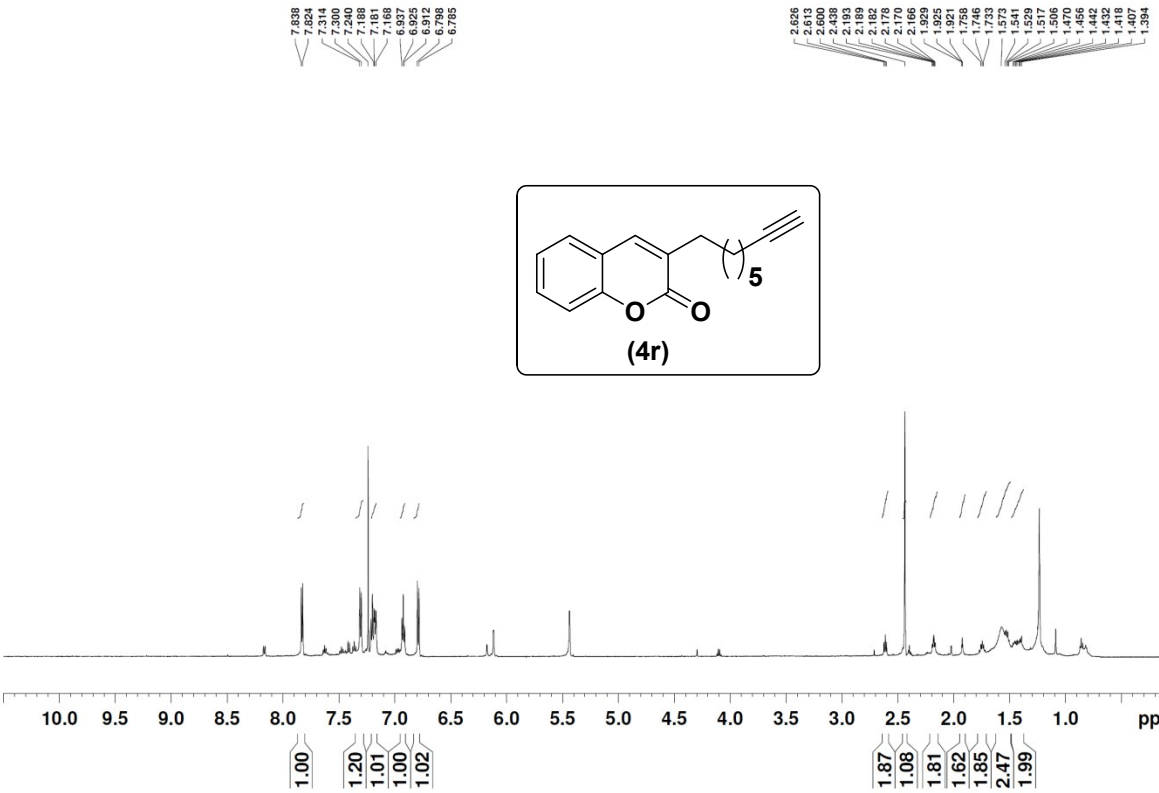
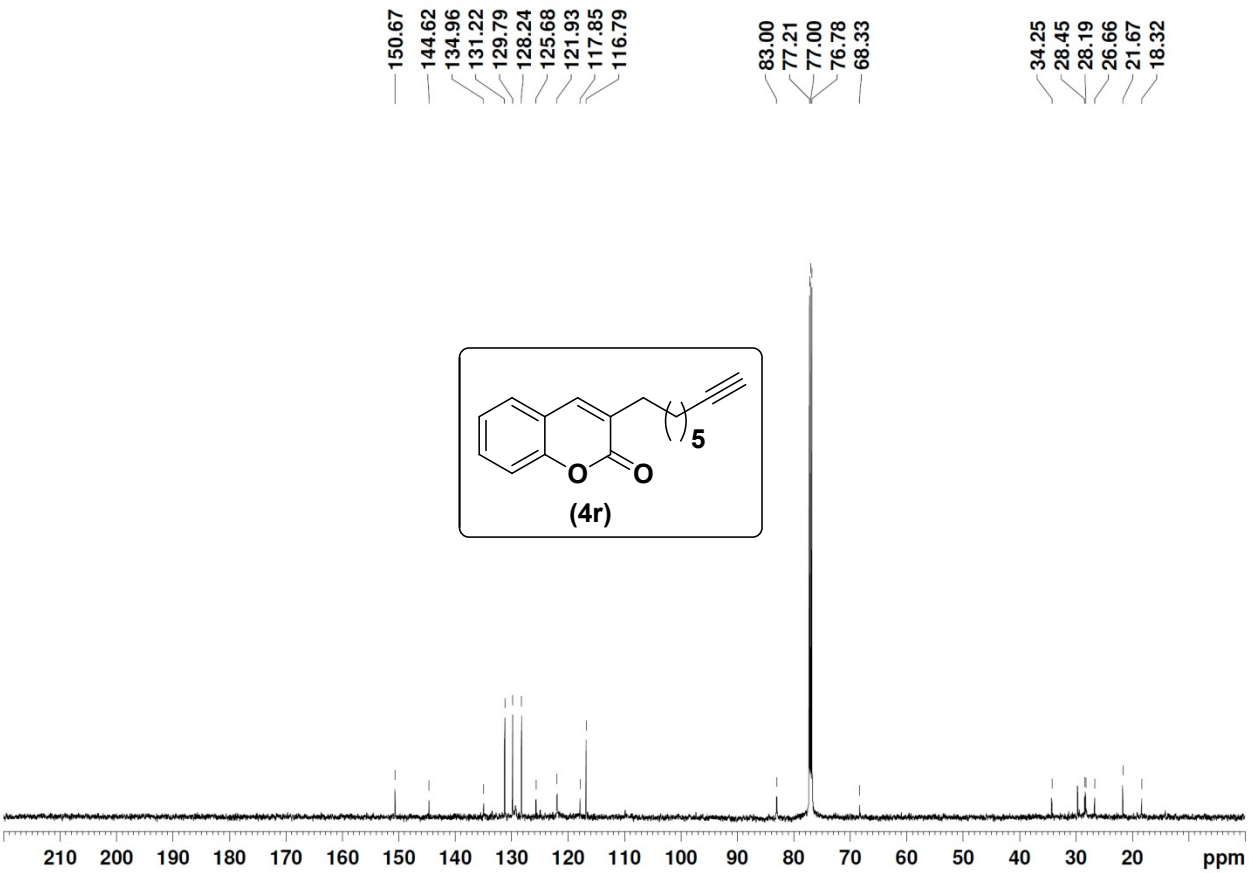
O

