Supporting Information

Photoredox Synthesis of Functionalized Quinazolines via Copper-catalyzed Aerobic Oxidative C_{sp2}-H Annulation of Amidines with Terminal alkynes

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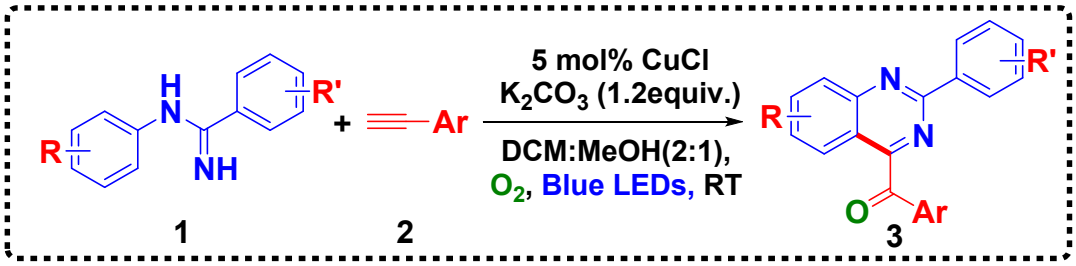
Experimental section

General procedure: All reactions were conducted in oven-dried glass wares. All reactions were conducted using a blue light-emitting diode (LED) array (30 lamps, power density: 40 mW/cm^2 at 460 nm) 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 solvents (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 2,4-disubstituted quinazolines:

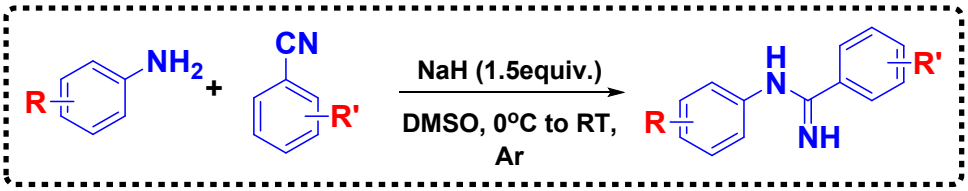
Scheme S1: Current photochemical process for the synthesis of 2,4-disubstituted quinazolines



A dry test tube (20 mL) containing 5 mol% CuCl, was added amidines (0.2 mmol), 6 mL of dry solvent (DCM: MeOH = 2:1), and terminal acetylene (0.4 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 2 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 product.

General procedure for the preparation of starting materials (N-phenylbenzimidamide substrates):

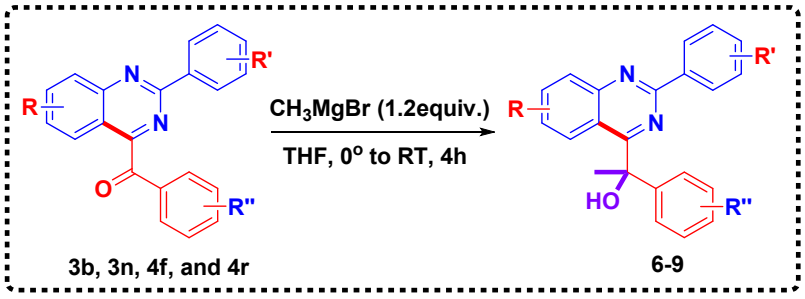
Scheme S2: Synthesis of N-phenylbenzimidamide substrates[S1]



A round bottom flask (50 mL in volume) was charged with NaH (60% in mineral oil) (360 mg, 15.0 mmol, 60%, 1.5 equiv). Under a stream of Ar, DMSO (5 mL) was added. The resulting suspension was cooled with an ice-water bath prior to the addition of the aniline (11.0 mmol, 1.1 equiv.) and the carbonitrile (10.0 mmol). The mixture was kept at 0 °C for 1 h and then stirred at room temperature until the starting material was consumed as monitored by TLC analysis. Ice-water (50 mL) was added while maintaining vigorous stirring. The aqueous layer was extracted with EtOAc (3 × 50 mL). The extracts were combined and washed with cold water (2 × 50 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to obtain the desired product (yield > 90%).

General procedure for the synthesis of anticancer compounds:

Scheme S3: Preparation of anticancer compounds[S2]



To a solution of 4-aroylquinazoline (0.5 mmol) in THF (15 mL), 1.2 equiv. of methyl magnesium bromide (3 M solution in diethyl ether) was added with stirring under argon atmosphere at 0 °C. The reaction mixture was then stirred at room temperature until the starting

material was consumed as monitored by TLC. Upon completion of reaction, the saturated solution of ammonium chloride was added to the reaction mixture. Subsequently, the product was extracted with ethyl acetate and washed with brine and dried over Na_2SO_4. The solvent was then evaporated and the residue was purified by column chromatography on silica gel to obtain the desired product (yield > 90%).

Preparation of copper(I)-phenylacetylide:[S3] CuI (1.0 g, 5.0 mmol) was dissolved in ammonium hydroxide to form a blue-colored 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 a bright yellow solid was obtained. The spectroscopic data for the yellow solid are shown below: IR (KBr, cm^{-1}) [S4:] 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]= $9.660469e^{+09}$; 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 superoxide.

The reaction under standard condition (**1a**, phenylacetylene, base, CuCl, O_2) in MeOH was irradiated with blue LED light for 30 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). This result indicates that superoxide free radical was formed in the reaction. No superoxide EPR signals were observed from the reaction solution under standard condition in the absence of CuCl (Figure 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

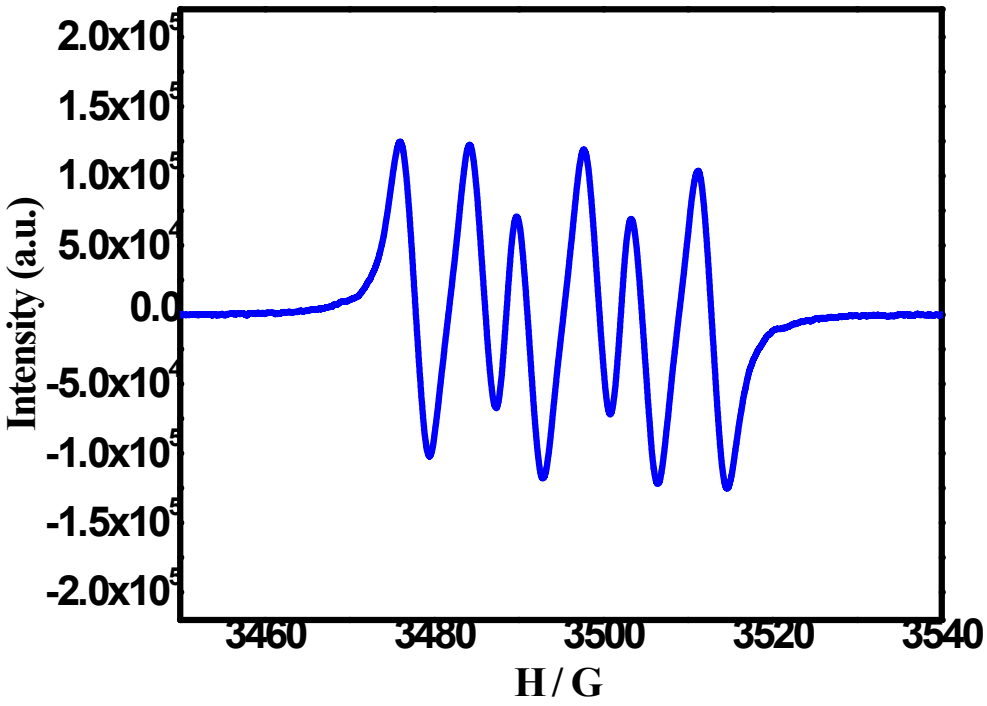


Figure S1: EPR spectra of the reaction mixture: 4-chloro-N-phenylbenzimidamide (**1a**) (0.2 mmol), phenylacetylene (0.4 mmol), K_2CO_3 (1.2 equiv.) and 5 mol% of CuCl in MeOH (5 mL), 0.5 mL of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5 x 10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere (1 atm) for 30 minutes. The reaction mixture was then analyzed by EPR. There are classical 6 peaks, the signals corresponding to (DMPO-OO(H))

EPR spectra of the reaction mixture in the absence of CuCl

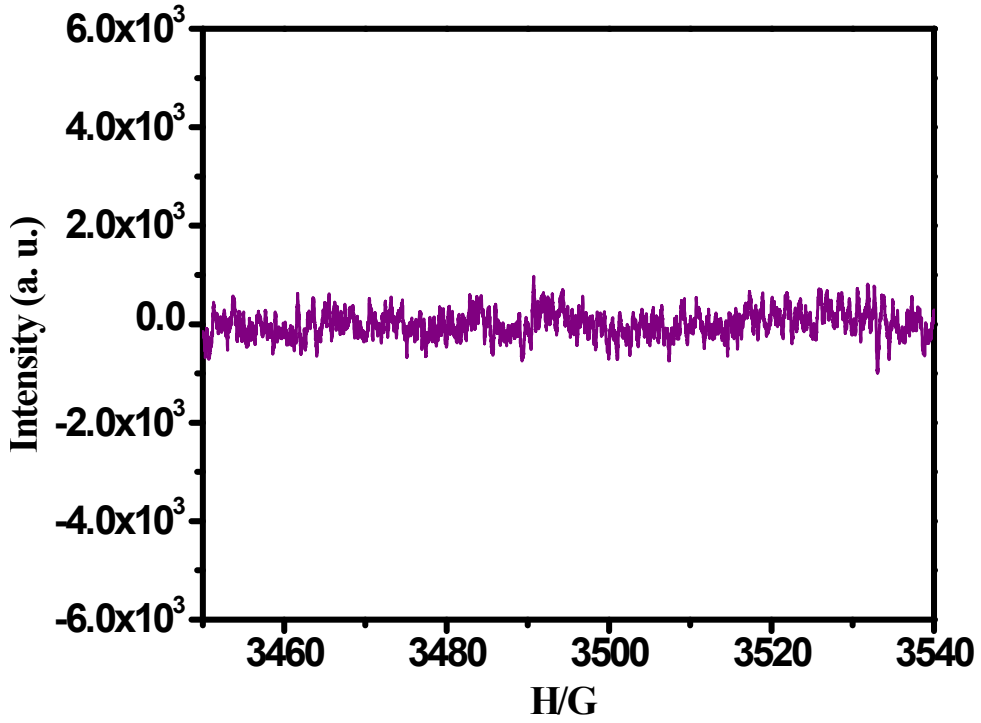


Figure S2: EPR spectra of the reaction mixture: 4-chloro-N-phenylbenzimidamide (**1a**) (0.2 mmol) phenylacetylene (0.4 mmol), K_2CO_3 (1.2 equiv.) in MeOH (5 mL), 0.5 mL of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5×10^{-2} M). The mixture was then irradiated with blue LEDs at room temperature under an oxygen atmosphere (1 atm) for 30 minutes (in the absence of CuCl). The reaction mixtures were analyzed by EPR spectra. No signals were detected.

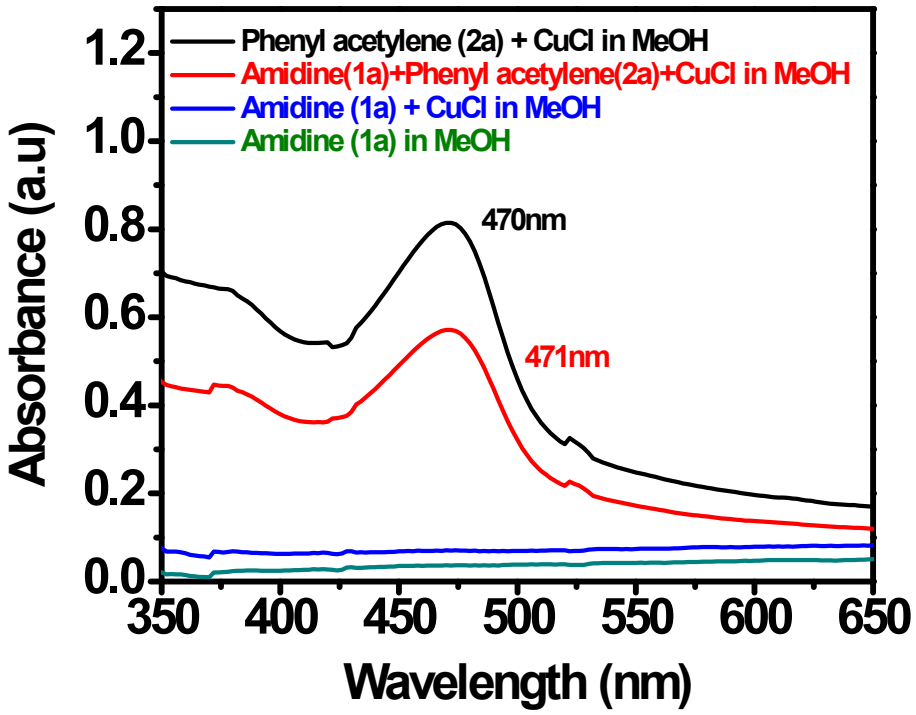
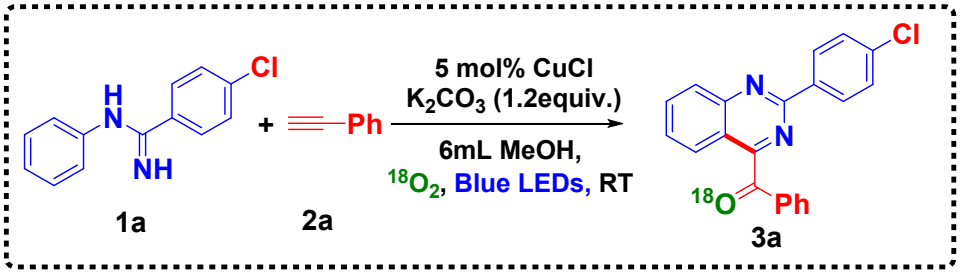


Figure S3: UV-visible spectra of the reaction mixture in MeOH

$^{18}O_2$ Labeling Experiment

We have performed an $^{18}O_2$ experiment under the standard condition (97% purity of $^{18}O_2$ gas was filled in the reaction system). ESI mass showed the formation of ^{18}O atom product (^{18}O% is 96%). Thus, O-atom in the product is from the molecular oxygen (O_2).

Scheme S4: $^{18}O_2$ Labeling Experiment



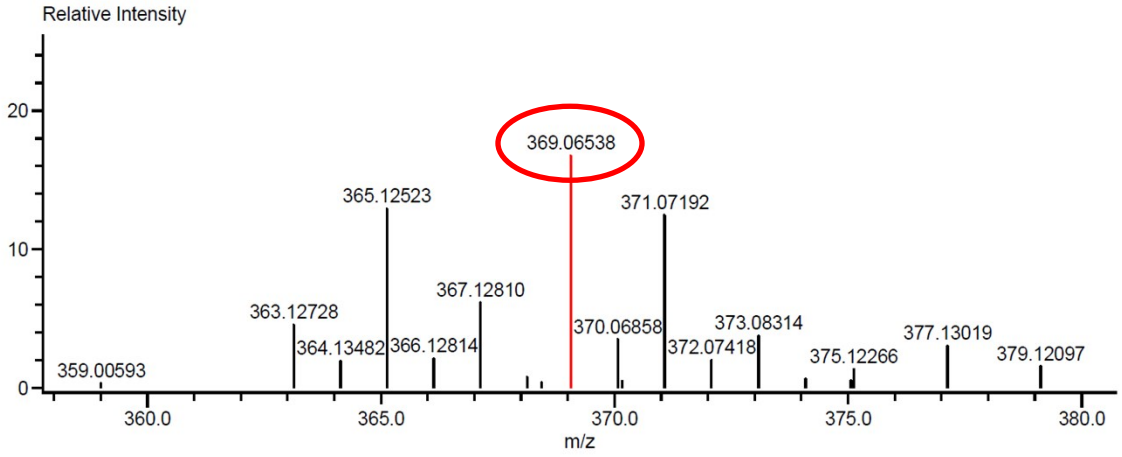
ESI-MS Calculated for $C_{21}H_{13}ClN_2{}^{18}O$ (M+Na)= 346.0759, found: 369.0653

Mass Data

Data:3 a
Comment:
Description:
Ionization Mode:ESI+
History:Average(MS[1] 0.29..0.70)

Acquired:5/14/2020 4:33:24 PM
Operator:AccuTOF
m/z Calibration File:20200102-1TFANa...
Created:5/14/2020 4:41:31 PM
Created by:AccuTOF

Charge number:1
Tolerance:250.00[ppm], 200.00 .. 200....
Unsaturation Number:-150.0 .. 200.0 (...
Element:^{12}C:21 .. 21, ^{1}H:13 .. 14, ^{35}Cl:1 .. 1, ^{14}N:2 .. 2, ^{23}Na:0 .. 3, ^{16}O:0 .. 1, ^{18}O:0 .. 1



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
369.06538	1142.73	369.06566	-0.28	-0.75	$^{12}C_{21}{}^{1}H_{13}{}^{35}Cl_1{}^{14}N_2{}^{23}Na_1{}^{18}O_1$

Table S1. Evaluation of green chemistry metrics of current photochemical method for the synthesis of **4e**

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

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

Reactant 1	*N*-phenylbenzimidamide	0.589g	3.0 mmol	FW 196.24
Reactant 2	1-ethynyl-4-methoxybenzene	0.79g	6.0 mmol	FW 132.15
Base	K_2CO_3 (1.2equiv.)	0.5g	3.61 mmol	FW 138.2
Solvent	DCM (12mL,15.96g) MeOH (6mL,4.75g)	20.71g	----	----
Auxiliary	----	----	----	----
Recycled Solvent	DCM+MeOH	8.43g	----	----
Product	(4-methoxyphenyl)(2-phenylquinazolin-4-yl)methanone	0.523g	1.536 mmol	FW 340.37

Product yield = 51.2%

$$\text{E-factor} = \frac{0.589 + 0.79 + 0.5 + 20.71 - (0.523 + 8.43)}{0.523\text{g}} = 26.07 \text{ Kg waste/ 1 Kg product}$$

$$\text{Atom economy} = \frac{340.37}{344.39} \times 100 = 98.83\%$$

$$\text{Atom efficiency} = 51.2\% \times 98.83\% / 100 = 50.6\%$$

$$\text{Carbon efficiency} = \frac{22}{13 + 9} \times 100 = 100\%$$

$$\text{Reaction mass efficiency} = \frac{0.523\text{g}}{0.589\text{g} + 0.79\text{g}} \times 100 = 37.9\%$$

Table S2. Evaluation of green chemistry metrics of the reported thermal method[S5]

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

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

Reactant 1	**4-chloro-2-phenylquinazoline**	**0.722g**	**3.0 mmol**	**FW 240.69**
Reactant 2	**4-methoxybenzaldehyde**	**0.49g**	**3.6 mmol**	**FW 136.14**
Additive	**1,3-dimethylimidazolium iodide**	**0.224g**	**1.0 mmol**	**FW 224.04**
Base	**NaH (50% oil dispersion)**	**0.173g**	**3.6 mmol**	**FW 23.99**
Solvent	**THF (20mL)**	**17.78g**	**----**	**----**
Auxiliary	**----**	**----**	**----**	**----**
Product	**(4-methoxyphenyl) (2-phenylquinazolin -4-yl) methanone**	**0.388g**	**1.14 mmol**	**FW 340.37**

Product yield = 38%

$$\text{E-factor} = \frac{0.722+0.49+0.224+0.173+17.78 - 0.388}{0.388\text{g}} = 48.97 \text{ Kg waste/ 1 Kg product}$$

$$\text{Atom economy} = \frac{340.37}{376.83} \times 100 = 90.32\%$$

$$\text{Atom efficiency} = 38\% \times 90.32\% / 100 = 34.32\%$$

$$\text{Carbon efficiency} = \frac{22}{14 + 8} \times 100 = 100\%$$

$$\text{Reaction mass efficiency} = \frac{0.388\text{g}}{0.722\text{g} + 0.49\text{g}} \times 100 = 32.01\%$$

To demonstrate and compare the practicality and efficiency of this photo-oxidative annulation reaction with the reported thermal[S5] reaction, a 3.0 mmol scale reaction was performed. The reaction of 0.589 g (3.0 mmol) of compound *N*-phenylbenzimidamide with 1-ethynyl-4-methoxybenzene (0.79g) (6.0 mmol) in presence of CuCl, K_2CO_3, and O_2 under photo irradiation for 24 h formed 0.523g of the product **4e** (51.2% yield). We have also calculated and compared the green chemistry metrics for this photo-oxidative annulation reaction and the reported thermal reaction. The green chemistry metric evaluation for the current green process has an E-factor of

26.07, 98.83% atom economy, 50.6 % atom efficiency, 100% carbon efficiency and 37.9% reaction mass efficiency. Whereas, the green chemistry metric evaluation for the reported thermal reaction has an E-factor of 48.97, 90.32% atom economy, 34.32 % atom efficiency, 100% carbon efficiency and 32.01% reaction mass efficiency. These green chemistry metrics evaluation results for the current method and thermal method are tabulated in **Table S3** and the results showed that the current organic photochemical method is ~1.9 times (in terms of E-factor) better than that of thermal method.

Table S3. Comparison of photochemical and thermal method[S5] green chemistry metrics evaluation

Parameters / **Method**	**E-factor (Kg waste/1Kg product)**	**Atom economy (%)**	**Atom efficiency (%)**	**Carbon efficiency (%)**	**Reaction mass efficiency (RME) (%)**
Photochemical	**26.07**	**98.83**	**50.6**	**100**	**37.9**
Thermal	**48.97**	**90.32**	**34.32**	**100**	**32.01**

Table S4. Evaluation of Eco-Scale of current photochemical method for the synthesis of **4e.**

EcoScale = 100 - Sum of individual penalties

Score on EcoScale: >75, Excellent; >50, Acceptable; <50, Inadequate

A) Calculation of penalty points:

Parameters		Penalty points
1. Yield	(100-%yield)/2 = (100-51.2)/2 = 24.4	24.4
2. Price of reaction components (To obtain 10 mmol of end product)		
a. *N*-phenylbenzimidamide = 2.3g = US$5.40 (synthesis cost)		
b. 1-Ethynyl-4-methoxybenzene = 2.6g = US$27.5 (synthesis cost)		
c. CuCl	= 0.05g = US$0.16	
d. K_2CO_3	= 1.66g = US$0.05	
e. DCM	= 30mL = US$1.50	
f. MeOH	= 15mL = US$1.20	
Total price (USD) = $35.81		
Thus, expensive (>$10 and <$50)		3
3. Safety		
Solvent: DCM and MeOH		
Toxic (T)		5
Highly flammable (F)		5
4. Technical Setup		
Inconventional activation technique (Photochemical activation)		2
5. Temperature and time		
Room temperature and <24h		1
6. Workup and purification		
Removal of solvent with bp <150^{o}C		0
Classical Chromatography		10
Total Penalty Points		50.4

B) EcoScale calculation:

EcoScale = 100- 50.4 = 49.6 ~ 50 (an acceptable synthesis)

Table S5. Evaluation of Eco-Scale of the reported thermal method[S5]

EcoScale = 100 - Sum of individual penalties

Score on EcoScale: >75, Excellent; >50, Acceptable; <50, Inadequate

A) Calculation of penalty points:

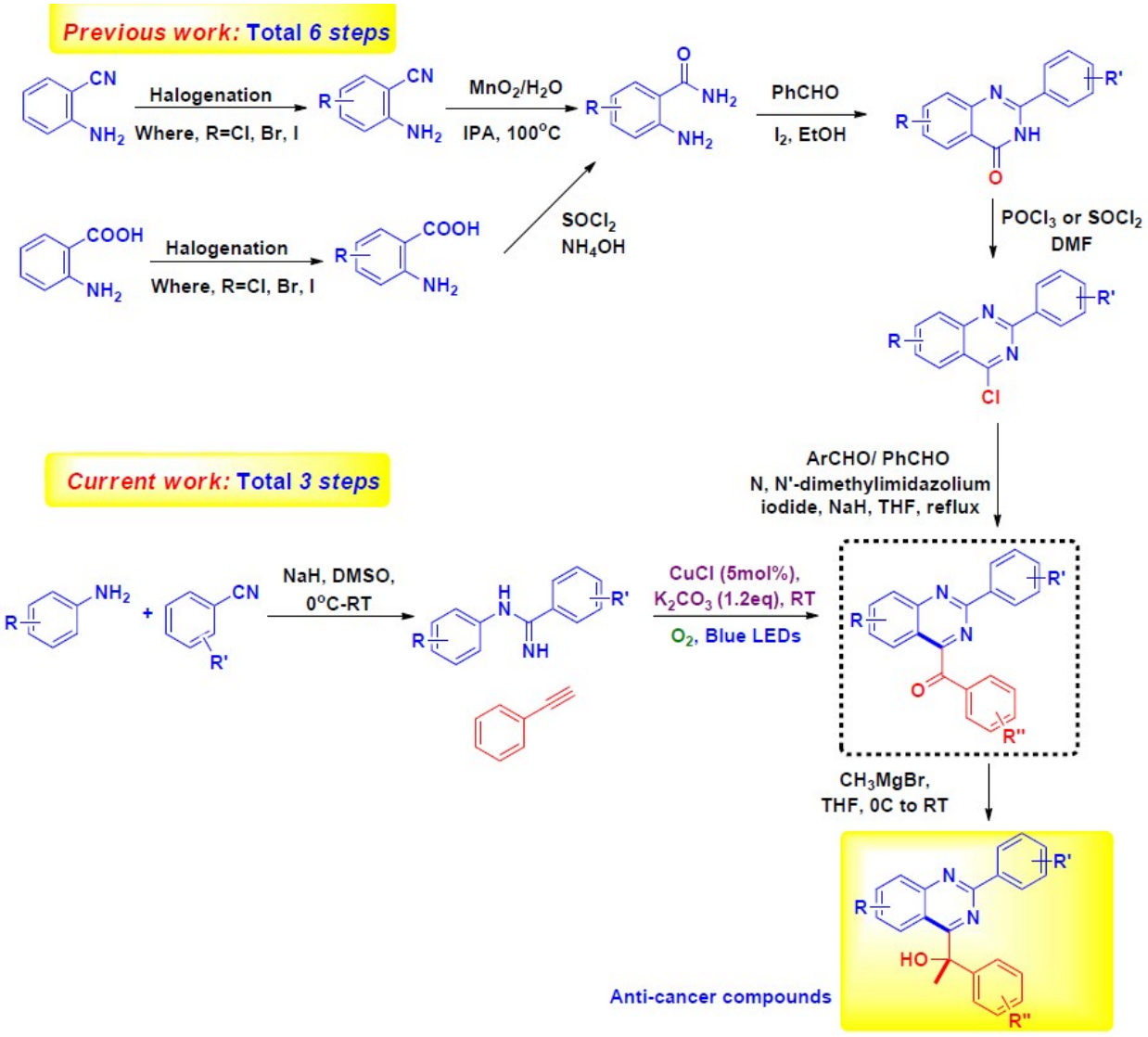
Parameters		Penalty points
1. Yield	(100-%yield)/2 = (100-38)/2 = 31	31
2. Price of reaction components (To obtain 10 mmol of end product)		
a. 4-Chloro-2-phenylquinazoline	= 2.4g = US$45.3	
b. 4-methoxybenzaldehyde	= 1.63g = US$12.71	
c. 1,3-dimethylimidazolium iodide	= 0.67g = US$8.79	
d. NaH (50% dispersion)	= 0.29g = US$4.06	
e. THF (anhydrous)	= 40mL = US$9.58	
f. $CHCl_3$ (For workup)	= 50mL = US$1.20	
Total price (USD) = $81.64		
Thus, very expensive (>$50)		5
3. Safety		
Solvent: THF and $CHCl_3$		
Toxic (T)		5
Highly flammable (F)		5
4. Technical Setup		
Common setup		0
(inert) gas atmosphere		1
5. Temperature and time		
Heating, <1h		2
6. Workup and purification		
Removal of solvent with bp <150^{o}C		0
Liquid-liquid extraction with $CHCl_3$		3
Classical Chromatography		10
Total Penalty Points		62

B) EcoScale calculation:

EcoScale = 100- 62 = 38 (inadequate synthesis)

The Eco-Scale evaluations for the current photochemical method (**Table S4**) and thermal method (**Table S5**) indicate that the current photochemical method is an **acceptable synthesis**; whereas, for the reported thermal method is at an inadequate level. Thus, the current synthetic organic reaction is simple, ecofriendly, and highly efficient.

Scheme S5: Synthesis of anti-cancer compounds by previous and current process[S2, S6]

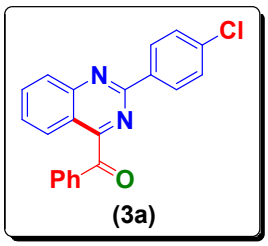


The current protocol could be used to synthesize these anti-cancer compounds in only 3 steps, whereas the reported various methods can form these compounds in 6 steps. Thus, the current method is 2 times better than that of reported thermal methods.[S6,S2]

Note: Here we have just compared the number of steps required for the formation of anti-cancer compounds as the several parameters such as reaction conditions, yield, etc. will vary the product yield depending upon the substrates.

Spectroscopic Data

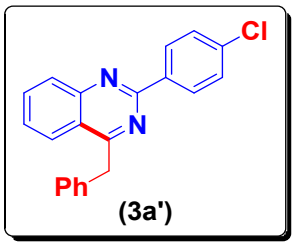
(2-(4-chlorophenyl)quinazolin-4-yl)(phenyl)methanone (3a)



(3a)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.54 (d, *J*= 9.6 Hz, 2 H), 8.14 (d, *J*= 7.8 Hz, 1 H), 8.03-8.01 (m, 3 H), 7.92 (t, *J*= 6.6 Hz, 1 H), 7.65 (t, *J*= 8.4 Hz, 1 H), 7.58 (t, *J*= 6.0 Hz, 1 H), 7.51 (d, *J*= 7.2 Hz, 2 H), 7.48-7.44 (m, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.9, 164.2, 158.6, 151.9, 137.1, 135.9, 135.3, 134.6, 134.3, 130.7, 130.0, 129.2, 128.8, 128.7, 128.1, 125.7, and 120.5; ESI-MS calcd for $C_{21}H_{13}ClN_2O$ (M+H): 344.0716, found: 345.0975.

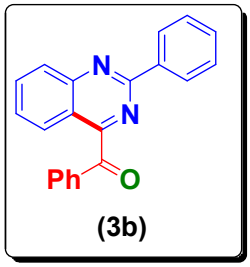
4-benzyl-2-(4-chlorophenyl)quinazoline (3a')



(3a')

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.58 (d, *J*= 9.0 Hz, 2 H), 8.11 (d, *J*= 8.4 Hz, 1 H), 8.04 (d, *J*= 8.4 Hz, 1 H), 7.81 (t, *J*= 7.2 Hz, 1 H), 7.52-7.46 (m, 5 H), 7.36 (d, *J*= 7.2 Hz, 2 H), 7.29-7.19 (m, 1 H), 4.65 (s, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 169.3, 159.1, 151.1, 137.7, 136.7, 136.6, 133.5, 129.9, 129.3, 128.8, 128.7, 128.6, 127.1, 126.6, 125.0, 122.4 and 41.4; ESI-MS calcd for $C_{21}H_{15}ClN_2$ (M+H): 330.0924, found: 331.1000.

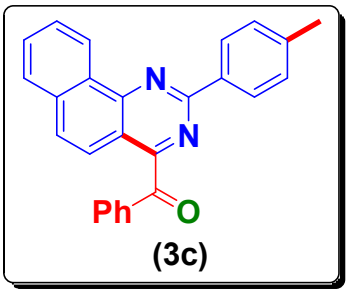
phenyl(2-phenylquinazolin-4-yl)methanone (3b)



(3b)

Pale yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.59 (d, *J*= 5.4 Hz, 2 H), 8.17 (d, *J*= 8.4 Hz, 1 H), 8.05-8.03 (m, 3 H), 7.92 (t, *J*= 7.2 Hz, 1 H), 7.65 (d, *J*= 7.2 Hz, 1 H), 7.57 (t, *J*= 7.2 Hz, 1 H), 7.51-7.48 (m, 5 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.0, 164.0, 159.5, 152.0, 137.4, 135.4, 134.4, 134.2, 130.8, 130.7, 129.2, 128.7, 128.6, 128.5, 127.9, 125.7 and 120.5; ESI-MS calcd for $C_{21}H_{14}N_2O$ (M+H): 310.1106, found: 311.1195.

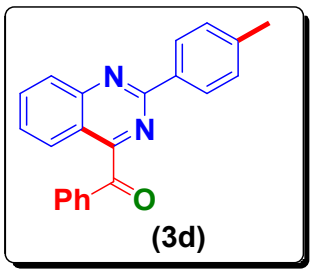
phenyl(2-p-tolylbenzo[h]quinazolin-4-yl) methanone (3c)



(3c)

Off white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.50 (d, J= 8.4 Hz, 2 H), 8.19 (d, J= 4.0 Hz, 2 H), 8.17(d, J= 5.2 Hz, 1 H), 8.00 (d, J= 8.8 Hz, 2 H), 7.90 (t, J= 8.0 Hz, 1 H), 7.65-7.43 (m, 5 H), 7.28 (d, J= 8.0 Hz, 2 H), 2.43 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 195.2, 163.1, 160.3, 154.2, 141.2, 136.4, 135.0, 134.5, 134.3, 132.3, 130.5, 129.3, 129.0, 128.6, 128.1, 127.7, 127.5, 127.4, 126.0, 117.7 and 21.5; ESI-MS calcd for $C_{26}H_{18}N_2O$ (M+H): 374.1419, found: 375.1497.

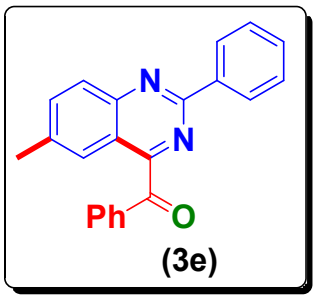
phenyl(2-p-tolylquinazolin-4-yl) methanone (3d)



(3d)

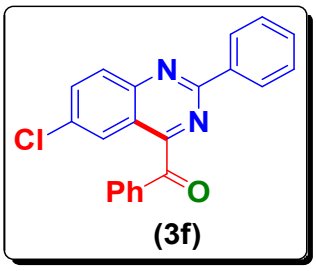
White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.47(d, J= 8.0Hz, 2 H), 8.14 (d, J= 8.4 Hz, 1 H), 8.02 (t, J= 8.0 Hz, 3 H), 7.90 (t, J= 8.4 Hz, 1 H), 7.64 (t, J= 7.6 Hz, 1 H), 7.54 (t, J= 7.6 Hz, 1 H), 7.48 (t, J= 7.6 Hz, 2 H), 7.28 (d, J= 8.0 Hz, 2 H), 2.41 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.1, 164.0, 159.6, 152.0, 141.2, 135.4, 134.7, 134.3, 134.2, 130.8, 129.4, 129.1, 128.7, 128.6, 127.7, 125.7, 120.4 and 21.5; ESI-MS calcd for $C_{22}H_{16}N_2O$ (M+H): 324.1263, found: 325.1345**.**

(6-methyl-2-phenylquinazolin-4-yl)(phenyl)methanone (3e)



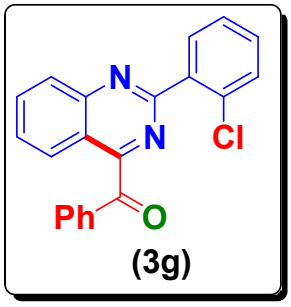
White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.56 (d, *J*= 3.6 Hz, 2 H), 8.07-8.03 (m, 3 H), 7.79-7.75 (m, 2 H), 7.65 (t, *J*= 7.8 Hz, 1 H), 7.51-7.47 (m, 5 H), 2.50 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.3, 163.2, 158.9, 150.7, 138.3, 137.6, 136.8, 135.4, 134.2, 130.8, 130.6, 128.9, 128.7, 128.6, 128.5, 124.2, 120.5 and 21.8; **ESI-MS** calcd for $C_{22}H_{16}N_2O$ (M+H): 324.1263, found: 325.1334.

(6-chloro-2-phenylquinazolin-4-yl)(phenyl)methanone (3f)



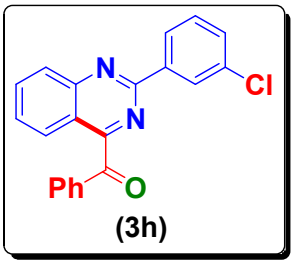
White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.56 (d, *J*= 4.2 Hz, 2 H), 8.11-8.05 (m, 4 H), 7.84 (t, *J*= 9.0 Hz, 1 H), 7.66 (t, *J*= 7.2 Hz, 1 H), 7.52-7.48 (m, 5 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.4, 162.7, 159.6, 150.6, 137.0, 135.5, 135.1, 134.4, 133.8, 131.1, 130.8, 128.7, 124.6 and 120.9; **ESI-MS** calcd for $C_{21}H_{13}ClN_2O$ (M+Na): 344.0716, found: 367.0610.

(2-(2-chlorophenyl)quinazolin-4-yl)(phenyl)methanone (3g)



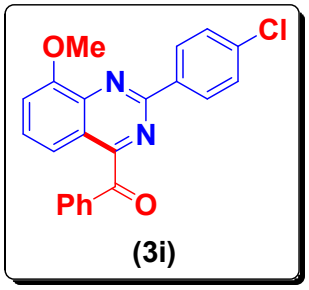
Light yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.21 (d, J= 8.0 Hz, 1 H), 8.09-7.96 (m, 4 H), 7.82 (d, J= 3.6 Hz, 1 H), 7.68-7.62 (m, 2 H), 7.51-7.47 (m, 3 H), 7.38 (d, J= 3.6 Hz, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.8, 164.3, 160.6, 151.6, 137.8, 135.2, 134.7, 134.4, 133.0, 131.9, 130.9, 130.6, 130.5, 129.3, 128.8, 128.7, 126.9, 125.8 and 120.3; **ESI-MS** calcd for $C_{21}H_{13}ClN_2O$ (M+Na): 344.0716, found: 367.0617.

(2-(3-chlorophenyl)quinazolin-4-yl)(phenyl)methanone (3h)



White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.59 (s, 1 H), 8.47 (d, *J*= 7.8 Hz, 1 H), 8.17 (d, *J*= 9.0 Hz, 1 H), 8.03-7.93 (m, 4 H), 7.66 (t, *J*= 6.6 Hz, 1 H), 7.60 (t, *J*= 7.2 Hz, 1 H), 7.50 (t, *J*= 7.8 Hz, 2 H), 7.43-7.40 (m, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.9, 164.3, 158.3, 151.9, 139.2, 135.2, 134.8, 134.7, 134.4, 130.8, 130.7, 129.8, 129.3, 128.7, 128.6, 128.3, 126.8, 125.8 and 120.7; **HRFD-MS** calcd for $C_{21}H_{13}ClN_2O$: 344.0716, found: 344.0706

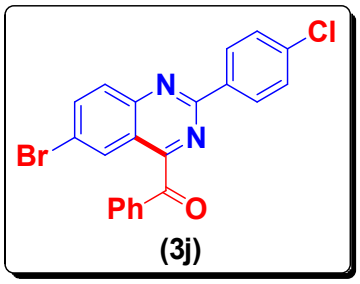
(2-(4-chlorophenyl)-8-methoxyquinazolin-4-yl)(phenyl)methanone (3i)



(3i)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.54 (d, *J*= 8.4 Hz, 2 H), 7.98 (d, *J*= 7.8 Hz, 2 H), 7.63 (t, *J*= 7.8 Hz, 1 H), 7.54-7.47 (m, 6 H), 7.43 (d, *J*= 8.4 Hz, 1 H), 4.11 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.0, 164.1, 157.9, 155.2, 144.1, 137.0, 135.9, 135.2, 134.3, 130.6, 130.0, 128.8, 128.7, 128.3, 121.3, 117.0, 112.4 and 56.3; **ESI-MS** calcd for $C_{22}H_{15}ClN_2O_2$ (M+H): 374.0822, found: 375.0916.

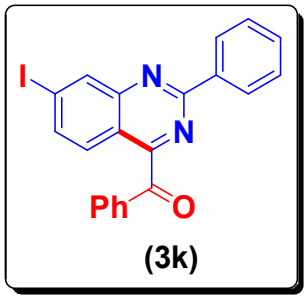
(6-bromo-2-(4-chlorophenyl)quinazolin-4-yl)(phenyl)methanone (3j)



(3j)

White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.51 (d, J= 8.4 Hz, 2 H), 8.23 (s, 1 H), 8.02 (d, J= 8.0 Hz, 4 H), 7.67 (t, J= 7.6 Hz, 1 H), 7.51 (t, J= 7.6 Hz, 2 H), 7.45 (d, J= 8.4 Hz, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.3, 162.9, 158.9, 150.9, 138.2, 137.6, 135.7, 135.3, 134.4, 130.9, 130.8, 130.1, 129.0, 128.7, 128.1, 122.2 and 121.6; **ESI-MS** calcd for $C_{21}H_{12}BrClN_2O$ (M+Na): 421.9822, found: 444.9730.

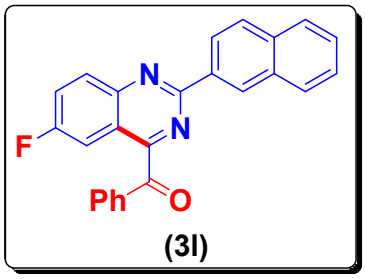
(7-iodo-2-phenylquinazolin-4-yl)(phenyl)methanone (3k)



(3k)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.59 (d, *J*= 7.2 Hz, 2 H), 8.17 (d, *J*= 8.4 Hz, 1 H), 8.04 (d, *J*= 8.4 Hz, 3 H), 7.92 (t, *J*= 6.6 Hz, 1 H), 7.65 (t, *J*= 7.2 Hz, 1 H), 7.57 (t, *J*= 7.2 Hz, 1 H), 7.51-7.48 (m, 4 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.1, 164.1, 159.6, 152.0, 137.4, 135.4, 134.4, 134.3, 130.9, 130.8, 129.3, 128.7, 128.6, 128.5, 127.9, 125.7 and 120.5.

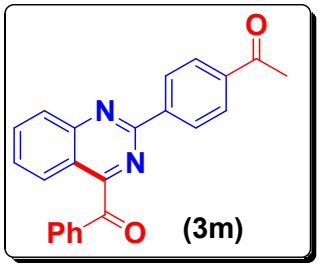
(6-fluoro-2-(naphthalen-2-yl) quinazolin-4-yl) (phenyl) methanone (3l)



(3l)

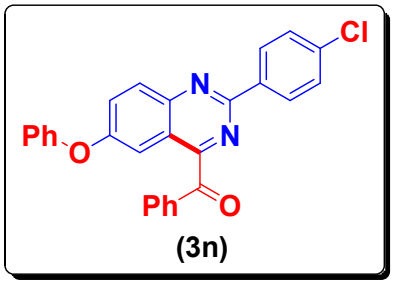
White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.08 (s, 1 H), 8.66 (d, J= 8.8 Hz, 1 H), 8.23 (d, J= 5.2 Hz, 1 H), 8.09 (d, J= 8.4 Hz, 2 H), 7.95 (t, J= 6.8 Hz, 2 H), 7.86 (t, J= 7.6 Hz, 2 H), 7.75-7.67 (m, 3 H), 7.55-7.49 (m, 4 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.7, 163.0, 161.6, 159.1, 149.5, 135.2, 134.8, 134.4, 133.3, 131.9, 131.9, 130.9, 129.2, 129.1, 128.7, 128.3, 127.7, 127.3, 127.0, 126.8, 125.3, 125.1, 121.0, and 109.5; **^{19}F NMR** (470 MHz, CCl_3F): δ -108.7 (s), **HRFD-MS** calcd for $C_{25}H_{15}FN_2O$: 378.1168, found: 378.1159.

1-(4-(4-benzoylquinazolin-2-yl)phenyl)ethanone (3m)



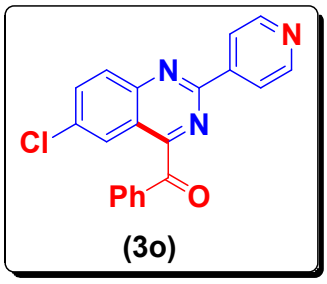
Light yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.68 (d, J= 7.6 Hz, 2 H), 8.19 (d, J= 9.6 Hz, 1 H), 8.06-7.94 (m, 6 H), 7.68-7.60 (m, 2 H), 7.50 (t, J= 8.0 Hz, 2 H), 2.64 (s,3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 197.9, 192.9, 164.3, 158.4, 151.9, 141.5, 138.6, 135.3, 134.7, 134.4, 130.7, 129.4, 128.8, 128.7, 128.5, 125.8, 120.7 and 26.8; **ESI-MS** calcd for $C_{23}H_{16}N_2O_2$ (M+H): 352.1212, found: 353.1283.

(2-(4-chlorophenyl)-6-phenoxyquinazolin-4-yl) (phenyl) methanone (3n)



White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.49 (d, *J*= 7.8 Hz, 2 H), 8.12 (d, *J*= 9.0 Hz, 1 H), 7.97 (d, *J*= 8.4 Hz, 2 H), 7.68-7.62 (m, 3 H), 7.51-7.34 (m, 6 H), 7.16(d, *J*= 7.8 Hz, 1 H), 7.04(d, *J*= 8.4 Hz, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.8, 162.4, 151.5, 156.8, 155.6, 149.0, 136.9, 135.9, 135.3, 134.2, 131.1, 130.7, 130.1, 128.8, 128.6, 128.1, 124.5, 121.4, 119.5 and 110.6; **ESI-MS** calcd for $C_{27}H_{17}ClN_2O_2$ (M+Na): 436.0979, found: 459.0876

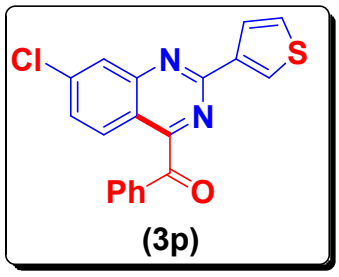
(6-chloro-2-(pyridin-4-yl) quinazolin-4-yl) (phenyl) methanone (3o)



(3o)

Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.78 (s, 2 H), 8.40 (d, *J*= 4.2 Hz, 2 H), 8.16 (d, *J*= 9.0 Hz, 1 H), 8.11 (d, *J*= 2.4 Hz, 1 H), 8.01 (d, *J*= 7.2 Hz, 2 H), 7.91 (t, *J*= 9.0 Hz, 1 H), 7.68(t, *J*= 6.6 Hz, 1 H), 7.52 (d, *J*= 7.8 Hz, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.2, 163.2, 157.6, 150.5, 144.3, 136.0, 135.1, 134.9, 134.7, 131.1, 130.8, 128.8, 124.8, 122.3 and 121.6; **ESI-MS** calcd for $C_{20}H_{12}ClN_3O$ (M+H): 345.0669, found: 346.0744.

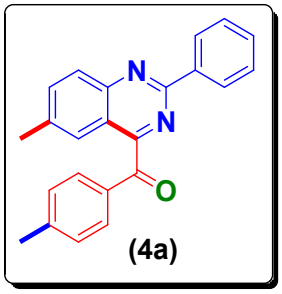
(7-chloro-2-(thiophen-3-yl) quinazolin-4-yl) (phenyl) methanone (3p)



(3p)

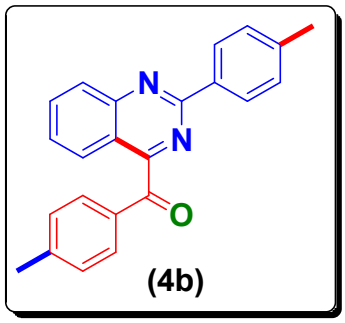
Brown solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.38 (d, *J*= 4.2 Hz, 1 H), 8.10 (s, 1 H), 8.02-7.95 (m, 4 H), 7.65 (t, *J*= 7.2 Hz, 1 H), 7.51-7.47 (m, 3 H), 7.38 (d, *J*= 7.8 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.5, 163.9, 157.6, 152.6, 141.2, 140.8, 135.1, 134.4, 130.7, 129.6, 128.7, 128.6, 127.9, 127.6, 127.1, 126.3 and 118.7; **HRFD-MS** calcd for $C_{19}H_{11}ClN_2OS$: 350.0281, found: 350.02767.

(6-methyl-2-phenylquinazolin-4-yl) (p-tolyl) methanone (4a)



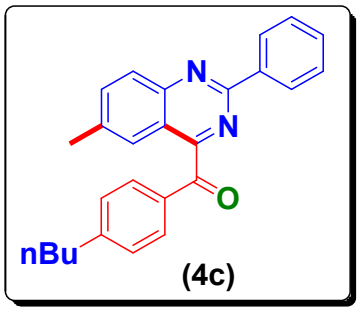
White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.05 (d, *J*= 8.4 Hz, 1 H), 7.92 (d, *J*= 8.0 Hz, 2 H), 7.74 (d, *J*= 8.8 Hz, 2 H), 7.47 (d, *J*= 4.8 Hz, 3 H), 7.28 (d, *J*= 8.4 Hz, 2 H), 2.49 (s, 3 H), 2.44 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.9, 163.6, 158.8, 150.6, 145.4, 138.2, 137.6, 136.7, 132.9, 130.9, 130.6, 129.4, 128.8, 128.6, 128.5, 124.3, 120.5, 21.9 and 21.8; **ESI-MS** calcd for $C_{23}H_{18}N_2O$ (M+H): 338.1419, found: 339.1488.

p-tolyl(2-p-tolylquinazolin-4-yl) methanone (4b)



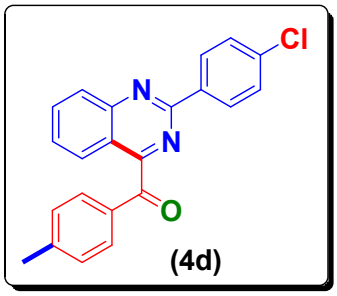
White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.48(d, J= 8.0 Hz, 2 H), 8.13 (d, J= 7.6 Hz, 1 H), 7.99 (d, J= 8.0 Hz, 1 H), 7.93-7.87 (m, 3 H), 7.53 (t, J= 7.2 Hz, 1 H), 7.28 (d, J= 7.2 Hz, 4 H), 2.43 (s, 3 H), 2.41 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.8, 164.3, 159.6, 151.9, 145.4, 141.1, 134.8, 134.3, 132.9, 130.9, 129.3, 129.1, 128.9, 128.6, 127.6, 125.7, 120.4, 21.8 and 21.5; **ESI-MS** calcd for $C_{23}H_{18}N_2O$ (M+H): 338.1419, found: 339.1479.

(4-butylphenyl) (6-methyl-2-phenylquinazolin-4-yl) methanone (4c)



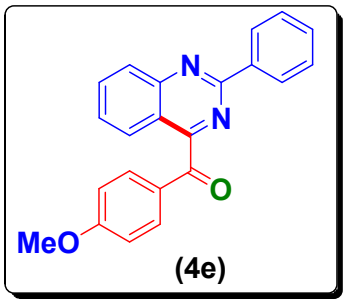
White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.57 (d, *J*= 7.8 Hz, 2 H), 8.04 (d, *J*= 8.4 Hz, 1 H), 7.93 (d, *J*= 8.4 Hz, 2 H), 7.75 (t, *J*= 10.8 Hz, 2 H), 7.47 (d, *J*= 6.0 Hz, 3 H), 7.29 (d, *J*= 7.8 Hz, 2 H), 2.68 (t, *J*= 7.8 Hz, 2 H), 2.48 (s, 3 H), 1.64-1.59 (m, 2 H), 1.37-1.33 (m, 2 H), 0.98 (t, *J*= 7.2 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.0, 163.7, 158.9, 150.6, 150.4, 138.2, 137.6, 136.7, 133.1, 130.9, 130.6, 128.8, 128.7, 128.6, 128.5, 124.3, 120.5, 35.8, 33.1, 22.3, 21.8 and 13.8; **ESI-MS** calcd for $C_{26}H_{24}N_2O$ (M+H): 380.1889, found: 381.1959.

(2-(4-chlorophenyl) quinazolin-4-yl) (p-tolyl) methanone (4d)



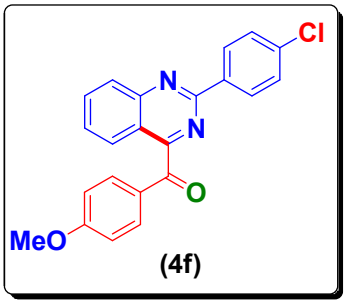
White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.54 (d, *J*= 8.4 Hz, 2 H), 8.13 (d, *J*= 8.4 Hz, 1 H), 7.99 (d, *J*= 8.4 Hz, 1 H), 7.91 (d, *J*= 7.8 Hz, 3 H), 7.56 (t, *J*= 7.2 Hz, 1 H), 7.44(d, *J*= 8.4 Hz, 2 H), 7.29 (d, *J*= 7.8 Hz, 2 H), 2.43 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.6, 164.5, 158.6, 151.8, 145.6, 137.0, 135.9, 134.5, 132.8, 130.0, 129.4, 129.1, 128.8, 128.0, 125.8, 120.5 and 21.8; **ESI-MS** calcd for $C_{22}H_{15}ClN_2O$ (M+H): 358.0873, found: 359.0951.

(4-methoxyphenyl) (2-phenylquinazolin-4-yl) methanone (4e)



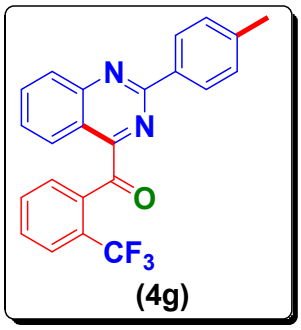
White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.59 (d, J= 3.2 Hz, 2 H), 8.14 (d, J= 8.0 Hz, 1 H), 8.00 (d, J= 8.0 Hz, 3 H), 7.90 (t, J= 8.8 Hz, 1 H), 7.55 (t, J= 8.0 Hz, 1 H), 7.48 (d, J= 5.4 Hz, 3 H), 6.96 (d, J= 7.6 Hz, 2 H), 3.87 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 191.6, 164.7, 164.6, 159.6, 151.9, 137.5, 134.3, 133.2, 130.8, 129.2, 128.7, 128.6, 128.4, 127.8, 125.8, 120.6, 114.0 and 55.6; **ESI-MS** calcd for $C_{22}H_{16}N_2O_2$ (M+Na): 340.1212, found: 363.1116.

(2-(4-chlorophenyl) quinazolin-4-yl) (4-methoxyphenyl) methanone (4f)



White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.54 (d, *J*= 8.4 Hz, 2 H), 8.13 (d, *J*= 8.4 Hz, 1 H), 7.98 (d, *J*= 7.2 Hz, 3 H), 7.91 (t, *J*= 7.2 Hz, 1 H), 7.56 (t, *J*= 8.4 Hz, 1 H), 7.44 (d, *J*= 8.4 Hz, 2 H), 6.96 (d, *J*= 9.0 Hz, 2 H), 3.87 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 191.5, 164.8, 164.6, 158.6, 151.8, 137.1, 136.0, 134.5, 133.1, 130.0, 129.1, 128.8, 128.3, 128.0, 125.9, 120.6, 114.0 and 55.6; **ESI-MS** calcd for $C_{22}H_{15}ClN_2O_2$ (M+Na): 374.0822, found: 397.0718.

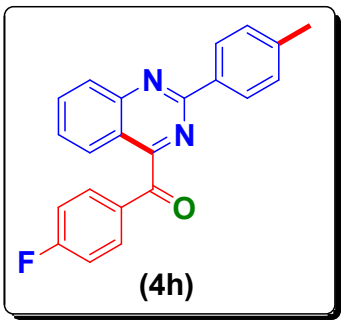
(2-p-tolylquinazolin-4-yl) (2-(trifluoromethyl) phenyl) methanone (4g)



(4g)

White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.78 (d, J= 8.8 Hz, 1 H), 8.21 (d, J= 8.4 Hz, 2 H), 8.14 (d, J= 9.2 Hz, 1 H), 7.94 (t, J= 7.2 Hz, 1 H), 7.78 (d, J= 5.6 Hz, 1 H), 7.71-7.65 (m, 4 H), 7.20 (d, J= 8.0 Hz, 2 H), 2.37 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 196.5, 159.5, 159.3, 152.9, 141.2, 138.2, 134.4, 134.3, 131.3, 130.5, 129.7, 129.3, 129.1, 128.7, 128.3, 126.4, 126.0, 120.1 and 21.4; **^{19}F NMR** (470 MHz, CCl_3F): δ -57.6 (s), **ESI-MS** calcd for $C_{23}H_{15}F_3N_2O$ (M+H): 392.1136, found: 393.1213.

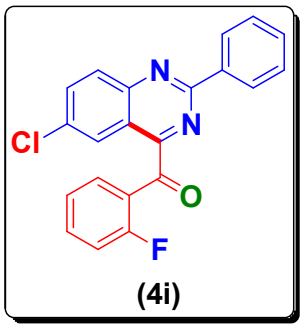
(4-fluorophenyl) (2-p-tolylquinazolin-4-yl) methanone (4h)



(4h)

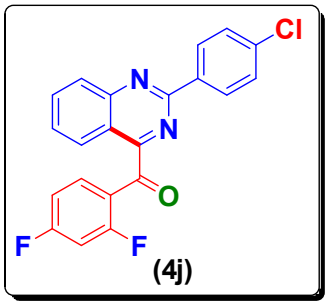
White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.46 (d, J= 8.0 Hz, 2 H), 8.14 (d, J= 8.8 Hz, 1 H), 8.10 (t, J= 5.6 Hz, 1 H), 8.02 (d, J= 8.0 Hz, 1 H), 7.91 (t, J= 7.2 Hz, 1 H), 7.56 (t, J= 7.2 Hz, 1 H), 7.29 (d, J= 8.4 Hz, 1 H), 7.16 (t, J= 8.8 Hz, 2 H), 2.42 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 191.5, 167.2, 165.7, 163.4, 159.6, 152.2, 141.3, 134.6, 134.4, 133.7, 133.6, 131.9, 129.4, 128.6, 127.8, 125.6, 120.4, 115.9 and 21.5; **^{19}F NMR** (470 MHz, CCl_3F): δ -102.6 (s), **ESI-MS** calcd for $C_{22}H_{15}FN_2O$ (M+H): 342.1168, found: 343.1239.

(6-chloro-2-phenylquinazolin-4-yl) (2-fluorophenyl) methanone (4i)



White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.47 (d, *J*= 7.8 Hz, 2 H), 8.29 (s, 3 H), 8.10 (d, *J*= 9.0 Hz, 1 H), 8.00 (t, *J*= 7.8 Hz, 1 H), 7.86 (t, *J*= 9.0 Hz, 1 H), 7.63 (t, *J*= 7.8 Hz, 1 H), 7.63 (t, *J*= 7.8 Hz, 1 H), 7.46 (d, *J*= 6.6 Hz, 3 H), 7.35 (t, *J*= 7.8 Hz, 1 H), 7.10 (d, *J*= 9.6 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 191.4, 162.9, 162.0, 161.2, 160.0, 150.9, 136.9, 135.8, 135.7, 135.3, 134.1, 131.6, 131.0, 130.8, 128.6, 128.5, 125.3, 125.2, 124.5, 120.0, 116.6 and 116.4; **^{19}F NMR** (563 MHz, CCl_3F): δ -106.7 (s), **ESI-MS** calcd for $C_{21}H_{12}ClFN_2O$ (M+H): 362.0622, found: 363.2391.

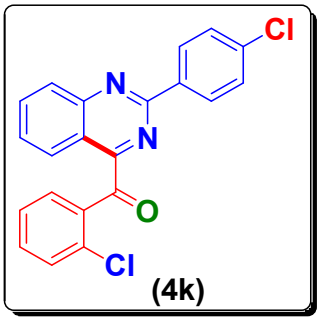
(2-(4-chlorophenyl) quinazolin-4-yl) (2,4-difluorophenyl) methanone (4j)



White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.44 (d, *J*= 8.4 Hz, 2 H), 8.20 (d, *J*= 8.4 Hz, 1 H), 8.15 (d, *J*= 8.4 Hz, 1 H), 8.09-8.03 (m, 1 H), 7.95 (t, *J*= 7.2 Hz, 1 H), 7.64 (t, *J*= 7.2 Hz, 1 H), 7.43 (d, *J*= 8.4 Hz, 2 H), 7.08 (t, *J*= 8.0 Hz, 1 H), 6.84 (d, *J*= 8.4 Hz, 1 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 190.2, 167.5, 167.4, 165.8, 165.7, 163.9, 163.1, 162.2, 162.1, 158.8, 152.3, 137.1, 135.8, 134.5, 133.7, 133.6, 129.9, 129.4, 129.2, 128.8, 128.4, 127.4, 125.5, 124.4, 122.2, 119.6,

112.5, 112.3, 105.1, 104.9 and 104.7; **^{19}F NMR** (470 MHz, CCl_3F): δ -99.2 (d) and -102.0 (d), **ESI-MS** calcd for $C_{21}H_{12}ClFN_2O$ (M+H): 380.0528, found: 381.0621.

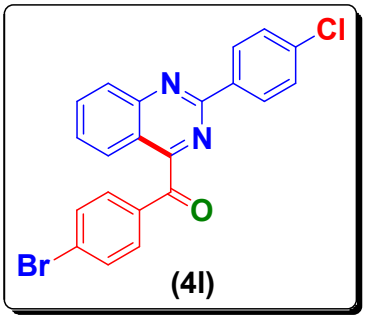
(2-chlorophenyl) (2-(4-chlorophenyl) quinazolin-4-yl) methanone (4k)



(4k)

Pale yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.48 (d, *J*= 7.8 Hz, 1 H), 8.36 (d, *J*= 9.0 Hz, 2 H), 8.14 (t, *J*= 8.4 Hz, 1 H), 7.95 (t, *J*= 8.4 Hz, 1 H), 7.79 (t, *J*= 7.8 Hz, 1 H), 7.67 (t, *J*= 9.6 Hz, 1 H), 7.51 (t, *J*= 7.8 Hz, 1 H), 7.46-7.38 (m, 4 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.8, 161.8, 158.6, 152.5, 137.3, 137.0, 135.7, 134.4, 133.0, 131.5, 130.2, 129.8, 129.1, 128.8, 128.7, 126.9, 125.9 and 120.1; **ESI-MS** calcd for $C_{21}H_{12}Cl_2N_2O$ (M+H): 378.0327, found: 379.0402.

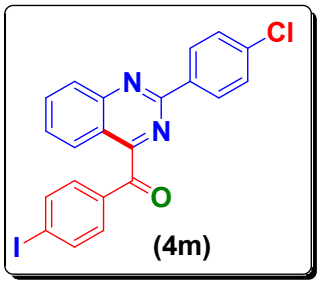
(4-bromophenyl) (2-(4-chlorophenyl) quinazolin-4-yl) methanone (4l)



(4l)

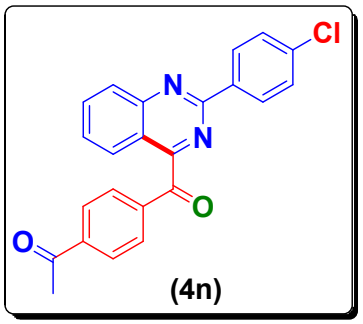
Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.52 (d, *J*= 9.0 Hz, 2 H), 8.15 (d, *J*= 9.0 Hz, 1 H), 8.06 (d, *J*= 8.4 Hz, 1 H), 7.95-7.89 (m, 3 H), 7.65-7.59 (m, 3 H), 7.45 (t, *J*= 8.4 Hz, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 191.9, 163.2, 158.5, 152.1, 137.3, 135.8, 134.7, 134.1, 132.1, 132.0, 129.9, 129.3, 128.9, 128.3, 125.7and 120.5; **HRFD-MS** calcd for $C_{21}H_{12}BrClN_2O$: 421.9822, found: 421.9826.

(2-(4-chlorophenyl) quinazolin-4-yl) (4-iodophenyl) methanone (4m)



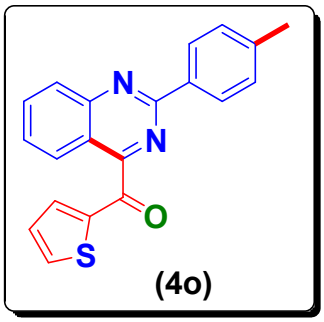
White solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.51 (d, J= 8.4 Hz, 2 H), 8.15 (d, J= 8.8 Hz, 1 H), 8.05 (d, J= 8.4 Hz, 1 H), 7.94 (t, J= 6.8 Hz, 1 H), 7.87 (d, J= 8.8 Hz, 2 H), 7.73 (d, J= 8.8 Hz, 2 H), 7.60 (t, J= 8.0 Hz, 1 H), 7.45 (d, J= 8.8 Hz, 2 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.2, 163.2, 158.5, 152.1, 138.0, 137.2, 135.7, 134.7, 134.6, 131.9, 129.9, 129.2, 128.9, 128.3, 125.6, 120.5 and 103.0; **HRFD-MS** calcd for $C_{21}H_{12}ClIN_2O$: 469.9683, found: 469.9683.

1-(4-(2-(4-chlorophenyl) quinazoline-4-carbonyl) phenyl) ethanone (4n)



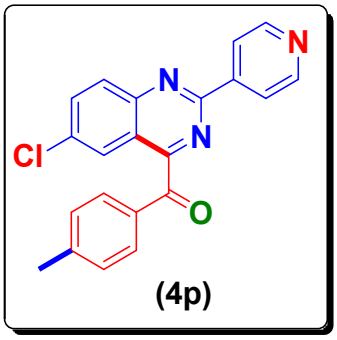
Light brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.50 (d, J= 8.4 Hz, 2 H), 8.16 (d, J= 8.8 Hz, 1 H), 8.11 (t, J= 8.4 Hz, 3 H), 8.05 (d, J= 8.0 Hz, 2 H), 7.94 (t, J= 7.2 Hz, 1 H), 7.62 (t, J= 7.2 Hz, 1 H), 7.45 (t, J= 8.8 Hz, 1 H), 2.65 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 197.4, 192.3, 162.9, 158.5, 152.2, 140.8, 138.5, 137.3, 135.7, 134.8, 130.9, 129.9, 129.3, 128.9, 128.4, 128.3, 125.6, 120.4 and 26.9; **ESI-MS** calcd for $C_{23}H_{15}ClN_2O_2$ (M+Na): 386.0822, found: 409.0724.

thiophen-2-yl (2-p-tolylquinazolin-4-yl) methanone (4o)



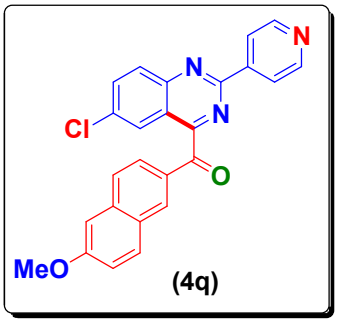
Light brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.55 (d, J= 8.4 Hz, 2 H), 8.41 (d, J= 9.2 Hz, 1 H), 8.13 (d, J= 8.4 Hz, 1 H), 8.04 (d, J= 3.6 Hz, 1 H), 7.91 (t, J= 8.4 Hz, 1 H), 7.82 (d, J= 3.6 Hz, 1 H), 7.80 (t, J= 4.8 Hz, 1 H), 7.60 (d, J= 7.2 Hz, 2 H), 7.19 (t, J= 3.6 Hz, 1 H), 2.44 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 184.7, 161.5, 159.6, 152.6, 141.2, 136.9, 136.8, 134.7, 134.3, 129.5, 129.1, 128.6, 128.3, 128.0, 126.1, 120.1 and 21.5; **ESI-MS** calcd for $C_{20}H_{14}N_2OS$ (M+Na): 330.0827, found: 353.0720.

(6-chloro-2-(pyridin-4-yl) quinazolin-4-yl) (p-tolyl) methanone (4p)



Light yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.78 (bs, 2 H), 8.40 (d, *J*= 5.4 Hz, 2 H), 8.14 (d, *J*= 9.6 Hz, 1 H), 8.08 (s, 1 H), 7.91 (d, *J*= 8.4 Hz, 3 H), 7.32 (d, *J*= 8.4 Hz, 2 H), 2.45 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 191.8, 163.6, 157.6, 150.5, 150.3, 146.0, 144.3, 135.9, 134.9, 132.4, 131.0, 130.9, 129.5, 124.8, 122.2, 121.6 and 21.9; **ESI-MS** calcd for $C_{21}H_{14}ClN_3O$ (M+H): 359.0825, found: 360.0895.

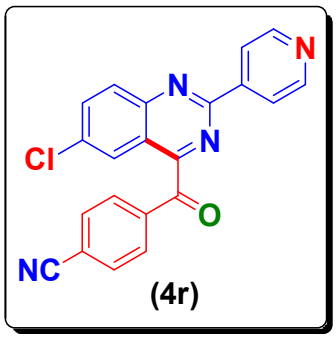
(6-chloro-2-(pyridin-4-yl) quinazolin-4-yl) (6-methoxynaphthalen-2-yl) methanone (4q)



(4q)

Light yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.77 (bs, 2 H), 8.43 (d, *J*= 4.8 Hz, 2 H), 8.32 (s, 1 H), 8.18-8.12 (m, 3 H), 7.92 (t, *J*= 8.4 Hz, 1 H), 7.85 (d, *J*= 9.0 Hz, 1 H), 7.74 (d, *J*= 8.4 Hz, 1 H), 7.17 (t, *J*= 9.0 Hz, 2 H), 3.95 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 191.8, 163.9, 160.7, 157.7, 150.6, 144.3, 138.2, 136.0, 135.0, 134.0, 131.6, 131.0, 130.3, 127.6, 127.5, 125.6, 124.9, 122.3, 121.8, 120.1, 105.9 and 55.5; **ESI-MS** calcd for $C_{25}H_{16}ClN_3O_2$ (M+H): 425.0931, found: 426.1047.

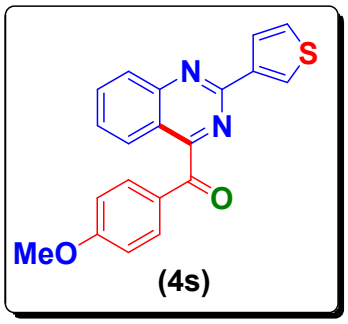
4-(6-chloro-2-(pyridin-4-yl) quinazoline-4-carbonyl) benzonitrile (4r)



(4r)

Light yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.80 (bs, 2 H), 8.35 (bs, 2 H), 8.26 (s, 1 H), 8.19 (d, *J*= 8.8 Hz, 2 H), 8.16 (d, *J*= 8.4 Hz, 2 H), 7.96 (d, *J*= 11.2 Hz, 1 H), 7.83 (d, *J*= 8.0 Hz, 1 H),; **^{13}C NMR** (150 MHz, $CDCl_3$): δ 190.8, 160.7, 157.5, 150.9, 150.7, 143.8, 138.1, 136.3, 135.8, 132.4, 131.2, 131.1, 124.6, 122.1, 121.5, 117.6 and 117.5; **ESI-MS** calcd for $C_{21}H_{11}ClN_4O$ (M+H): 370.0621, found: 371.0684.

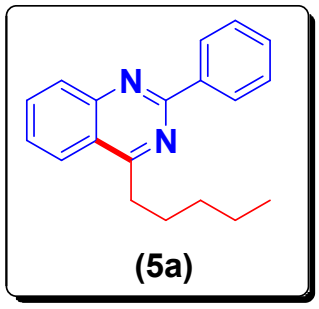
(4-methoxyphenyl) (2-(thiophen-3-yl) quinazolin-4-yl) methanone (4s)



(4s)

Light brown solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.39 (d, *J*= 3.0 Hz, 1 H), 8.08 (d, *J*= 9.6 Hz, 1 H), 8.03-7.96 (m, 4 H), 7.88 (t, *J*= 6.6 Hz, 1 H), 7.52 (t, *J*= 7.2 Hz, 1 H), 7.38 (d, *J*= 8.4 Hz, 1 H), 6.95 (t, *J*= 6.6 Hz, 1 H), 3.87 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 191.5, 164.8, 164.6, 156.8, 151.8, 141.6, 134.3, 133.2, 128.9, 128.4, 127.7, 127.5, 126.1, 125.9, 120.3, 114.0 and 55.6; **ESI-MS** calcd for $C_{20}H_{14}N_2O_2S$ (M+H): 346.0776, found: 347.0845.

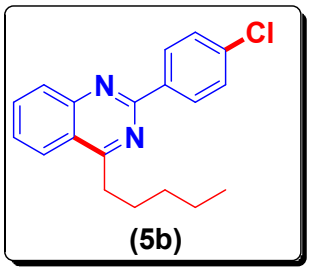
4-pentyl-2-phenylquinazoline (5a)



(5a)

Light yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): 8.57 (d, J= 9.0 Hz, 2 H), 8.10 (d, J= 9.0 Hz, 1 H), 7.83 (t, J= 7.8 Hz, 1 H), 7.56 (t, J= 4.2 Hz, 1 H), 7.47 (d, J= 9.0 Hz, 2 H), 3.29 (t, J= 7.8 Hz, 2 H), 1.98-1.93 (m, 2 H), 1.49-1.40 (m, 4 H), 0.92 (t, J= 7.2 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.5, 160.1, 150.7, 138.4, 133.2, 130.2, 129.3, 128.5, 128.4, 126.6, 124.6, 122.5, 34.5, 31.8, 28.2, 22.5 and 14.0; **ESI-MS** calcd for $C_{19}H_{20}N_2$ (M+H): 276.1626, found: 277.1714.

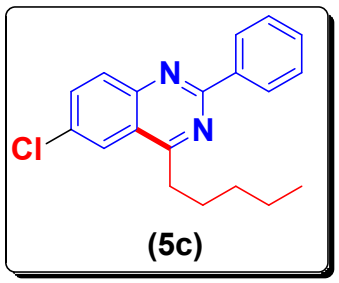
2-(4-chlorophenyl)-4-pentyl quinazoline (5b)



(5b)

Light yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.57 (d, *J*= 9.0 Hz, 2 H), 8.10 (d, *J*= 9.0 Hz, 1 H), 7.83 (t, *J*= 7.8 Hz, 1 H), 7.56 (t, *J*= 4.2 Hz, 1 H), 7.47 (d, *J*= 9.0 Hz, 2 H), 3.29 (t, *J*= 7.8 Hz, 2 H), 1.98-1.93 (m, 2 H), 1.49-1.40 (m, 4 H), 0.92 (t, *J*= 7.2 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.6, 159.0, 150.6, 136.9, 136.5, 133.4, 129.9, 129.3, 128.6, 126.9, 124.6, 122.5, 34.5, 31.8, 28.2 , 22.5 and 14.0; **ESI-MS** calcd for $C_{19}H_{19}ClN_2$ (M+H): 310.1237, found: 311.1331.

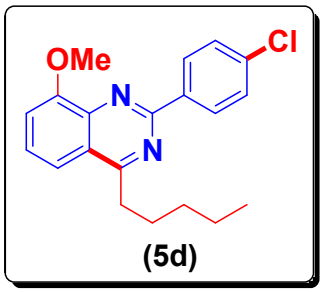
6-chloro-4-pentyl-2-phenyl quinazoline (5c)



(5c)

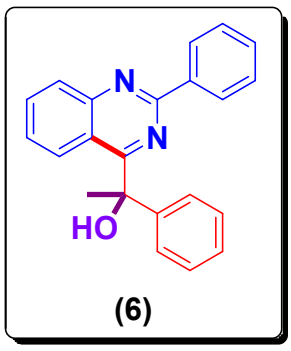
Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.59 (d, *J*= 7.8 Hz, 2 H), 8.05 (s, 1 H), 7.99 (d, *J*= 9.0 Hz, 1 H), 7.75 (t, *J*= 9.0 Hz, 1 H), 7.52-7.48 (m, 3 H), 3.25 (t, *J*= 7.8 Hz, 2 H), 1.98-1.94 (m, 2 H), 1.49-1.40 (m, 4 H), 0.92 (t, *J*= 7.2 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 170.7, 160.3, 149.2, 138.0, 134.1, 132.2, 131.0, 130.5, 128.5, 123.6, 123.0, 34.4, 31.7, 27.9, 22.5 and 14.0; **ESI-MS** calcd for $C_{19}H_{19}ClN_2$ (M+H): 310.1237, found: 311.1317.

2-(4-chlorophenyl)-8-methoxy-4-pentyl quinazoline (5d)



Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.58 (d, *J*= 8.8 Hz, 2 H), 7.65 (d, *J*= 8.0 Hz, 1 H), 7.48 (d, *J*= 8.0 Hz, 1 H), 7.45 (d, *J*= 8.4 Hz, 2 H), 7.17 (d, *J*= 7.6 Hz, 1 H), 4.08 (s, 3 H), 3.27 (t, *J*= 7.6 Hz, 2 H), 1.99-1.91 (m, 2 H), 1.48-1.38 (m, 4 H), 0.92 (t, *J*= 7.2 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.4, 158.3, 155.4, 142.8, 137.0, 136.4, 130.0, 128.6, 126.9, 123.4, 116.1, 111.3, 56.3, 34.9, 31.8, 28.1, 22.5 and 14.0; **ESI-MS** calcd for $C_{20}H_{21}ClN_2O$ (M+H): 340.1342, found: 341.1412.

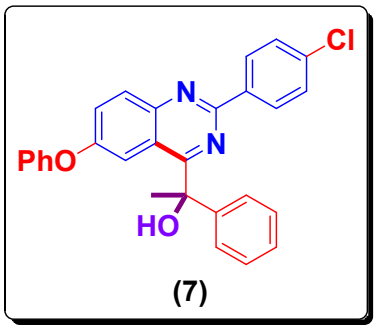
1-phenyl-1-(2-phenylquinazolin-4-yl) ethanol (6)



Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.66(d, *J*= 6.6 Hz, 2 H), 8.08 (d, *J*= 8.4 Hz, 1 H), 7.76-7.74 (m, 2 H), 7.73-7.69 (m, 3 H), 7.56 (t, *J*= 7.2 Hz, 2 H), 7.44-7.26 (m, 4 H), 6.63 (bs, 3 H), 2.16 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 172.3, 157.8, 152.1, 145.2, 137.3, 133.4,

130.9, 129.6, 128.7, 128.6, 128.5, 127.8, 126.7, 126.4, 119.8, 75.5 and 28.4; **ESI-MS** calcd for $C_{22}H_{18}N_2O$ (M+H): 326.1419, found: 327.1479.

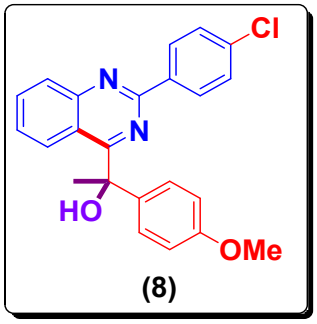
1-(2-(4-chlorophenyl)-6-phenoxyquinazolin-4-yl)-1-phenylethanol (7)



(7)

Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.58 (d, *J*= 8.4 Hz, 2 H), 8.04 (d, *J*= 9.6 Hz, 1 H), 7.57-7.51 (m, 3 H), 7.37 (t, *J*= 7.8 Hz, 2 H), 7.25 (t, *J*= 8.4 Hz, 1 H), 7.18-7.15 (m, 4 H), 6.98 (s, 1 H), 6.85 (d, *J*= 8.4 Hz, 2 H), 6.41 (s, 1 H), 1.98 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.1, 156.3, 155.7, 154.7, 148.5, 144.5, 136.8, 135.8, 131.3, 130.2, 129.5, 128.9, 128.6, 127.5, 127.0, 126.1, 124.7, 120.2, 109.9, 75.3 and 27.9; **ESI-MS** calcd for $C_{28}H_{21}ClN_2O_2$ (M+H): 452.1292, found: 453.1362.

1-(2-(4-chlorophenyl) quinazolin-4-yl)-1-(4-methoxyphenyl) ethanol (8)

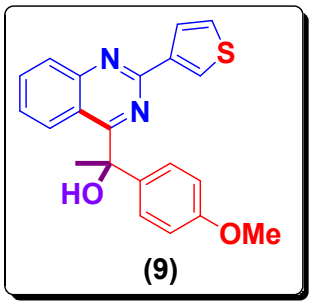


(8)

Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.61 (d, *J*= 8.4 Hz, 2 H), 8.05 (d, *J*= 8.4 Hz, 1 H), 7.77-7.70 (m, 2 H), 7.52 (t, *J*= 8.4 Hz, 2 H), 7.32 (d, *J*= 9.0 Hz, 2 H), 6.83 (d, *J*= 9.0 Hz, 2 H), 6.52 (s, 1 H), 3.76 (s, 3 H), 2.12 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 172.8, 159.0, 156.8,

152.0, 137.3, 137.1, 135.7, 133.6, 129.8, 129.5, 128.9, 127.7, 126.9, 126.6, 119.8, 113.9, 75.1, 55.2 and 28.7; **ESI-MS** calcd for $C_{23}H_{19}ClN_2O_2$ (M+H): 390.1135, found: 391.1227.

1-(4-methoxyphenyl)-1-(2-(thiophen-3-yl) quinazolin-4-yl) ethanol (9)



(9)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.48 (s, 2 H), 8.08 (d, *J*= 6.0 Hz, 1 H), 8.01 (d, *J*= 8.4 Hz, 1 H), 7.72 (t, *J*= 8.4 Hz, 1 H), 7.66 (t, *J*= 9.0 Hz, 1 H), 7.44 (t, *J*= 4.8 Hz, 1 H), 7.32 (t, *J*= 9.0 Hz, 1 H), 7.28 (t, *J*= 7.2 Hz, 1 H), 6.83 (d, *J*= 8.4 Hz, 2 H), 6.66 (s, 1 H), 3.75 (s, 3 H), 2.11 (s, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 172.6, 158.9, 154.9, 152.0, 141.2, 137.4, 133.4, 129.3, 128.4, 127.7, 127.5, 126.6, 126.5, 126.3, 119.5, 113.9, 74.8, 55.2 and 28.5; **ESI-MS** calcd for $C_{21}H_{18}N_2O_2S$ (M+H): 362.1089, found: 363.1150.