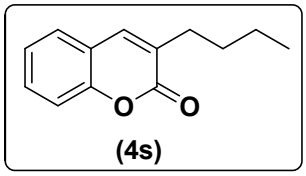
(4q)


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

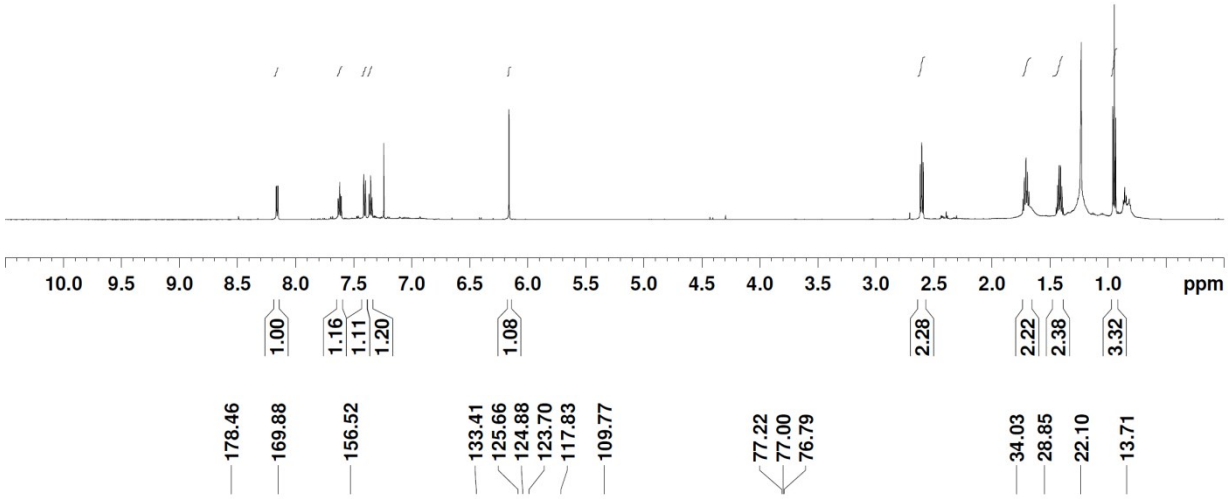

7.838
7.824
7.314
7.300
7.240
7.188
7.181
7.168
6.937
6.925
6.912
6.798
6.785
2.626
2.613
2.600
2.438
2.193
2.189
2.182
2.178
2.170
2.166
1.929
1.925
1.921
1.758
1.746
1.733
1.573
1.541
1.529
1.517
1.506
1.470
1.456
1.442
1.432
1.418
1.407
1.394
5
O
O
(4r)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.20
1.01
1.00
1.02
1.87
1.08
1.81
1.62
1.85
2.47
1.99

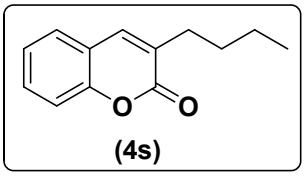

150.67
144.62
134.96
131.22
129.79
128.24
125.68
121.93
117.85
116.79
83.00
77.21
77.00
76.78
68.33
34.25
28.45
28.19
26.66
21.67
18.32
5
O
O
(4r)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.168
8.165
8.155
8.152
7.634
7.632
7.622
7.620
7.617
7.608
7.606
7.412
7.398
7.367
7.366
7.354
7.342
7.341
7.240
6.161
2.618
2.605
2.592
1.733
1.720
1.707
1.695
1.682
1.447
1.435
1.422
1.409
1.397
1.385
0.958
0.946
0.933

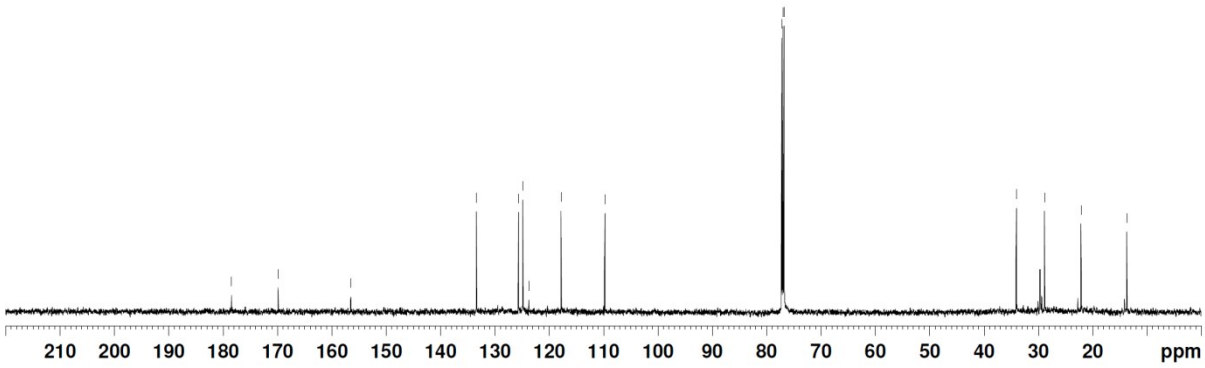

O
O

(4s)