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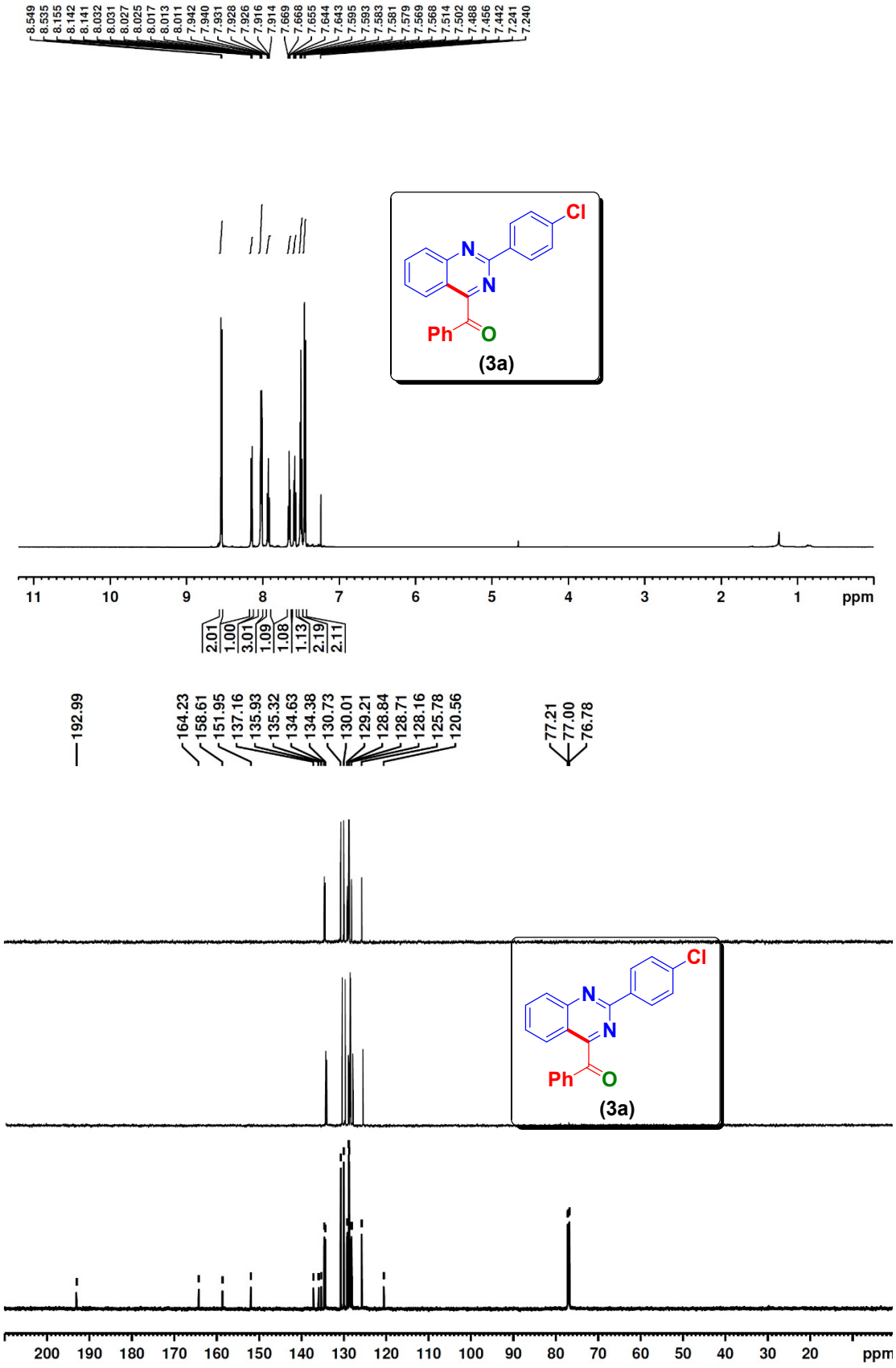
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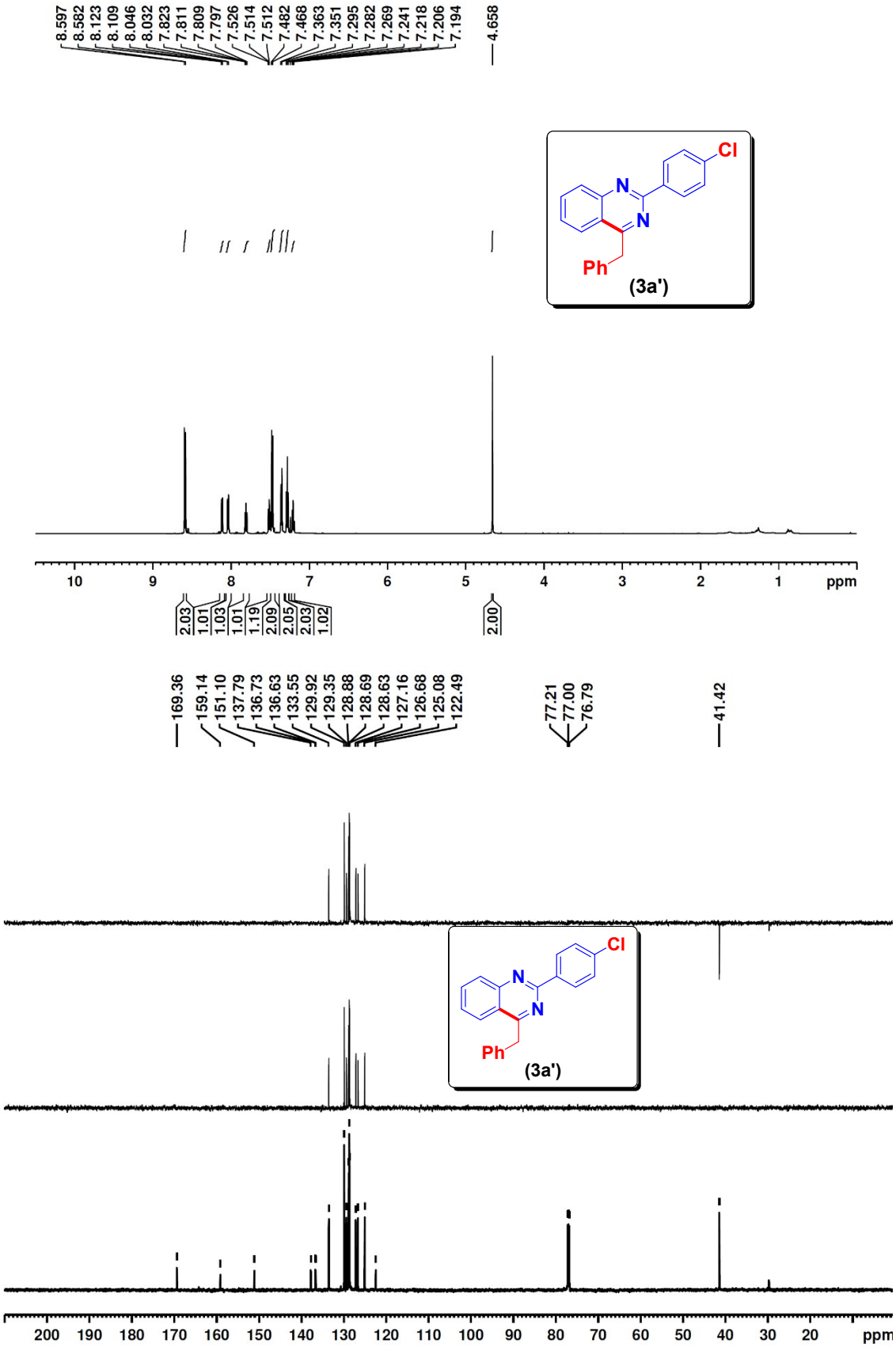
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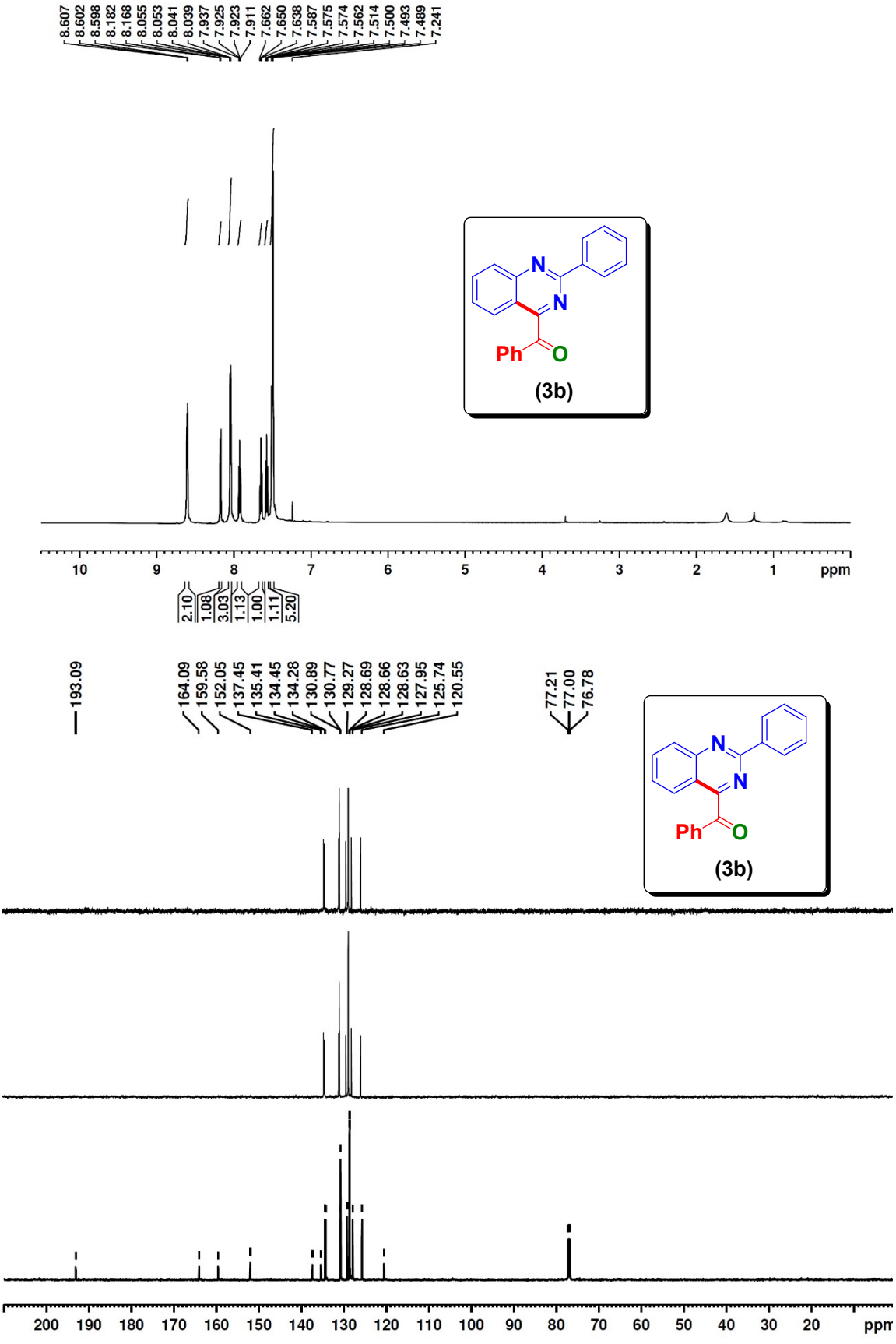
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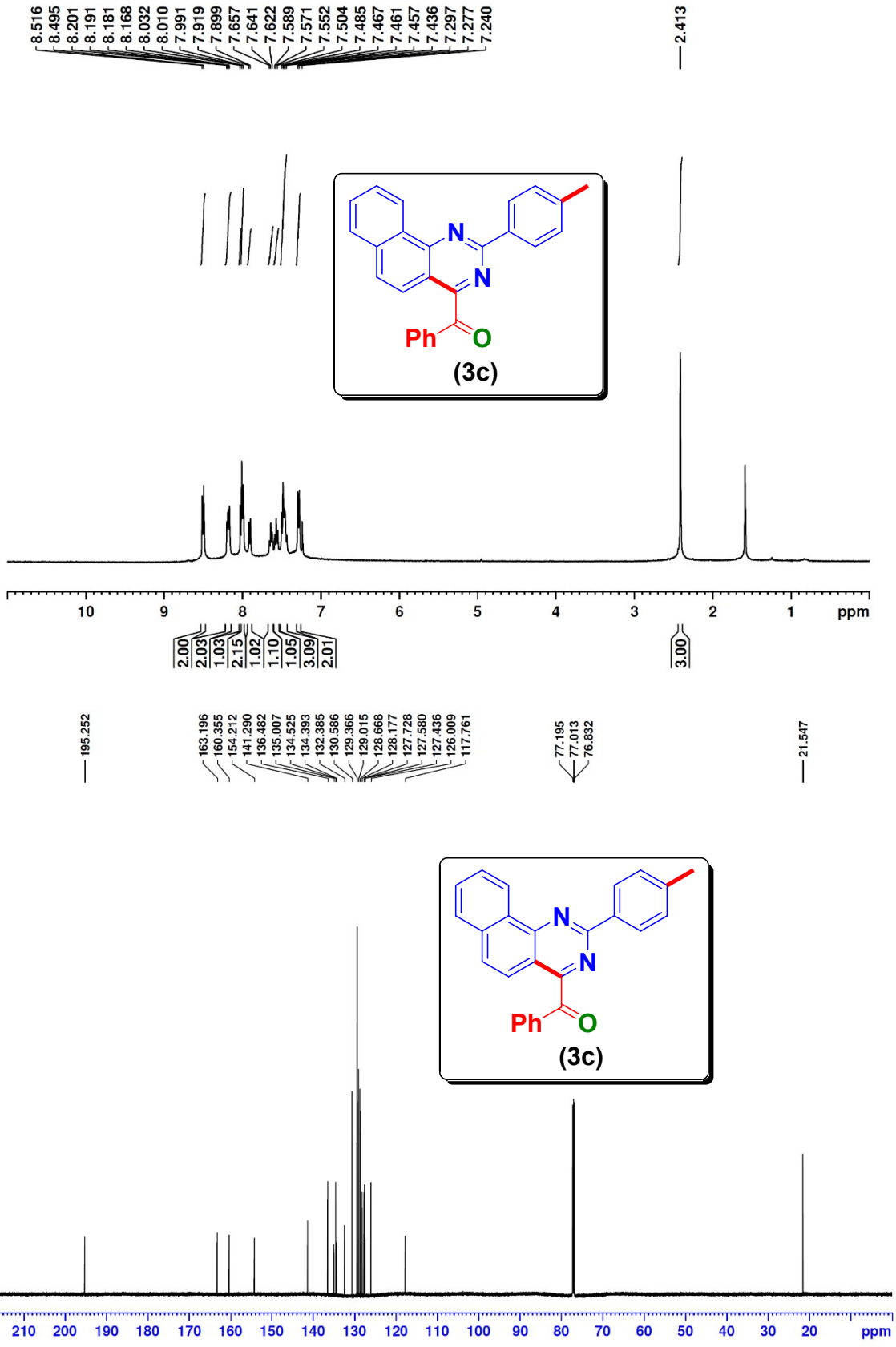
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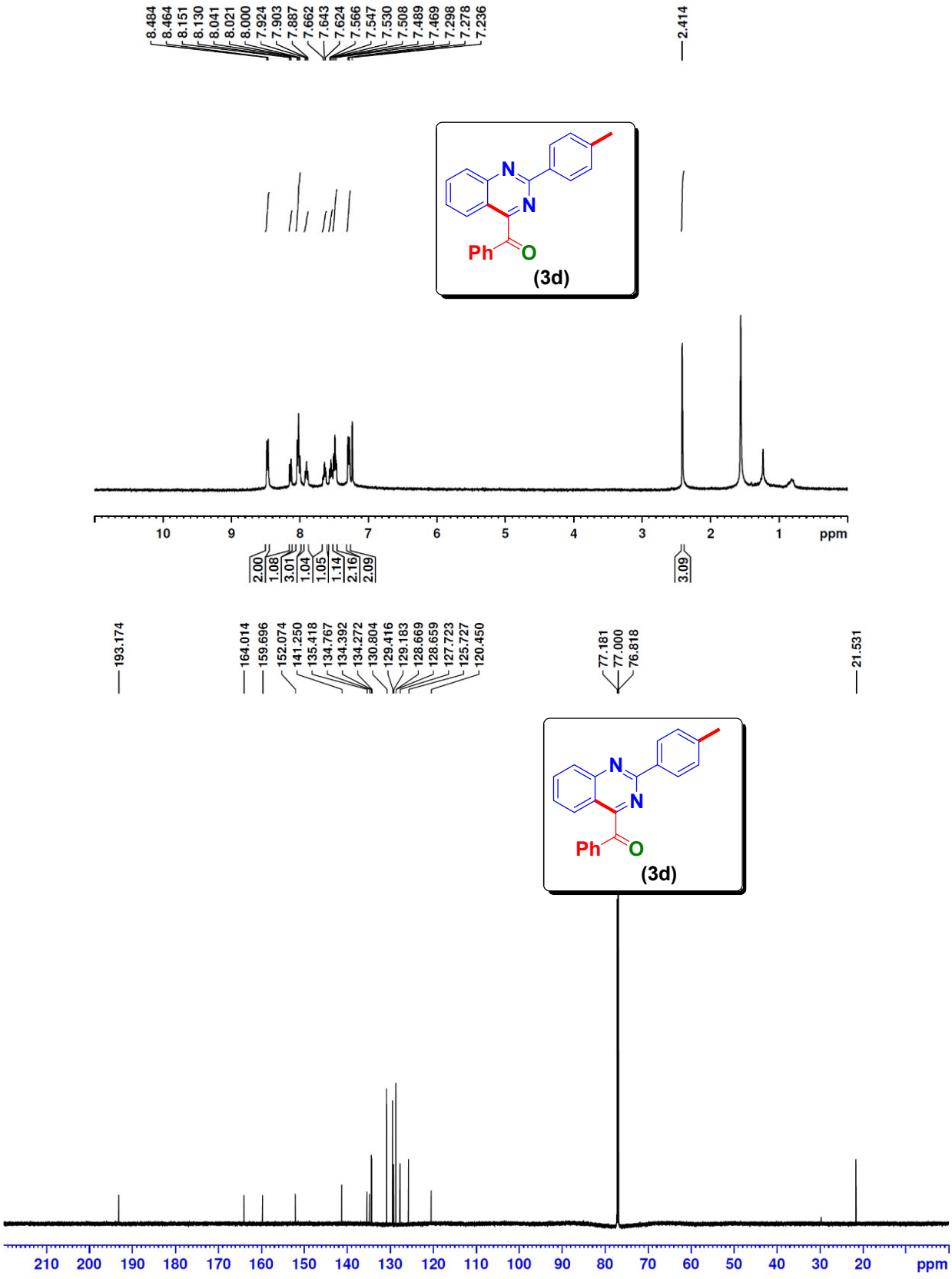
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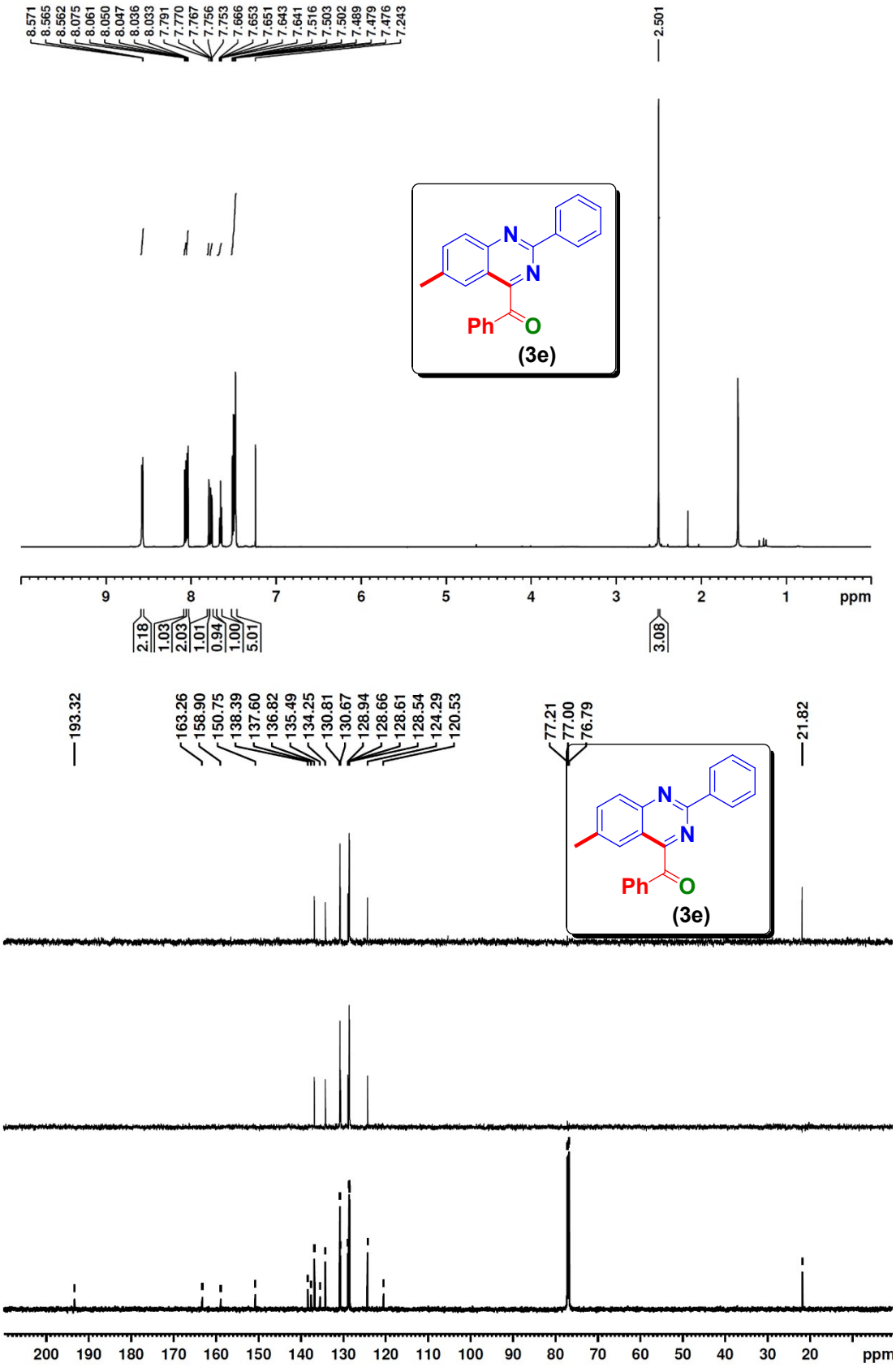
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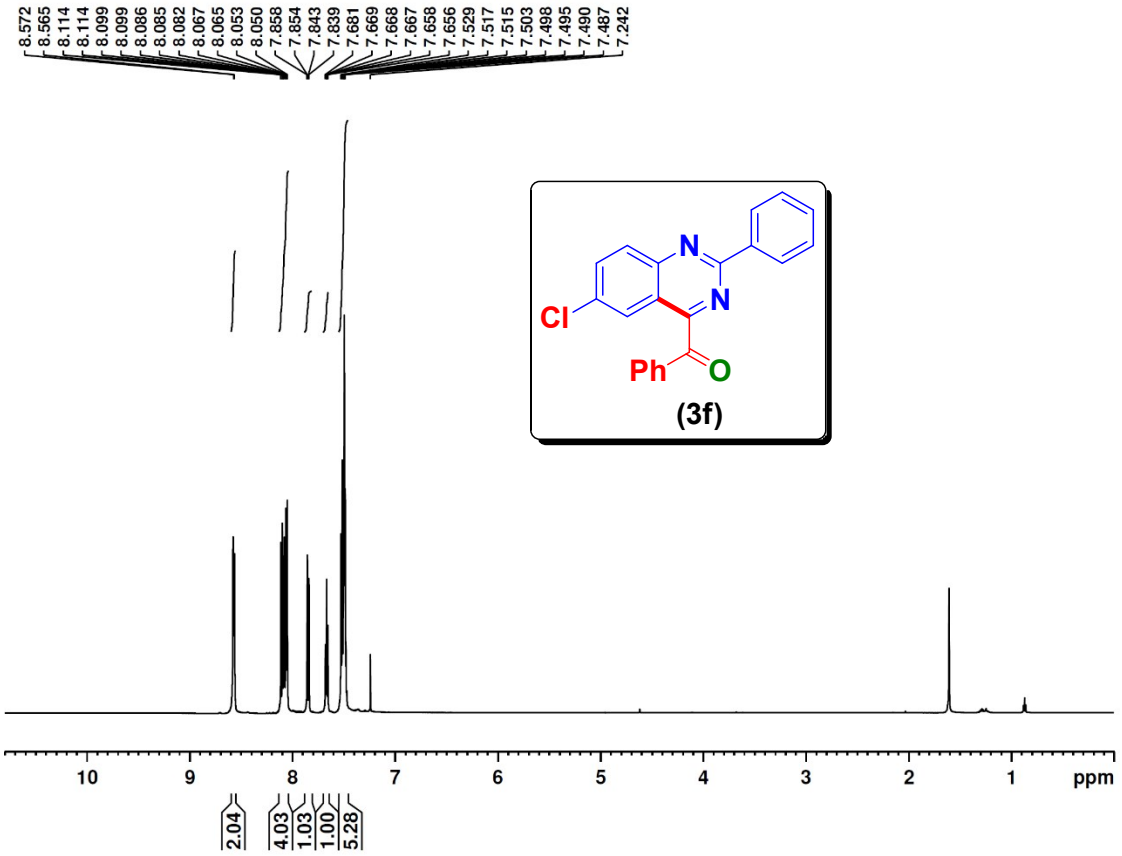
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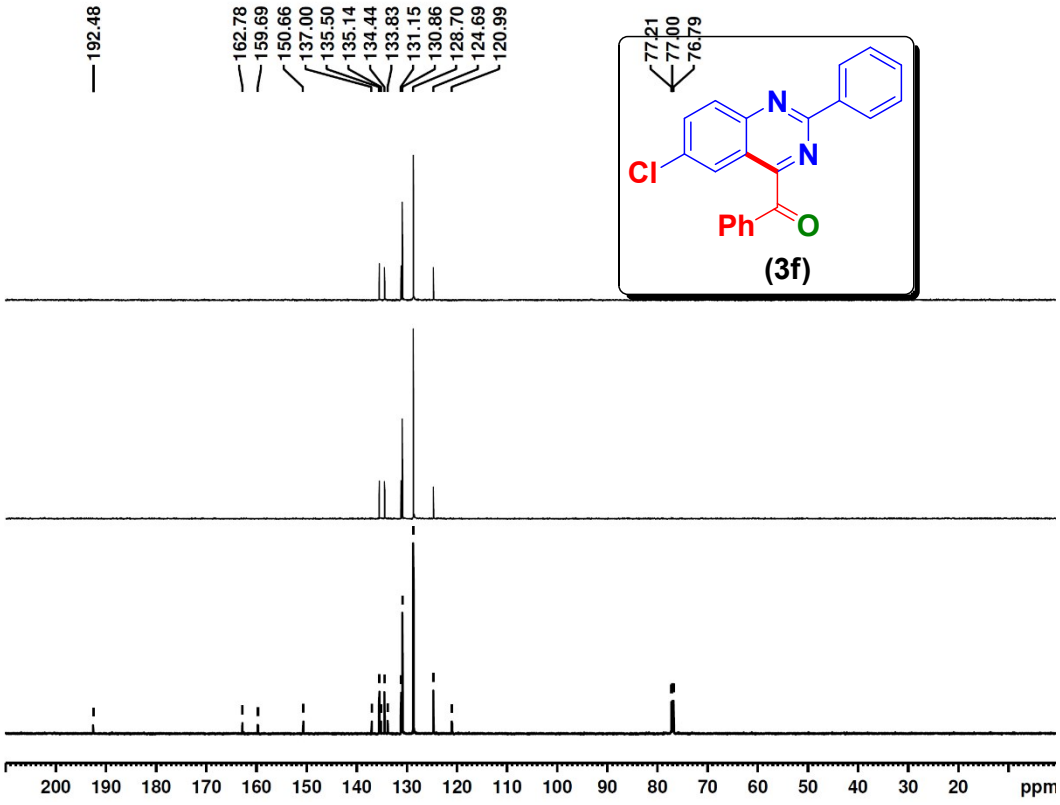
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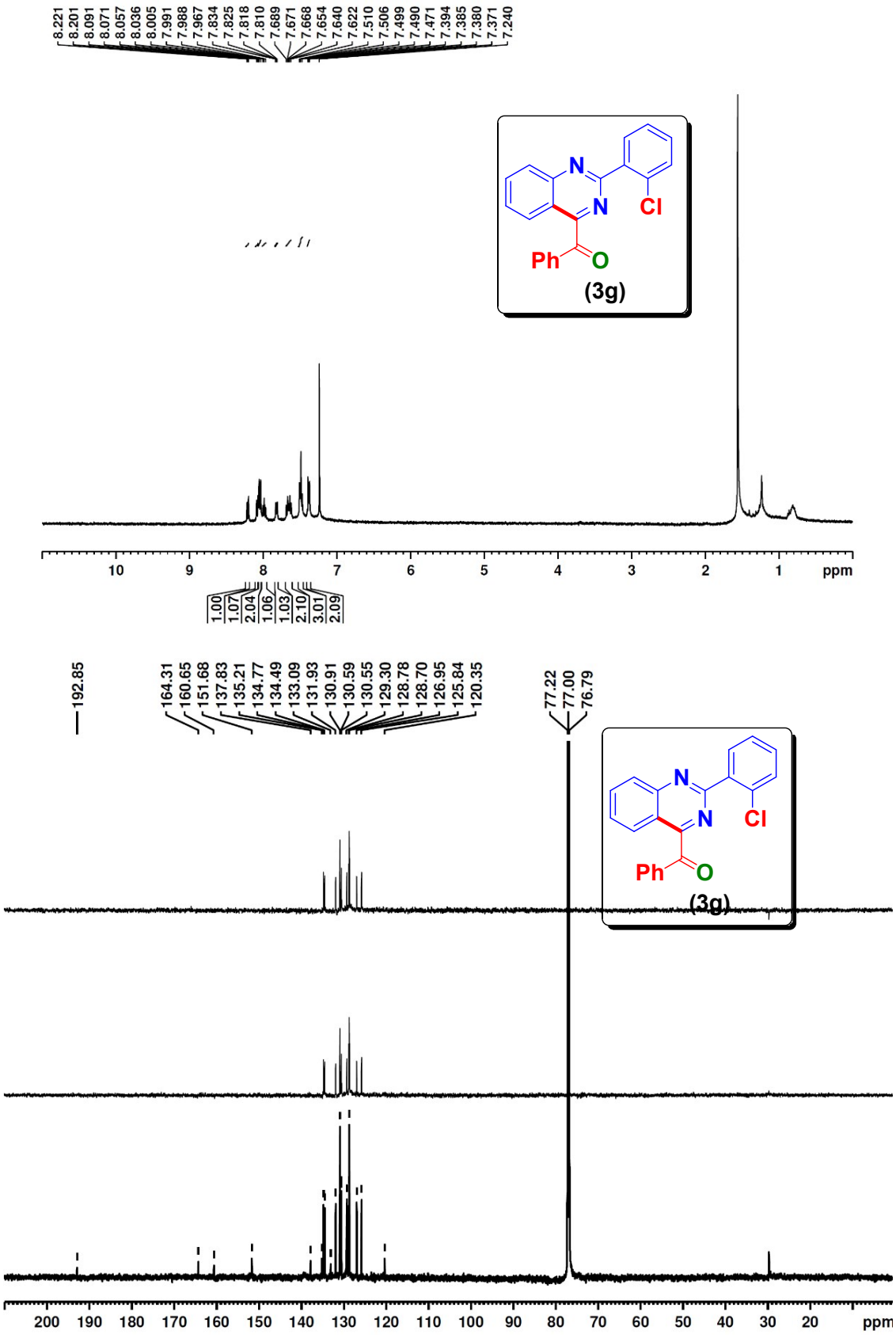
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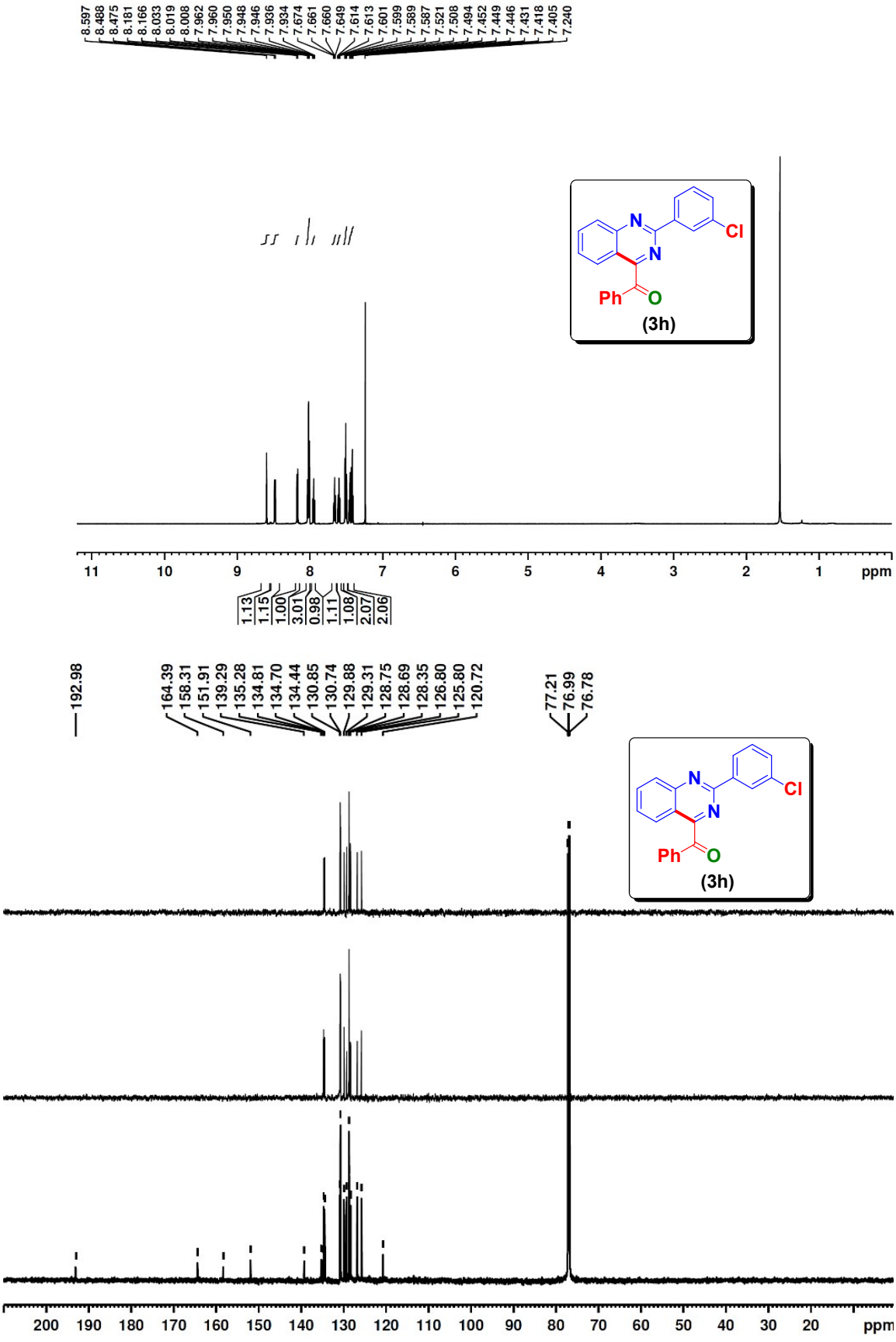
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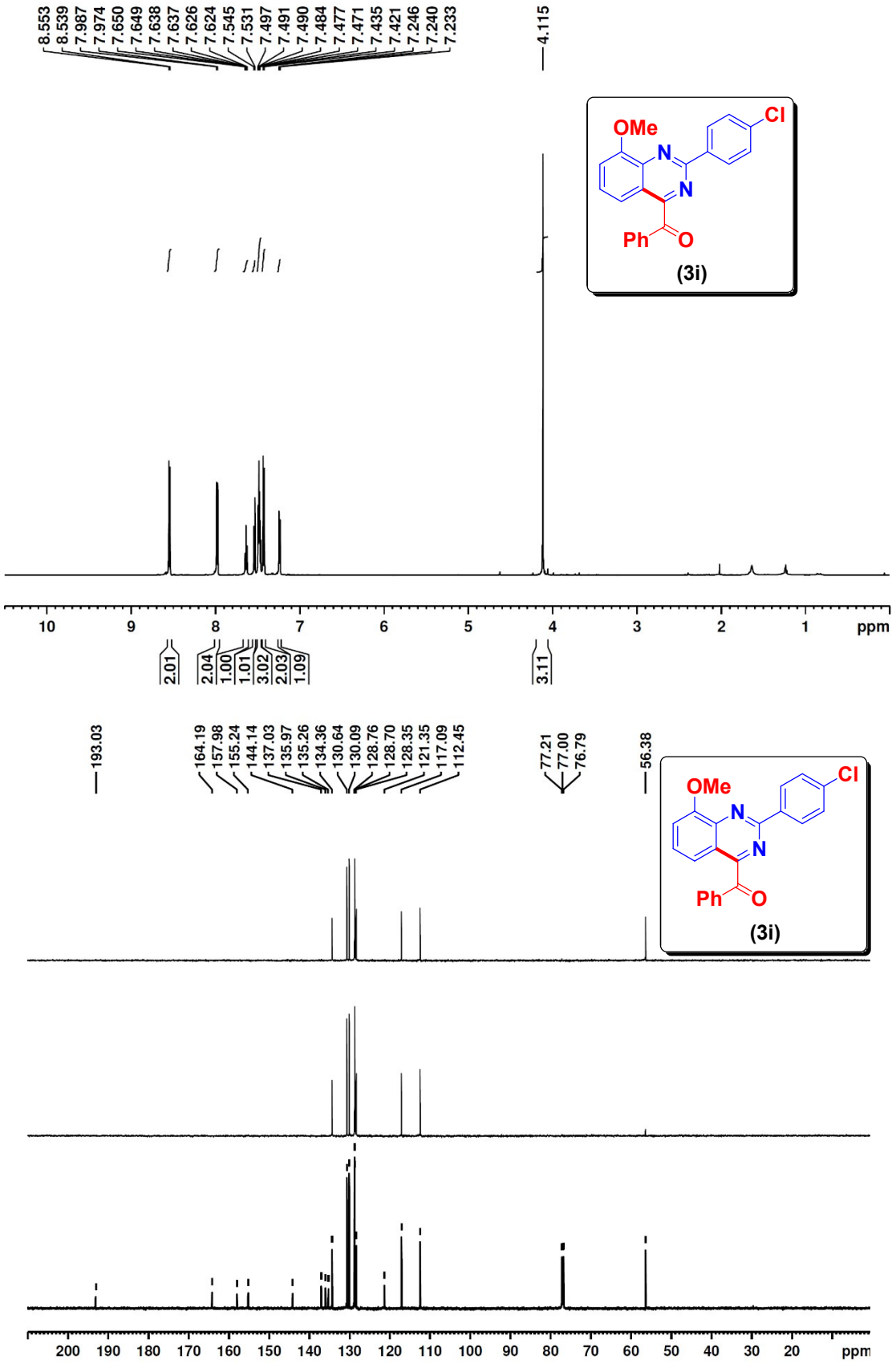
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7.987
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7.638
7.637
7.626
7.624
7.545
7.531
7.497
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7.490
7.484
7.477
7.471
7.435
7.421
7.246
7.240
7.233
4.115
OMe
N
N
Cl
Ph
O
(3i)
10
9
8
7
6
5
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ppm
2.01
2.04
1.00
1.01
3.02
2.03
1.09
3.11
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130.09
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128.35
121.35
117.09
112.45
77.21
77.00
76.79
56.38
OMe
N
N
Cl
Ph
O
(3i)
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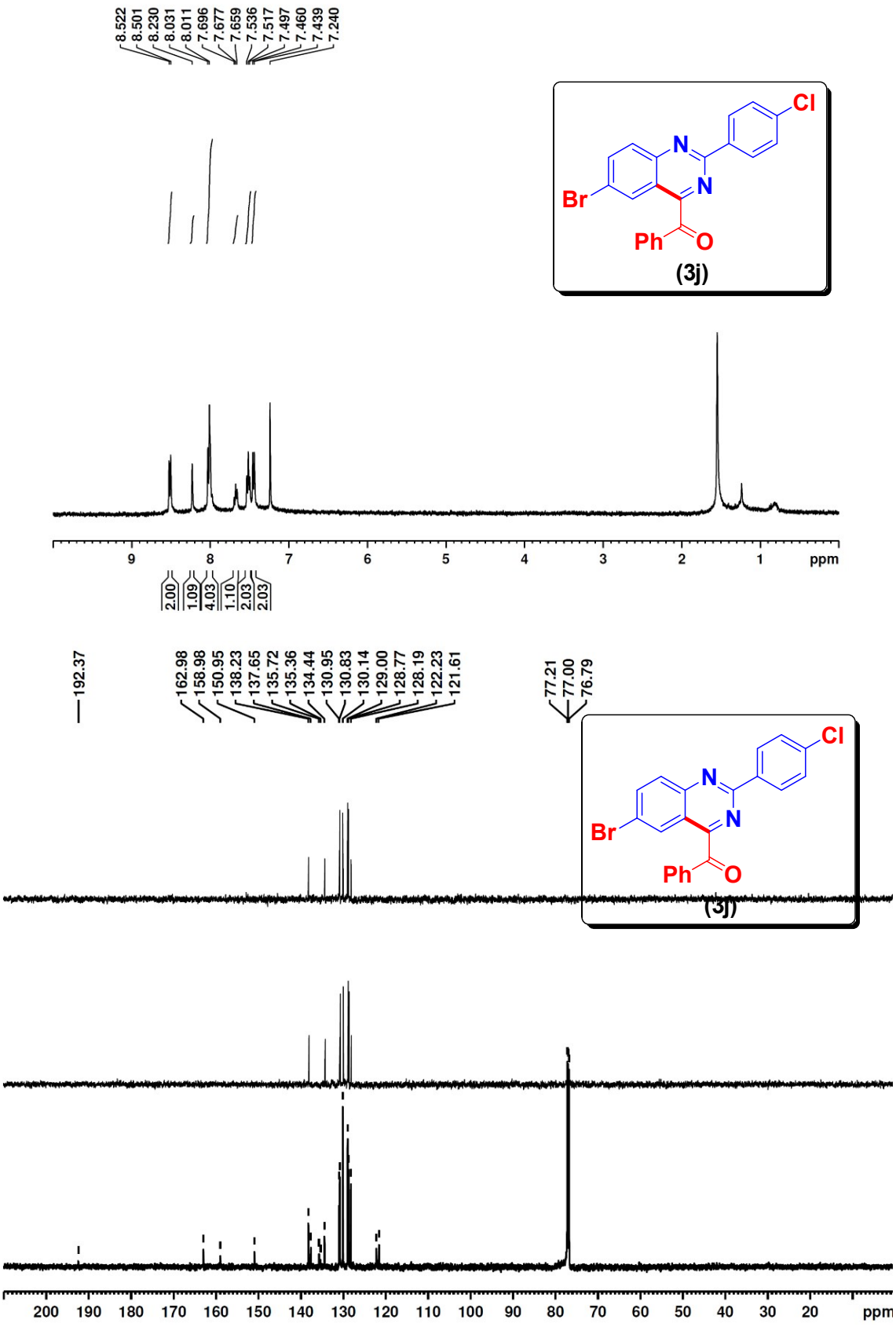
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7.240
Cl
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N
Br
Ph
O
(3j)
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5
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ppm
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2.03
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128.19
122.23
121.61
77.21
77.00
76.79
Cl
N
N
Br
Ph
O
(3j)
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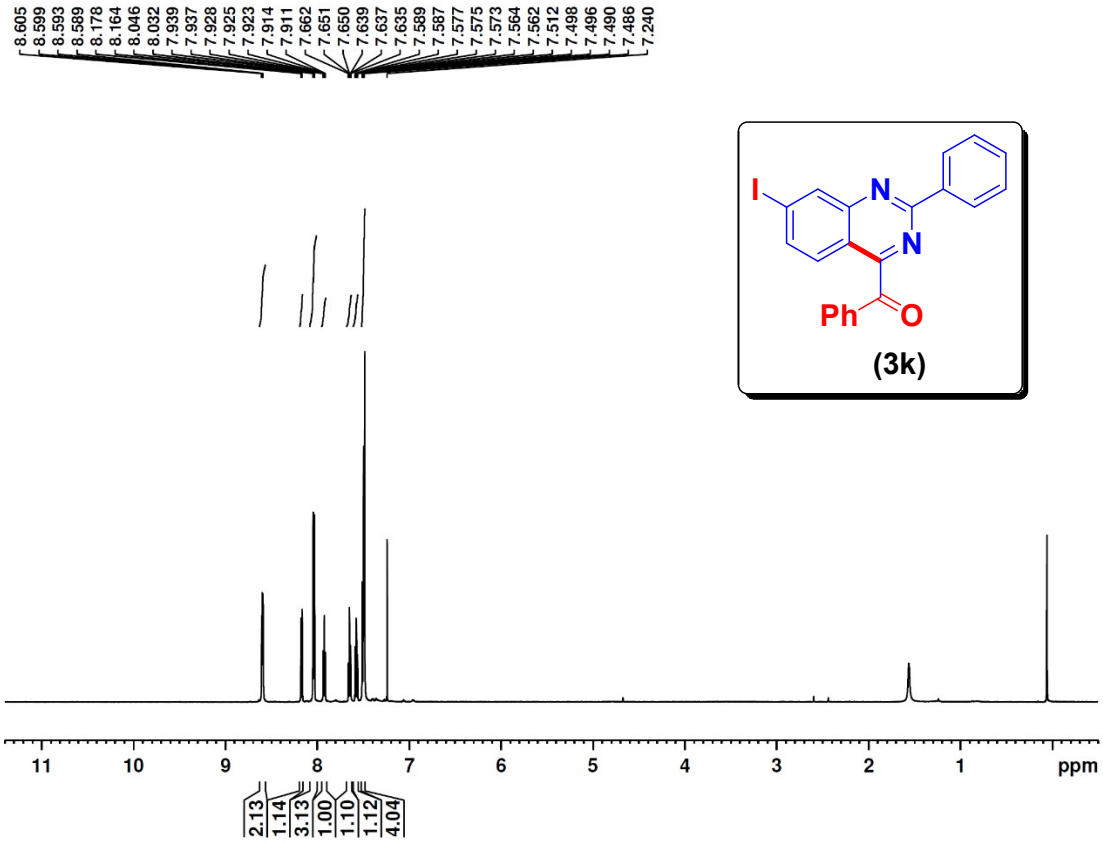
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7.928
7.925
7.923
7.914
7.911
7.662
7.651
7.650
7.639
7.637
7.635
7.589
7.587
7.577
7.575
7.573
7.564
7.562
7.512
7.498
7.496
7.490
7.486
7.240
I
N
N
Ph
O
(3k)
11
10
9
8
7
6
5
4
3
2
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ppm
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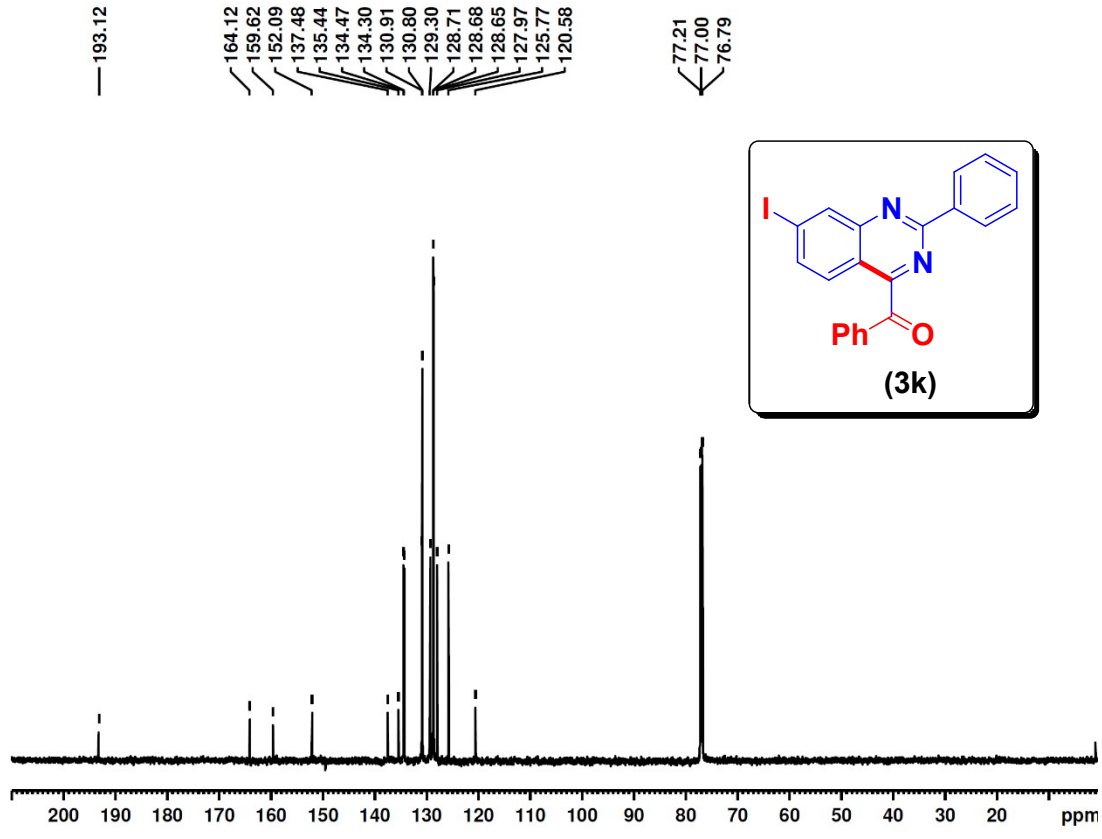
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130.80
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128.71
128.68
128.65
127.97
125.77
120.58
77.21
77.00
76.79
I
N
N
Ph
O
(3k)
200
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180
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160
150
140
130
120
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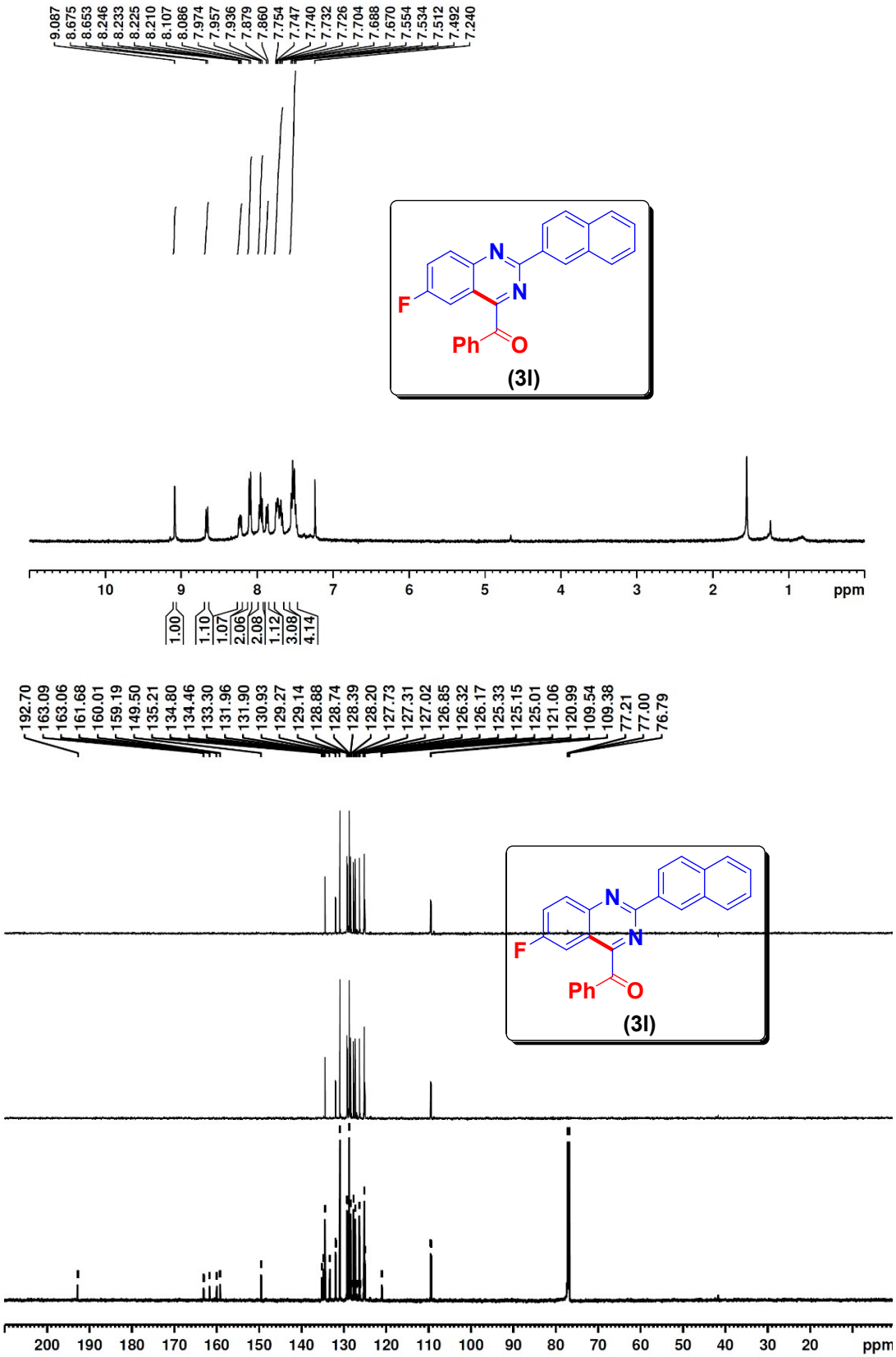
80
70
60
50
40
30
20
ppm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7.957
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7.879
7.860
7.754
7.747
7.740
7.732
7.726
7.704
7.688
7.670
7.554
7.534
7.512
7.492
7.240
N
N
F
Ph
O
(3l)
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.10
1.07
2.06
2.08
1.12
3.08
4.14
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163.09
163.06
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135.21
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125.15
125.01
121.06
120.99
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109.38
77.21
77.00
76.79
N
N
F
Ph
O
(3l)
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150
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130
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80
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40
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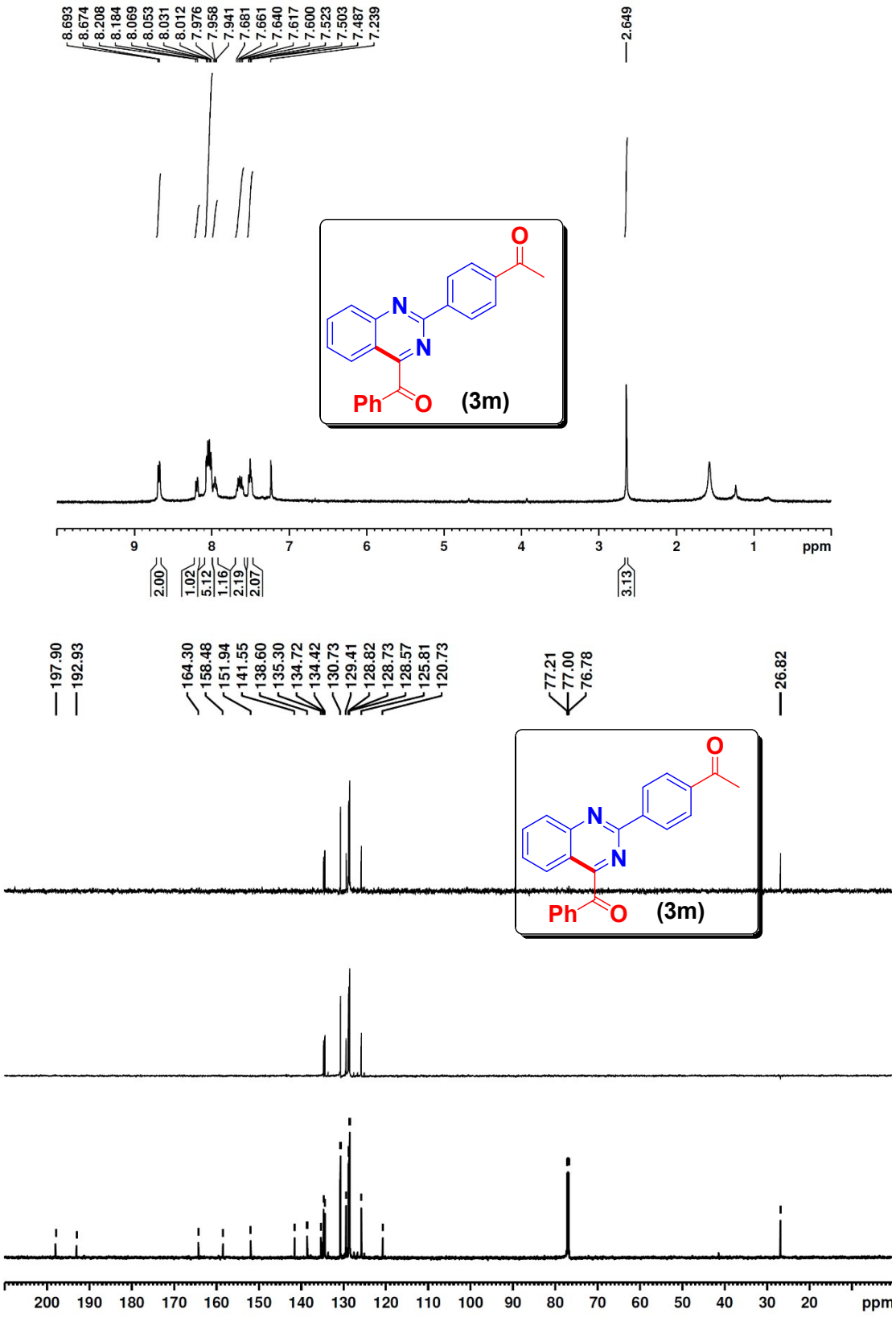
ppm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8.031
8.012
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7.941
7.681
7.661
7.640
7.617
7.600
7.523
7.503
7.487
7.239
2.649
O
N
N
Ph
O
(3m)
9
8
7
6
5
4
3
2
1
ppm
2.00
1.02
5.12
1.16
2.19
2.07
3.13
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141.55
138.60
135.30
134.72
134.42
130.73
129.41
128.82
128.73
128.57
125.81
120.73
77.21
77.00
76.78
26.82
O
N
N
Ph
O
(3m)
200
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180
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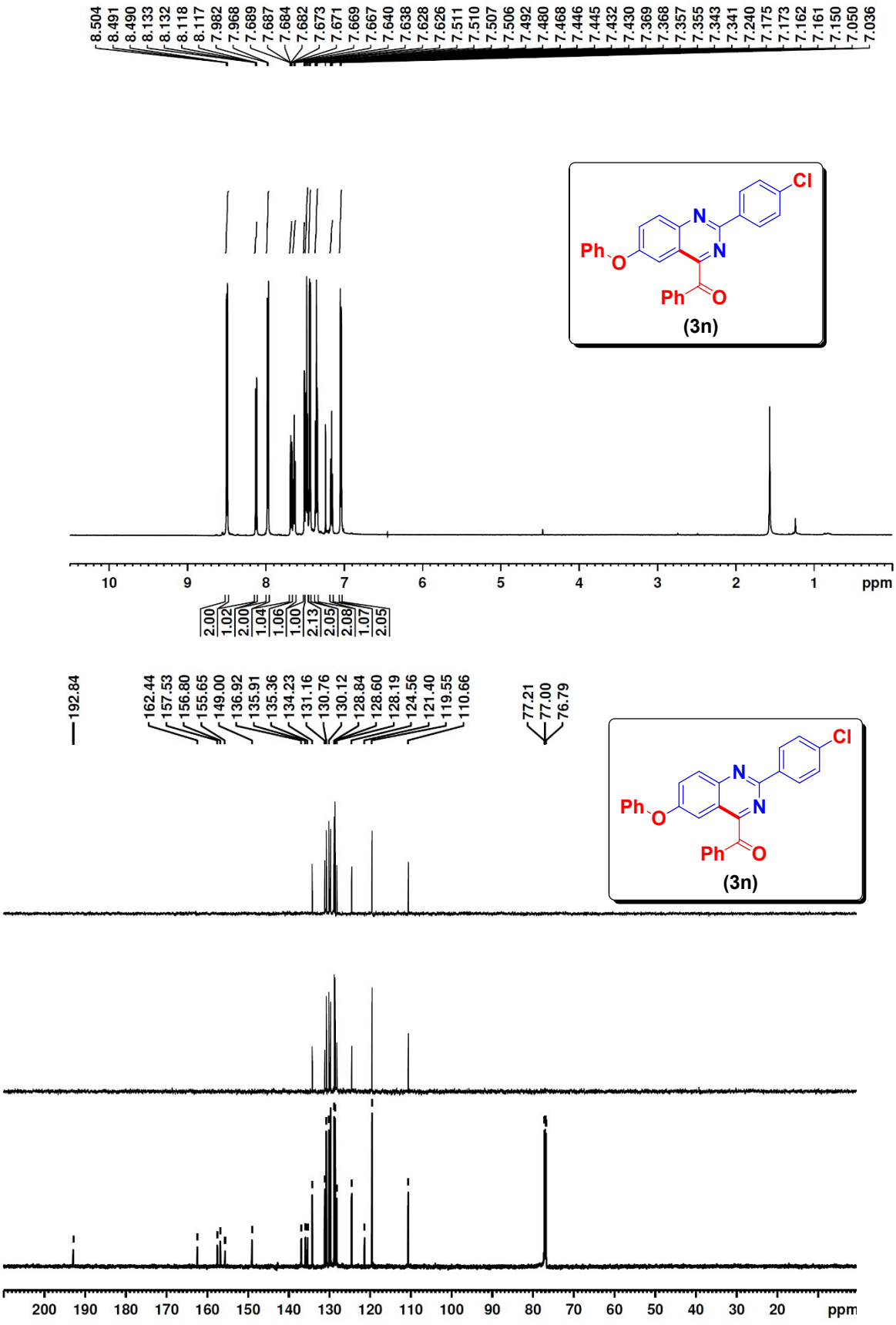
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.117
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7.687
7.684
7.682
7.673
7.671
7.669
7.667
7.640
7.638
7.628
7.626
7.511
7.510
7.507
7.506
7.492
7.480
7.468
7.446
7.445
7.432
7.430
7.369
7.368
7.357
7.355
7.343
7.341
7.240
7.175
7.173
7.162
7.161
7.150
7.050
7.036
Cl
N
N
Ph
O
Ph
O
(3n)
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.02
2.00
1.04
1.06
1.00
2.13
2.05
2.08
1.07
2.05
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156.80
155.65
149.00
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135.36
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131.16
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130.12
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128.19
124.56
121.40
119.55
110.66
77.21
77.00
76.79
Cl
N
N
Ph
O
Ph
O
(3n)
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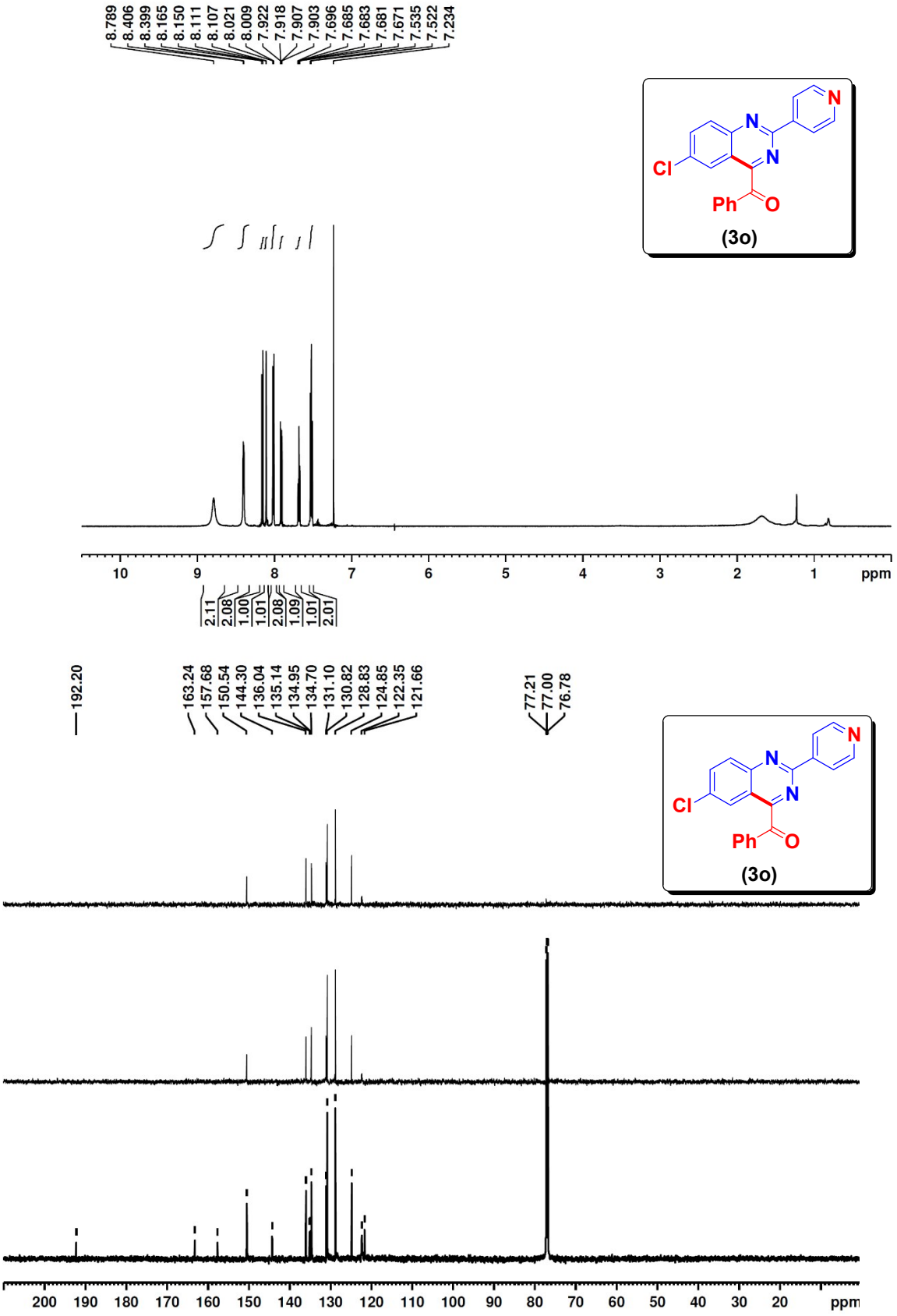
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.111
8.107
8.021
8.009
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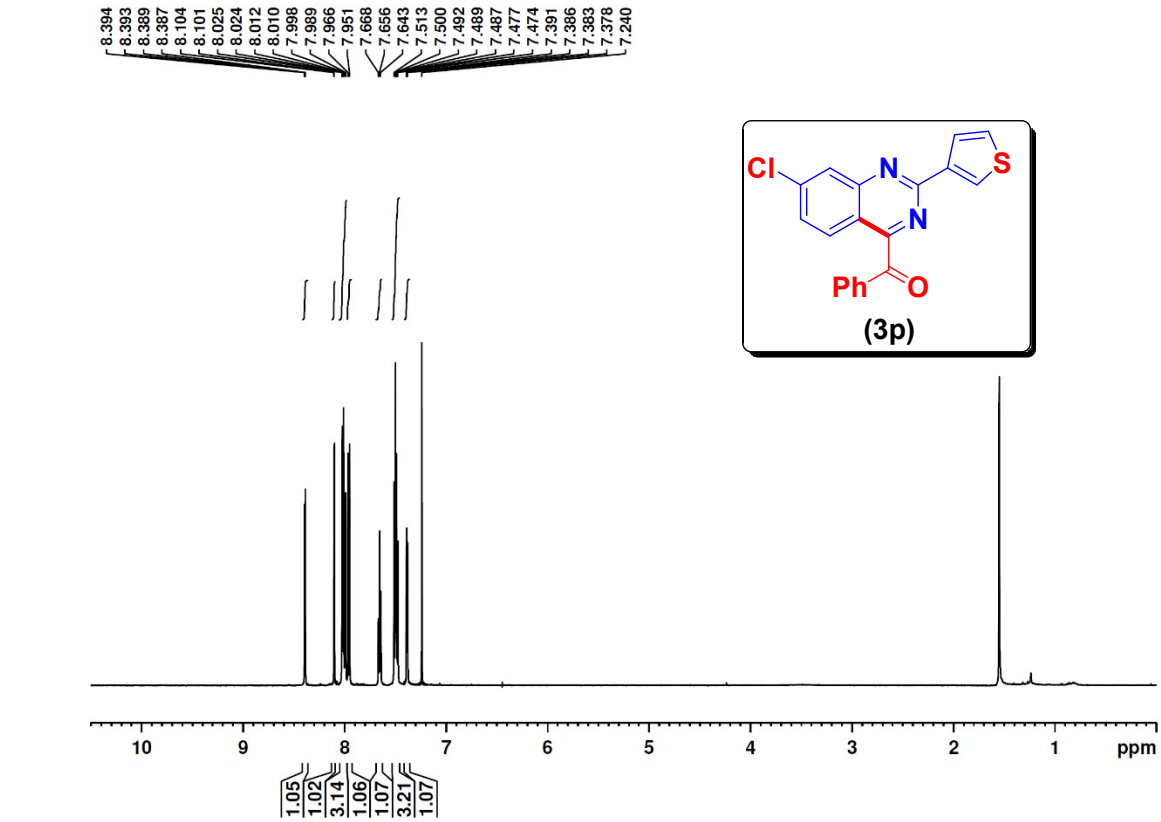
7.918
7.907
7.903
7.696
7.685
7.683
7.681
7.671
7.535
7.522
7.234
Cl
N
N
Ph
O
(3o)
10
9
8
7
6
5
4
3
2
1
ppm
2.11
2.08
1.00
1.01
2.08
1.09
1.01
2.01
192.20
163.24
157.68
150.54
144.30
136.04
135.14
134.95
134.70
131.10
130.82
128.83
124.85
122.35
121.66
77.21
77.00
76.78
(3o)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.024
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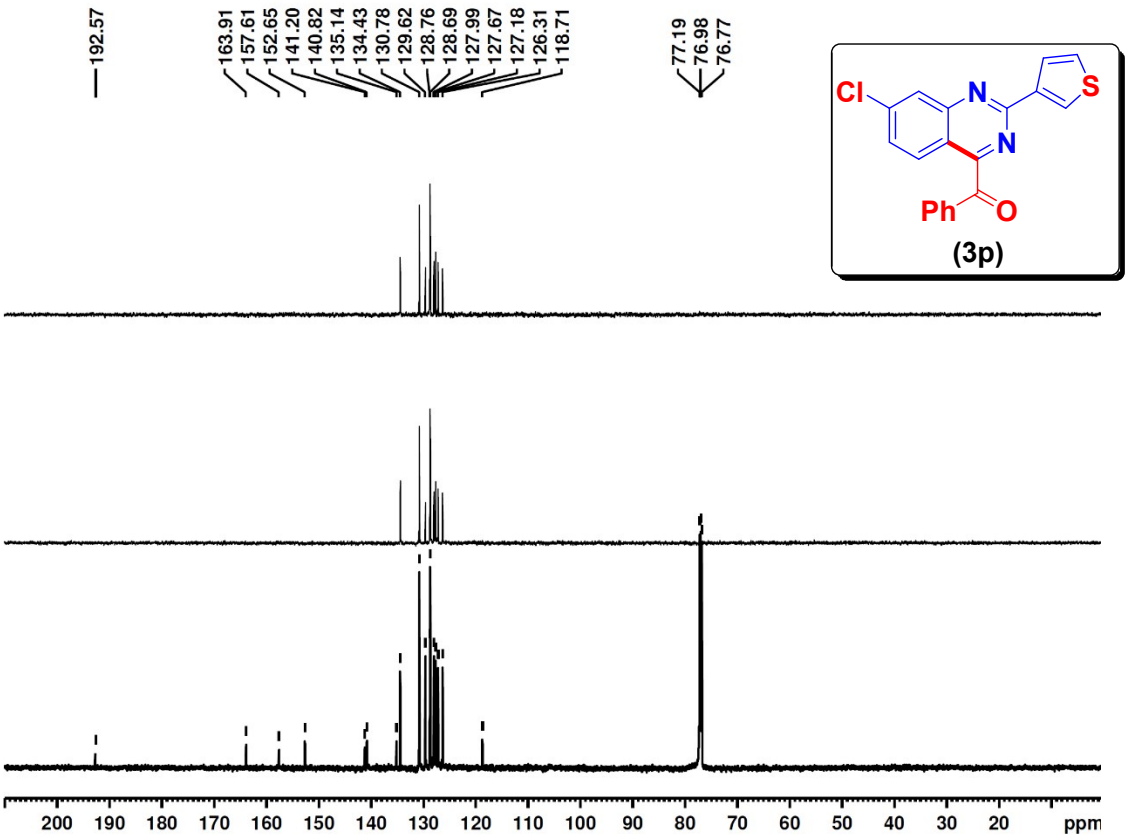
7.966
7.951
7.668
7.656
7.643
7.513
7.500
7.492
7.489
7.487
7.477
7.474
7.391
7.386
7.383
7.378
7.240
Cl
N
S
N
Ph
O
(3p)
10
9
8
7
6
5
4
3
2
1
ppm
1.05
1.02
3.14
1.06
1.07
3.21
1.07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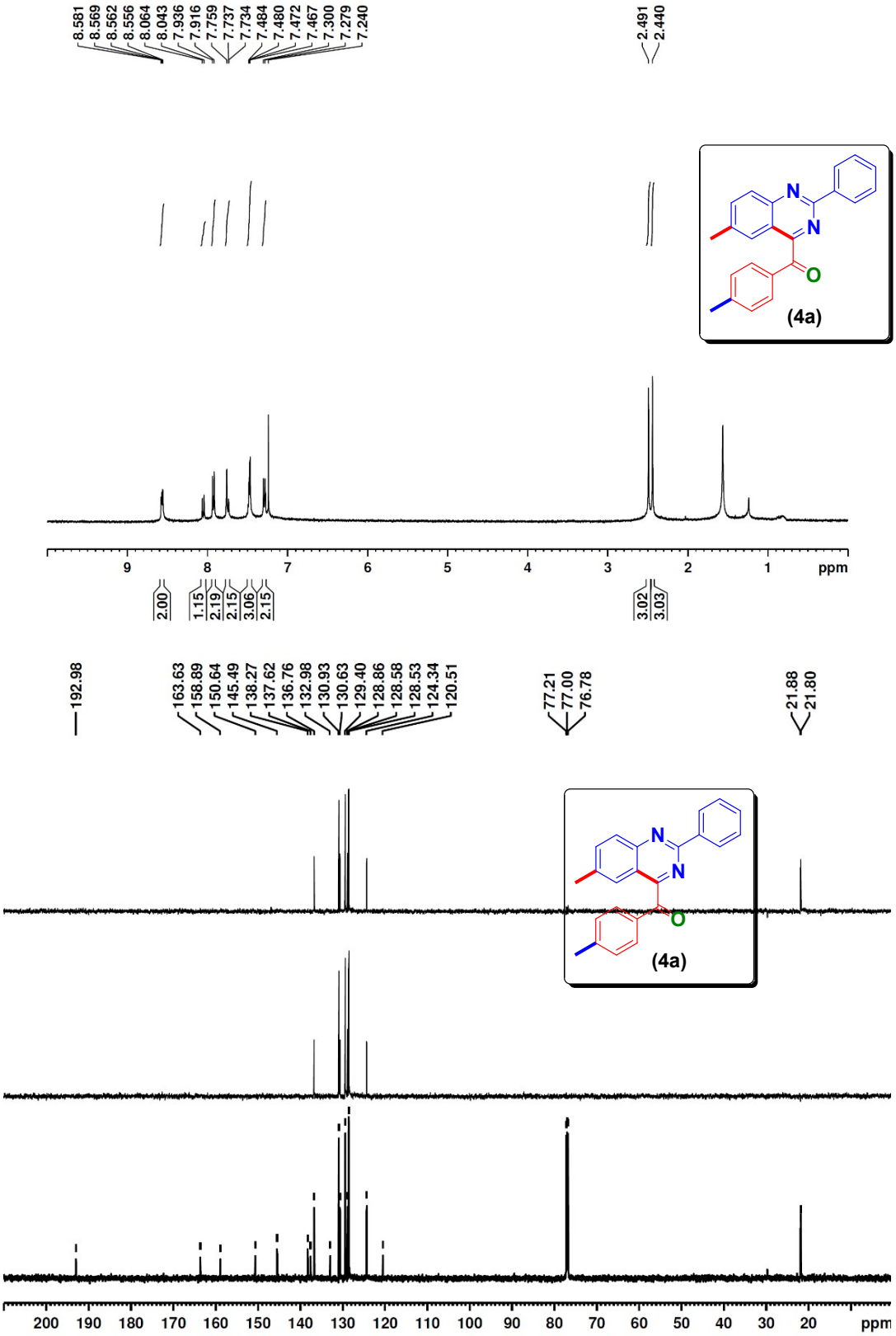