10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.16
1.11
1.20
1.08
2.28
2.22
2.38
3.32
178.46
169.88
156.52
133.41
125.66
124.88
123.70
117.83
109.77
77.22
77.00
76.79
34.03
28.85
22.10
13.71


O
O

(4s)


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.950
7.949
7.947
7.435
7.431
7.421
7.417
7.309
7.294
7.241
6.136
2.605
2.596
2.592
2.583
2.579
2.571
2.422
2.316
2.313
2.289
1.730
1.726
1.716
1.714
1.710
1.704
1.701
1.697
1.688
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1.675
1.430
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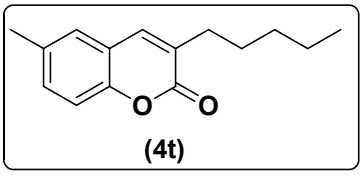
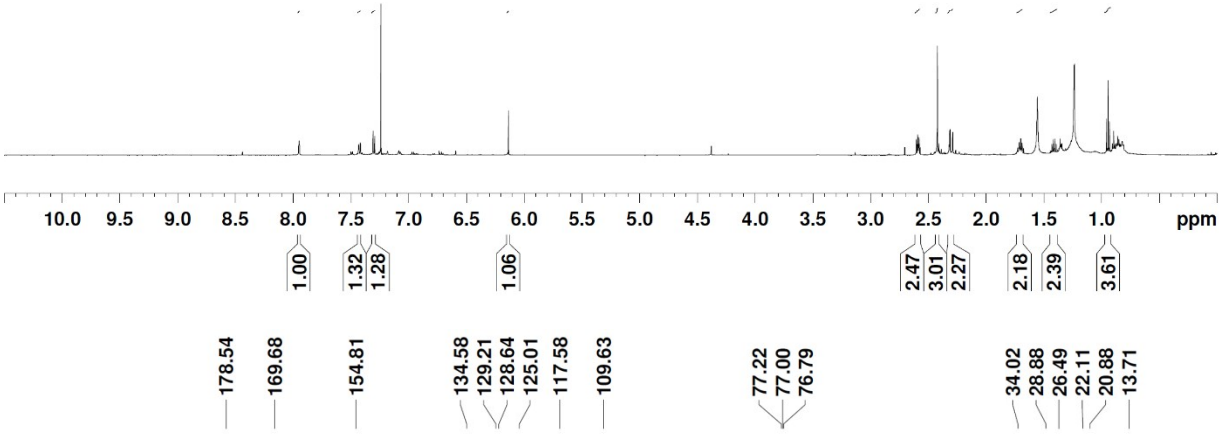
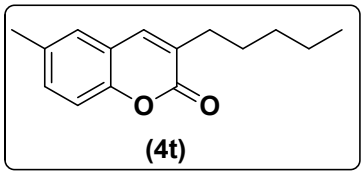
1.405
1.393
1.381
0.956
0.944
0.931


O
O

(4t)


10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.32
1.28
1.06
2.47
3.01
2.27
2.18
2.39
3.61
178.54
169.68
154.81
134.58
129.21
128.64
125.01
117.58
109.63
77.22
77.00
76.79
34.02
28.88
26.49
22.11
20.88
13.71


O
O

(4t)

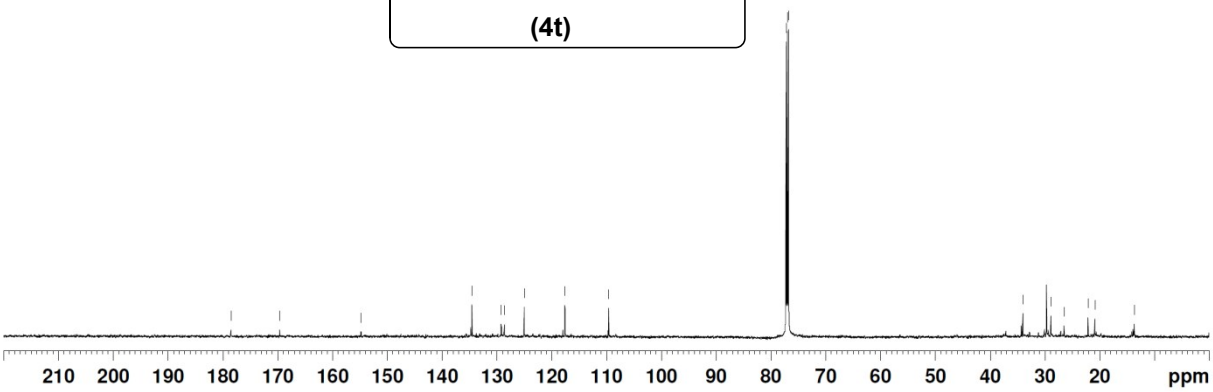
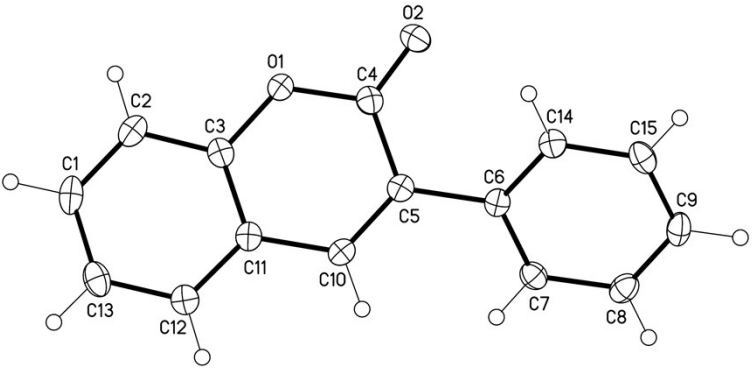

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

Figure S5: ORTEP diagram of compound **3a (CCDC No. 1841164)**



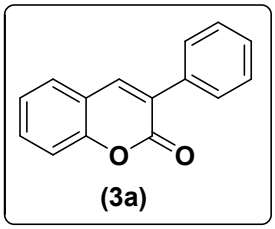


Table S2. Crystal data and structure refinement for 170725LT_0M.

Identification code	170725lt_0m	
Empirical formula	C15 H10 O2	
Formula weight	222.23	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 18.4742(8) Å	a= 90°.
	b = 5.9923(2) Å	b= 98.981(2)°.
	c = 19.2732(9) Å	g = 90°.
Volume	2107.44(15) $Å^3$	
Z	8	
Density (calculated)	1.401 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	928	
Crystal size	0.25 x 0.03 x 0.03 mm^3	
Theta range for data collection	2.140 to 26.395°.	

Index ranges	-22<=h<=22, -7<=k<=5, -24<=l<=24
Reflections collected	8563
Independent reflections	2159 [R(int) = 0.0298]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8877
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2159 / 0 / 154
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0383, wR2 = 0.0945
R indices (all data)	R1 = 0.0495, wR2 = 0.1025
Extinction coefficient	n/a
Largest diff. peak and hole	0.211 and -0.209 e.Å^{-3}

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 170725LT_0M. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4293(1)	2089(2)	5025(1)	18(1)
O(2)	3619(1)	609(2)	4099(1)	24(1)
C(1)	5250(1)	5158(3)	6507(1)	22(1)
C(2)	5072(1)	3484(2)	6015(1)	20(1)
C(3)	4465(1)	3797(2)	5503(1)	16(1)
C(4)	3707(1)	2196(2)	4491(1)	17(1)
C(5)	3253(1)	4220(2)	4437(1)	16(1)
C(6)	2634(1)	4352(2)	3842(1)	16(1)
C(7)	2550(1)	6247(2)	3416(1)	18(1)
C(8)	1988(1)	6357(2)	2844(1)	20(1)
C(9)	1497(1)	4598(2)	2705(1)	20(1)
C(10)	3429(1)	5892(2)	4901(1)	15(1)
C(11)	4041(1)	5732(2)	5461(1)	16(1)
C(12)	4234(1)	7390(2)	5967(1)	19(1)
C(13)	4831(1)	7100(3)	6488(1)	22(1)
C(14)	2138(1)	2598(2)	3697(1)	18(1)

C(15)	1567(1)	2736(2)	3137(1)	20(1)

Table S4. Bond lengths [Å] and angles [°] for 170725LT_0M.

O(1)-C(4)	1.3741(16)
O(1)-C(3)	1.3795(16)
O(2)-C(4)	1.2089(16)
C(1)-C(2)	1.384(2)
C(1)-C(13)	1.394(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.3865(18)
C(2)-H(10)	0.9500
C(3)-C(11)	1.3942(19)
C(4)-C(5)	1.4695(19)
C(5)-C(10)	1.3490(19)
C(5)-C(6)	1.4892(18)
C(6)-C(14)	1.3951(19)
C(6)-C(7)	1.3957(19)
C(7)-C(8)	1.3929(18)
C(7)-H(7)	0.9500
C(8)-C(9)	1.389(2)
C(8)-H(8)	0.9500
C(9)-C(15)	1.387(2)
C(9)-H(2)	0.9500
C(10)-C(11)	1.4392(18)
C(10)-H(5)	0.9500
C(11)-C(12)	1.3993(19)
C(12)-C(13)	1.3815(19)
C(12)-H(3)	0.9500
C(13)-H(4)	0.9500
C(14)-C(15)	1.3876(18)
C(14)-H(6)	0.9500
C(15)-H(9)	0.9500
C(4)-O(1)-C(3)	122.56(10)
C(2)-C(1)-C(13)	120.96(13)
C(2)-C(1)-H(1)	119.5
C(13)-C(1)-H(1)	119.5
C(1)-C(2)-C(3)	118.01(13)

C(1)-C(2)-H(10)	121.0
C(3)-C(2)-H(10)	121.0
O(1)-C(3)-C(2)	116.84(12)
O(1)-C(3)-C(11)	120.63(12)
C(2)-C(3)-C(11)	122.53(13)
O(2)-C(4)-O(1)	116.44(12)
O(2)-C(4)-C(5)	125.82(12)
O(1)-C(4)-C(5)	117.74(11)
C(10)-C(5)-C(4)	119.35(12)
C(10)-C(5)-C(6)	123.24(12)
C(4)-C(5)-C(6)	117.34(12)
C(14)-C(6)-C(7)	119.07(12)
C(14)-C(6)-C(5)	121.03(12)
C(7)-C(6)-C(5)	119.90(12)
C(8)-C(7)-C(6)	120.30(13)
C(8)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(9)-C(8)-C(7)	120.09(13)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(15)-C(9)-C(8)	119.80(13)
C(15)-C(9)-H(2)	120.1
C(8)-C(9)-H(2)	120.1
C(5)-C(10)-C(11)	121.85(12)
C(5)-C(10)-H(5)	119.1
C(11)-C(10)-H(5)	119.1
C(3)-C(11)-C(12)	118.10(12)
C(3)-C(11)-C(10)	117.85(12)
C(12)-C(11)-C(10)	124.05(12)
C(13)-C(12)-C(11)	120.27(13)
C(13)-C(12)-H(3)	119.9
C(11)-C(12)-H(3)	119.9
C(12)-C(13)-C(1)	120.12(13)
C(12)-C(13)-H(4)	119.9
C(1)-C(13)-H(4)	119.9
C(15)-C(14)-C(6)	120.44(13)