134.43
130.78
129.62
128.76
128.69
127.99
127.67
127.18
126.31
118.71
77.19
76.98
76.77
Cl
N
S
N
Ph
O
(3p)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.737
7.734
7.484
7.480
7.472
7.467
7.300
7.279
7.240
2.491
2.440
(4a)
9
8
7
6
5
4
3
2
1
ppm
2.00
1.15
2.19
2.15
3.06
2.15
3.02
3.03
192.98
163.63
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150.64
145.49
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137.62
136.76
132.98
130.93
130.63
129.40
128.86
128.58
128.53
124.34
120.51
77.21
77.00
76.78
21.88
21.80
(4a)
200
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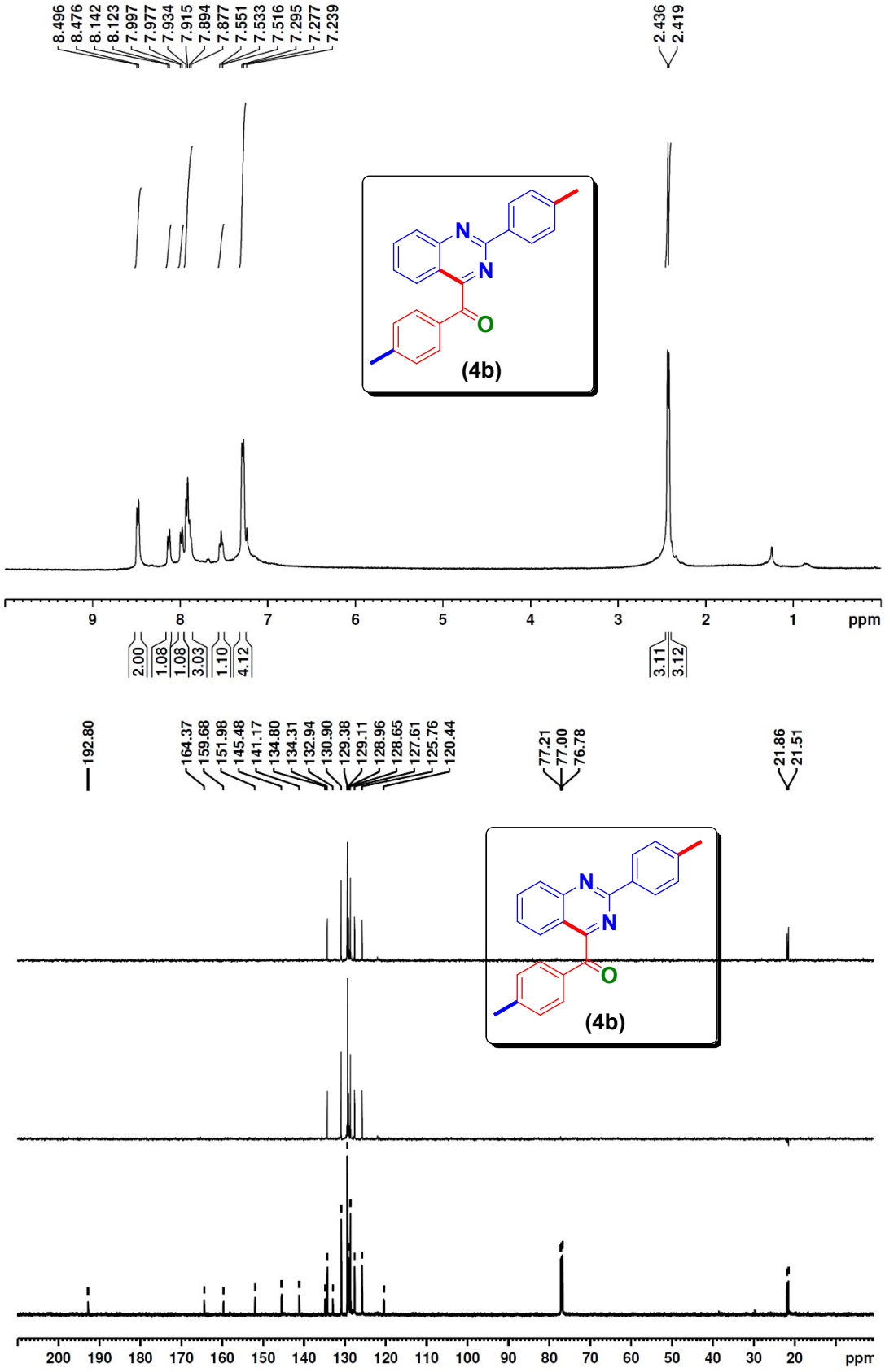
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.877
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7.516
7.295
7.277
7.239
2.436
2.419
N
N
O
(4b)
9
8
7
6
5
4
3
2
1
ppm
2.00
1.08
1.08
3.03
1.10
4.12
3.11
3.12
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159.68
151.98
145.48
141.17
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134.31
132.94
130.90
129.38
129.11
128.96
128.65
127.61
125.76
120.44
77.21
77.00
76.78
21.86
21.51
N
N
O
(4b)
200
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180
170
160
150
140
130
120
110
100
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80
70
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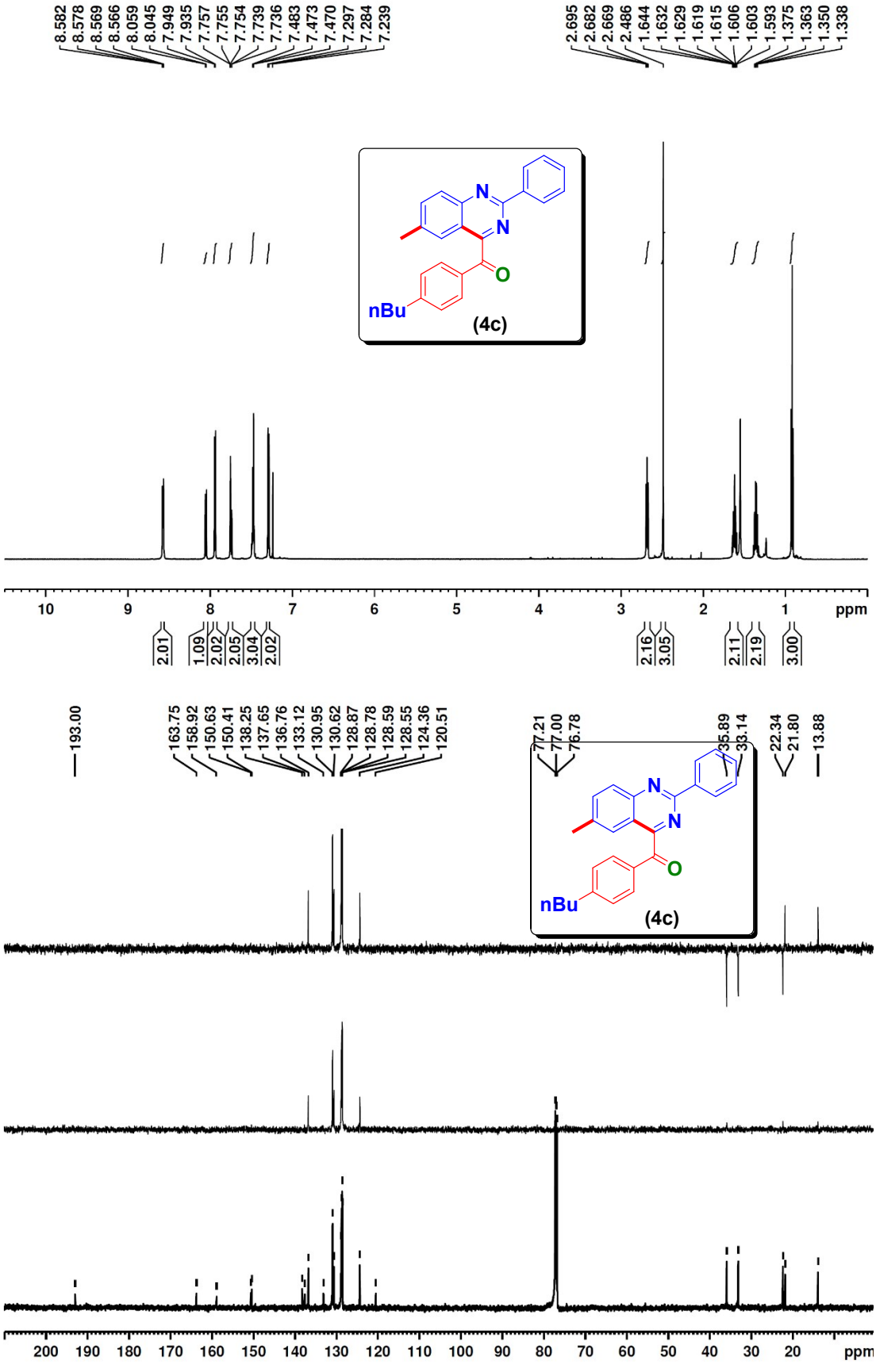
30
20
ppm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7.755
7.754
7.739
7.736
7.483
7.473
7.470
7.297
7.284
7.239
2.695
2.682
2.669
2.486
1.644
1.632
1.629
1.619
1.615
1.606
1.603
1.593
1.375
1.363
1.350
1.338
N
N
O
nBu
(4c)
10
9
8
7
6
5
4
3
2
1
ppm
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1.09
2.02
2.05
3.04
2.02
2.16
3.05
2.11
2.19
3.00
193.00
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158.92
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150.41
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130.62
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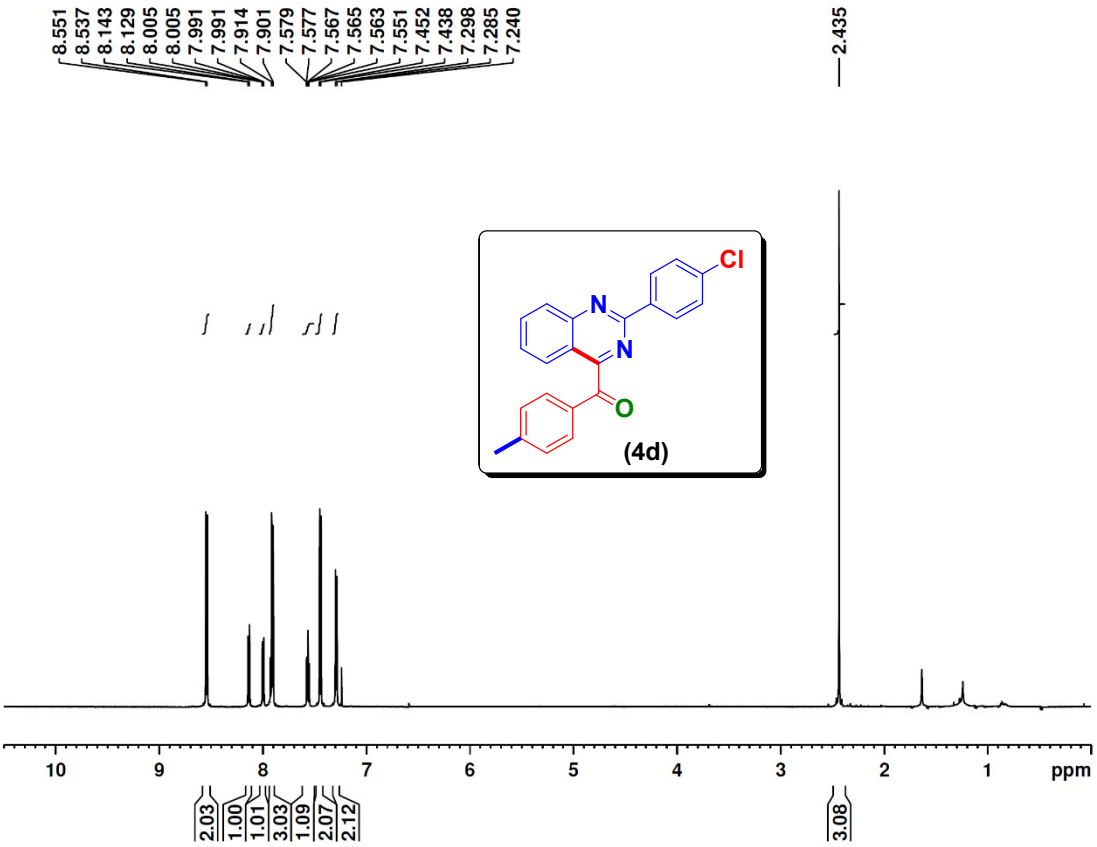
128.55
124.36
120.51
77.21
77.00
76.78
35.89
33.14
22.34
21.80
13.88
N
N
O
nBu
(4c)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.005
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7.991
7.914
7.901
7.579
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7.567
7.565
7.563
7.551
7.452
7.438
7.298
7.285
7.240
2.435
Cl
N
N
O
(4d)
10
9
8
7
6
5
4
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2
1
ppm
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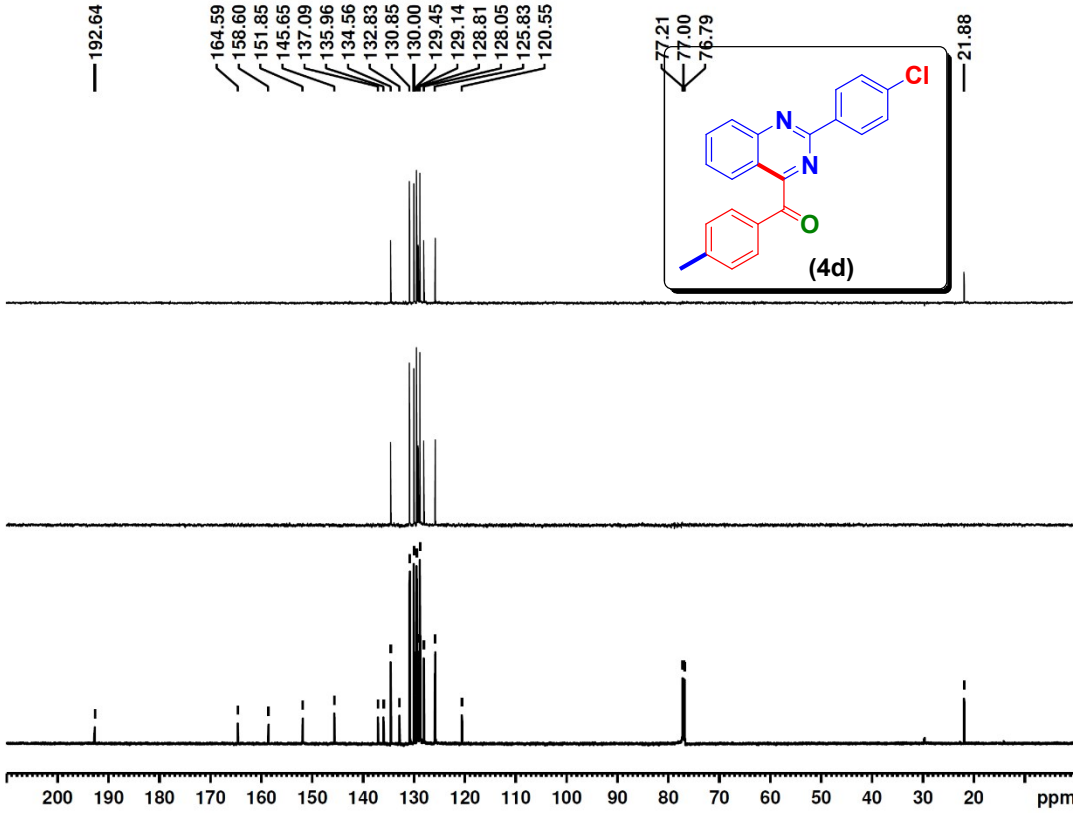
1.00
1.01
3.03
1.09
2.07
2.12
3.08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137.09
135.96
134.56
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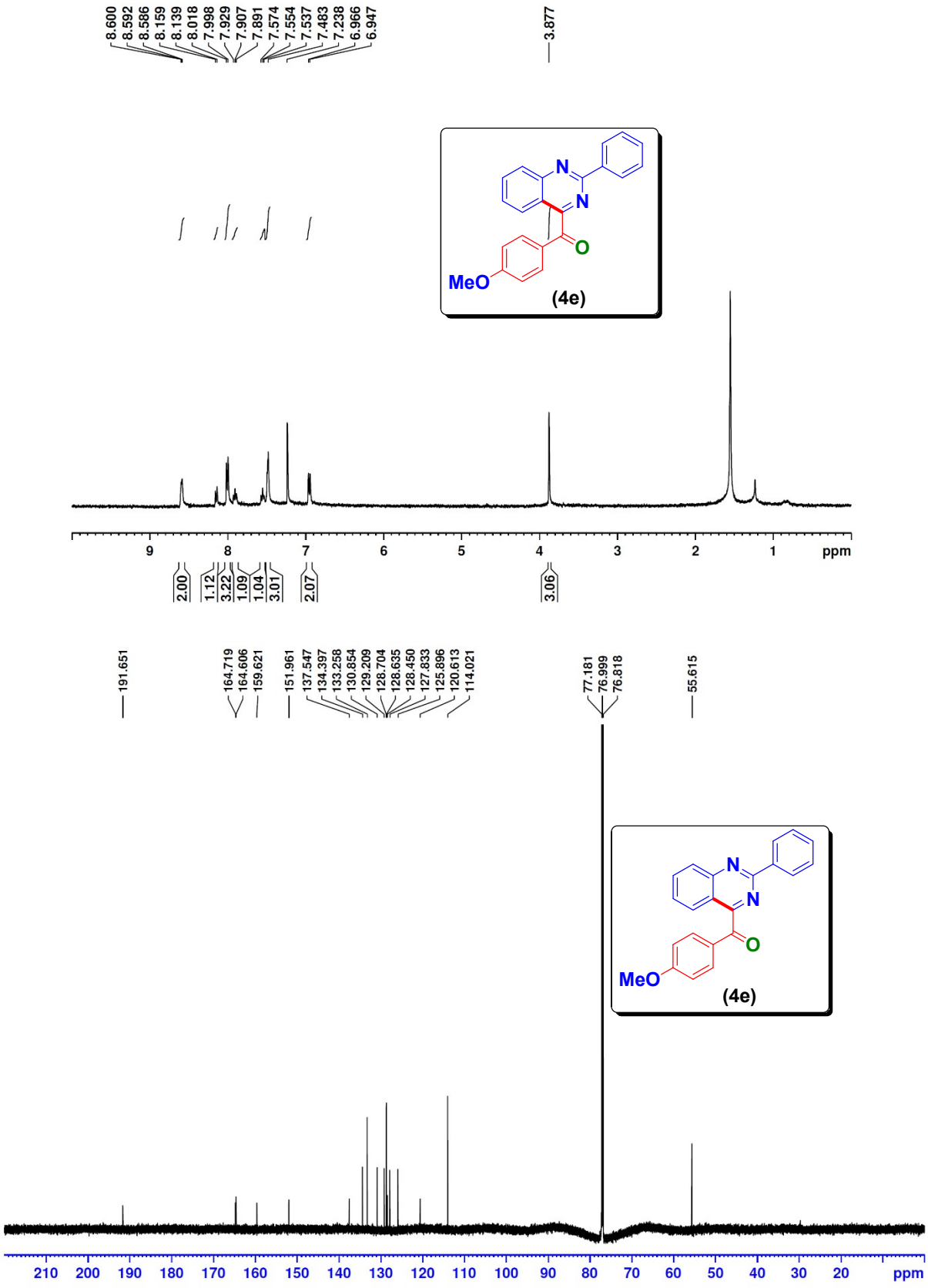
130.85
130.00
129.45
129.14
128.81
128.05
125.83
120.55
77.21
77.00
76.79
21.88
Cl
N
N
O
(4d)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.159
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8.018
7.998
7.929
7.907
7.891
7.574
7.554
7.537
7.483
7.238
6.966
6.947
3.877
N
N
O
MeO
(4e)
9
8
7
6
5
4
3
2
1
ppm
2.00
1.12
3.22
1.09
1.04
3.01
2.07
3.06
191.651
164.719
164.606
159.621
151.961
137.547
134.397
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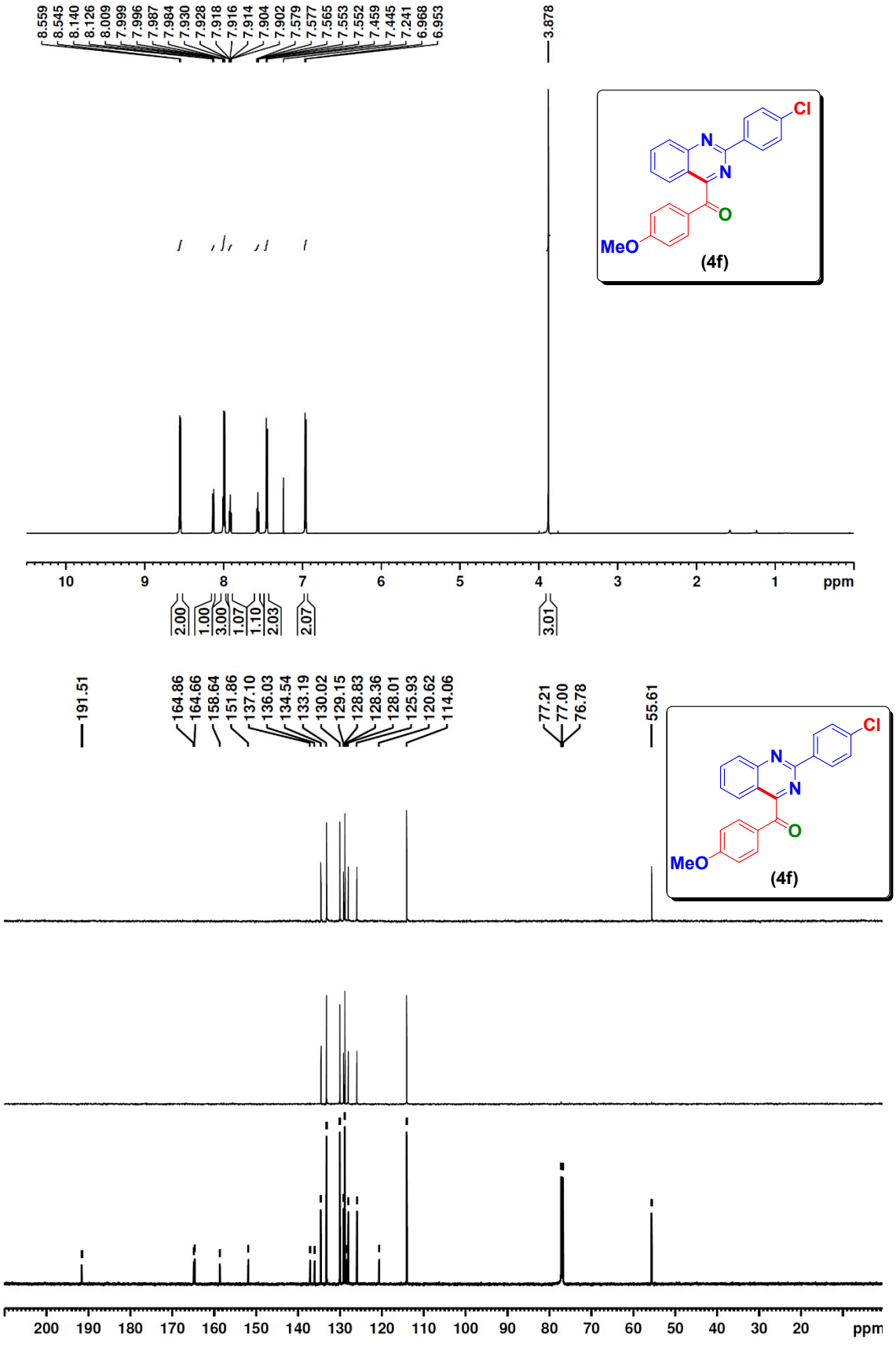
130.854
129.209
128.704
128.635
128.450
127.833
125.896
120.613
114.021
77.181
76.999
76.818
55.615
N
N
O
MeO
(4e)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.987
7.984
7.930
7.928
7.918
7.916
7.914
7.904
7.902
7.579
7.577
7.565
7.553
7.552
7.459
7.445
7.241
6.968
6.953
3.878
Cl
N
N
O
MeO
(4f)
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.00
3.00
1.07
1.10
2.03
2.07
3.01
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136.03
134.54
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128.36
128.01
125.93
120.62
114.06
77.21
77.00
76.78
55.61
Cl
N
N
O
MeO
(4f)
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190
180
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160
150
140
130
120
110
100
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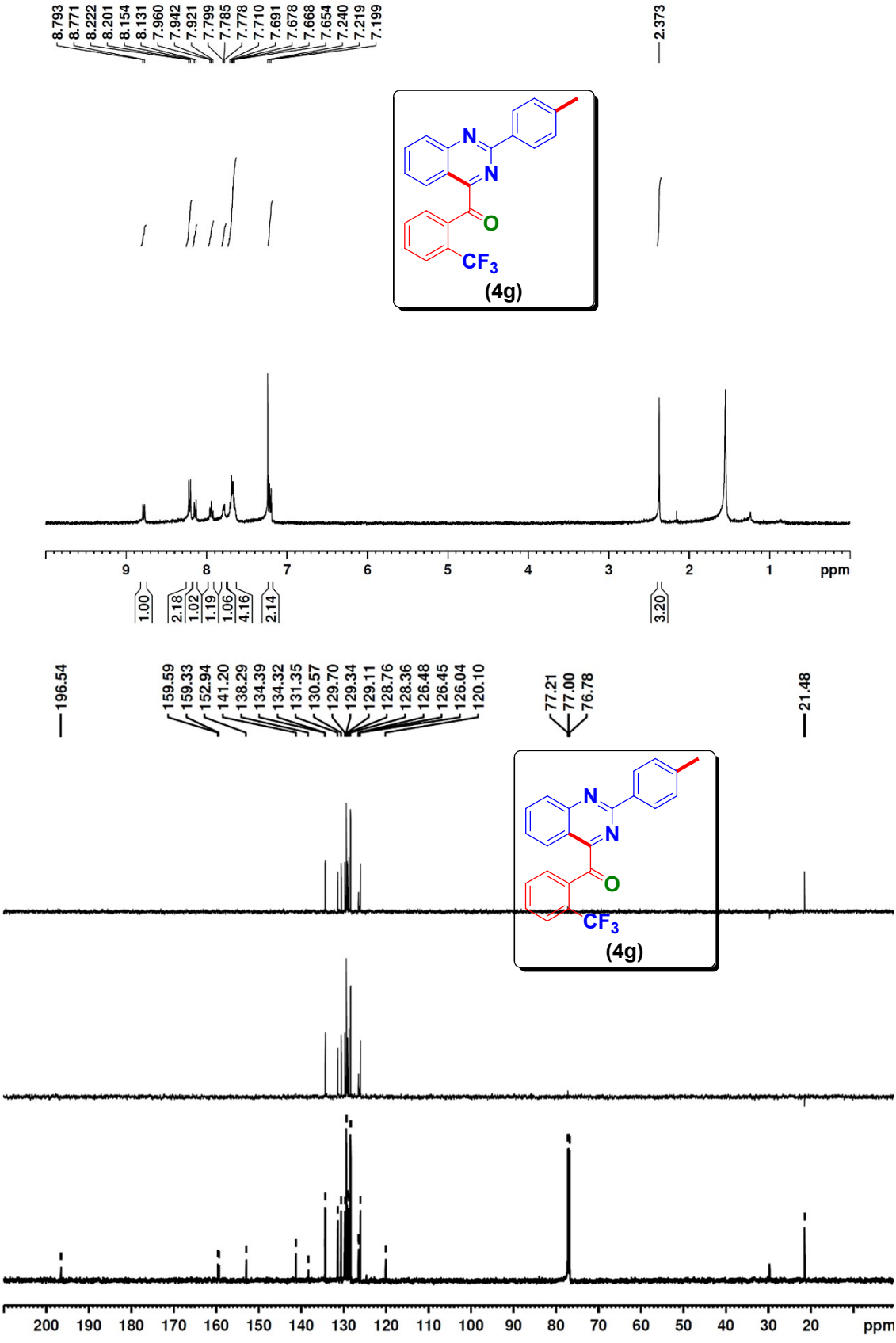
80
70
60
50
40
30
20
ppm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7.799
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7.778
7.710
7.691
7.678
7.668
7.654
7.240
7.219
7.199
2.373
N
N
O
CF3
(4g)
9
8
7
6
5
4
3
2
1
ppm
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2.18
1.02
1.19
1.06
4.16
2.14
3.20
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159.33
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128.36
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126.45
126.04
120.10
77.21
77.00
76.78
21.48
N
N
O
CF3
(4g)
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80
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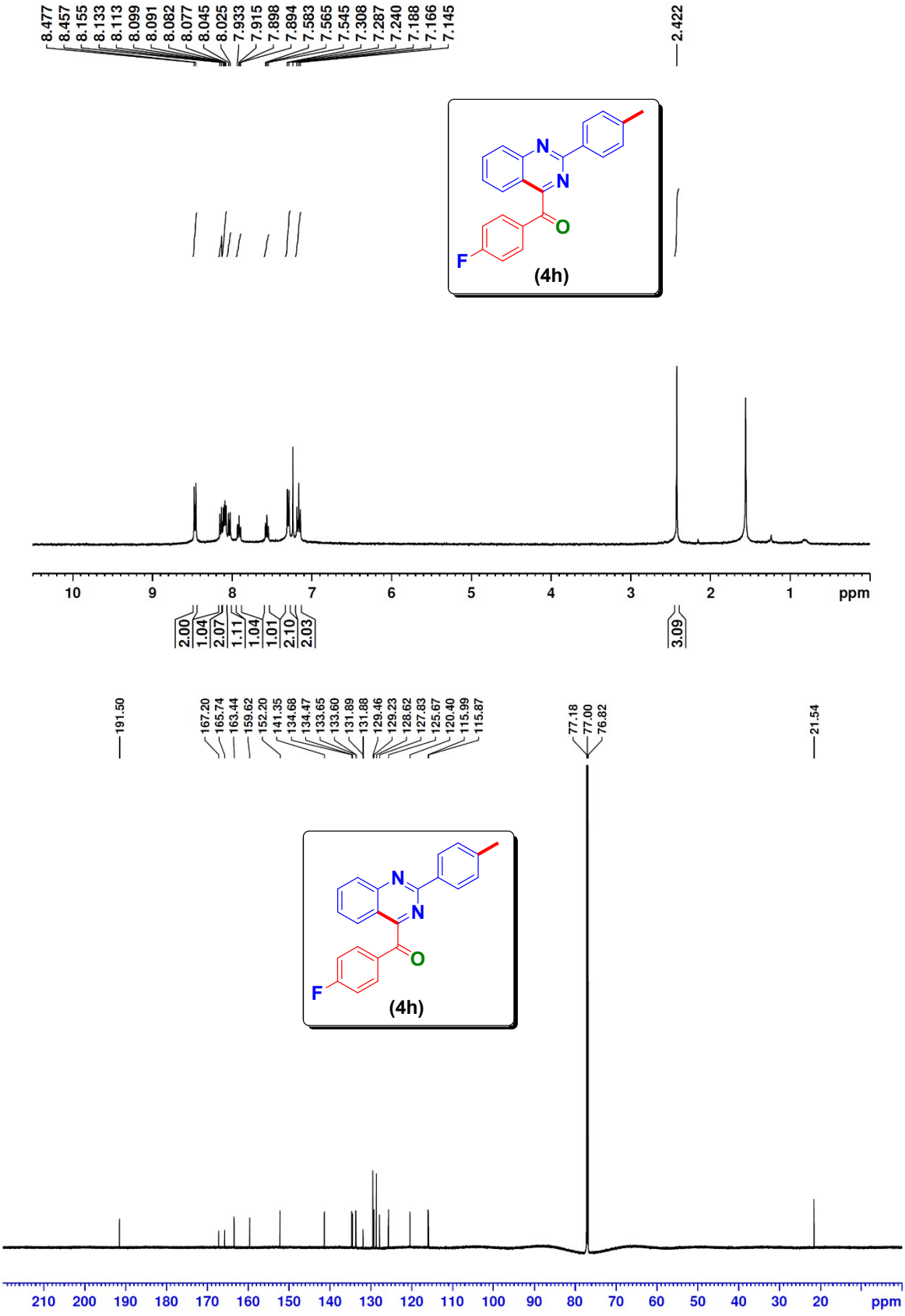
ppm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7.898
7.894
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7.545
7.308
7.287
7.240
7.188
7.166
7.145
2.422
N
N
O
F
(4h)
10
9
8
7
6
5
4
3
2
1
ppm
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115.87
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77.00
76.82
21.54
N
N
O
F
(4h)
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150
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120
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80
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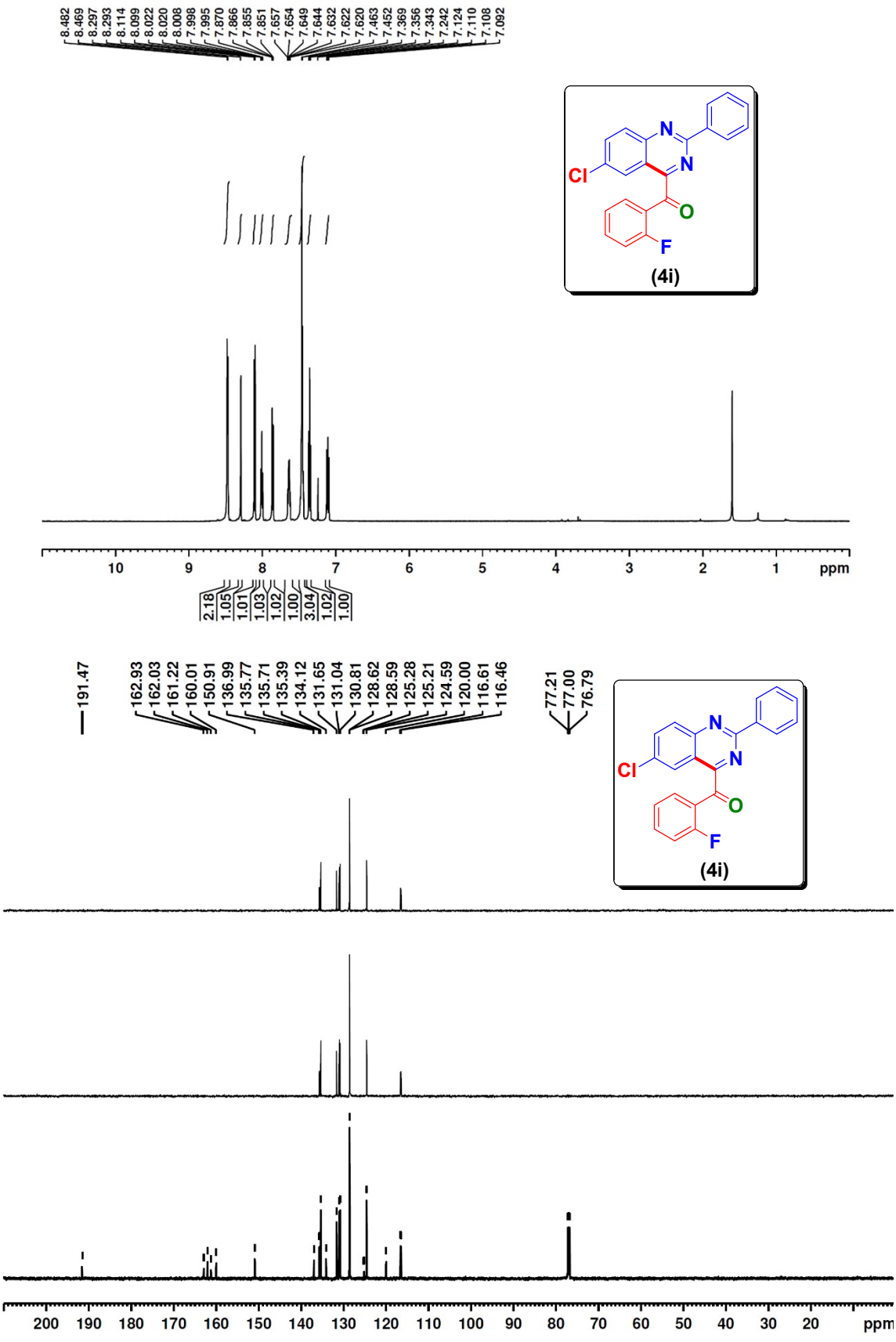
30
20
ppm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7.855
7.851
7.657
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7.644
7.632
7.622
7.620
7.463
7.452
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7.356
7.343
7.242
7.124
7.110
7.108
7.092
N
N
Cl
O
F
(4i)
10
9
8
7
6
5
4
3
2
1
ppm
2.18
1.05
1.01
1.03
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124.59
120.00
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77.21
77.00
76.79
N
N
Cl
O
F
(4i)
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130
120
110
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80
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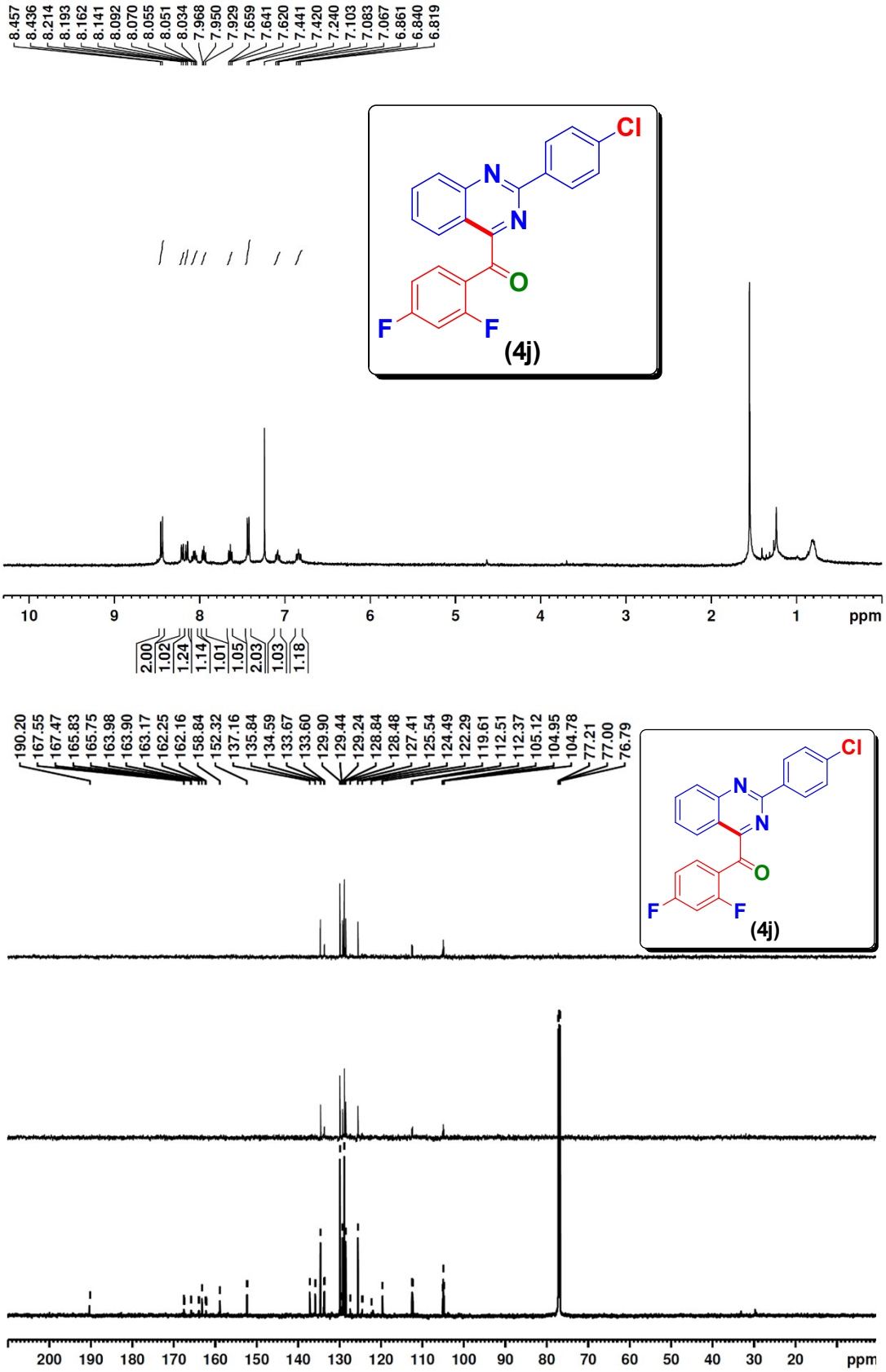
50
40
30
20
ppm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8.092
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7.968
7.950
7.929
7.659
7.641
7.620
7.441
7.420
7.240
7.103
7.083
7.067
6.861
6.840
6.819
Cl
N
N
O
F
F
(4j)
10
9
8
7
6
5
4
3
2
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ppm