C(15)-C(14)-H(6)	119.8
C(6)-C(14)-H(6)	119.8
C(9)-C(15)-C(14)	120.27(13)
C(9)-C(15)-H(9)	119.9
C(14)-C(15)-H(9)	119.9

Symmetry transformations used to generate equivalent atoms:

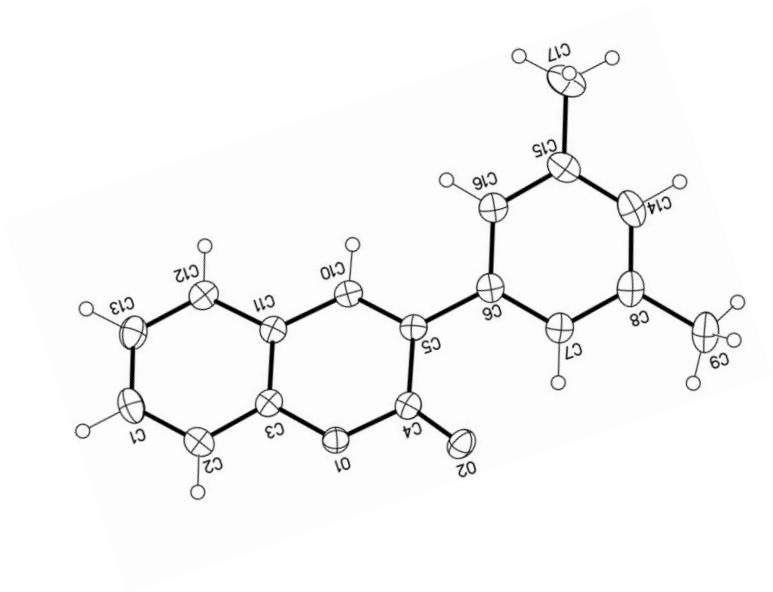
Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 170725LT_0M. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	18(1)	18(1)	18(1)	0(1)	0(1)	2(1)
O(2)	25(1)	19(1)	28(1)	-5(1)	0(1)	0(1)
C(1)	16(1)	35(1)	16(1)	3(1)	0(1)	-4(1)
C(2)	16(1)	24(1)	20(1)	6(1)	4(1)	2(1)
C(3)	16(1)	20(1)	14(1)	1(1)	5(1)	-4(1)
C(4)	17(1)	18(1)	17(1)	1(1)	4(1)	-3(1)
C(5)	14(1)	17(1)	15(1)	2(1)	5(1)	-2(1)
C(6)	14(1)	20(1)	14(1)	0(1)	4(1)	1(1)
C(7)	17(1)	18(1)	18(1)	-2(1)	4(1)	-1(1)
C(8)	22(1)	22(1)	16(1)	2(1)	4(1)	5(1)
C(9)	16(1)	29(1)	14(1)	-3(1)	1(1)	4(1)
C(10)	15(1)	17(1)	15(1)	3(1)	5(1)	1(1)
C(11)	14(1)	19(1)	14(1)	2(1)	5(1)	-2(1)
C(12)	18(1)	21(1)	17(1)	0(1)	4(1)	-1(1)
C(13)	22(1)	28(1)	16(1)	-2(1)	4(1)	-6(1)
C(14)	18(1)	19(1)	16(1)	1(1)	4(1)	-1(1)
C(15)	16(1)	24(1)	19(1)	-6(1)	5(1)	-4(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 170725LT_0M.

	x	y	z	U(eq)
H(1)	5663	4981	6863	27
H(10)	5357	2161	6028	24
H(7)	2878	7468	3516	21
H(8)	1940	7636	2549	24
H(2)	1114	4671	2314	24
H(5)	3141	7213	4857	18
H(3)	3952	8721	5953	22
H(4)	4957	8225	6833	26
H(6)	2190	1300	3983	21
H(9)	1224	1550	3050	24

Figure S6: ORTEP diagram of compound **4f (CCDC No**. **1841166)**



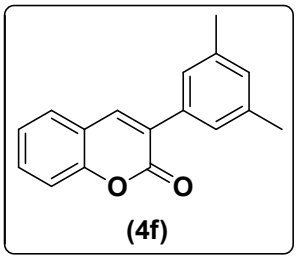


Table S7. Crystal data and structure refinement for 170926LT_0M_A.

Identification code	170926lt_0m_a	
Empirical formula	C17 H14 O2	
Formula weight	250.28	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 13.4167(12) Å	a= 90°.
	b = 7.2031(8) Å	b= 106.425(5)°.
	c = 13.9328(15) Å	g = 90°.
Volume	1291.5(2) $Å^3$	
Z	4	
Density (calculated)	1.287 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	528	

Crystal size	? x ? x ? mm^3
Theta range for data collection	1.861 to 26.450°.
Index ranges	-16<=h<=16, -6<=k<=8, -16<=l<=17
Reflections collected	7027
Independent reflections	2464 [R(int) = 0.0239]
Completeness to theta = 25.000°	93.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2464 / 0 / 174
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.1065
R indices (all data)	R1 = 0.0540, wR2 = 0.1166
Extinction coefficient	n/a
Largest diff. peak and hole	0.259 and -0.175 $e.Å^{-3}$

Table S8. Atomic coordinates (1×10^4) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for 170926LT_0M_A. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4265(1)	9144(2)	919(1)	21(1)
O(2)	2585(1)	9561(2)	306(1)	26(1)
C(1)	6971(1)	8446(2)	2254(1)	29(1)
C(2)	6090(1)	8944(2)	1508(1)	24(1)
C(3)	5132(1)	8632(2)	1671(1)	19(1)
C(4)	3270(1)	9015(2)	1013(1)	19(1)
C(5)	3149(1)	8212(2)	1942(1)	19(1)
C(6)	2094(1)	8085(2)	2081(1)	20(1)
C(7)	1218(1)	7618(2)	1298(1)	22(1)
C(8)	242(1)	7482(2)	1457(1)	25(1)
C(9)	-705(1)	6999(3)	606(1)	34(1)
C(10)	4000(1)	7618(2)	2650(1)	20(1)
C(11)	5029(1)	7832(2)	2548(1)	19(1)
C(12)	5938(1)	7308(2)	3282(1)	23(1)
C(13)	6900(1)	7631(2)	3138(1)	27(1)
C(14)	150(1)	7827(2)	2408(1)	27(1)
C(15)	1003(1)	8300(2)	3201(1)	24(1)
C(16)	1975(1)	8414(2)	3027(1)	22(1)
C(17)	882(1)	8754(3)	4220(1)	35(1)

Table S9. Bond lengths [Å] and angles [°] for 170926LT_0M_A.

O(1)-C(3)	1.3780(16)
O(1)-C(4)	1.3808(16)
O(2)-C(4)	1.2081(16)
C(1)-C(2)	1.383(2)
C(1)-C(13)	1.391(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.3855(19)
C(2)-H(14)	0.9500
C(3)-C(11)	1.392(2)
C(4)-C(5)	1.4680(19)
C(5)-C(10)	1.3500(19)
C(5)-C(6)	1.4849(18)
C(6)-C(16)	1.392(2)
C(6)-C(7)	1.3999(19)
C(7)-C(8)	1.3926(19)
C(7)-H(13)	0.9500
C(8)-C(14)	1.387(2)
C(8)-C(9)	1.513(2)
C(9)-H(2)	0.9800
C(9)-H(11)	0.9800
C(9)-H(12)	0.9800
C(10)-C(11)	1.4355(18)
C(10)-H(5)	0.9500
C(11)-C(12)	1.4043(19)
C(12)-C(13)	1.381(2)
C(12)-H(4)	0.9500
C(13)-H(3)	0.9500
C(14)-C(15)	1.390(2)
C(14)-H(10)	0.9500
C(15)-C(16)	1.3943(19)
C(15)-C(17)	1.509(2)
C(16)-H(6)	0.9500
C(17)-H(7)	0.9800
C(17)-H(9)	0.9800

C(17)-H(8)	0.9800
C(3)-O(1)-C(4)	122.73(11)
C(2)-C(1)-C(13)	121.12(13)
C(2)-C(1)-H(1)	119.4
C(13)-C(1)-H(1)	119.4
C(1)-C(2)-C(3)	118.00(14)
C(1)-C(2)-H(14)	121.0
C(3)-C(2)-H(14)	121.0
O(1)-C(3)-C(2)	117.03(13)
O(1)-C(3)-C(11)	120.39(12)
C(2)-C(3)-C(11)	122.58(13)
O(2)-C(4)-O(1)	115.70(12)
O(2)-C(4)-C(5)	126.81(12)
O(1)-C(4)-C(5)	117.48(11)
C(10)-C(5)-C(4)	119.16(12)
C(10)-C(5)-C(6)	121.71(13)
C(4)-C(5)-C(6)	119.13(12)
C(16)-C(6)-C(7)	118.90(13)
C(16)-C(6)-C(5)	118.84(12)
C(7)-C(6)-C(5)	122.26(13)
C(8)-C(7)-C(6)	120.83(14)
C(8)-C(7)-H(13)	119.6
C(6)-C(7)-H(13)	119.6
C(14)-C(8)-C(7)	118.73(14)
C(14)-C(8)-C(9)	120.58(13)
C(7)-C(8)-C(9)	120.68(14)
C(8)-C(9)-H(2)	109.5
C(8)-C(9)-H(11)	109.5
H(2)-C(9)-H(11)	109.5
C(8)-C(9)-H(12)	109.5
H(2)-C(9)-H(12)	109.5
H(11)-C(9)-H(12)	109.5
C(5)-C(10)-C(11)	122.14(13)
C(5)-C(10)-H(5)	118.9
C(11)-C(10)-H(5)	118.9
C(3)-C(11)-C(12)	117.97(12)

C(3)-C(11)-C(10)	117.94(12)
C(12)-C(11)-C(10)	124.09(13)
C(13)-C(12)-C(11)	120.24(14)
C(13)-C(12)-H(4)	119.9
C(11)-C(12)-H(4)	119.9
C(12)-C(13)-C(1)	120.07(14)
C(12)-C(13)-H(3)	120.0
C(1)-C(13)-H(3)	120.0
C(8)-C(14)-C(15)	121.89(13)
C(8)-C(14)-H(10)	119.1
C(15)-C(14)-H(10)	119.1
C(14)-C(15)-C(16)	118.41(14)
C(14)-C(15)-C(17)	121.20(13)
C(16)-C(15)-C(17)	120.35(14)
C(6)-C(16)-C(15)	121.23(14)
C(6)-C(16)-H(6)	119.4
C(15)-C(16)-H(6)	119.4
C(15)-C(17)-H(7)	109.5
C(15)-C(17)-H(9)	109.5
H(7)-C(17)-H(9)	109.5
C(15)-C(17)-H(8)	109.5
H(7)-C(17)-H(8)	109.5
H(9)-C(17)-H(8)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 170926LT_0M_A. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