2.00
1.02
1.24
1.14
1.01
1.05
2.03
1.03
1.18
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167.55
167.47
165.83
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163.90
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128.48
127.41
125.54
124.49
122.29
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112.51
112.37
105.12
104.95
104.78
77.21
77.00
76.79
Cl
N
N
O
F
F
(4j)
200
190
180
170
160
150
140
130
120
110
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80
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50
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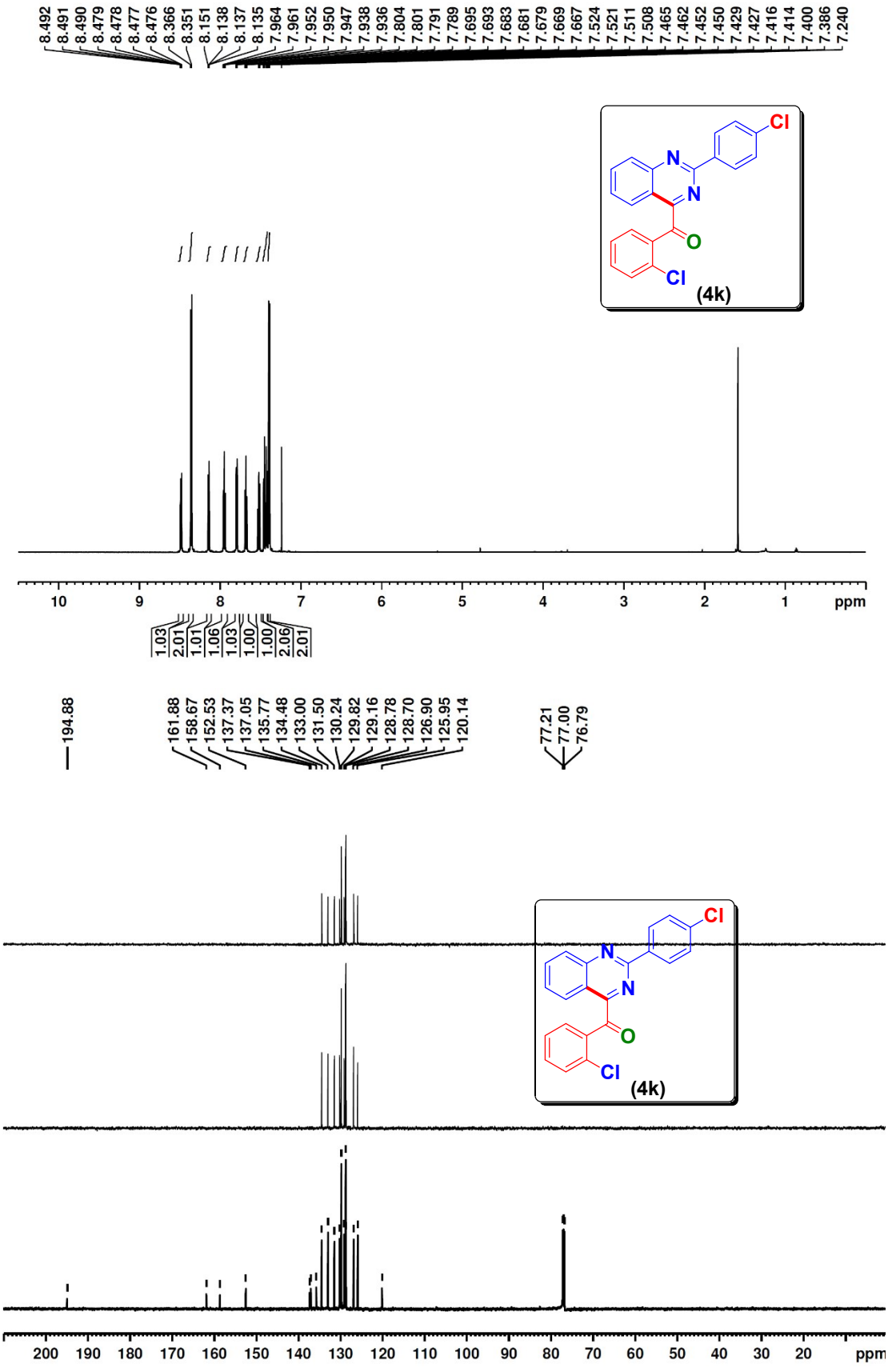
30
20
ppm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7.961
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7.950
7.947
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7.936
7.804
7.801
7.791
7.789
7.695
7.693
7.683
7.681
7.679
7.669
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7.524
7.521
7.511
7.508
7.465
7.462
7.452
7.450
7.429
7.427
7.416
7.414
7.400
7.386
7.240
Cl
N
N
O
Cl
(4k)
10
9
8
7
6
5
4
3
2
1
ppm
1.03
2.01
1.01
1.06
1.03
1.00
1.00
2.06
2.01
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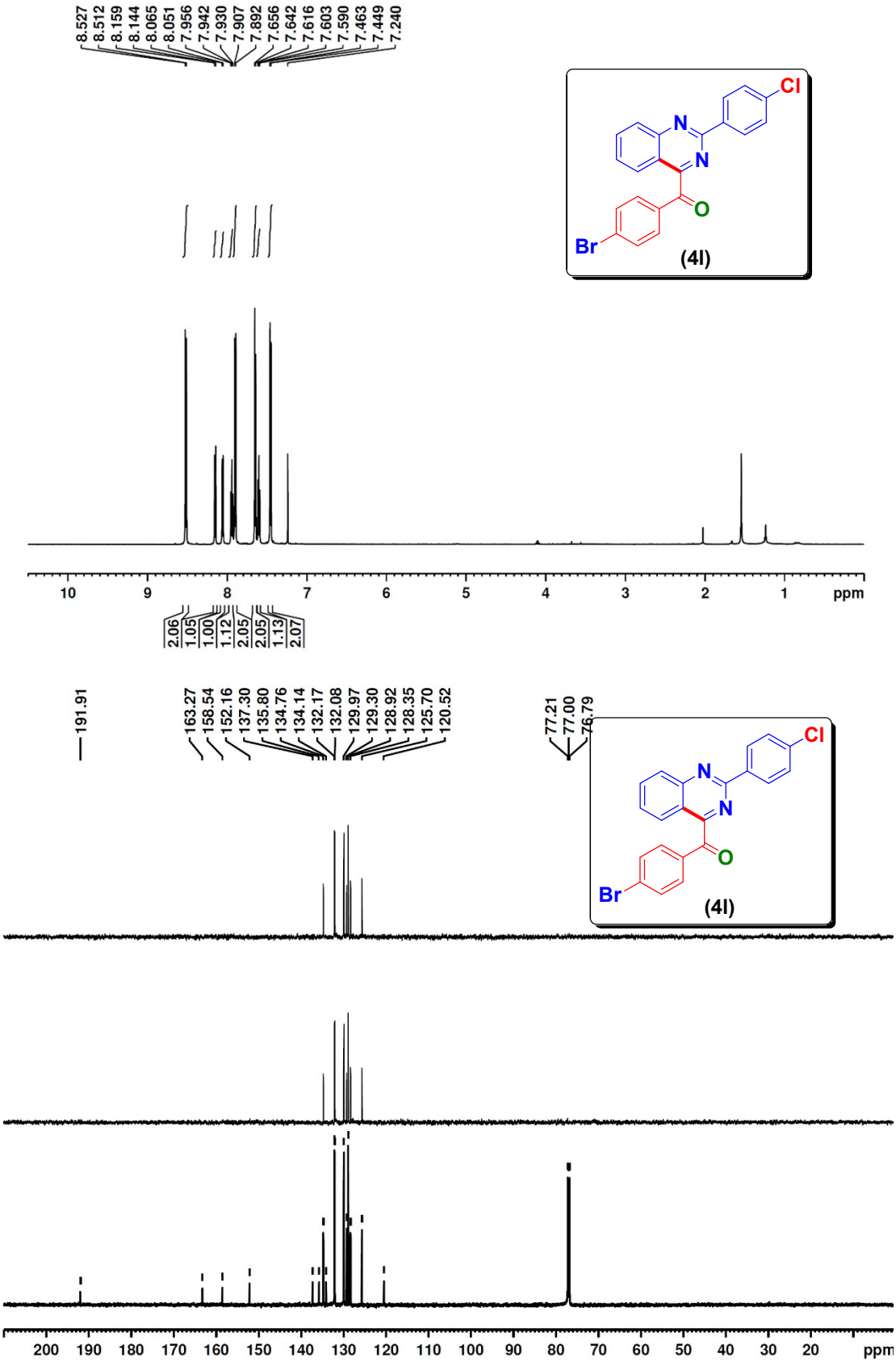
152.53
137.37
137.05
135.77
134.48
133.00
131.50
130.24
129.82
129.16
128.78
128.70
126.90
125.95
120.14
77.21
77.00
76.79
Cl
N
N
O
Cl
(4k)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.892
7.656
7.642
7.616
7.603
7.590
7.463
7.449
7.240
Cl
N
N
O
Br
(4l)
10
9
8
7
6
5
4
3
2
1
ppm
2.06
1.05
1.00
1.12
2.05
2.05
1.13
2.07
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152.16
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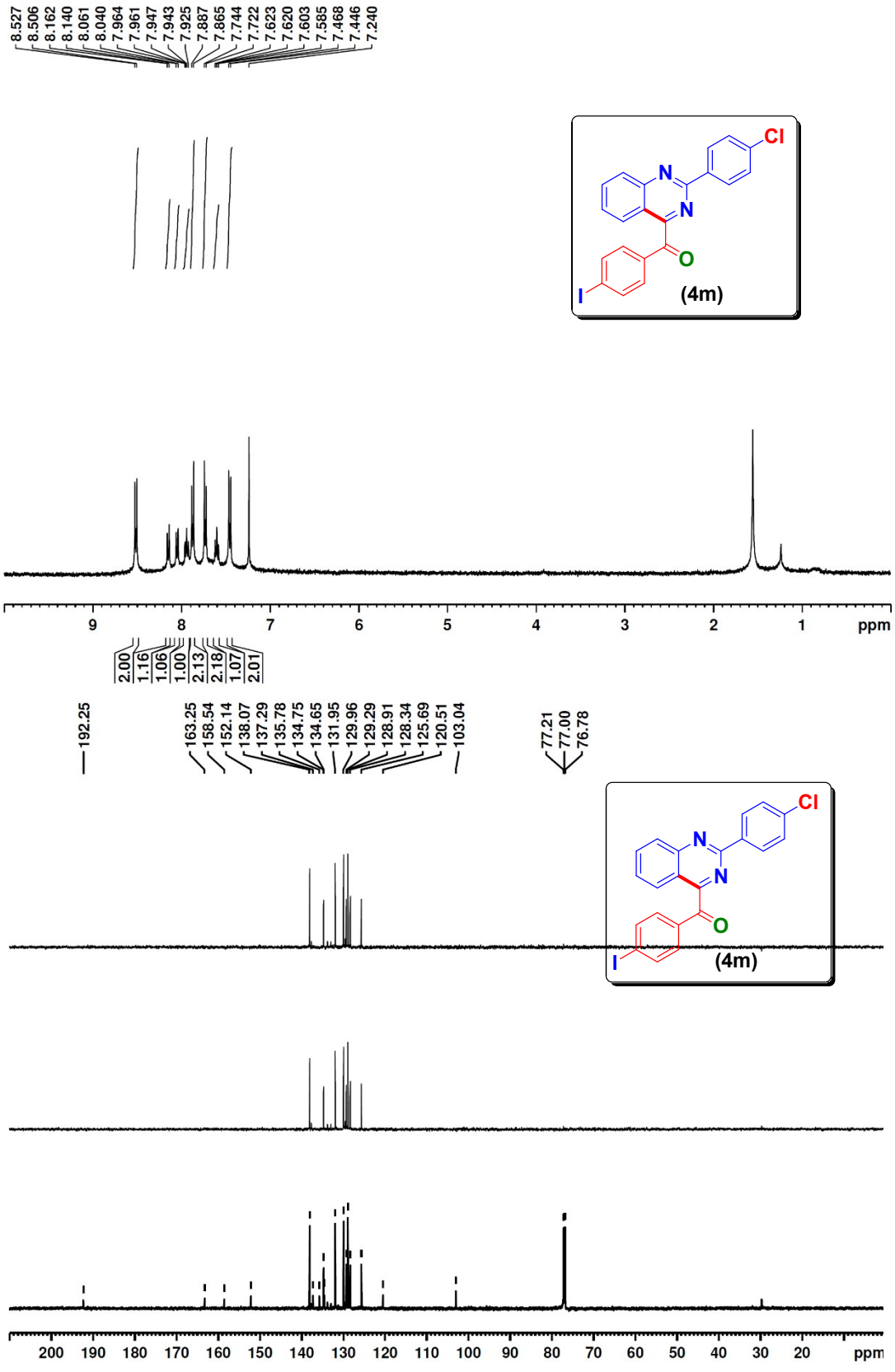
134.76
134.14
132.17
132.08
129.97
129.30
128.92
128.35
125.70
120.52
77.21
77.00
76.79
Cl
N
N
O
Br
(4l)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.061
8.040
7.964
7.961
7.947
7.943
7.925
7.887
7.865
7.744
7.722
7.623
7.620
7.603
7.585
7.468
7.446
7.240
Cl
N
N
O
I
(4m)
9
8
7
6
5
4
3
2
1
ppm
2.00
1.16
1.06
1.00
2.13
2.18
1.07
2.01
192.25
163.25
158.54
152.14
138.07
137.29
135.78
134.75
134.65
131.95
129.96
129.29
128.91
128.34
125.69
120.51
103.04
77.21
77.00
76.78
Cl
N
N
O
I
(4m)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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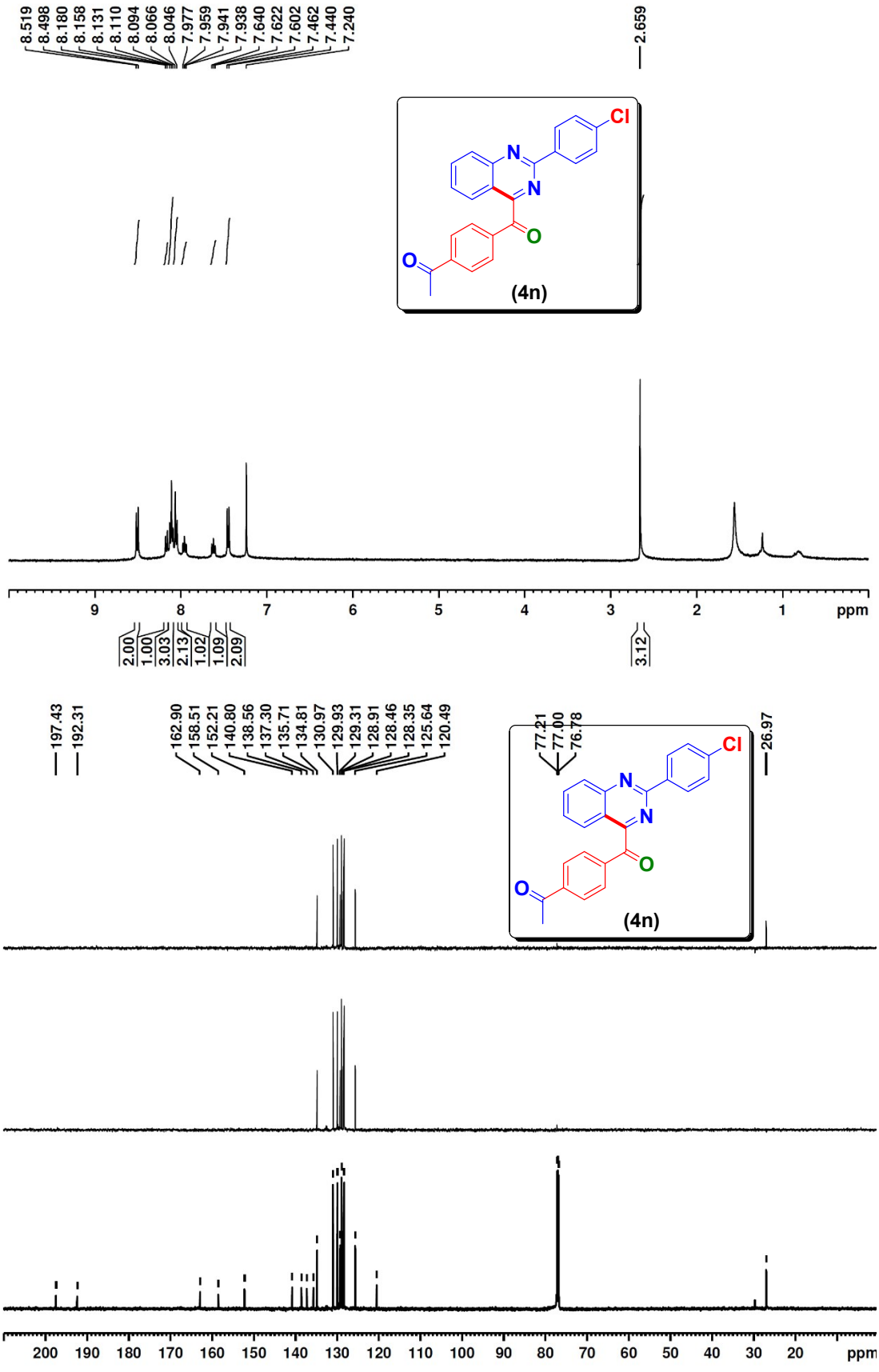
50
40
30
20
ppm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8.066
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7.959
7.941
7.938
7.640
7.622
7.602
7.462
7.440
7.240
2.659
Cl
N
N
O
O
(4n)
9
8
7
6
5
4
3
2
1
ppm
2.00
1.00
3.03
2.13
1.02
1.09
2.09
3.12
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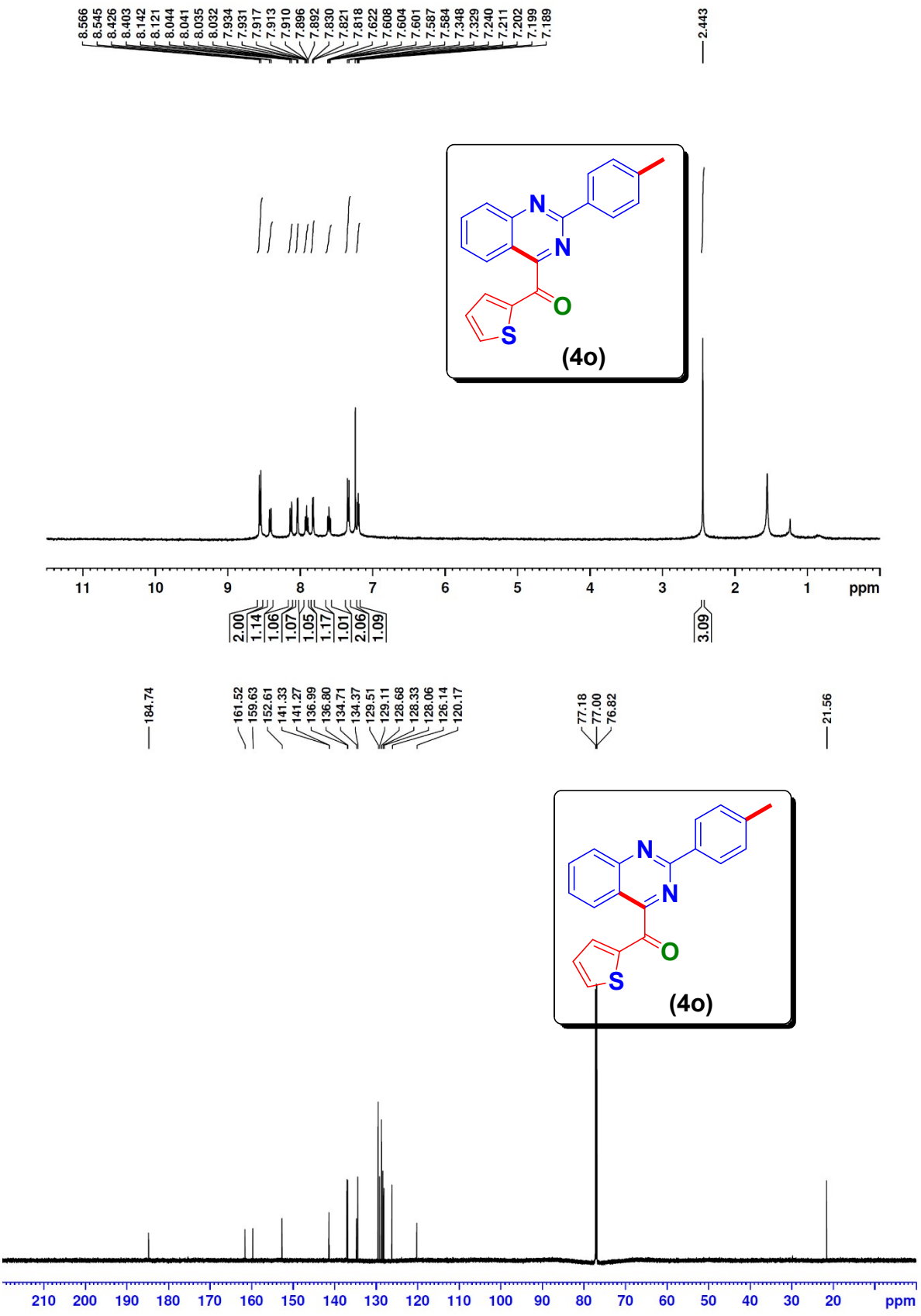
135.71
134.81
130.97
129.93
129.31
128.91
128.46
128.35
125.64
120.49
77.21
77.00
76.78
26.97
Cl
N
N
O
O
(4n)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.121
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8.041
8.035
8.032
7.934
7.931
7.917
7.913
7.910
7.896
7.892
7.830
7.821
7.818
7.622
7.608
7.604
7.601
7.587
7.584
7.348
7.329
7.240
7.211
7.202
7.199
7.189
2.443
N
N
O
S
(4o)
11
10
9
8
7
6
5
4
3
2
1
ppm
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1.14
1.06
1.07
1.05
1.17
1.01
2.06
1.09
3.09
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152.61
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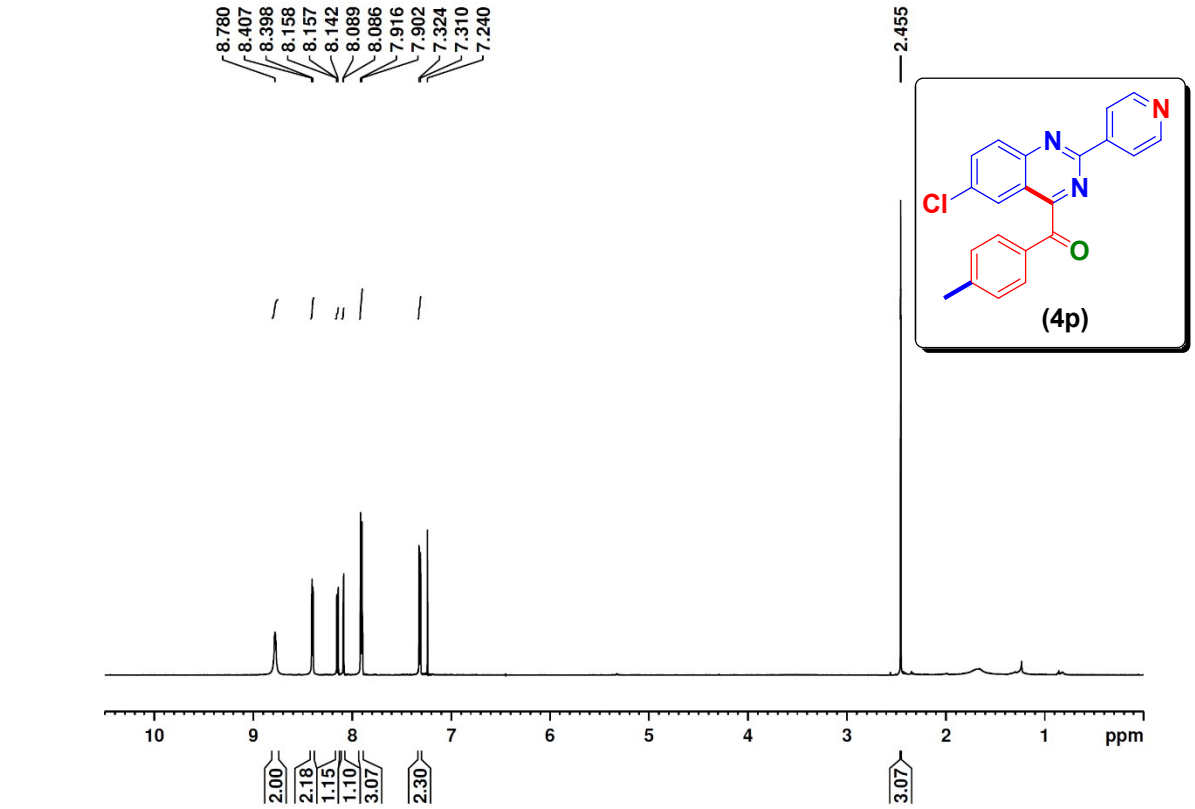
141.27
136.99
136.80
134.71
134.37
129.51
129.11
128.68
128.33
128.06
126.14
120.17
77.18
77.00
76.82
21.56
N
N
O
S
(4o)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.086
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7.324
7.310
7.240
2.455
Cl
N
N
N
O
(4p)
10
9
8
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6
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3
2
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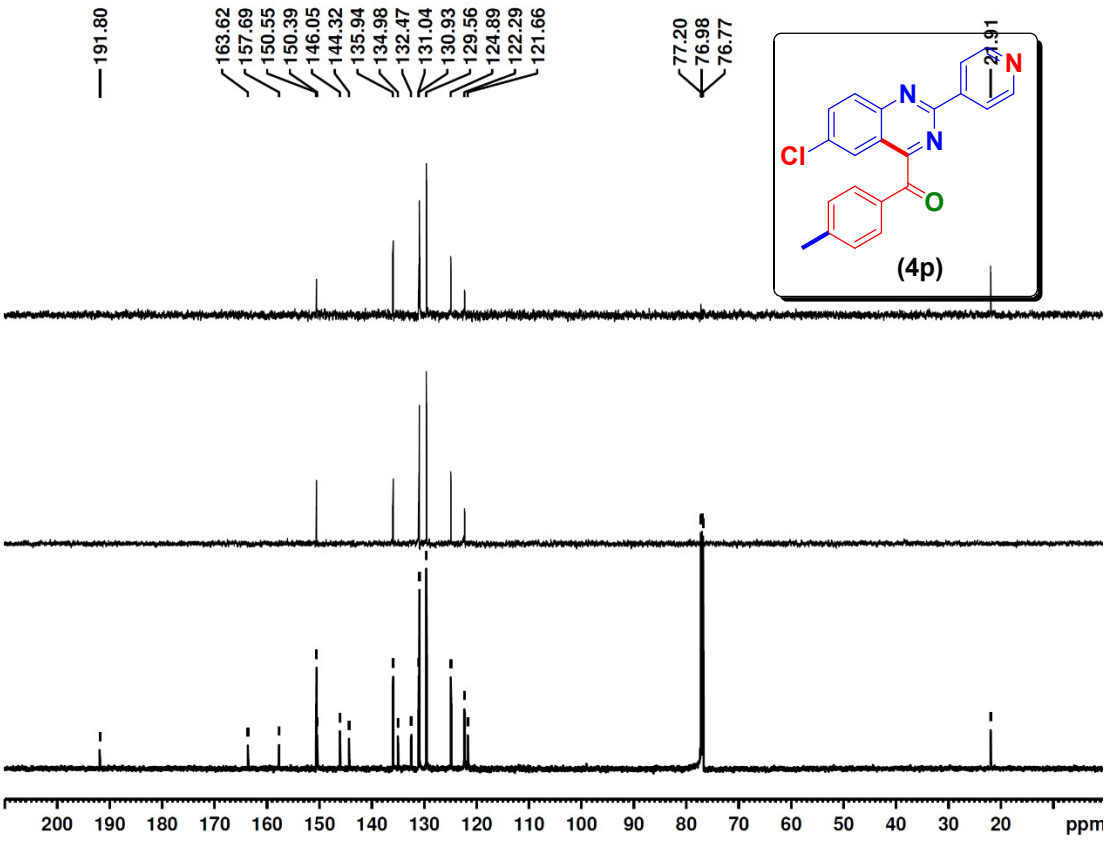
3.07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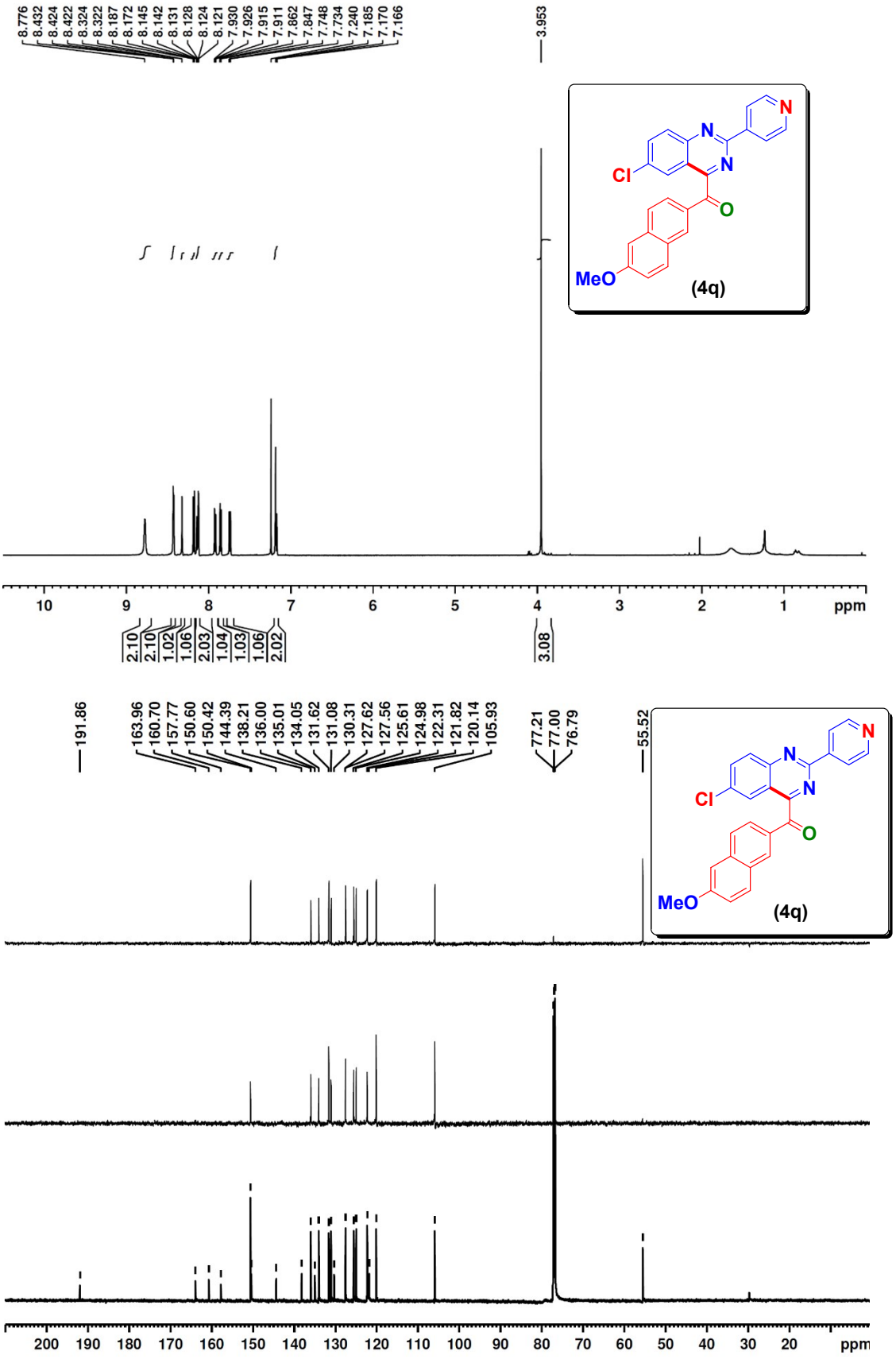
129.56
124.89
122.29
121.66
77.20
76.98
76.77
21.91
Cl
N
N
N
O
(4p)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.124
8.121
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7.926
7.915
7.911
7.862
7.847
7.748
7.734
7.240
7.185
7.170
7.166
3.953
Cl
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N
O
MeO
(4q)
10
9
8
7
6
5
4
3
2
1
ppm
2.10
2.10
1.02
1.06
2.03
1.04
1.03
1.06
2.02
3.08
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136.00
135.01
134.05
131.62
131.08
130.31
127.62
127.56
125.61
124.98
122.31
121.82
120.14
105.93
77.21
77.00
76.79
55.52
200
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180
170
160
150
140
130
120
110
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80
70
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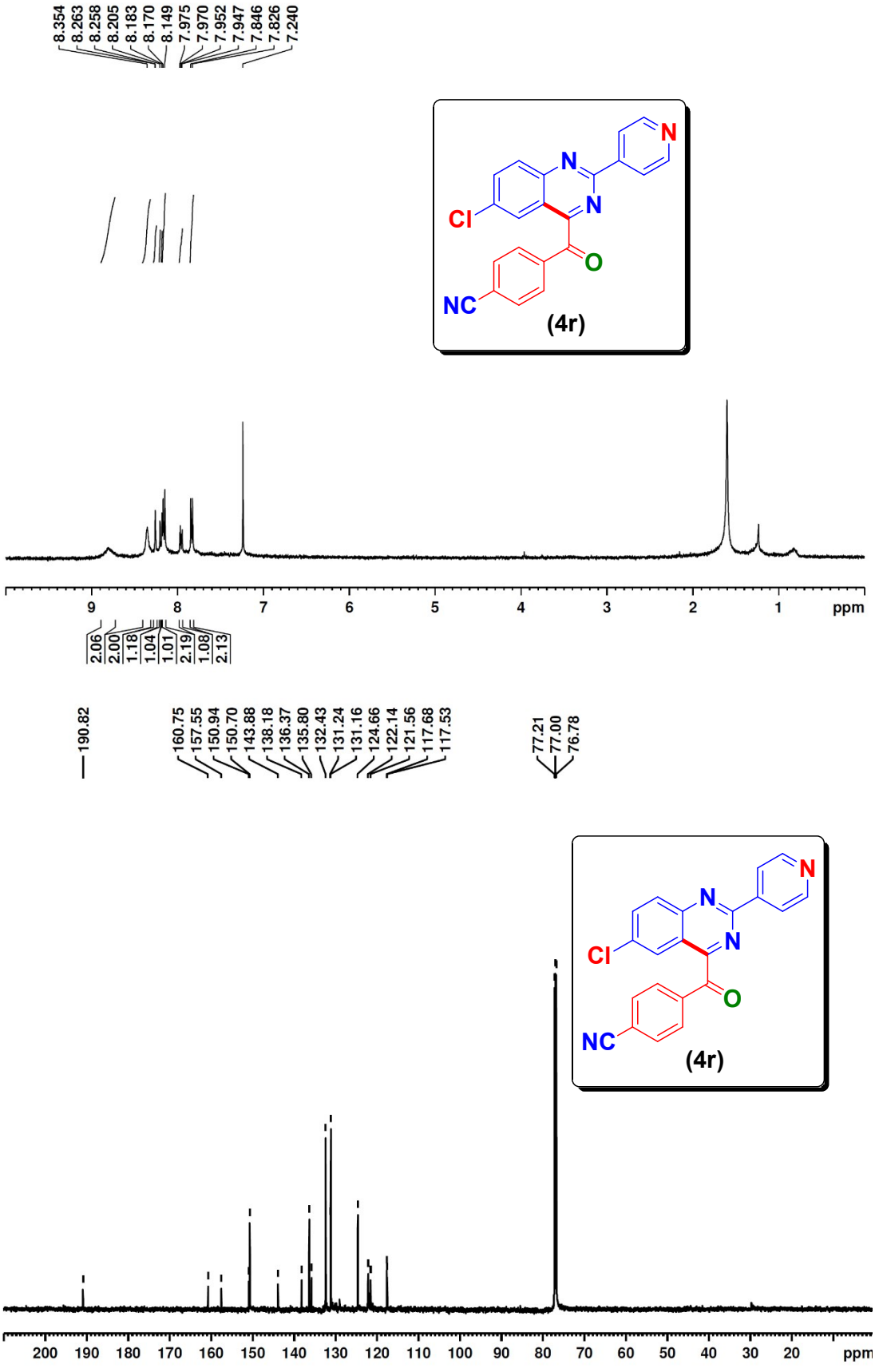
50
40
30
20
ppm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7.947
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7.826
7.240
Cl
N
N
N
O
NC
(4r)
9
8
7
6
5
4
3
2
1
ppm
2.06
2.00
1.18
1.04
1.01
2.19
1.08
2.13
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131.24
131.16
124.66
122.14
121.56
117.68
117.53
77.21
77.00
76.78
Cl
N
N
N
O
NC
(4r)
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160
150
140
130
120
110
100
90
80
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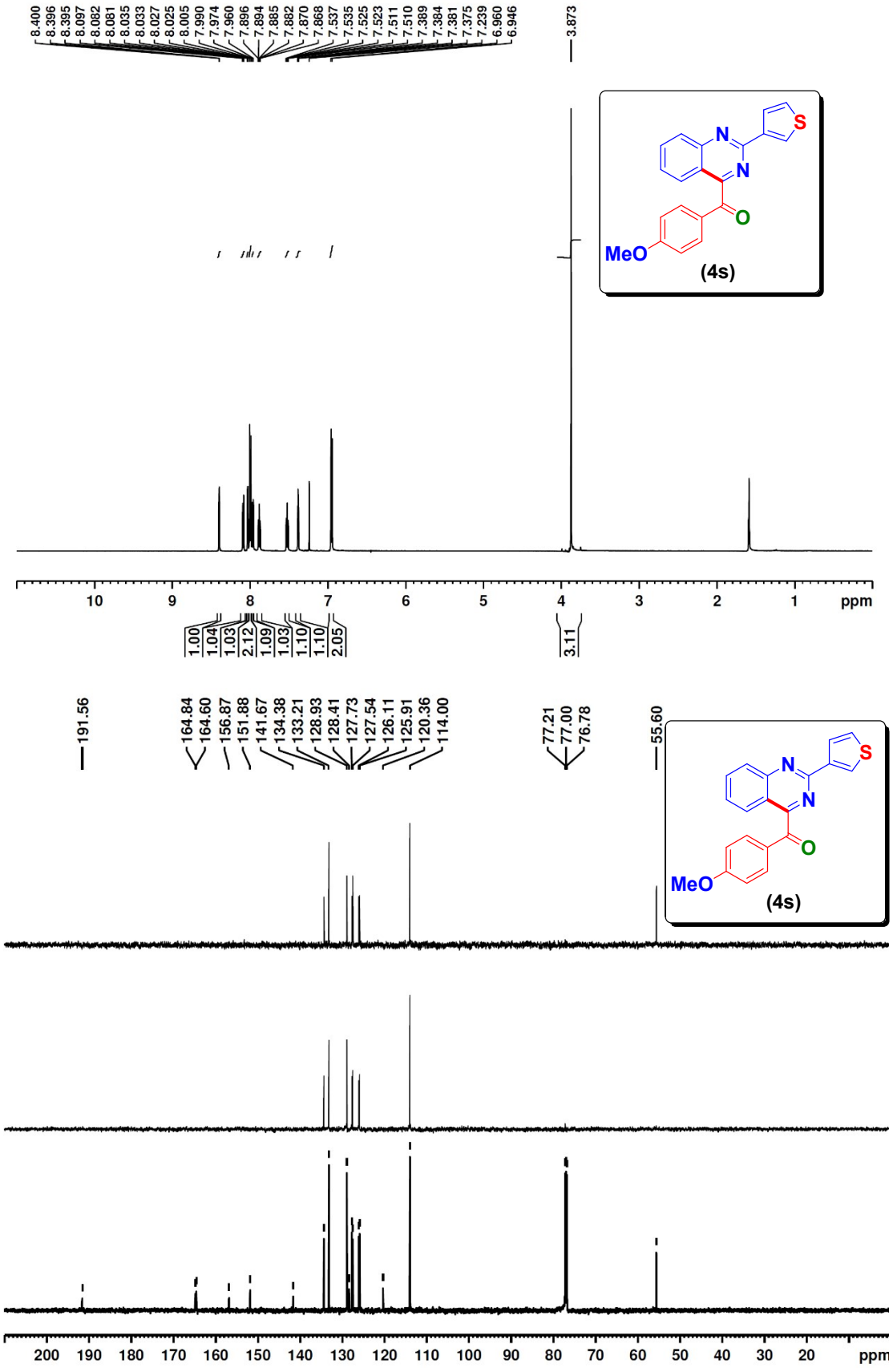
50
40
30
20
ppm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8.033
8.027
8.025
8.005
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7.974
7.960
7.896
7.894
7.885
7.882
7.870
7.868
7.537
7.535
7.525
7.523
7.511
7.510
7.389
7.384
7.381
7.375
7.239
6.960
6.946
3.873
N
S
N
O
MeO
(4s)
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.04
1.03
2.12
1.09
1.03
1.10
1.10
2.05
3.11
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164.84
164.60
156.87
151.88
141.67
134.38
133.21
128.93
128.41
127.73
127.54
126.11
125.91
120.36
114.00
77.21
77.00
76.78
55.60
200
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180
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160
150
140
130
120
110
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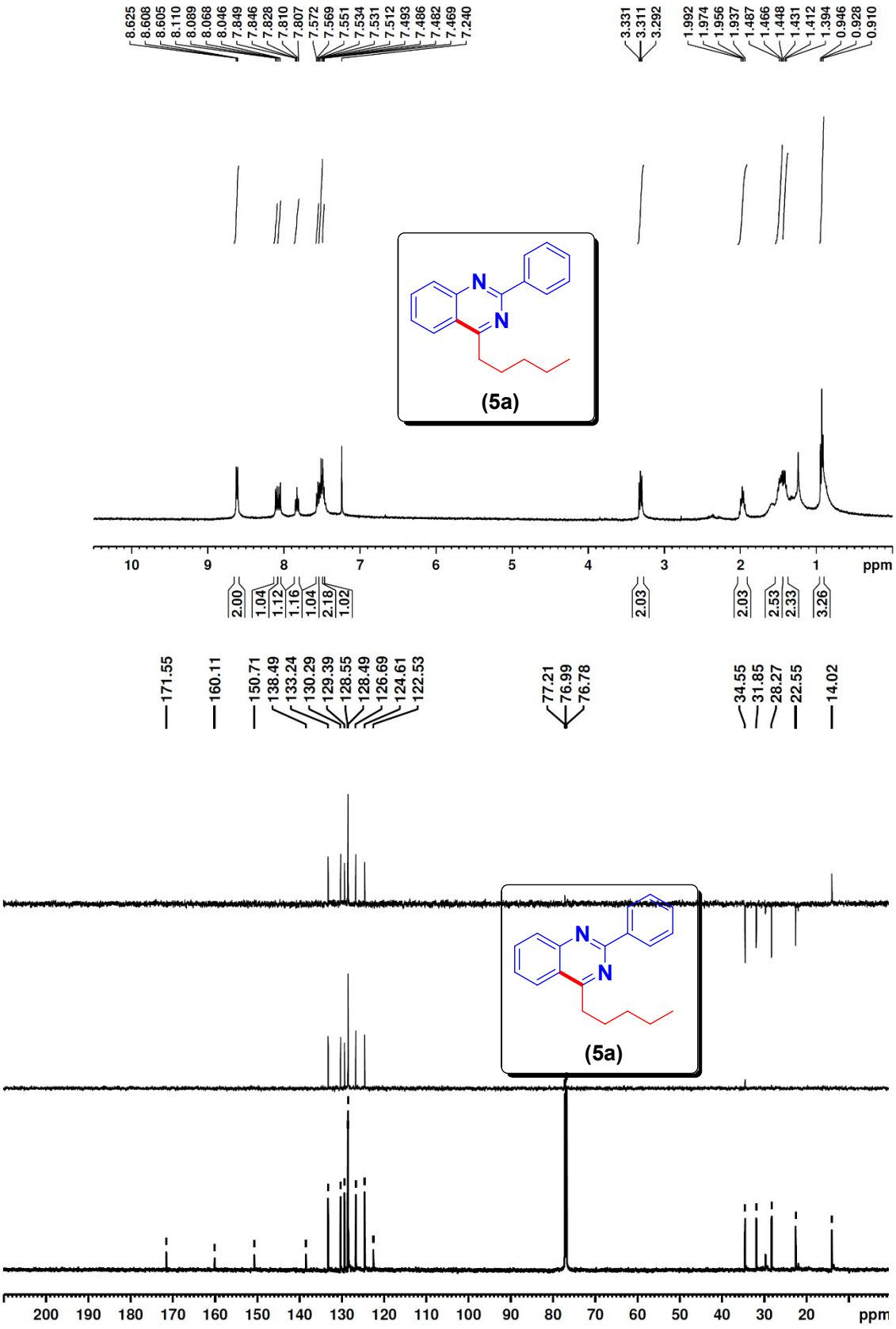
80
70
60
50
40
30
20
ppm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7.846
7.828
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7.572
7.569
7.551
7.534
7.531
7.512
7.493
7.486
7.482
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7.240