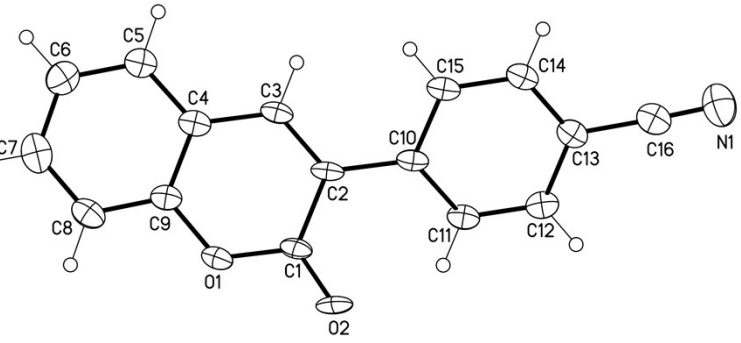
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	22(1)	21(1)	20(1)	2(1)	6(1)	0(1)
O(2)	25(1)	26(1)	22(1)	5(1)	2(1)	-1(1)
C(1)	22(1)	27(1)	40(1)	-2(1)	12(1)	2(1)
C(2)	27(1)	18(1)	28(1)	0(1)	12(1)	1(1)

C(3)	23(1)	13(1)	21(1)	-2(1)	4(1)	1(1)
C(4)	22(1)	13(1)	22(1)	-2(1)	5(1)	-2(1)
C(5)	23(1)	12(1)	21(1)	-3(1)	6(1)	-2(1)
C(6)	23(1)	11(1)	26(1)	4(1)	6(1)	2(1)
C(7)	24(1)	16(1)	26(1)	3(1)	6(1)	1(1)
C(8)	22(1)	14(1)	37(1)	7(1)	4(1)	2(1)
C(9)	22(1)	30(1)	46(1)	7(1)	2(1)	-1(1)
C(10)	25(1)	14(1)	21(1)	0(1)	6(1)	-1(1)
C(11)	22(1)	13(1)	22(1)	-2(1)	6(1)	0(1)
C(12)	26(1)	17(1)	24(1)	0(1)	5(1)	2(1)
C(13)	23(1)	23(1)	32(1)	0(1)	3(1)	5(1)
C(14)	23(1)	17(1)	44(1)	11(1)	14(1)	6(1)
C(15)	32(1)	13(1)	32(1)	8(1)	15(1)	6(1)
C(16)	25(1)	14(1)	26(1)	5(1)	7(1)	2(1)
C(17)	44(1)	28(1)	40(1)	6(1)	24(1)	6(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 170926LT_0M_A.

	x	y	z	U(eq)
H(1)	7637	8663	2162	35
H(14)	6140	9485	901	29
H(13)	1291	7390	650	27
H(2)	-1139	6115	842	51
H(11)	-484	6439	58	51
H(12)	-1104	8128	366	51
H(5)	3915	7040	3235	24
H(4)	5891	6730	3881	27
H(3)	7514	7296	3642	32
H(10)	-514	7736	2521	33
H(6)	2566	8721	3564	26
H(7)	804	10098	4278	52
H(9)	1499	8333	4739	52
H(8)	266	8124	4306	52

Figure S7: ORTEP diagram of compound **4k (CCDC No. 1841165)**



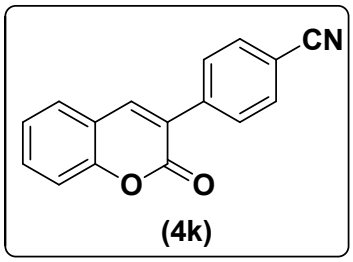


Table S12. Crystal data and structure refinement for 170811LT_A.

Identification code	170811LT_a	
Empirical formula	C16 H9 N O2	
Formula weight	247.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 13.795(7) Å	a= 90°.
	b = 7.246(4) Å	b= 105.255(11)°.
	c = 12.168(6) Å	g = 90°.
Volume	1173.5(10) $Å^3$	
Z	4	
Density (calculated)	1.399 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	512	
Crystal size	0.15 x 0.05 x 0.05 mm^3	
Theta range for data collection	1.530 to 26.396°.	

Index ranges	-17<=h<=17, -8<=k<=9, -15<=l<=14
Reflections collected	10299
Independent reflections	2329 [R(int) = 0.0741]
Completeness to theta = 25.242°	98.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.7321
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2329 / 0 / 173
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0912, wR2 = 0.2398
R indices (all data)	R1 = 0.1394, wR2 = 0.2722
Extinction coefficient	0.028(8)
Largest diff. peak and hole	0.604 and -0.371 e.$Å^{-3}$

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 170811LT_A. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4468(3)	6715(5)	8646(4)	20(1)
C(2)	4936(3)	6214(5)	7729(3)	18(1)
C(3)	4328(3)	5868(5)	6682(3)	20(1)
C(4)	3259(3)	5944(5)	6438(4)	21(1)
C(5)	2608(3)	5645(5)	5351(4)	26(1)
C(6)	1587(3)	5754(5)	5188(4)	31(1)
C(7)	1190(3)	6159(6)	6099(4)	33(1)
C(8)	1810(3)	6449(5)	7176(4)	27(1)
C(9)	2829(3)	6356(5)	7328(4)	21(1)
C(10)	6044(3)	6185(5)	7983(3)	18(1)
C(11)	6655(3)	5554(5)	9017(4)	21(1)
C(12)	7684(3)	5523(5)	9224(4)	24(1)
C(13)	8130(3)	6126(5)	8372(4)	23(1)
C(14)	7531(3)	6766(5)	7338(4)	23(1)
C(15)	6504(3)	6783(5)	7133(4)	21(1)
C(16)	9196(3)	6053(5)	8557(4)	30(1)
N(1)	10054(3)	5978(6)	8678(4)	46(1)

O(1)	3439(2)	6691(4)	8403(2)	23(1)
O(2)	4916(2)	7163(4)	9604(2)	27(1)

Table S14. Bond lengths [Å] and angles [°] for 170811LT_A.