3.331
3.311
3.292
1.992
1.974
1.956
1.937
1.487
1.466
1.448
1.431
1.412
1.394
0.946
0.928
0.910
N
N
(5a)
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.04
1.12
1.16
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2.18
1.02
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2.03
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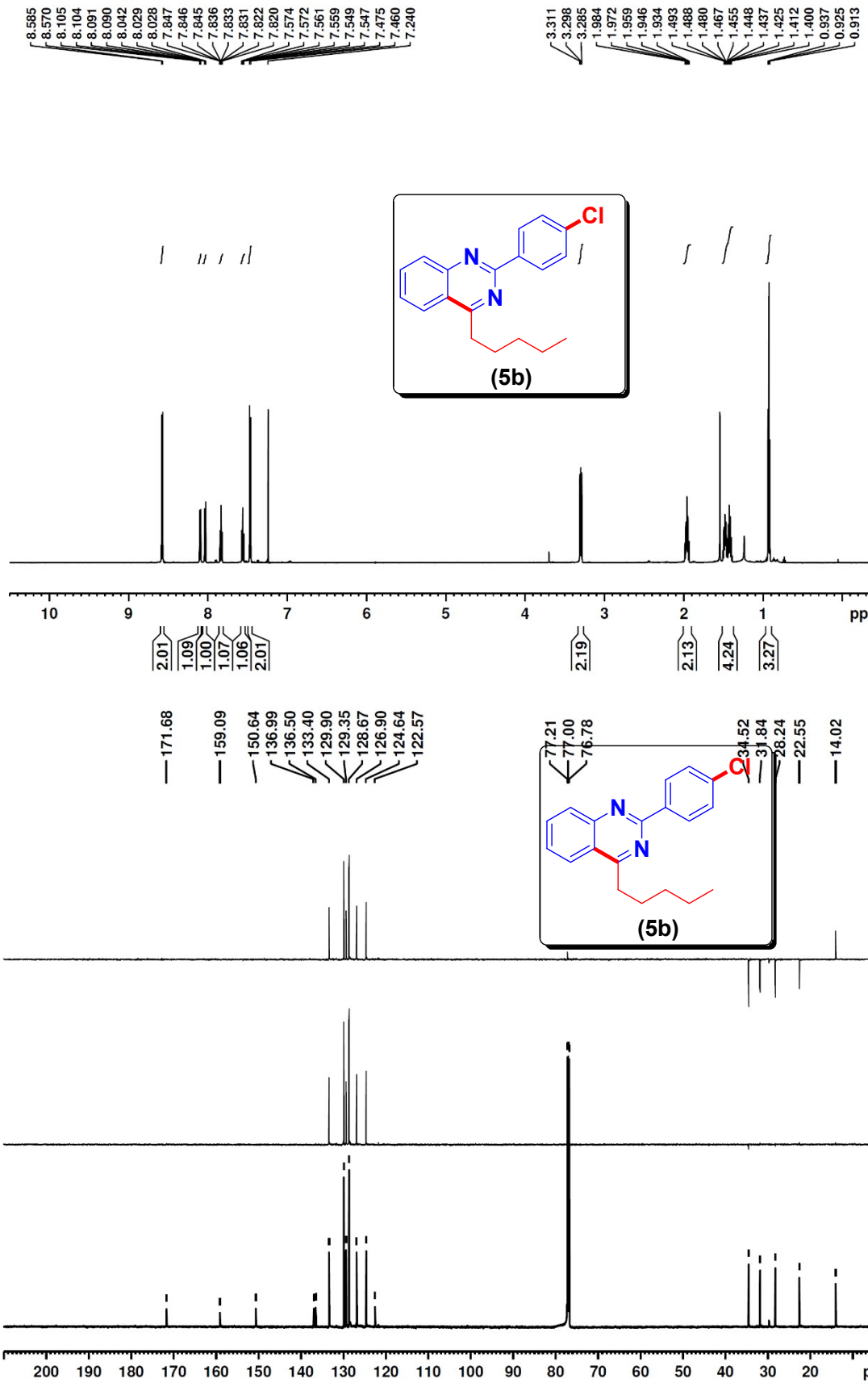
150.71
138.49
133.24
130.29
129.39
128.55
128.49
126.69
124.61
122.53
77.21
76.99
76.78
34.55
31.85
28.27
22.55
14.02
N
N
(5a)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.846
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7.836
7.833
7.831
7.822
7.820
7.574
7.572
7.561
7.559
7.549
7.547
7.475
7.460
7.240
3.311
3.298
3.285
1.984
1.972
1.959
1.946
1.934
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1.455
1.448
1.437
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1.400
0.937
0.925
0.913
Cl
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N
(5b)
10
9
8
7
6
5
4
3
2
1
ppm
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1.09
1.00
1.07
1.06
2.01
2.19
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4.24
3.27
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124.64
122.57
77.21
77.00
76.78
34.52
31.84
28.24
22.55
14.02
Cl
N
N
(5b)
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140
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100
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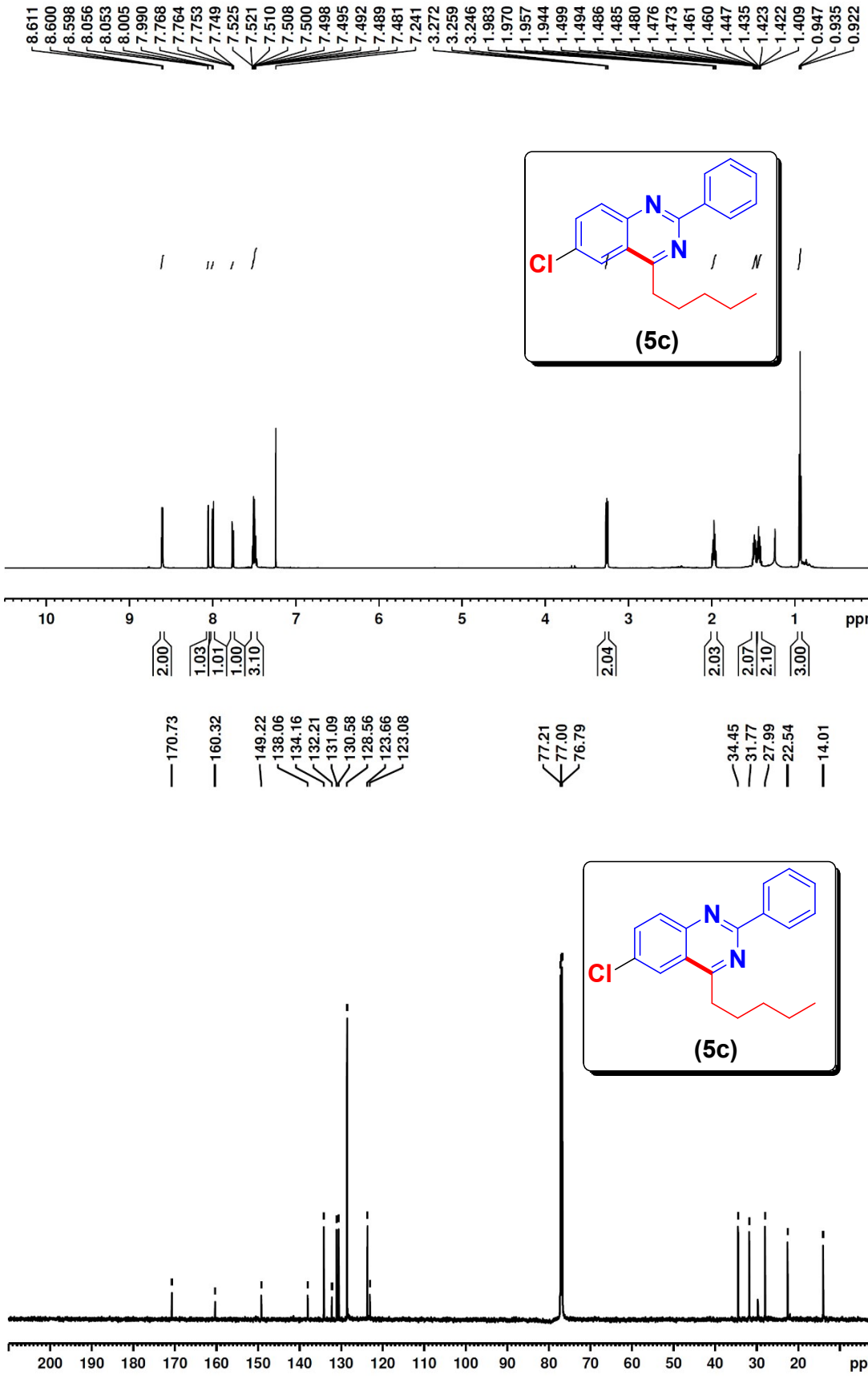
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7.521
7.510
7.508
7.500
7.498
7.495
7.492
7.489
7.481
7.241
3.272
3.259
3.246
1.983
1.970
1.957
1.944
1.499
1.494
1.486
1.485
1.480
1.476
1.473
1.461
1.460
1.447
1.435
1.423
1.422
1.409
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0.935
0.922
Cl
N
N
(5c)
10
9
8
7
6
5
4
3
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1
ppm
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1.00
3.10
2.04
2.03
2.07
2.10
3.00
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132.21
131.09
130.58
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123.66
123.08
77.21
77.00
76.79
34.45
31.77
27.99
22.54
14.01
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N
N
(5c)
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150
140
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120
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50
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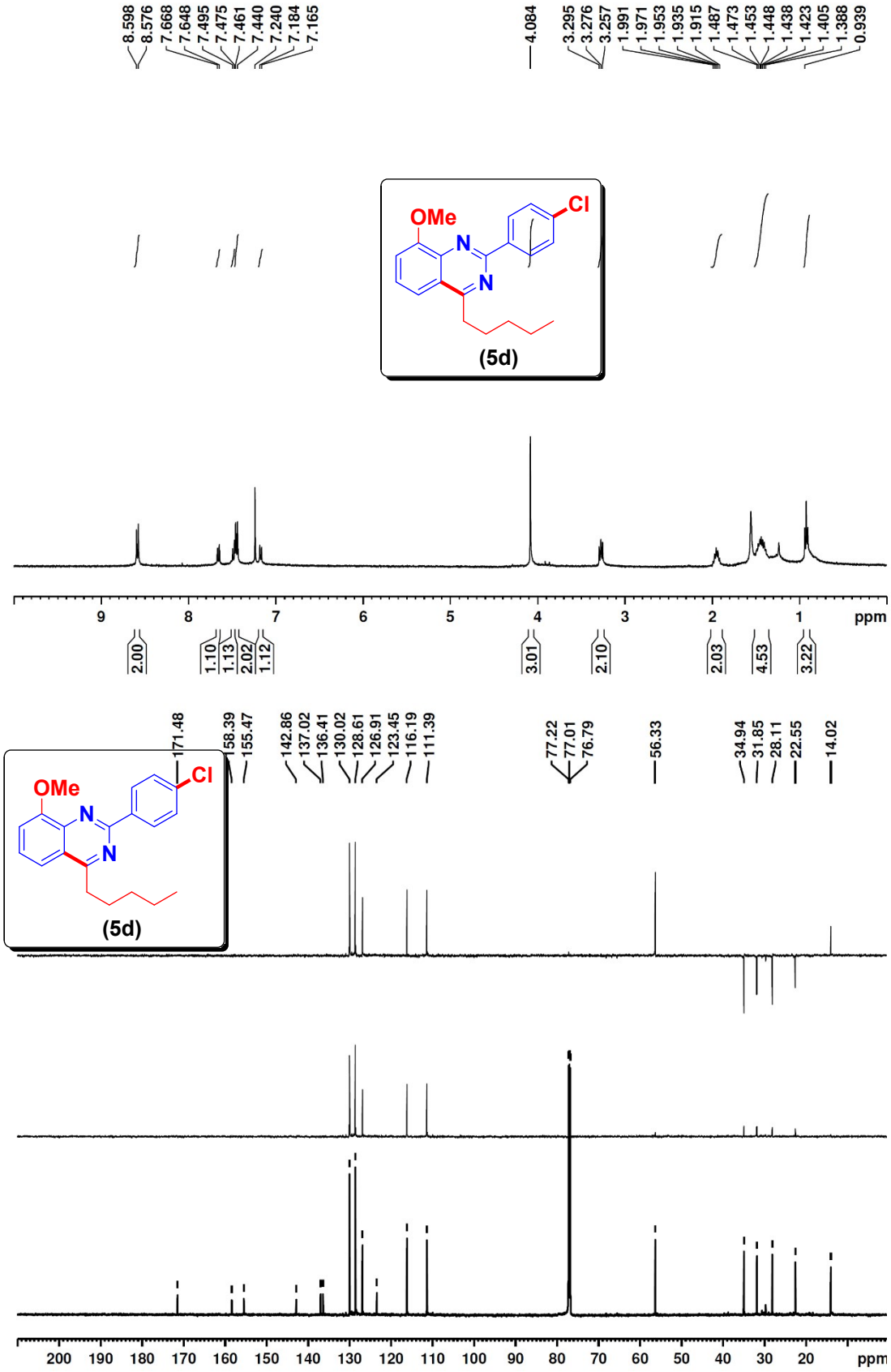
ppm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3.295
3.276
3.257
1.991
1.971
1.953
1.935
1.915
1.487
1.473
1.453
1.448
1.438
1.423
1.405
1.388
0.939
OMe
N
N
Cl
(5d)
9
8
7
6
5
4
3
2
1
ppm
2.00
1.10
1.13
2.02
1.12
3.01
2.10
2.03
4.53
3.22
171.48
158.39
155.47
142.86
137.02
136.41
130.02
128.61
126.91
123.45
116.19
111.39
77.22
77.01
76.79
56.33
34.94
31.85
28.11
22.55
14.02
OMe
N
N
Cl
(5d)
200
190
180
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160
150
140
130
120
110
100
90
80
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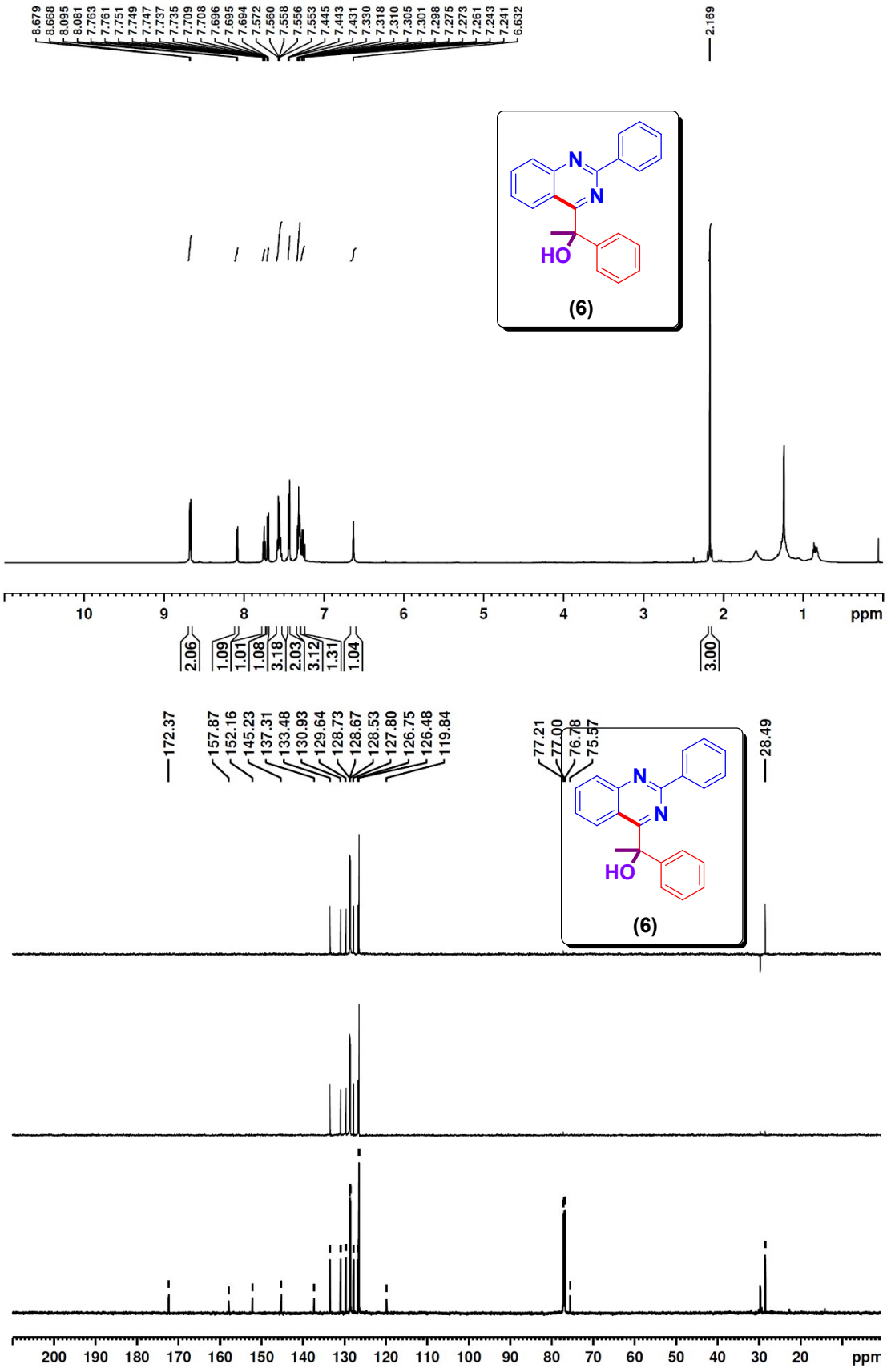
60
50
40
30
20
ppm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7.708
7.696
7.695
7.694
7.572
7.560
7.558
7.556
7.553
7.445
7.443
7.431
7.330
7.318
7.310
7.305
7.301
7.298
7.275
7.273
7.261
7.243
7.241
6.632
2.169
N
N
HO
(6)
10
9
8
7
6
5
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3
2
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ppm
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1.01
1.08
3.18
2.03
3.12
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1.04
3.00
172.37
157.87
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145.23
137.31
133.48
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129.64
128.73
128.67
128.53
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126.48
119.84
77.21
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75.57
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N
N
HO
(6)
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150
140
130
120
110
100
90
80
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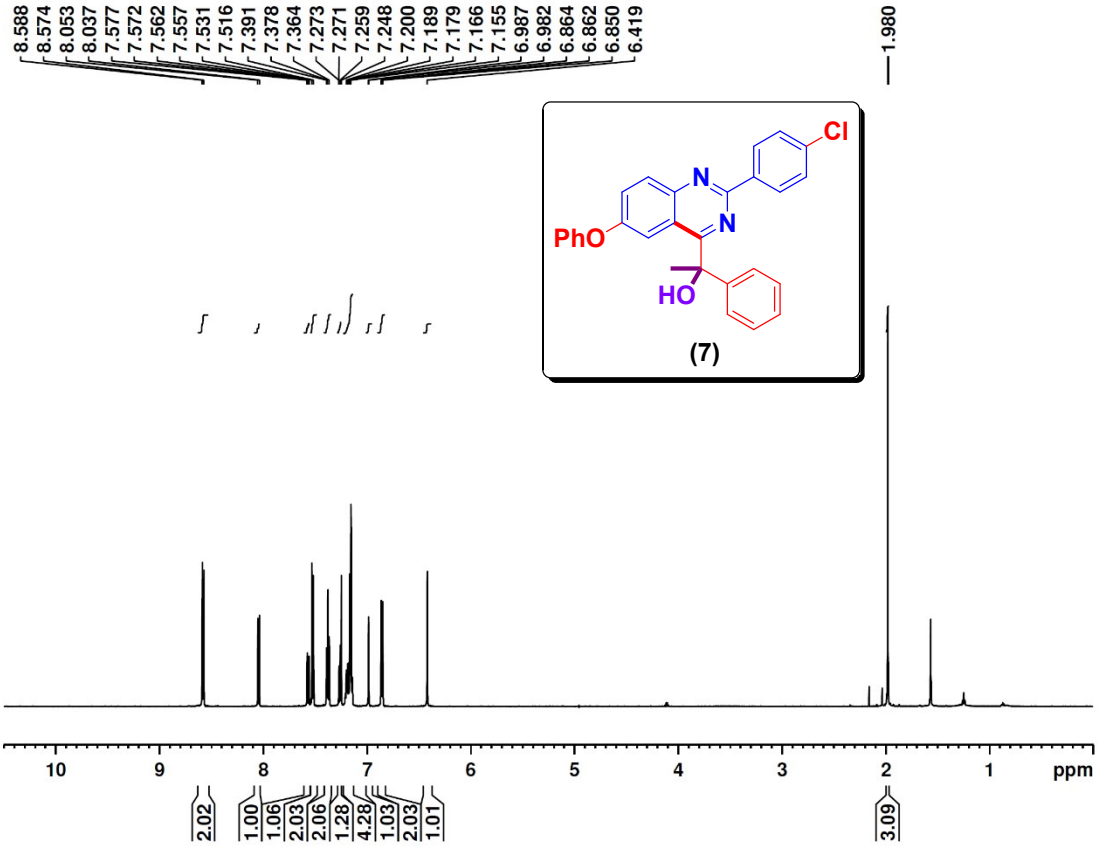
40
30
20
ppm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7.557
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7.516
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7.364
7.273
7.271
7.259
7.248
7.200
7.189
7.179
7.166
7.155
6.987
6.982
6.864
6.862
6.850
6.419
1.980
Cl
N
N
PhO
HO
(7)
10
9
8
7
6
5
4
3
2
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1.06
2.03
2.06
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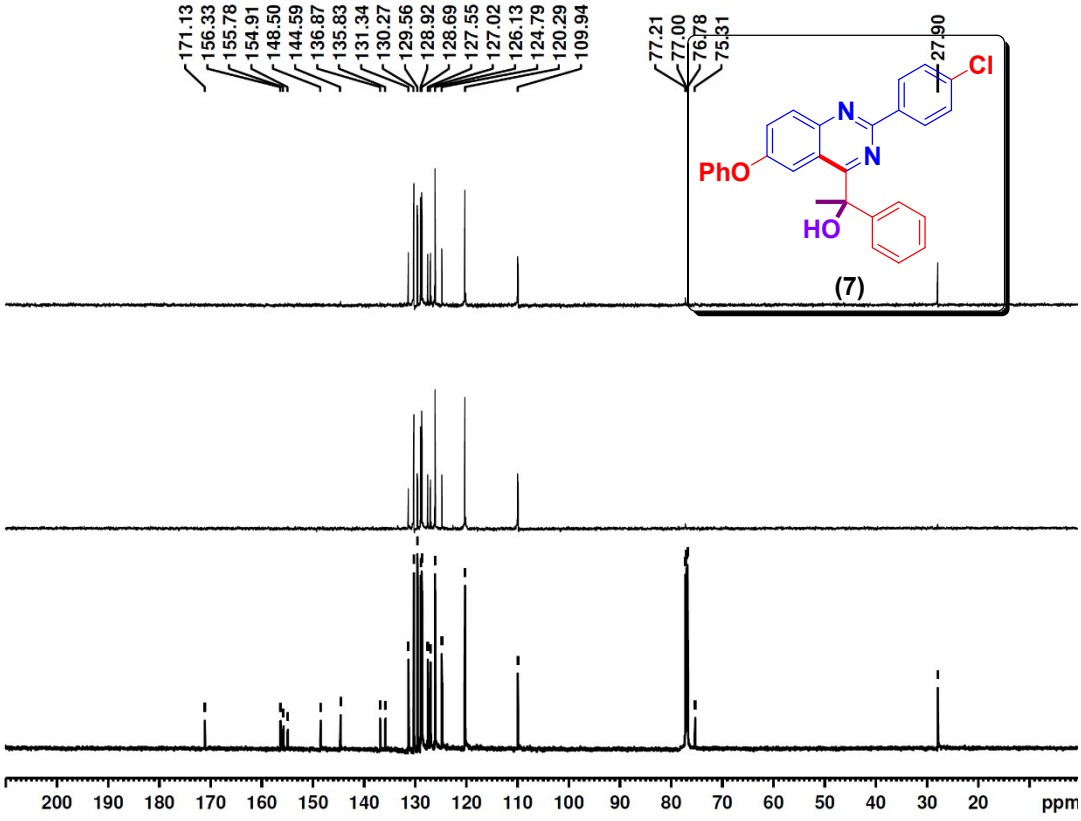
4.28
1.03
2.03
1.01
3.09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136.87
135.83
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130.27
129.56
128.92
128.69
127.55
127.02
126.13
124.79
120.29
109.94
77.21
77.00
76.78
75.31
27.90
Cl
N
N
PhO
HO
(7)
200
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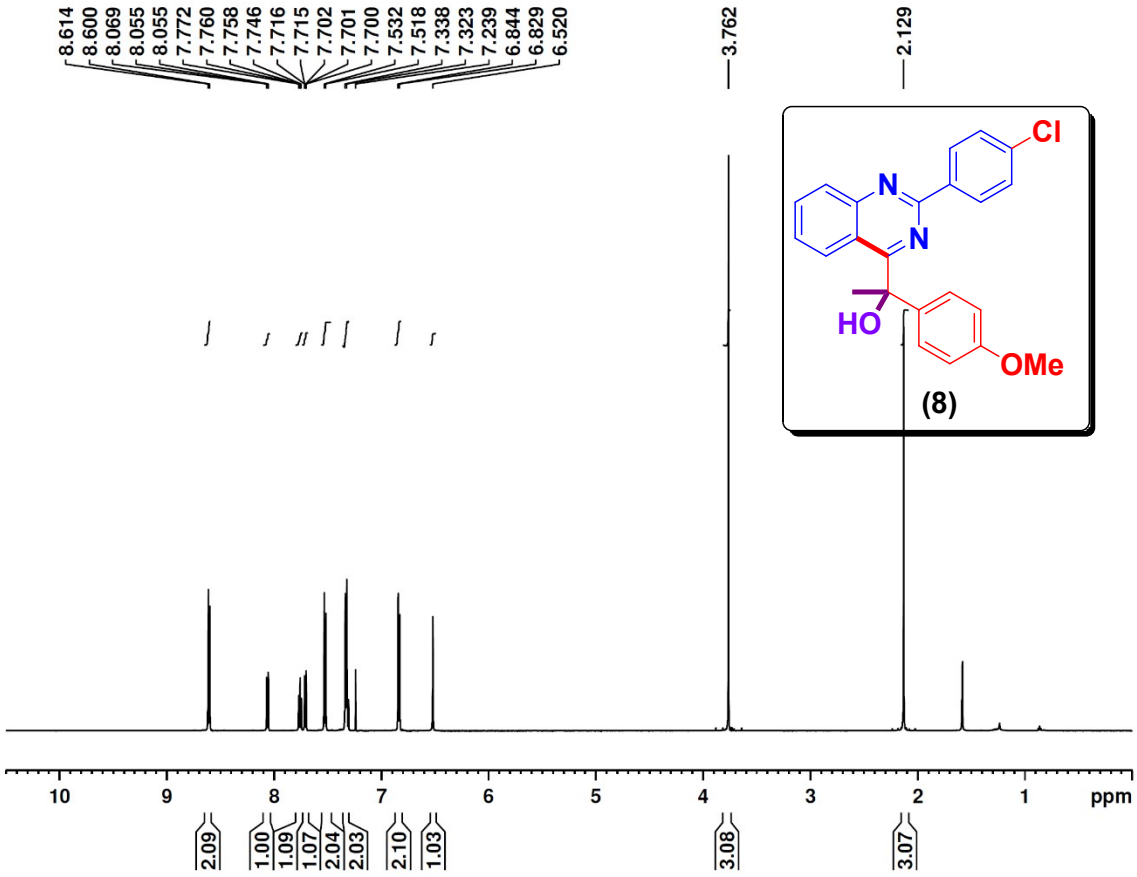
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.055
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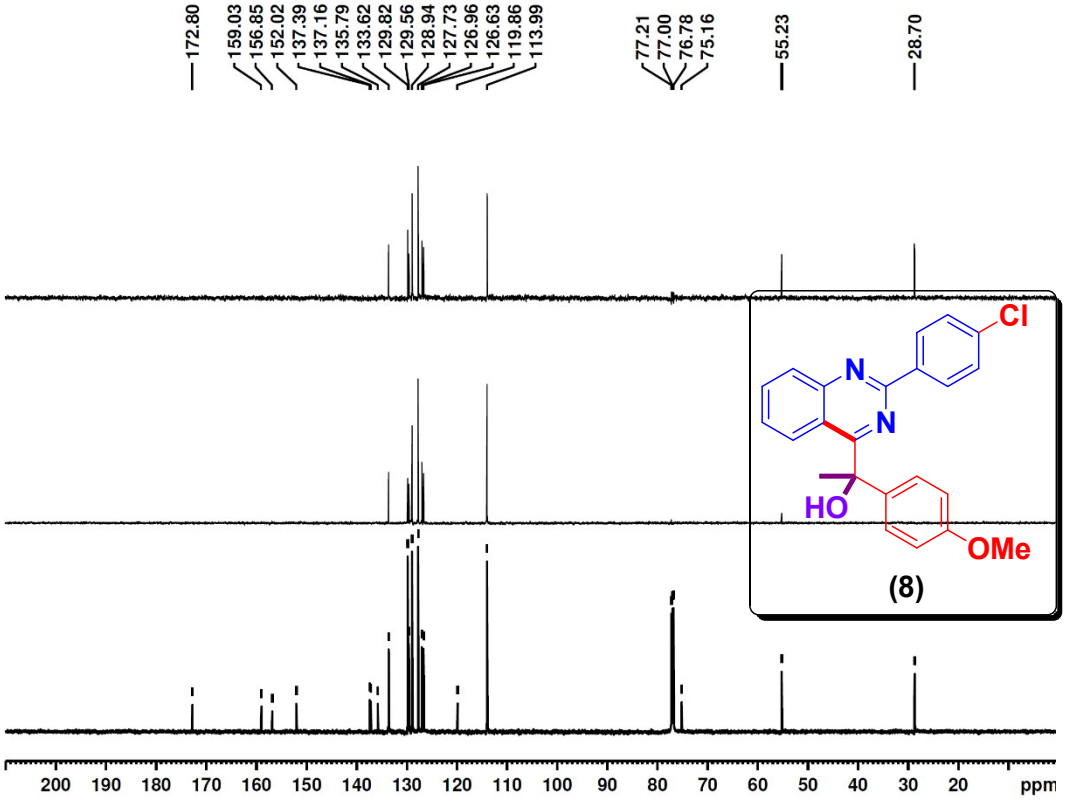
7.760
7.758
7.746
7.716
7.715
7.702
7.701
7.700
7.532
7.518
7.338
7.323
7.239
6.844
6.829
6.520
3.762
2.129
Cl
N
N
HO
OMe
(8)
10
9
8
7
6
5
4
3
2
1
ppm
2.09
1.00
1.09
1.07
2.04
2.03
2.10
1.03
3.08
3.07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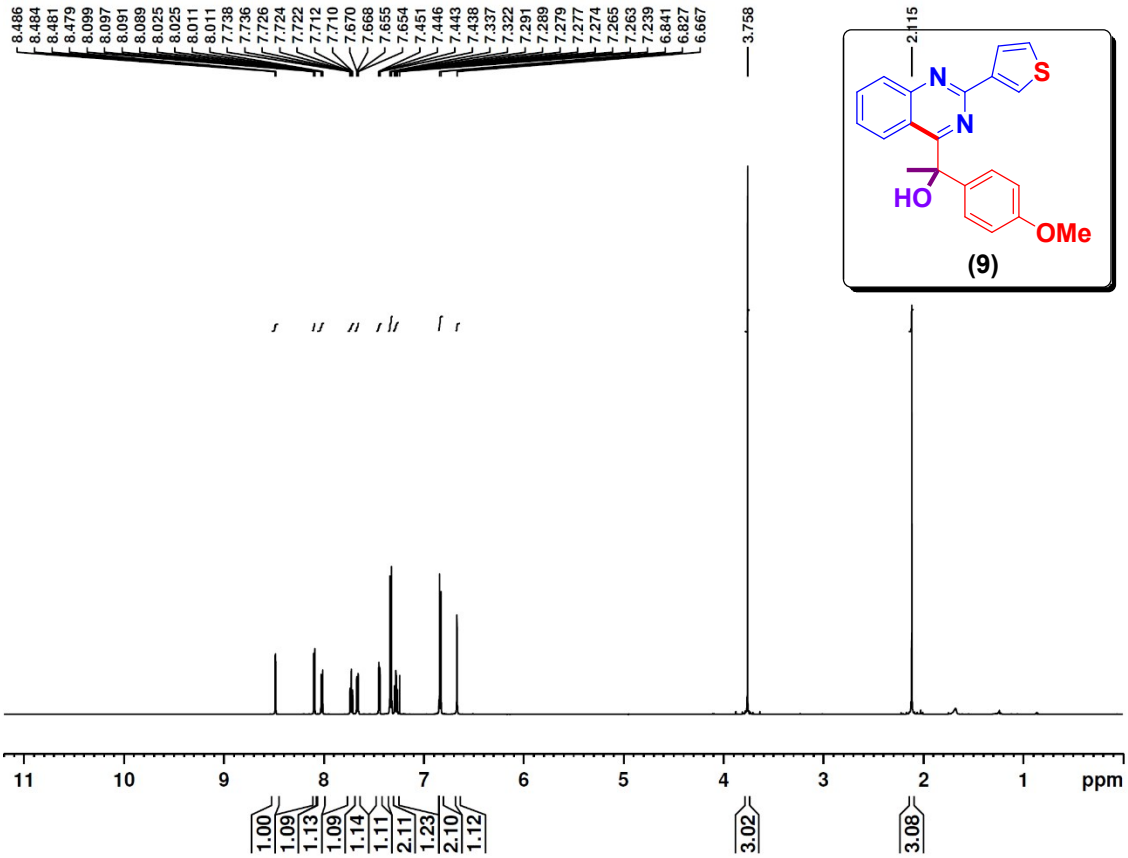
159.03
156.85
152.02
137.39
137.16
135.79
133.62
129.82
129.56
128.94
127.73
126.96
126.63
119.86
113.99
77.21
77.00
76.78
75.16
55.23
28.70
Cl
N
N
HO
OMe
(8)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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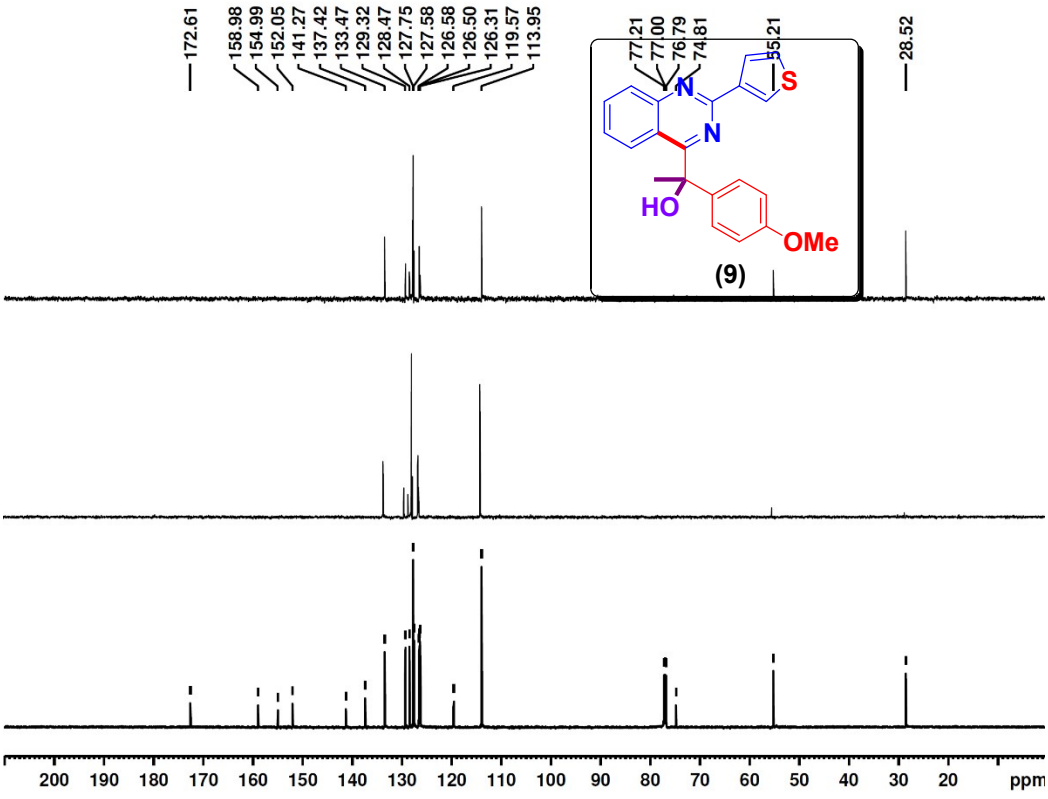
8.481
8.479
8.099
8.097
8.091
8.089
8.025
8.025
8.011
8.011
7.738
7.736
7.726
7.724
7.722
7.712
7.710
7.670
7.668
7.655
7.654
7.451
7.446
7.443
7.438
7.337
7.322
7.291
7.289
7.279
7.277
7.274
7.265
7.263
7.239
6.841
6.827
6.667
3.758
2.115
N
S
N
HO
OMe
(9)
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.09
1.13
1.09
1.14
1.11
2.11
1.23
2.10
1.12
3.02
3.08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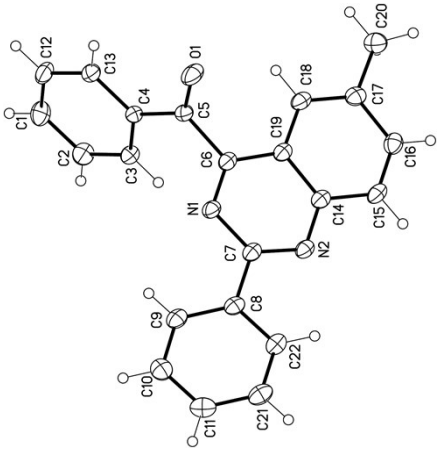
152.05
141.27
137.42
133.47
129.32
128.47
127.75
127.58
126.58
126.50
126.31
119.57
113.95
77.21
77.00
76.79
74.81
55.21
28.52
N
S
N
HO
OMe
(9)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

Figure S4: ORTEP diagram of compound **3e (CCDC No. 2003609)**



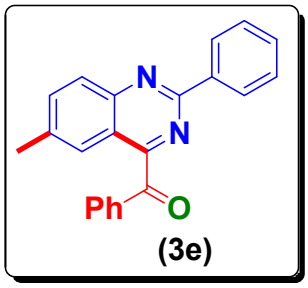


Table S6. Crystal data and structure refinement for 160224LT_0M.

Identification code	160224LT_0m	
Empirical formula	C22 H16 N2 O	
Formula weight	324.37	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 28.4647(16) Å	a= 90°.
	b = 8.4046(4) Å	b= 126.515(2)°.
	c = 17.4446(9) Å	g = 90°.
Volume	3354.1(3) $Å^3$	
Z	8	
Density (calculated)	1.285 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	1360	
Crystal size	0.20 x 0.15 x 0.15 mm^3	
Theta range for data collection	1.780 to 26.419°.	
Index ranges	-35<=h<=32, -8<=k<=10, -18<=l<=21	
Reflections collected	13500	
Independent reflections	3443 [R(int) = 0.0290]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.9048	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3443 / 0 / 227	

Goodness-of-fit on F^2	1.115
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.1086
R indices (all data)	R1 = 0.0473, wR2 = 0.1231
Extinction coefficient	n/a
Largest diff. peak and hole	0.336 and -0.283 e.$Å^{-3}$

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 160224LT_0M. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	388(1)	3410(1)	8816(1)	32(1)
N(2)	2422(1)	4726(1)	10193(1)	20(1)
N(1)	1774(1)	3131(1)	10327(1)	20(1)
C(1)	552(1)	-2520(2)	8735(1)	27(1)
C(2)	1068(1)	-1857(2)	8966(1)	25(1)
C(3)	1152(1)	-218(2)	9079(1)	20(1)
C(4)	714(1)	759(2)	8946(1)	17(1)
C(5)	783(1)	2506(2)	9029(1)	19(1)
C(6)	1372(1)	3236(1)	9400(1)	18(1)
C(7)	2293(1)	3910(2)	10691(1)	19(1)
C(8)	2739(1)	3833(2)	11742(1)	19(1)
C(9)	2708(1)	2687(2)	12290(1)	22(1)
C(10)	3134(1)	2627(2)	13270(1)	25(1)
C(11)	3591(1)	3713(2)	13716(1)	27(1)
C(12)	114(1)	-1547(2)	8604(1)	26(1)
C(13)	190(1)	86(2)	8703(1)	21(1)
C(14)	2005(1)	4811(2)	9227(1)	19(1)
C(15)	2119(1)	5685(2)	8663(1)	22(1)
C(16)	1702(1)	5781(2)	7696(1)	23(1)
C(17)	1148(1)	5025(2)	7230(1)	22(1)
C(18)	1029(1)	4185(2)	7772(1)	21(1)
C(19)	1452(1)	4063(1)	8775(1)	18(1)
C(20)	712(1)	5135(2)	6160(1)	27(1)
C(21)	3621(1)	4869(2)	13177(1)	27(1)
C(22)	3201(1)	4930(2)	12198(1)	23(1)

Table S8. Bond lengths [Å] and angles [°] for 160224LT_0M.

O(1)-C(5)	1.2171(16)
N(2)-C(7)	1.3193(17)
N(2)-C(14)	1.3693(17)
N(1)-C(6)	1.3149(17)
N(1)-C(7)	1.3773(16)
C(1)-C(2)	1.3862(19)
C(1)-C(12)	1.391(2)
C(1)-H(1)	0.9300
C(2)-C(3)	1.3913(19)
C(2)-H(3)	0.9300
C(3)-C(4)	1.3916(18)
C(3)-H(4)	0.9300
C(4)-C(13)	1.4049(17)
C(4)-C(5)	1.4775(18)
C(5)-C(6)	1.5223(17)
C(6)-C(19)	1.4211(18)
C(7)-C(8)	1.4866(18)
C(8)-C(9)	1.3964(19)
C(8)-C(22)	1.4020(18)
C(9)-C(10)	1.3899(19)
C(9)-H(14)	0.9300
C(10)-C(11)	1.389(2)
C(10)-H(11)	0.9300
C(11)-C(21)	1.389(2)
C(11)-H(2)	0.9300
C(12)-C(13)	1.3836(19)
C(12)-H(16)	0.9300
C(13)-H(15)	0.9300
C(14)-C(15)	1.4117(19)
C(14)-C(19)	1.4210(17)
C(15)-C(16)	1.3700(19)
C(15)-H(10)	0.9300
C(16)-C(17)	1.4239(18)
C(16)-H(9)	0.9300
C(17)-C(18)	1.3726(19)
C(17)-C(20)	1.5090(18)
C(18)-C(19)	1.4192(18)
C(18)-H(5)	0.9300

C(20)-H(6)	0.9600
C(20)-H(7)	0.9600
C(20)-H(8)	0.9600
C(21)-C(22)	1.386(2)
C(21)-H(13)	0.9300
C(22)-H(12)	0.9300

C(7)-N(2)-C(14)	117.42(11)
C(6)-N(1)-C(7)	116.36(11)
C(2)-C(1)-C(12)	120.09(12)
C(2)-C(1)-H(1)	120.0
C(12)-C(1)-H(1)	120.0
C(1)-C(2)-C(3)	120.20(12)
C(1)-C(2)-H(3)	119.9
C(3)-C(2)-H(3)	119.9
C(2)-C(3)-C(4)	119.86(12)
C(2)-C(3)-H(4)	120.1
C(4)-C(3)-H(4)	120.1
C(3)-C(4)-C(13)	119.85(12)
C(3)-C(4)-C(5)	121.16(11)
C(13)-C(4)-C(5)	118.96(11)
O(1)-C(5)-C(4)	123.14(12)
O(1)-C(5)-C(6)	117.53(11)
C(4)-C(5)-C(6)	119.32(11)
N(1)-C(6)-C(19)	123.89(11)
N(1)-C(6)-C(5)	115.35(11)
C(19)-C(6)-C(5)	120.61(11)
N(2)-C(7)-N(1)	125.93(12)
N(2)-C(7)-C(8)	117.80(11)
N(1)-C(7)-C(8)	116.26(11)
C(9)-C(8)-C(22)	119.11(13)
C(9)-C(8)-C(7)	121.22(12)
C(22)-C(8)-C(7)	119.67(12)
C(10)-C(9)-C(8)	120.15(12)
C(10)-C(9)-H(14)	119.9
C(8)-C(9)-H(14)	119.9
C(11)-C(10)-C(9)	120.40(13)
C(11)-C(10)-H(11)	119.8
C(9)-C(10)-H(11)	119.8
C(10)-C(11)-C(21)	119.74(13)

C(10)-C(11)-H(2)	120.1
C(21)-C(11)-H(2)	120.1
C(13)-C(12)-C(1)	120.26(12)
C(13)-C(12)-H(16)	119.9
C(1)-C(12)-H(16)	119.9
C(12)-C(13)-C(4)	119.73(12)
C(12)-C(13)-H(15)	120.1
C(4)-C(13)-H(15)	120.1
N(2)-C(14)-C(15)	119.68(11)
N(2)-C(14)-C(19)	121.49(12)
C(15)-C(14)-C(19)	118.82(12)
C(16)-C(15)-C(14)	119.84(12)
C(16)-C(15)-H(10)	120.1
C(14)-C(15)-H(10)	120.1
C(15)-C(16)-C(17)	122.09(13)
C(15)-C(16)-H(9)	119.0
C(17)-C(16)-H(9)	119.0
C(18)-C(17)-C(16)	118.65(12)
C(18)-C(17)-C(20)	121.73(12)
C(16)-C(17)-C(20)	119.61(12)
C(17)-C(18)-C(19)	120.65(12)
C(17)-C(18)-H(5)	119.7
C(19)-C(18)-H(5)	119.7
C(18)-C(19)-C(14)	119.96(12)
C(18)-C(19)-C(6)	125.14(11)
C(14)-C(19)-C(6)	114.90(12)
C(17)-C(20)-H(6)	109.5
C(17)-C(20)-H(7)	109.5
H(6)-C(20)-H(7)	109.5
C(17)-C(20)-H(8)	109.5
H(6)-C(20)-H(8)	109.5
H(7)-C(20)-H(8)	109.5
C(22)-C(21)-C(11)	120.26(13)
C(22)-C(21)-H(13)	119.9
C(11)-C(21)-H(13)	119.9
C(21)-C(22)-C(8)	120.32(13)
C(21)-C(22)-H(12)	119.8
C(8)-C(22)-H(12)	119.8

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 160224LT_0M. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

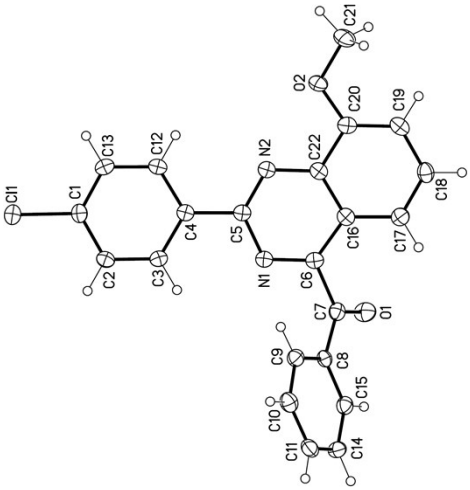
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	20(1)	21(1)	54(1)	2(1)	20(1)	1(1)
N(2)	16(1)	18(1)	25(1)	-2(1)	13(1)	-1(1)
N(1)	15(1)	18(1)	26(1)	0(1)	12(1)	0(1)
C(1)	33(1)	16(1)	34(1)	-4(1)	21(1)	-4(1)
C(2)	26(1)	20(1)	32(1)	-1(1)	19(1)	3(1)
C(3)	18(1)	21(1)	22(1)	-1(1)	12(1)	-1(1)
C(4)	16(1)	18(1)	16(1)	0(1)	9(1)	-1(1)
C(5)	15(1)	19(1)	22(1)	2(1)	10(1)	1(1)
C(6)	16(1)	13(1)	27(1)	-2(1)	13(1)	0(1)
C(7)	16(1)	15(1)	26(1)	-2(1)	14(1)	1(1)
C(8)	16(1)	20(1)	25(1)	-3(1)	13(1)	2(1)
C(9)	18(1)	21(1)	29(1)	-3(1)	16(1)	1(1)
C(10)	26(1)	27(1)	28(1)	2(1)	19(1)	5(1)
C(11)	23(1)	33(1)	22(1)	-5(1)	12(1)	3(1)
C(12)	23(1)	23(1)	31(1)	-2(1)	17(1)	-7(1)
C(13)	18(1)	21(1)	24(1)	1(1)	12(1)	0(1)
C(14)	17(1)	16(1)	25(1)	-3(1)	13(1)	1(1)
C(15)	17(1)	22(1)	30(1)	-4(1)	16(1)	-3(1)
C(16)	24(1)	21(1)	29(1)	0(1)	19(1)	0(1)
C(17)	19(1)	20(1)	25(1)	-1(1)	13(1)	3(1)
C(18)	16(1)	19(1)	27(1)	-3(1)	12(1)	-1(1)
C(19)	16(1)	14(1)	26(1)	-2(1)	13(1)	1(1)
C(20)	23(1)	31(1)	26(1)	0(1)	14(1)	2(1)
C(21)	22(1)	29(1)	28(1)	-10(1)	14(1)	-5(1)
C(22)	22(1)	23(1)	27(1)	-4(1)	16(1)	-3(1)

Table S10. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for 160224LT_0M.

	x	y	z	U(eq)
H(1)	499	-3616	8667	33
H(3)	1358	-2509	9046	31
H(4)	1500	223	9242	24
H(14)	2401	1961	11997	26

H(11)	3113	1856	13631	30
H(2)	3876	3667	14372	32
H(16)	-231	-1995	8451	31
H(15)	-105	735	8608	25
H(10)	2477	6194	8946	26
H(9)	1783	6359	7333	27
H(5)	668	3691	7479	25
H(6)	831	4445	5866	41
H(7)	695	6211	5961	41
H(8)	333	4817	5973	41
H(13)	3925	5605	13475	32
H(12)	3225	5703	11840	28

Figure S5: ORTEP diagram of compound **3i (CCDC No. 2003611)**



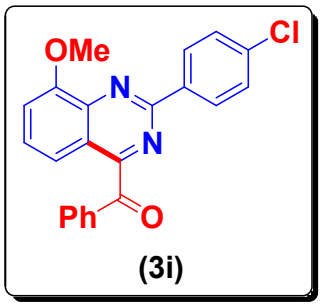


Table S11. Crystal data and structure refinement for mo_200215lt_0m.

Identification code	mo_200215LT_0m	
Empirical formula	C22 H15 Cl N2 O2	
Formula weight	374.81	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 14.020(4) Å	a= 90°.
	b = 8.187(2) Å	b= 104.692(8)°.
	c = 15.972(4) Å	g = 90°.
Volume	1773.3(8) $Å^3$	
Z	4	
Density (calculated)	1.404 Mg/m^3	
Absorption coefficient	0.236 mm^{-1}	
F(000)	776	
Crystal size	0.15 x 0.12 x 0.04 mm^3	
Theta range for data collection	1.729 to 26.390°.	
Index ranges	-17<=h<=17, -10<=k<=8, -19<=l<=19	
Reflections collected	24604	
Independent reflections	3630 [R(int) = 0.0521]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6987	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3630 / 0 / 245	

Goodness-of-fit on F^2	1.008
Final R indices [I>2sigma(I)]	R1 = 0.0354, wR2 = 0.0811
R indices (all data)	R1 = 0.0553, wR2 = 0.0907
Extinction coefficient	n/a
Largest diff. peak and hole	0.251 and -0.244 e.$Å^{-3}$

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_200215lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Cl(1)	11371(1)	6189(1)	1538(1)	28(1)
O(1)	6587(1)	1988(2)	4493(1)	28(1)
O(2)	11323(1)	787(2)	6234(1)	25(1)
N(1)	8636(1)	3610(2)	4163(1)	19(1)
N(2)	10199(1)	2485(2)	4922(1)	18(1)
C(1)	10882(1)	5358(2)	2348(1)	20(1)
C(2)	9961(1)	5886(2)	2408(1)	19(1)
C(3)	9565(1)	5225(2)	3046(1)	18(1)
C(4)	10073(1)	4036(2)	3614(1)	17(1)
C(5)	9628(1)	3323(2)	4282(1)	17(1)
C(6)	8215(1)	2970(2)	4739(1)	18(1)
C(7)	7101(1)	3209(2)	4542(1)	20(1)
C(8)	6676(1)	4878(2)	4411(1)	18(1)
C(9)	7260(1)	6283(2)	4526(1)	21(1)
C(10)	6825(1)	7816(2)	4471(1)	25(1)
C(11)	5800(1)	7957(2)	4276(1)	25(1)
C(12)	11004(1)	3529(2)	3535(1)	20(1)
C(13)	11412(1)	4191(2)	2904(1)	22(1)
C(14)	5214(1)	6573(2)	4135(1)	26(1)
C(15)	5640(1)	5041(2)	4204(1)	22(1)
C(16)	8738(1)	2036(2)	5460(1)	19(1)
C(17)	8316(1)	1361(2)	6104(1)	22(1)
C(18)	8907(1)	516(2)	6772(1)	23(1)
C(19)	9927(1)	286(2)	6843(1)	22(1)
C(20)	10351(1)	922(2)	6228(1)	20(1)
C(21)	11975(1)	84(3)	6991(1)	32(1)
C(22)	9762(1)	1829(2)	5516(1)	18(1)

Table S13. Bond lengths [Å] and angles [°] for mo_200215lt_0m.

Cl(1)-C(1)	1.7491(16)
O(1)-C(7)	1.223(2)
O(2)-C(20)	1.3639(19)
O(2)-C(21)	1.439(2)
N(1)-C(6)	1.321(2)
N(1)-C(5)	1.375(2)
N(2)-C(5)	1.320(2)
N(2)-C(22)	1.364(2)
C(1)-C(13)	1.385(2)
C(1)-C(2)	1.388(2)
C(2)-C(3)	1.388(2)
C(2)-H(15)	0.9500
C(3)-C(4)	1.396(2)
C(3)-H(14)	0.9500
C(4)-C(12)	1.406(2)
C(4)-C(5)	1.485(2)
C(6)-C(16)	1.422(2)
C(6)-C(7)	1.526(2)
C(7)-C(8)	1.484(2)
C(8)-C(9)	1.397(2)
C(8)-C(15)	1.411(2)
C(9)-C(10)	1.388(2)
C(9)-H(7)	0.9500
C(10)-C(11)	1.395(2)
C(10)-H(6)	0.9500
C(11)-C(14)	1.385(3)
C(11)-H(1)	0.9500
C(12)-C(13)	1.389(2)
C(12)-H(3)	0.9500
C(13)-H(2)	0.9500
C(14)-C(15)	1.381(2)
C(14)-H(5)	0.9500
C(15)-H(4)	0.9500
C(16)-C(17)	1.421(2)
C(16)-C(22)	1.425(2)
C(17)-C(18)	1.362(2)
C(17)-H(13)	0.9500
C(18)-C(19)	1.419(2)
C(18)-H(12)	0.9500

C(19)-C(20)	1.373(2)
C(19)-H(11)	0.9500
C(20)-C(22)	1.432(2)
C(21)-H(8)	0.9800
C(21)-H(9)	0.9800
C(21)-H(10)	0.9800

C(20)-O(2)-C(21)	117.34(13)
C(6)-N(1)-C(5)	116.80(14)
C(5)-N(2)-C(22)	116.92(14)
C(13)-C(1)-C(2)	121.94(15)
C(13)-C(1)-Cl(1)	119.65(13)
C(2)-C(1)-Cl(1)	118.41(13)
C(1)-C(2)-C(3)	118.73(16)
C(1)-C(2)-H(15)	120.6
C(3)-C(2)-H(15)	120.6
C(2)-C(3)-C(4)	121.05(15)
C(2)-C(3)-H(14)	119.5
C(4)-C(3)-H(14)	119.5
C(3)-C(4)-C(12)	118.73(14)
C(3)-C(4)-C(5)	120.18(14)
C(12)-C(4)-C(5)	121.09(15)
N(2)-C(5)-N(1)	126.09(15)
N(2)-C(5)-C(4)	118.59(14)
N(1)-C(5)-C(4)	115.32(14)
N(1)-C(6)-C(16)	123.21(15)
N(1)-C(6)-C(7)	114.87(14)
C(16)-C(6)-C(7)	121.79(14)
O(1)-C(7)-C(8)	122.31(15)
O(1)-C(7)-C(6)	117.66(15)
C(8)-C(7)-C(6)	120.03(14)
C(9)-C(8)-C(15)	119.13(16)
C(9)-C(8)-C(7)	122.56(15)
C(15)-C(8)-C(7)	118.23(15)
C(10)-C(9)-C(8)	120.15(16)
C(10)-C(9)-H(7)	119.9
C(8)-C(9)-H(7)	119.9
C(9)-C(10)-C(11)	119.99(17)
C(9)-C(10)-H(6)	120.0
C(11)-C(10)-H(6)	120.0

C(14)-C(11)-C(10)	120.29(17)
C(14)-C(11)-H(1)	119.9
C(10)-C(11)-H(1)	119.9
C(13)-C(12)-C(4)	120.81(16)
C(13)-C(12)-H(3)	119.6
C(4)-C(12)-H(3)	119.6
C(1)-C(13)-C(12)	118.75(15)
C(1)-C(13)-H(2)	120.6
C(12)-C(13)-H(2)	120.6
C(15)-C(14)-C(11)	120.13(16)
C(15)-C(14)-H(5)	119.9
C(11)-C(14)-H(5)	119.9
C(14)-C(15)-C(8)	120.27(16)
C(14)-C(15)-H(4)	119.9
C(8)-C(15)-H(4)	119.9
C(17)-C(16)-C(6)	124.84(15)
C(17)-C(16)-C(22)	120.34(15)
C(6)-C(16)-C(22)	114.81(14)
C(18)-C(17)-C(16)	118.85(16)
C(18)-C(17)-H(13)	120.6
C(16)-C(17)-H(13)	120.6
C(17)-C(18)-C(19)	122.04(16)
C(17)-C(18)-H(12)	119.0
C(19)-C(18)-H(12)	119.0
C(20)-C(19)-C(18)	120.20(16)
C(20)-C(19)-H(11)	119.9
C(18)-C(19)-H(11)	119.9
O(2)-C(20)-C(19)	125.24(16)
O(2)-C(20)-C(22)	114.95(14)
C(19)-C(20)-C(22)	119.81(15)
O(2)-C(21)-H(8)	109.5
O(2)-C(21)-H(9)	109.5
H(8)-C(21)-H(9)	109.5
O(2)-C(21)-H(10)	109.5
H(8)-C(21)-H(10)	109.5
H(9)-C(21)-H(10)	109.5
N(2)-C(22)-C(16)	122.17(15)
N(2)-C(22)-C(20)	119.06(14)
C(16)-C(22)-C(20)	118.76(14)

Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_200215lt_0m. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

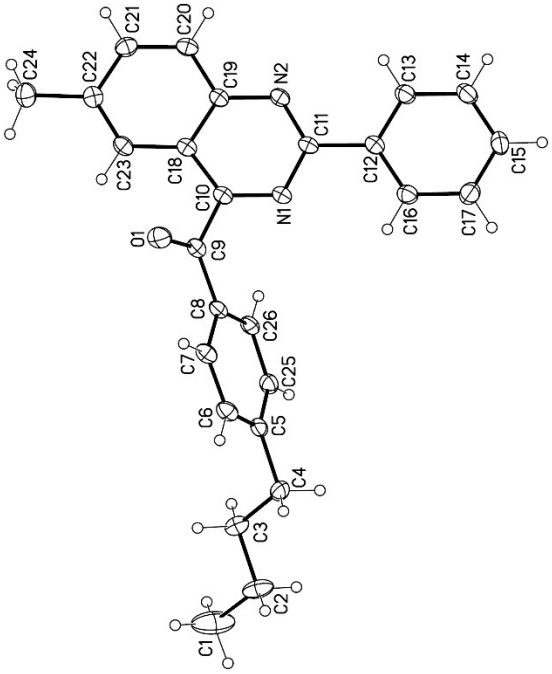
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	28(1)	31(1)	27(1)	5(1)	12(1)	1(1)
O(1)	22(1)	23(1)	37(1)	-2(1)	4(1)	-5(1)
O(2)	21(1)	34(1)	20(1)	5(1)	1(1)	6(1)
N(1)	18(1)	18(1)	19(1)	-1(1)	3(1)	-1(1)
N(2)	20(1)	16(1)	17(1)	-3(1)	3(1)	0(1)
C(1)	22(1)	19(1)	18(1)	-2(1)	6(1)	-4(1)
C(2)	19(1)	18(1)	18(1)	-1(1)	1(1)	0(1)
C(3)	17(1)	19(1)	18(1)	-4(1)	2(1)	0(1)
C(4)	18(1)	15(1)	17(1)	-4(1)	2(1)	-2(1)
C(5)	19(1)	14(1)	18(1)	-4(1)	3(1)	-1(1)
C(6)	18(1)	14(1)	21(1)	-4(1)	3(1)	-1(1)
C(7)	20(1)	23(1)	16(1)	-2(1)	4(1)	-2(1)
C(8)	21(1)	22(1)	12(1)	1(1)	4(1)	1(1)
C(9)	21(1)	24(1)	18(1)	0(1)	4(1)	0(1)
C(10)	31(1)	21(1)	24(1)	1(1)	7(1)	-1(1)
C(11)	33(1)	25(1)	20(1)	5(1)	9(1)	7(1)
C(12)	20(1)	18(1)	20(1)	0(1)	2(1)	2(1)
C(13)	18(1)	22(1)	26(1)	-3(1)	5(1)	2(1)
C(14)	20(1)	36(1)	23(1)	4(1)	6(1)	7(1)
C(15)	21(1)	26(1)	18(1)	0(1)	5(1)	-2(1)
C(16)	22(1)	14(1)	19(1)	-3(1)	4(1)	-2(1)
C(17)	22(1)	19(1)	25(1)	-1(1)	6(1)	-1(1)
C(18)	30(1)	19(1)	22(1)	-1(1)	9(1)	-3(1)
C(19)	28(1)	17(1)	18(1)	-1(1)	1(1)	1(1)
C(20)	22(1)	18(1)	19(1)	-5(1)	2(1)	1(1)
C(21)	27(1)	42(1)	22(1)	6(1)	-2(1)	7(1)
C(22)	22(1)	14(1)	16(1)	-4(1)	2(1)	-2(1)

Table S15. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$)

for mo_200215lt_0m.

	x	y	z	U(eq)
H(15)	9607	6685	2019	23
H(14)	8939	5587	3097	22
H(7)	7957	6189	4644	25
H(6)	7224	8769	4565	30
H(1)	5504	9007	4240	31
H(3)	11359	2723	3919	24
H(2)	12044	3850	2855	26
H(5)	4516	6676	3990	31
H(4)	5235	4095	4111	26
H(13)	7634	1497	6068	26
H(12)	8627	66	7203	28
H(11)	10318	-310	7318	27
H(8)	11958	741	7500	48
H(9)	12649	66	6919	48
H(10)	11764	-1034	7070	48

Figure S6: ORTEP diagram of compound **4c (CCDC No. 2003610)**



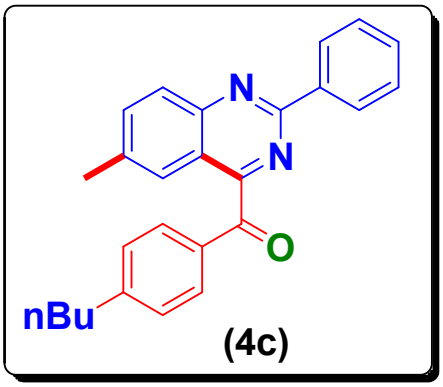


Table S16. Crystal data and structure refinement for mo_170408lt_0m.

Identification code	mo_170408LT_0m	
Empirical formula	C26 H24 N2 O	
Formula weight	380.47	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R -3 :H	
Unit cell dimensions	a = 36.593(4) Å	a= 90°.
	b = 36.593(4) Å	b= 90°.
	c = 7.8611(8) Å	g = 120°.
Volume	9116(2) $Å^3$	
Z	18	
Density (calculated)	1.247 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	3636	
Crystal size	0.12 x 0.04 x 0.03 mm^3	
Theta range for data collection	1.113 to 26.391°.	
Index ranges	-45<=h<=45, -45<=k<=45, -6<=l<=9	
Reflections collected	46493	
Independent reflections	4153 [R(int) = 0.0596]	
Completeness to theta = 25.242°	100.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8467
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4153 / 0 / 264
Goodness-of-fit on F^2	1.132
Final R indices [I>2sigma(I)]	R1 = 0.0436, wR2 = 0.1159
R indices (all data)	R1 = 0.0634, wR2 = 0.1362
Extinction coefficient	n/a
Largest diff. peak and hole	0.365 and -0.338 e.$Å^{-3}$

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_170408lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4530(1)	8761(1)	3901(2)	26(1)
N(1)	5206(1)	9626(1)	1710(2)	16(1)
N(2)	5198(1)	10262(1)	2337(2)	17(1)
C(1)	4072(1)	7214(1)	-6289(3)	56(1)
C(2)	4491(1)	7481(1)	-5426(2)	30(1)
C(3)	4454(1)	7721(1)	-3912(2)	23(1)
C(4)	4868(1)	7980(1)	-2950(2)	23(1)
C(5)	4824(1)	8232(1)	-1528(2)	19(1)
C(6)	4750(1)	8085(1)	138(2)	21(1)
C(7)	4693(1)	8310(1)	1423(2)	20(1)
C(8)	4720(1)	8699(1)	1081(2)	17(1)
C(9)	4672(1)	8930(1)	2535(2)	18(1)
C(10)	4826(1)	9400(1)	2374(2)	16(1)
C(11)	5379(1)	10057(1)	1713(2)	16(1)
C(12)	5810(1)	10309(1)	989(2)	17(1)
C(13)	6020(1)	10750(1)	1045(2)	21(1)
C(14)	6423(1)	10986(1)	385(2)	24(1)
C(15)	6627(1)	10789(1)	-329(2)	23(1)
C(16)	6015(1)	10113(1)	263(2)	21(1)
C(17)	6422(1)	10352(1)	-388(2)	25(1)
C(18)	4591(1)	9580(1)	3055(2)	16(1)
C(19)	4804(1)	10028(1)	3018(2)	16(1)
C(20)	4603(1)	10239(1)	3712(2)	20(1)
C(21)	4205(1)	10011(1)	4361(2)	22(1)

C(22)	3981(1)	9563(1)	4357(2)	20(1)
C(23)	4176(1)	9354(1)	3726(2)	19(1)
C(24)	3536(1)	9330(1)	5029(2)	26(1)
C(25)	4833(1)	8612(1)	-1879(2)	20(1)
C(26)	4791(1)	8848(1)	-592(2)	18(1)

Table S18. Bond lengths [Å] and angles [°] for mo_170408lt_0m.