C(1)-O(2)	1.212(5)
C(1)-O(1)	1.372(5)
C(1)-C(2)	1.474(5)
C(2)-C(3)	1.352(6)
C(2)-C(10)	1.477(5)
C(3)-C(4)	1.427(5)
C(3)-H(3)	0.9500
C(4)-C(9)	1.396(6)
C(4)-C(5)	1.406(6)
C(5)-C(6)	1.372(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.391(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.380(7)
C(7)-H(7)	0.9500
C(8)-C(9)	1.371(5)
C(8)-H(8)	0.9500
C(9)-O(1)	1.378(5)
C(10)-C(11)	1.395(6)
C(10)-C(15)	1.416(5)
C(11)-C(12)	1.374(5)
C(11)-H(11)	0.9500
C(12)-C(13)	1.408(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.390(6)
C(13)-C(16)	1.429(6)
C(14)-C(15)	1.372(5)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-N(1)	1.154(5)
O(2)-C(1)-O(1)	116.6(3)
O(2)-C(1)-C(2)	125.5(3)
O(1)-C(1)-C(2)	118.0(4)
C(3)-C(2)-C(1)	118.2(3)

C(3)-C(2)-C(10)	123.1(3)
C(1)-C(2)-C(10)	118.7(3)
C(2)-C(3)-C(4)	122.7(4)
C(2)-C(3)-H(3)	118.7
C(4)-C(3)-H(3)	118.7
C(9)-C(4)-C(5)	117.8(4)
C(9)-C(4)-C(3)	118.3(4)
C(5)-C(4)-C(3)	124.0(4)
C(6)-C(5)-C(4)	120.3(4)
C(6)-C(5)-H(5)	119.9
C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(7)	120.1(4)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	120.9(4)
C(8)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
C(9)-C(8)-C(7)	118.6(4)
C(9)-C(8)-H(8)	120.7
C(7)-C(8)-H(8)	120.7
C(8)-C(9)-O(1)	117.9(3)
C(8)-C(9)-C(4)	122.4(4)
O(1)-C(9)-C(4)	119.7(3)
C(11)-C(10)-C(15)	118.6(4)
C(11)-C(10)-C(2)	122.7(3)
C(15)-C(10)-C(2)	118.7(4)
C(12)-C(11)-C(10)	121.4(4)
C(12)-C(11)-H(11)	119.3
C(10)-C(11)-H(11)	119.3
C(11)-C(12)-C(13)	119.4(4)
C(11)-C(12)-H(12)	120.3
C(13)-C(12)-H(12)	120.3
C(14)-C(13)-C(12)	119.9(4)
C(14)-C(13)-C(16)	119.8(4)
C(12)-C(13)-C(16)	120.3(4)
C(15)-C(14)-C(13)	120.5(4)

C(15)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(14)-C(15)-C(10)	120.2(4)
C(14)-C(15)-H(15)	119.9
C(10)-C(15)-H(15)	119.9
N(1)-C(16)-C(13)	178.2(5)
C(1)-O(1)-C(9)	123.0(3)

Symmetry transformations used to generate equivalent atoms:

Table S15. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 170811LT_A. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	31(2)	15(2)	18(2)	6(2)	14(2)	3(2)
C(2)	34(2)	9(2)	15(2)	1(1)	13(2)	2(1)
C(3)	32(2)	12(2)	19(2)	2(2)	14(2)	1(1)
C(4)	32(2)	10(2)	23(2)	2(2)	12(2)	0(2)
C(5)	32(2)	22(2)	27(3)	-1(2)	10(2)	-2(2)
C(6)	36(2)	22(2)	33(3)	-3(2)	6(2)	-7(2)
C(7)	29(2)	21(2)	50(3)	4(2)	11(2)	1(2)
C(8)	34(2)	19(2)	33(3)	5(2)	18(2)	2(2)
C(9)	30(2)	12(2)	21(2)	4(2)	10(2)	0(1)
C(10)	32(2)	9(2)	17(2)	-3(1)	12(2)	-2(1)
C(11)	33(2)	12(2)	21(2)	4(2)	12(2)	-1(1)
C(12)	34(2)	15(2)	22(2)	2(2)	8(2)	1(2)
C(13)	29(2)	15(2)	27(3)	-4(2)	12(2)	-2(2)
C(14)	31(2)	16(2)	25(2)	-4(2)	14(2)	-5(2)
C(15)	34(2)	12(2)	20(2)	0(2)	13(2)	0(1)
C(16)	36(3)	23(2)	33(3)	1(2)	14(2)	0(2)
N(1)	35(2)	45(2)	59(3)	5(2)	15(2)	-2(2)
O(1)	30(2)	23(1)	21(2)	1(1)	14(1)	3(1)
O(2)	43(2)	28(2)	12(2)	-4(1)	11(1)	3(1)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 170811LT_A.

	x	y	z	U(eq)
H(3)	4625	5562	6084	23
H(5)	2877	5367	4727	32
H(6)	1151	5552	4452	37
H(7)	482	6238	5978	40
H(8)	1536	6707	7799	32
H(11)	6355	5137	9591	25
H(12)	8090	5099	9936	28
H(14)	7835	7195	6770	27
H(15)	6100	7197	6417	25