O(1)-C(9)	1.219(2)
N(1)-C(10)	1.320(2)
N(1)-C(11)	1.373(2)
N(2)-C(11)	1.320(2)
N(2)-C(19)	1.365(2)
C(1)-C(2)	1.506(3)
C(1)-H(16)	0.9800
C(1)-H(1)	0.9800
C(1)-H(17)	0.9800
C(2)-C(3)	1.524(2)
C(2)-H(15)	0.9900
C(2)-H(18)	0.9900
C(3)-C(4)	1.525(3)
C(3)-H(13)	0.9900
C(3)-H(14)	0.9900
C(4)-C(5)	1.508(2)
C(4)-H(20)	0.9900
C(4)-H(19)	0.9900
C(5)-C(6)	1.391(2)
C(5)-C(25)	1.402(2)
C(6)-C(7)	1.384(3)
C(6)-H(12)	0.9500
C(7)-C(8)	1.402(2)
C(7)-H(23)	0.9500
C(8)-C(26)	1.398(2)
C(8)-C(9)	1.485(2)
C(9)-C(10)	1.521(2)
C(10)-C(18)	1.424(2)
C(11)-C(12)	1.487(2)
C(12)-C(16)	1.392(2)
C(12)-C(13)	1.400(2)
C(13)-C(14)	1.384(3)

C(13)-H(3)	0.9500
C(14)-C(15)	1.389(3)
C(14)-H(24)	0.9500
C(15)-C(17)	1.386(3)
C(15)-H(2)	0.9500
C(16)-C(17)	1.394(3)
C(16)-H(5)	0.9500
C(17)-H(4)	0.9500
C(18)-C(19)	1.419(2)
C(18)-C(23)	1.421(2)
C(19)-C(20)	1.416(2)
C(20)-C(21)	1.365(3)
C(20)-H(11)	0.9500
C(21)-C(22)	1.421(2)
C(21)-H(10)	0.9500
C(22)-C(23)	1.373(2)
C(22)-C(24)	1.505(2)
C(23)-H(6)	0.9500
C(24)-H(7)	0.9800
C(24)-H(8)	0.9800
C(24)-H(9)	0.9800
C(25)-C(26)	1.388(2)
C(25)-H(22)	0.9500
C(26)-H(21)	0.9500

C(10)-N(1)-C(11)	117.18(14)
C(11)-N(2)-C(19)	117.40(14)
C(2)-C(1)-H(16)	109.5
C(2)-C(1)-H(1)	109.5
H(16)-C(1)-H(1)	109.5
C(2)-C(1)-H(17)	109.5
H(16)-C(1)-H(17)	109.5
H(1)-C(1)-H(17)	109.5
C(1)-C(2)-C(3)	111.76(18)
C(1)-C(2)-H(15)	109.3
C(3)-C(2)-H(15)	109.3
C(1)-C(2)-H(18)	109.3
C(3)-C(2)-H(18)	109.3
H(15)-C(2)-H(18)	107.9
C(2)-C(3)-C(4)	113.54(16)

C(2)-C(3)-H(13)	108.9
C(4)-C(3)-H(13)	108.9
C(2)-C(3)-H(14)	108.9
C(4)-C(3)-H(14)	108.9
H(13)-C(3)-H(14)	107.7
C(5)-C(4)-C(3)	111.83(14)
C(5)-C(4)-H(20)	109.2
C(3)-C(4)-H(20)	109.2
C(5)-C(4)-H(19)	109.2
C(3)-C(4)-H(19)	109.2
H(20)-C(4)-H(19)	107.9
C(6)-C(5)-C(25)	118.28(16)
C(6)-C(5)-C(4)	121.40(16)
C(25)-C(5)-C(4)	120.22(16)
C(7)-C(6)-C(5)	120.98(16)
C(7)-C(6)-H(12)	119.5
C(5)-C(6)-H(12)	119.5
C(6)-C(7)-C(8)	120.58(16)
C(6)-C(7)-H(23)	119.7
C(8)-C(7)-H(23)	119.7
C(26)-C(8)-C(7)	118.87(16)
C(26)-C(8)-C(9)	123.57(15)
C(7)-C(8)-C(9)	117.56(15)
O(1)-C(9)-C(8)	121.95(15)
O(1)-C(9)-C(10)	118.14(15)
C(8)-C(9)-C(10)	119.80(14)
N(1)-C(10)-C(18)	123.17(15)
N(1)-C(10)-C(9)	114.93(14)
C(18)-C(10)-C(9)	121.60(15)
N(2)-C(11)-N(1)	125.45(15)
N(2)-C(11)-C(12)	117.84(14)
N(1)-C(11)-C(12)	116.70(14)
C(16)-C(12)-C(13)	118.82(16)
C(16)-C(12)-C(11)	120.95(15)
C(13)-C(12)-C(11)	120.22(15)
C(14)-C(13)-C(12)	120.28(17)
C(14)-C(13)-H(3)	119.9
C(12)-C(13)-H(3)	119.9
C(13)-C(14)-C(15)	120.74(17)
C(13)-C(14)-H(24)	119.6

C(15)-C(14)-H(24)	119.6
C(17)-C(15)-C(14)	119.31(17)
C(17)-C(15)-H(2)	120.3
C(14)-C(15)-H(2)	120.3
C(12)-C(16)-C(17)	120.54(16)
C(12)-C(16)-H(5)	119.7
C(17)-C(16)-H(5)	119.7
C(15)-C(17)-C(16)	120.31(17)
C(15)-C(17)-H(4)	119.8
C(16)-C(17)-H(4)	119.8
C(19)-C(18)-C(23)	119.44(15)
C(19)-C(18)-C(10)	114.68(15)
C(23)-C(18)-C(10)	125.87(15)
N(2)-C(19)-C(20)	118.79(15)
N(2)-C(19)-C(18)	122.09(15)
C(20)-C(19)-C(18)	119.13(15)
C(21)-C(20)-C(19)	119.78(16)
C(21)-C(20)-H(11)	120.1
C(19)-C(20)-H(11)	120.1
C(20)-C(21)-C(22)	121.99(16)
C(20)-C(21)-H(10)	119.0
C(22)-C(21)-H(10)	119.0
C(23)-C(22)-C(21)	118.89(16)
C(23)-C(22)-C(24)	121.82(16)
C(21)-C(22)-C(24)	119.29(16)
C(22)-C(23)-C(18)	120.71(16)
C(22)-C(23)-H(6)	119.6
C(18)-C(23)-H(6)	119.6
C(22)-C(24)-H(7)	109.5
C(22)-C(24)-H(8)	109.5
H(7)-C(24)-H(8)	109.5
C(22)-C(24)-H(9)	109.5
H(7)-C(24)-H(9)	109.5
H(8)-C(24)-H(9)	109.5
C(26)-C(25)-C(5)	121.24(16)
C(26)-C(25)-H(22)	119.4
C(5)-C(25)-H(22)	119.4
C(25)-C(26)-C(8)	119.96(15)
C(25)-C(26)-H(21)	120.0
C(8)-C(26)-H(21)	120.0

Symmetry transformations used to generate equivalent atoms:

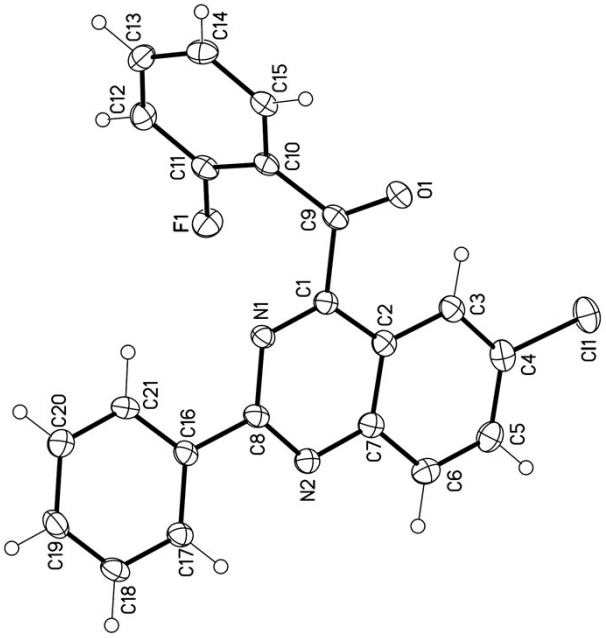
Table S19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_170408lt_0m. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	37(1)	19(1)	23(1)	6(1)	6(1)	14(1)
N(1)	18(1)	13(1)	16(1)	0(1)	-3(1)	7(1)
N(2)	19(1)	14(1)	17(1)	0(1)	-3(1)	7(1)
C(1)	85(2)	63(2)	40(1)	-29(1)	-30(1)	51(2)
C(2)	55(1)	29(1)	19(1)	0(1)	0(1)	31(1)
C(3)	31(1)	25(1)	20(1)	-1(1)	1(1)	19(1)
C(4)	22(1)	20(1)	29(1)	1(1)	7(1)	12(1)
C(5)	13(1)	16(1)	27(1)	-3(1)	-1(1)	6(1)
C(6)	21(1)	15(1)	29(1)	1(1)	-4(1)	10(1)
C(7)	21(1)	15(1)	22(1)	1(1)	-4(1)	8(1)
C(8)	14(1)	12(1)	22(1)	-2(1)	-4(1)	5(1)
C(9)	16(1)	15(1)	21(1)	0(1)	-3(1)	7(1)
C(10)	18(1)	15(1)	14(1)	0(1)	-4(1)	7(1)
C(11)	19(1)	14(1)	14(1)	-1(1)	-5(1)	8(1)
C(12)	18(1)	16(1)	15(1)	0(1)	-4(1)	7(1)
C(13)	21(1)	17(1)	24(1)	-1(1)	-1(1)	9(1)
C(14)	23(1)	16(1)	25(1)	-1(1)	-1(1)	5(1)
C(15)	17(1)	25(1)	21(1)	2(1)	2(1)	5(1)
C(16)	24(1)	17(1)	21(1)	0(1)	0(1)	9(1)
C(17)	25(1)	26(1)	26(1)	2(1)	4(1)	14(1)
C(18)	18(1)	16(1)	13(1)	0(1)	-4(1)	8(1)
C(19)	18(1)	16(1)	14(1)	0(1)	-4(1)	7(1)
C(20)	24(1)	15(1)	22(1)	-1(1)	-2(1)	10(1)
C(21)	24(1)	24(1)	20(1)	-1(1)	-1(1)	15(1)
C(22)	19(1)	22(1)	17(1)	2(1)	-3(1)	10(1)
C(23)	19(1)	15(1)	20(1)	1(1)	-4(1)	7(1)
C(24)	21(1)	28(1)	30(1)	2(1)	0(1)	12(1)
C(25)	19(1)	17(1)	22(1)	2(1)	2(1)	7(1)
C(26)	18(1)	12(1)	23(1)	2(1)	-1(1)	6(1)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for mo_170408lt_0m.

	x	y	z	U(eq)
H(16)	3871	7010	-5475	85
H(1)	4108	7064	-7249	85
H(17)	3965	7396	-6706	85
H(15)	4695	7685	-6255	36
H(18)	4602	7298	-5033	36
H(13)	4239	7516	-3118	28
H(14)	4354	7912	-4321	28
H(20)	4960	7789	-2473	28
H(19)	5088	8175	-3752	28
H(12)	4738	7826	398	26
H(23)	4635	8200	2548	24
H(3)	5885	10889	1539	25
H(24)	6561	11285	420	29
H(2)	6904	10952	-771	28
H(5)	5876	9814	210	25
H(4)	6559	10215	-875	30
H(11)	4745	10539	3726	24
H(10)	4074	10156	4829	26
H(6)	4031	9054	3739	22
H(7)	3414	9028	4816	39
H(8)	3367	9433	4452	39
H(9)	3539	9380	6255	39
H(22)	4870	8711	-3019	24
H(21)	4810	9111	-848	22

Figure S7: ORTEP diagram of compound **4i (CCDC No. 2003606)**



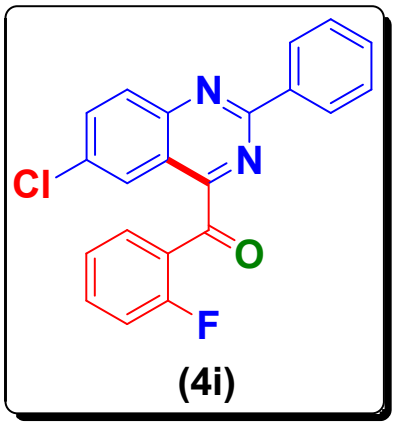


Table S21. Crystal data and structure refinement for 190921lt_a.

Identification code	190921LT_a	
Empirical formula	C21 H12 Cl F N2 O	
Formula weight	362.78	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.1316(6) Å	a= 90°.
	b = 18.1683(10) Å	b= 112.003(3)°.
	c = 8.7769(5) Å	g = 90°.
Volume	1645.77(16) $Å^3$	
Z	4	
Density (calculated)	1.464 Mg/m^3	
Absorption coefficient	0.255 mm^{-1}	
F(000)	744	
Crystal size	0.20 x 0.15 x 0.04 mm^3	
Theta range for data collection	1.973 to 26.411°.	
Index ranges	-13<=h<=13, -22<=k<=13, -10<=l<=10	
Reflections collected	14119	

Independent reflections	3372 [R(int) = 0.0303]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6293
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3372 / 0 / 235
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0369, wR2 = 0.0854
R indices (all data)	R1 = 0.0482, wR2 = 0.0942
Extinction coefficient	n/a
Largest diff. peak and hole	0.262 and -0.357 e.$Å^{-3}$

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 190921lt_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3167(1)	4179(1)	6561(2)	17(1)
C(2)	3222(2)	4841(1)	5736(2)	18(1)
C(3)	2224(2)	5112(1)	4300(2)	20(1)
C(4)	2415(2)	5756(1)	3642(2)	22(1)
C(5)	3576(2)	6158(1)	4334(2)	24(1)
C(6)	4539(2)	5914(1)	5720(2)	22(1)
C(7)	4386(2)	5246(1)	6458(2)	18(1)
C(8)	5209(1)	4376(1)	8466(2)	17(1)
C(9)	1935(2)	3730(1)	6104(2)	18(1)
C(10)	1999(1)	2914(1)	6179(2)	17(1)
C(11)	2885(2)	2495(1)	5789(2)	18(1)
C(12)	2895(2)	1739(1)	5810(2)	22(1)
C(13)	1987(2)	1379(1)	6270(2)	22(1)
C(14)	1074(2)	1778(1)	6659(2)	23(1)
C(15)	1078(2)	2533(1)	6605(2)	20(1)
C(16)	6267(1)	4101(1)	9960(2)	17(1)
C(17)	7308(2)	4556(1)	10823(2)	19(1)
C(18)	8282(2)	4308(1)	12247(2)	21(1)
C(19)	8226(2)	3610(1)	12830(2)	25(1)
C(20)	7202(2)	3154(1)	11976(2)	31(1)
C(21)	6227(2)	3394(1)	10544(2)	25(1)
Cl(1)	1197(1)	6105(1)	1904(1)	29(1)

F(1)	3755(1)	2845(1)	5293(1)	25(1)
N(1)	4130(1)	3940(1)	7865(2)	17(1)
N(2)	5369(1)	5010(1)	7843(2)	18(1)
O(1)	909(1)	4050(1)	5778(2)	25(1)

Table S23. Bond lengths [Å] and angles [°] for 190921lt_a.

C(1)-N(1)	1.315(2)
C(1)-C(2)	1.416(2)
C(1)-C(9)	1.515(2)
C(2)-C(7)	1.417(2)
C(2)-C(3)	1.420(2)
C(3)-C(4)	1.356(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.410(2)
C(4)-Cl(1)	1.7366(17)
C(5)-C(6)	1.360(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.416(2)
C(6)-H(6)	0.9500
C(7)-N(2)	1.364(2)
C(8)-N(2)	1.316(2)
C(8)-N(1)	1.369(2)
C(8)-C(16)	1.483(2)
C(9)-O(1)	1.2164(19)
C(9)-C(10)	1.484(2)
C(10)-C(11)	1.386(2)
C(10)-C(15)	1.399(2)
C(11)-F(1)	1.3586(18)
C(11)-C(12)	1.373(2)
C(12)-C(13)	1.386(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.391(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.374(2)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.389(2)

C(16)-C(17)	1.395(2)
C(17)-C(18)	1.387(2)
C(17)-H(17)	0.9500
C(18)-C(19)	1.378(2)
C(18)-H(18)	0.9500
C(19)-C(20)	1.382(2)
C(19)-H(19)	0.9500
C(20)-C(21)	1.388(2)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500

N(1)-C(1)-C(2)	123.26(14)
N(1)-C(1)-C(9)	114.47(14)
C(2)-C(1)-C(9)	121.99(14)
C(1)-C(2)-C(7)	114.80(14)
C(1)-C(2)-C(3)	125.40(15)
C(7)-C(2)-C(3)	119.80(15)
C(4)-C(3)-C(2)	118.85(15)
C(4)-C(3)-H(3)	120.6
C(2)-C(3)-H(3)	120.6
C(3)-C(4)-C(5)	121.90(15)
C(3)-C(4)-Cl(1)	119.63(13)
C(5)-C(4)-Cl(1)	118.47(13)
C(6)-C(5)-C(4)	120.28(16)
C(6)-C(5)-H(5)	119.9
C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(7)	119.99(16)
C(5)-C(6)-H(6)	120.0
C(7)-C(6)-H(6)	120.0
N(2)-C(7)-C(6)	118.86(14)
N(2)-C(7)-C(2)	121.97(15)
C(6)-C(7)-C(2)	119.17(15)
N(2)-C(8)-N(1)	125.61(14)
N(2)-C(8)-C(16)	118.44(14)
N(1)-C(8)-C(16)	115.95(14)
O(1)-C(9)-C(10)	120.88(14)
O(1)-C(9)-C(1)	118.79(15)
C(10)-C(9)-C(1)	120.17(13)
C(11)-C(10)-C(15)	117.06(16)
C(11)-C(10)-C(9)	124.35(14)

C(15)-C(10)-C(9)	118.54(14)
F(1)-C(11)-C(12)	117.97(14)
F(1)-C(11)-C(10)	118.71(15)
C(12)-C(11)-C(10)	123.27(15)
C(11)-C(12)-C(13)	118.28(15)
C(11)-C(12)-H(12)	120.9
C(13)-C(12)-H(12)	120.9
C(12)-C(13)-C(14)	120.32(16)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	120.03(15)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(14)-C(15)-C(10)	121.02(15)
C(14)-C(15)-H(15)	119.5
C(10)-C(15)-H(15)	119.5
C(21)-C(16)-C(17)	118.89(15)
C(21)-C(16)-C(8)	120.86(14)
C(17)-C(16)-C(8)	120.24(15)
C(18)-C(17)-C(16)	120.39(16)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(19)-C(18)-C(17)	120.36(15)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(18)-C(19)-C(20)	119.57(16)
C(18)-C(19)-H(19)	120.2
C(20)-C(19)-H(19)	120.2
C(19)-C(20)-C(21)	120.58(17)
C(19)-C(20)-H(20)	119.7
C(21)-C(20)-H(20)	119.7
C(20)-C(21)-C(16)	120.20(16)
C(20)-C(21)-H(21)	119.9
C(16)-C(21)-H(21)	119.9
C(1)-N(1)-C(8)	117.12(14)
C(8)-N(2)-C(7)	117.19(13)

Symmetry transformations used to generate equivalent atoms:

Table S24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 190921lt_a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

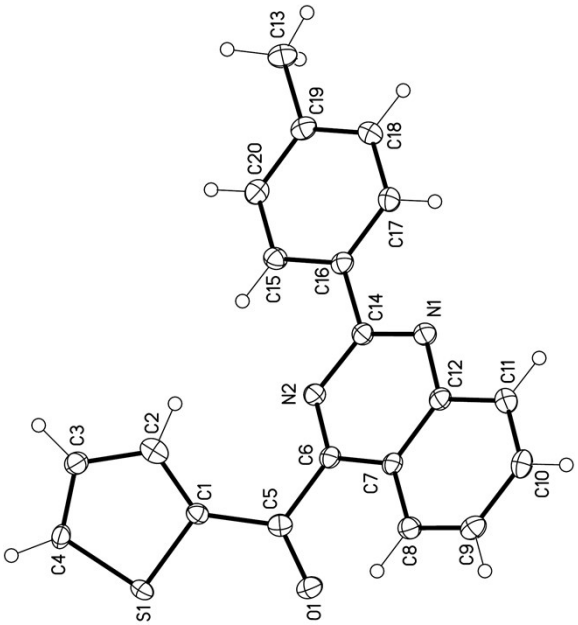
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	15(1)	18(1)	18(1)	-3(1)	8(1)	0(1)
C(2)	17(1)	20(1)	18(1)	-2(1)	9(1)	2(1)
C(3)	18(1)	23(1)	19(1)	-2(1)	8(1)	2(1)
C(4)	24(1)	26(1)	15(1)	0(1)	8(1)	6(1)
C(5)	30(1)	20(1)	23(1)	3(1)	12(1)	2(1)
C(6)	23(1)	21(1)	23(1)	-2(1)	10(1)	-2(1)
C(7)	19(1)	20(1)	18(1)	-3(1)	9(1)	0(1)
C(8)	14(1)	20(1)	19(1)	-4(1)	8(1)	-1(1)
C(9)	16(1)	24(1)	15(1)	0(1)	4(1)	-1(1)
C(10)	15(1)	22(1)	12(1)	-1(1)	2(1)	-1(1)
C(11)	15(1)	25(1)	16(1)	1(1)	6(1)	-2(1)
C(12)	22(1)	22(1)	21(1)	-2(1)	9(1)	2(1)
C(13)	28(1)	17(1)	21(1)	0(1)	8(1)	-1(1)
C(14)	23(1)	25(1)	21(1)	0(1)	10(1)	-7(1)
C(15)	15(1)	25(1)	18(1)	-2(1)	6(1)	-1(1)
C(16)	15(1)	20(1)	19(1)	-2(1)	8(1)	2(1)
C(17)	17(1)	21(1)	21(1)	-2(1)	8(1)	-1(1)
C(18)	14(1)	27(1)	23(1)	-7(1)	7(1)	-2(1)
C(19)	18(1)	29(1)	22(1)	0(1)	1(1)	3(1)
C(20)	28(1)	21(1)	33(1)	4(1)	0(1)	-1(1)
C(21)	19(1)	22(1)	29(1)	-1(1)	2(1)	-5(1)
Cl(1)	28(1)	35(1)	20(1)	7(1)	7(1)	8(1)
F(1)	25(1)	24(1)	32(1)	0(1)	18(1)	-2(1)
N(1)	14(1)	18(1)	18(1)	-2(1)	6(1)	0(1)
N(2)	18(1)	19(1)	19(1)	-1(1)	8(1)	0(1)
O(1)	15(1)	25(1)	31(1)	0(1)	5(1)	2(1)

Table S25. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for 190921lt_a.

	x	y	z	U(eq)

H(3)	1437	4847	3810	23
H(5)	3687	6603	3831	28
H(6)	5314	6191	6193	26
H(12)	3508	1471	5516	26
H(13)	1988	856	6321	27
H(14)	448	1527	6962	27
H(15)	445	2801	6861	24
H(17)	7352	5040	10434	23
H(18)	8990	4621	12824	26
H(19)	8889	3443	13812	30
H(20)	7164	2671	12373	37
H(21)	5531	3075	9961	30

Figure S8: ORTEP diagram of compound **4o (CCDC No. 2003605)**



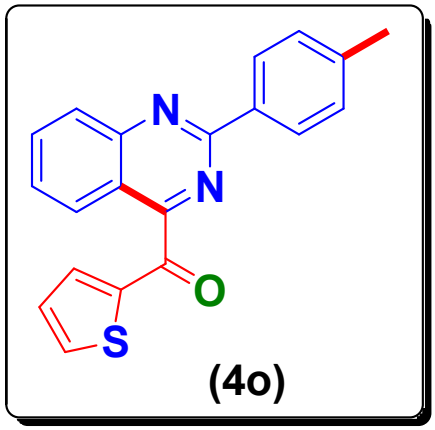


Table S26. Crystal data and structure refinement for 190416lt_0m_a.

Identification code	190416lt_0m_a	
Empirical formula	C20 H14 N2 O S	
Formula weight	330.39	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 3.8618(3) Å	a= 90°.
	b = 33.708(3) Å	b= 98.934(3)°.
	c = 11.8039(12) Å	g = 90°.
Volume	1517.9(2) $Å^3$	
Z	4	
Density (calculated)	1.446 Mg/m^3	
Absorption coefficient	0.222 mm^{-1}	
F(000)	688	
Crystal size	0.15 x 0.05 x 0.05 mm^3	
Theta range for data collection	1.208 to 26.386°.	
Index ranges	-4<=h<=3, -42<=k<=42, -13<=l<=14	
Reflections collected	10411	
Independent reflections	3072 [R(int) = 0.0329]	
Completeness to theta = 25.242°	99.2 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.7454 and 0.7130
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3072 / 180 / 264
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0346, wR2 = 0.0802
R indices (all data)	R1 = 0.0440, wR2 = 0.0856
Extinction coefficient	n/a
Largest diff. peak and hole	0.263 and -0.209 e.$Å^{-3}$

Table S27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 190416lt_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	1055(2)	2784(1)	305(1)	17(1)
C(1)	1370(30)	3180(2)	1220(5)	14(1)
C(2)	-248(18)	3509(1)	703(6)	24(1)
C(3)	-1696(17)	3443(1)	-440(4)	18(1)
C(4)	-1209(14)	3061(1)	-779(3)	17(1)
S(1')	140(20)	3621(2)	658(7)	22(1)
C(1')	1540(190)	3186(8)	1310(30)	19(5)
C(2')	820(60)	2898(5)	514(16)	37(4)
C(3')	-740(90)	3005(6)	-588(18)	22(4)
C(4')	-1380(100)	3404(7)	-620(19)	20(4)
C(5)	3085(4)	3121(1)	2411(1)	16(1)
C(6)	3546(4)	3474(1)	3215(1)	15(1)
C(7)	3025(4)	3440(1)	4376(1)	15(1)
C(8)	1642(4)	3106(1)	4877(1)	17(1)
C(9)	1403(4)	3107(1)	6020(1)	19(1)
C(10)	2510(4)	3440(1)	6706(1)	20(1)
C(11)	3797(4)	3769(1)	6243(1)	18(1)
C(12)	4045(4)	3778(1)	5061(1)	16(1)
N(1)	5259(3)	4116(1)	4619(1)	17(1)
C(14)	5421(4)	4117(1)	3512(1)	15(1)
N(2)	4662(3)	3801(1)	2784(1)	16(1)
C(16)	6555(4)	4486(1)	2991(1)	16(1)
C(17)	7534(4)	4818(1)	3668(1)	20(1)

C(18)	8582(4)	5163(1)	3185(1)	21(1)
C(19)	8661(4)	5188(1)	2014(1)	18(1)
C(20)	7665(4)	4857(1)	1344(1)	18(1)
C(15)	6622(4)	4511(1)	1818(1)	17(1)
C(13)	9779(4)	5565(1)	1482(1)	22(1)
O(1)	4196(3)	2795(1)	2764(1)	24(1)

Table S28. Bond lengths [Å] and angles [°] for 190416lt_0m_a.

S(1)-C(1)	1.711(5)
S(1)-C(4)	1.711(3)
C(1)-C(2)	1.367(7)
C(1)-C(5)	1.472(4)
C(2)-C(3)	1.396(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.371(4)
C(3)-H(3)	0.9500
C(4)-H(4)	0.9500
S(1')-C(4')	1.697(18)
S(1')-C(1')	1.70(2)
C(1')-C(2')	1.35(2)
C(1')-C(5)	1.36(2)
C(2')-C(3')	1.394(17)
C(2')-H(2')	0.9500
C(3')-C(4')	1.367(16)
C(3')-H(3')	0.9500
C(4')-H(4')	0.9500
C(5)-O(1)	1.2267(18)
C(5)-C(6)	1.516(2)
C(6)-N(2)	1.3147(19)
C(6)-C(7)	1.420(2)
C(7)-C(8)	1.415(2)
C(7)-C(12)	1.417(2)
C(8)-C(9)	1.366(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.410(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.364(2)

C(10)-H(10)	0.9500
C(11)-C(12)	1.414(2)
C(11)-H(11)	0.9500
C(12)-N(1)	1.3648(19)
N(1)-C(14)	1.3181(19)
C(14)-N(2)	1.3717(19)
C(14)-C(16)	1.482(2)
C(16)-C(15)	1.392(2)
C(16)-C(17)	1.392(2)
C(17)-C(18)	1.384(2)
C(17)-H(17)	0.9500
C(18)-C(19)	1.390(2)
C(18)-H(18)	0.9500
C(19)-C(20)	1.388(2)
C(19)-C(13)	1.510(2)
C(20)-C(15)	1.382(2)
C(20)-H(20)	0.9500
C(15)-H(15)	0.9500
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800

C(1)-S(1)-C(4)	91.4(2)
C(2)-C(1)-C(5)	130.0(5)
C(2)-C(1)-S(1)	111.6(3)
C(5)-C(1)-S(1)	118.3(3)
C(1)-C(2)-C(3)	112.9(5)
C(1)-C(2)-H(2)	123.5
C(3)-C(2)-H(2)	123.5
C(4)-C(3)-C(2)	112.2(4)
C(4)-C(3)-H(3)	123.9
C(2)-C(3)-H(3)	123.9
C(3)-C(4)-S(1)	111.8(3)
C(3)-C(4)-H(4)	124.1
S(1)-C(4)-H(4)	124.1
C(4')-S(1')-C(1')	94.3(11)
C(2')-C(1')-C(5)	124.1(19)
C(2')-C(1')-S(1')	106.5(13)
C(5)-C(1')-S(1')	129.5(18)
C(1')-C(2')-C(3')	118.5(16)

C(1')-C(2')-H(2')	120.7
C(3')-C(2')-H(2')	120.7
C(4')-C(3')-C(2')	109.3(17)
C(4')-C(3')-H(3')	125.4
C(2')-C(3')-H(3')	125.4
C(3')-C(4')-S(1')	111.3(16)
C(3')-C(4')-H(4')	124.3
S(1')-C(4')-H(4')	124.3
O(1)-C(5)-C(1')	123.3(12)
O(1)-C(5)-C(1)	121.9(3)
O(1)-C(5)-C(6)	119.27(13)
C(1')-C(5)-C(6)	117.4(11)
C(1)-C(5)-C(6)	118.8(2)
N(2)-C(6)-C(7)	122.93(13)
N(2)-C(6)-C(5)	115.53(12)
C(7)-C(6)-C(5)	121.41(13)
C(8)-C(7)-C(12)	119.41(13)
C(8)-C(7)-C(6)	125.86(14)
C(12)-C(7)-C(6)	114.72(13)
C(9)-C(8)-C(7)	119.90(14)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(8)-C(9)-C(10)	120.55(14)
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7
C(11)-C(10)-C(9)	120.86(14)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6
C(10)-C(11)-C(12)	119.91(14)
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0
N(1)-C(12)-C(11)	118.41(13)
N(1)-C(12)-C(7)	122.28(13)
C(11)-C(12)-C(7)	119.31(14)
C(14)-N(1)-C(12)	116.98(13)
N(1)-C(14)-N(2)	125.42(14)
N(1)-C(14)-C(16)	118.44(13)
N(2)-C(14)-C(16)	116.13(13)
C(6)-N(2)-C(14)	117.45(12)
C(15)-C(16)-C(17)	118.51(14)

C(15)-C(16)-C(14)	121.00(13)
C(17)-C(16)-C(14)	120.49(13)
C(18)-C(17)-C(16)	120.66(14)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(19)	120.99(14)
C(17)-C(18)-H(18)	119.5
C(19)-C(18)-H(18)	119.5
C(20)-C(19)-C(18)	118.08(14)
C(20)-C(19)-C(13)	120.75(14)
C(18)-C(19)-C(13)	121.17(14)
C(15)-C(20)-C(19)	121.37(14)
C(15)-C(20)-H(20)	119.3
C(19)-C(20)-H(20)	119.3
C(20)-C(15)-C(16)	120.39(14)
C(20)-C(15)-H(15)	119.8
C(16)-C(15)-H(15)	119.8
C(19)-C(13)-H(13A)	109.5
C(19)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(19)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S29. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 190416lt_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}
S(1)	20(1)	13(1)	16(1)	-4(1)	2(1)	-1(1)
C(1)	16(2)	14(2)	14(2)	-1(1)	3(1)	-2(1)
C(2)	23(2)	24(3)	27(2)	-6(2)	5(1)	-2(2)
C(3)	18(2)	16(1)	20(2)	2(1)	2(1)	0(1)
C(4)	17(2)	20(2)	12(1)	4(1)	-1(1)	-3(1)
S(1')	22(3)	31(4)	13(2)	-3(2)	-2(2)	8(2)
C(1')	18(8)	13(8)	26(8)	-6(7)	9(7)	4(7)

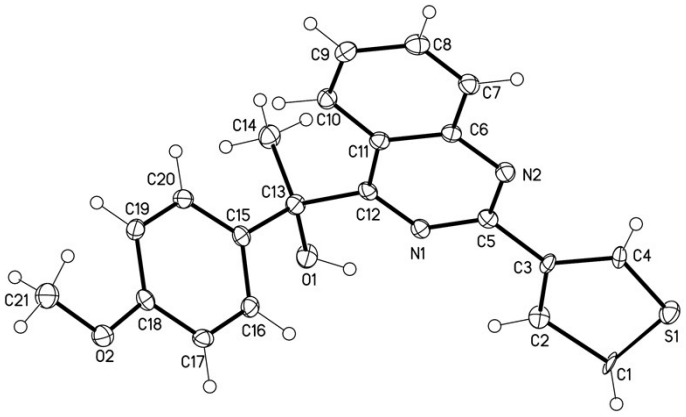
C(2')	39(7)	34(7)	39(7)	6(6)	6(6)	3(7)
C(3')	29(8)	20(7)	17(7)	-14(6)	5(6)	-3(6)
C(4')	23(8)	25(7)	10(6)	-4(5)	-5(7)	-2(6)
C(5)	15(1)	16(1)	18(1)	1(1)	5(1)	-1(1)
C(6)	12(1)	15(1)	17(1)	1(1)	-1(1)	2(1)
C(7)	12(1)	15(1)	16(1)	1(1)	-1(1)	2(1)
C(8)	15(1)	16(1)	20(1)	1(1)	1(1)	-1(1)
C(9)	18(1)	18(1)	22(1)	4(1)	4(1)	0(1)
C(10)	18(1)	26(1)	14(1)	2(1)	3(1)	2(1)
C(11)	18(1)	20(1)	17(1)	-2(1)	2(1)	0(1)
C(12)	14(1)	16(1)	17(1)	1(1)	1(1)	3(1)
N(1)	18(1)	16(1)	16(1)	0(1)	3(1)	-1(1)
C(14)	13(1)	16(1)	16(1)	0(1)	1(1)	2(1)
N(2)	16(1)	15(1)	16(1)	0(1)	1(1)	1(1)
C(16)	12(1)	16(1)	18(1)	1(1)	1(1)	2(1)
C(17)	25(1)	19(1)	15(1)	1(1)	1(1)	-2(1)
C(18)	25(1)	17(1)	21(1)	-2(1)	1(1)	-3(1)
C(19)	13(1)	17(1)	23(1)	3(1)	3(1)	2(1)
C(20)	19(1)	20(1)	17(1)	1(1)	5(1)	3(1)
C(15)	18(1)	16(1)	18(1)	-2(1)	3(1)	1(1)
C(13)	22(1)	18(1)	26(1)	3(1)	7(1)	-1(1)
O(1)	33(1)	16(1)	21(1)	2(1)	2(1)	4(1)

Table S30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 190416lt_0m_a.

	x	y	z	U(eq)
H(2)	-374	3756	1083	29
H(3)	-2882	3641	-927	22
H(4)	-2030	2962	-1526	20
H(2')	1377	2629	699	45
H(3')	-1271	2828	-1219	26
H(4')	-2537	3542	-1273	24
H(8)	882	2881	4420	21
H(9)	484	2882	6355	23
H(10)	2356	3435	7502	23

H(11)	4525	3992	6714	22
H(17)	7483	4807	4469	24
H(18)	9257	5386	3661	25
H(20)	7700	4869	541	22
H(15)	5947	4288	1341	21
H(13A)	12273	5549	1416	32
H(13B)	9389	5792	1967	32
H(13C)	8400	5600	719	32

Figure S9: ORTEP diagram of compound **9 (CCDC No. 2006219)**



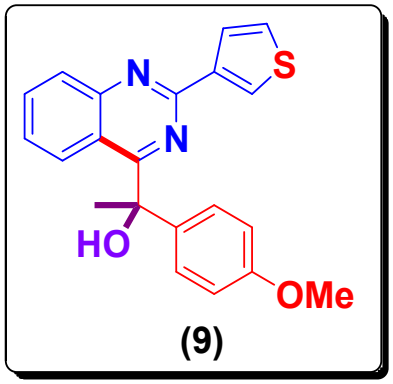


Table S31. Crystal data and structure refinement for 200542lt_0m_a.

Identification code	200542LT_0m_a
Empirical formula	C21 H18 N2 O2 S
Formula weight	362.43
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$

Unit cell dimensions	a = 9.3403(6) Å	a= 90°.
	b = 17.0872(9) Å	b= 106.207(3)°.
	c = 10.8820(7) Å	g = 90°.
Volume	1667.74(18) $Å^3$	
Z	4	
Density (calculated)	1.443 Mg/m^3	
Absorption coefficient	0.213 mm^{-1}	
F(000)	760	
Crystal size	0.18 x 0.05 x 0.05 mm^3	
Theta range for data collection	2.271 to 26.406°.	
Index ranges	-11<=h<=11, -21<=k<=20, -13<=l<=13	
Reflections collected	14781	
Independent reflections	3421 [R(int) = 0.0303]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6989	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3421 / 438 / 284	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0359, wR2 = 0.0878	
R indices (all data)	R1 = 0.0428, wR2 = 0.0924	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.313 and -0.340 $e.Å^{-3}$	

Table S32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 200542lt_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	5176(2)	7918(1)	6316(2)	18(1)
C(1)	7066(12)	7888(7)	6372(11)	16(1)
C(2)	6938(13)	7163(5)	5378(13)	16(1)
C(3)	5546(16)	6792(6)	4975(12)	12(1)
C(4)	4491(12)	7179(5)	5457(11)	14(1)
S(1')	6975(5)	7824(3)	6244(5)	28(1)
C(1')	5122(14)	7773(6)	6229(13)	20(1)

C(2')	4506(19)	7084(8)	5368(17)	15(1)
C(3')	5550(20)	6711(9)	4901(18)	13(1)
C(4')	6972(19)	7062(8)	5340(19)	15(1)
C(5)	5209(2)	6054(1)	4150(1)	13(1)
C(6)	3560(2)	5101(1)	3184(1)	13(1)
C(7)	2112(2)	4778(1)	2928(1)	16(1)
C(8)	1767(2)	4107(1)	2231(1)	18(1)
C(9)	2844(2)	3732(1)	1758(1)	17(1)
C(10)	4255(2)	4029(1)	1991(1)	15(1)
C(11)	4654(2)	4728(1)	2708(1)	13(1)
C(12)	6073(2)	5111(1)	3005(1)	13(1)
C(13)	7406(2)	4854(1)	2512(1)	14(1)
C(14)	6981(2)	4899(1)	1051(1)	19(1)
C(15)	7988(2)	4048(1)	3042(1)	14(1)
C(16)	8780(2)	3989(1)	4335(1)	15(1)
C(17)	9339(2)	3282(1)	4866(1)	15(1)
C(18)	9117(2)	2605(1)	4122(1)	15(1)
C(19)	8340(2)	2650(1)	2831(1)	16(1)
C(20)	7801(2)	3371(1)	2309(1)	16(1)
C(21)	9380(2)	1222(1)	4032(2)	23(1)
N(1)	6332(1)	5749(1)	3712(1)	13(1)
N(2)	3850(1)	5771(1)	3899(1)	14(1)
O(1)	8584(1)	5407(1)	2979(1)	18(1)
O(2)	9704(1)	1936(1)	4745(1)	19(1)

Table S33. Bond lengths [Å] and angles [°] for 200542lt_0m_a.

S(1)-C(4)	1.596(7)
S(1)-C(1)	1.751(10)
C(1)-C(2)	1.627(10)
C(1)-H(1)	0.9500
C(2)-C(3)	1.401(12)
C(2)-H(2)	0.9500
C(3)-C(4)	1.404(11)
C(3)-C(5)	1.528(7)
C(4)-H(4)	0.9500
S(1')-C(4')	1.630(11)

S(1')-C(1')	1.728(12)
C(1')-C(2')	1.515(12)
C(1')-H(1')	0.9500
C(2')-C(3')	1.378(17)
C(2')-H(2')	0.9500
C(3')-C(5)	1.373(12)
C(3')-C(4')	1.410(18)
C(4')-H(4')	0.9500
C(5)-N(2)	1.3147(18)
C(5)-N(1)	1.3710(18)
C(6)-N(2)	1.3676(18)
C(6)-C(7)	1.4142(19)
C(6)-C(11)	1.420(2)
C(7)-C(8)	1.363(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.405(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.368(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.417(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.4329(19)
C(12)-N(1)	1.3169(18)
C(12)-C(13)	1.5496(19)
C(13)-O(1)	1.4314(16)
C(13)-C(14)	1.5292(19)
C(13)-C(15)	1.5337(19)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(20)	1.387(2)
C(15)-C(16)	1.399(2)
C(16)-C(17)	1.377(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.394(2)
C(17)-H(17)	0.9500
C(18)-O(2)	1.3643(17)
C(18)-C(19)	1.392(2)
C(19)-C(20)	1.392(2)
C(19)-H(19)	0.9500

C(20)-H(20)	0.9500
C(21)-O(2)	1.4315(18)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
O(1)-H(1A)	0.8400

C(4)-S(1)-C(1)	103.4(5)
C(2)-C(1)-S(1)	96.5(6)
C(2)-C(1)-H(1)	131.8
S(1)-C(1)-H(1)	131.8
C(3)-C(2)-C(1)	116.2(8)
C(3)-C(2)-H(2)	121.9
C(1)-C(2)-H(2)	121.9
C(2)-C(3)-C(4)	110.9(5)
C(2)-C(3)-C(5)	125.3(9)
C(4)-C(3)-C(5)	123.8(9)
C(3)-C(4)-S(1)	112.5(7)
C(3)-C(4)-H(4)	123.7
S(1)-C(4)-H(4)	123.7
C(4')-S(1')-C(1')	97.0(7)
C(2')-C(1')-S(1')	104.5(9)
C(2')-C(1')-H(1')	127.7
S(1')-C(1')-H(1')	127.7
C(3')-C(2')-C(1')	113.7(11)
C(3')-C(2')-H(2')	123.2
C(1')-C(2')-H(2')	123.2
C(5)-C(3')-C(2')	121.6(14)
C(5)-C(3')-C(4')	126.3(14)
C(2')-C(3')-C(4')	112.0(8)
C(3')-C(4')-S(1')	112.8(10)
C(3')-C(4')-H(4')	123.6
S(1')-C(4')-H(4')	123.6
N(2)-C(5)-N(1)	125.13(13)
N(2)-C(5)-C(3')	118.6(9)
N(1)-C(5)-C(3')	116.3(9)
N(2)-C(5)-C(3)	117.1(6)
N(1)-C(5)-C(3)	117.8(6)
N(2)-C(6)-C(7)	117.76(13)
N(2)-C(6)-C(11)	122.35(12)

C(7)-C(6)-C(11)	119.88(13)
C(8)-C(7)-C(6)	120.22(13)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(7)-C(8)-C(9)	120.26(13)
C(7)-C(8)-H(8)	119.9
C(9)-C(8)-H(8)	119.9
C(10)-C(9)-C(8)	120.97(14)
C(10)-C(9)-H(9)	119.5
C(8)-C(9)-H(9)	119.5
C(9)-C(10)-C(11)	120.37(13)
C(9)-C(10)-H(10)	119.8
C(11)-C(10)-H(10)	119.8
C(10)-C(11)-C(6)	118.29(13)
C(10)-C(11)-C(12)	126.43(13)
C(6)-C(11)-C(12)	115.28(13)
N(1)-C(12)-C(11)	121.19(13)
N(1)-C(12)-C(13)	113.73(12)
C(11)-C(12)-C(13)	125.05(12)
O(1)-C(13)-C(14)	106.64(11)
O(1)-C(13)-C(15)	107.63(11)
C(14)-C(13)-C(15)	113.40(12)
O(1)-C(13)-C(12)	107.61(11)
C(14)-C(13)-C(12)	110.20(11)
C(15)-C(13)-C(12)	111.06(11)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(20)-C(15)-C(16)	117.68(13)
C(20)-C(15)-C(13)	123.95(12)
C(16)-C(15)-C(13)	118.37(12)
C(17)-C(16)-C(15)	121.16(13)
C(17)-C(16)-H(16)	119.4
C(15)-C(16)-H(16)	119.4
C(16)-C(17)-C(18)	120.41(13)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8

O(2)-C(18)-C(19)	124.81(13)
O(2)-C(18)-C(17)	115.68(12)
C(19)-C(18)-C(17)	119.51(13)
C(20)-C(19)-C(18)	119.15(13)
C(20)-C(19)-H(19)	120.4
C(18)-C(19)-H(19)	120.4
C(15)-C(20)-C(19)	122.07(13)
C(15)-C(20)-H(20)	119.0
C(19)-C(20)-H(20)	119.0
O(2)-C(21)-H(21A)	109.5
O(2)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(2)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(12)-N(1)-C(5)	119.00(12)
C(5)-N(2)-C(6)	116.97(12)
C(13)-O(1)-H(1A)	109.5
C(18)-O(2)-C(21)	116.79(11)

Symmetry transformations used to generate equivalent atoms:

Table S34. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 200542lt_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}
S(1)	20(1)	14(1)	20(1)	-4(1)	6(1)	-2(1)
C(1)	20(2)	11(2)	16(2)	-11(1)	6(1)	-1(1)
C(2)	16(1)	15(2)	19(1)	0(2)	7(1)	-2(2)
C(3)	17(1)	8(2)	11(2)	-3(1)	4(1)	0(2)
C(4)	16(1)	12(2)	15(2)	-3(1)	7(1)	3(1)
S(1')	25(1)	23(1)	39(2)	7(1)	12(1)	-4(1)
C(1')	21(2)	17(2)	23(2)	0(2)	8(2)	0(2)
C(2')	18(2)	11(2)	16(2)	-4(2)	4(2)	-2(2)
C(3')	15(2)	12(2)	14(2)	3(2)	7(2)	2(2)
C(4')	18(2)	11(2)	18(2)	-1(2)	8(2)	0(2)
C(5)	14(1)	13(1)	12(1)	3(1)	4(1)	1(1)

C(6)	14(1)	14(1)	11(1)	2(1)	2(1)	1(1)
C(7)	13(1)	20(1)	16(1)	1(1)	5(1)	1(1)
C(8)	14(1)	22(1)	17(1)	1(1)	4(1)	-4(1)
C(9)	19(1)	17(1)	14(1)	-2(1)	4(1)	-1(1)
C(10)	16(1)	16(1)	14(1)	0(1)	5(1)	2(1)
C(11)	14(1)	14(1)	11(1)	2(1)	3(1)	1(1)
C(12)	13(1)	14(1)	11(1)	4(1)	3(1)	3(1)
C(13)	12(1)	16(1)	16(1)	-1(1)	5(1)	-2(1)
C(14)	20(1)	21(1)	17(1)	1(1)	8(1)	2(1)
C(15)	9(1)	17(1)	17(1)	-1(1)	6(1)	1(1)
C(16)	12(1)	17(1)	17(1)	-4(1)	6(1)	-1(1)
C(17)	11(1)	22(1)	13(1)	-1(1)	3(1)	-1(1)
C(18)	10(1)	17(1)	18(1)	1(1)	6(1)	2(1)
C(19)	14(1)	18(1)	17(1)	-5(1)	5(1)	0(1)
C(20)	13(1)	22(1)	13(1)	-1(1)	3(1)	2(1)
C(21)	26(1)	16(1)	24(1)	-1(1)	4(1)	2(1)
N(1)	13(1)	12(1)	13(1)	2(1)	4(1)	1(1)
N(2)	14(1)	15(1)	15(1)	0(1)	4(1)	1(1)
O(1)	15(1)	18(1)	24(1)	-5(1)	8(1)	-4(1)
O(2)	20(1)	16(1)	20(1)	-1(1)	2(1)	3(1)

Table S35. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 200542lt_0m_a.

	x	y	z	U(eq)
H(1)	7893	8193	6830	19
H(2)	7760	7000	5087	20
H(4)	3481	7017	5290	17
H(1')	4606	8104	6663	24
H(2')	3494	6924	5169	18
H(4')	7833	6875	5131	18
H(7)	1379	5029	3243	19
H(8)	794	3891	2064	21
H(9)	2589	3267	1269	20
H(10)	4972	3766	1671	18
H(14A)	6630	5428	774	28

H(14B)	6187	4521	689	28
H(14C)	7855	4776	755	28
H(16)	8936	4445	4856	18
H(17)	9879	3256	5746	18
H(19)	8180	2193	2312	19
H(20)	7289	3402	1424	19
H(21A)	8299	1145	3738	34
H(21B)	9840	782	4579	34
H(21C)	9781	1250	3291	34
H(1A)	8319	5740	3439	27