Supporting Information

Synthesis of Quinazolin-4(1*H*)-ones via Amination and Annulation of Amidines and Benzamides

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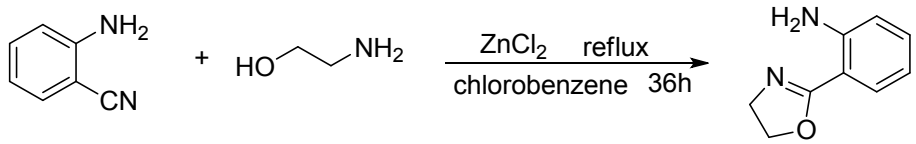
1. General information

^{1}H NMR, and ^{13}C NMR spectra were recorded on Mercury 400M in $CDCl_3$. All ^{1}H NMR and ^{13}C NMR chemical shifts were given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. Copies of their ^{1}H NMR and ^{13}C NMR spectra were provided. Products were purified by flash chromatography on 200–300 mesh silica gels. All melting points were determined without correction. All reactions were carried out in oven-dried glassware, unless otherwise noted. Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification

2. Experimental section

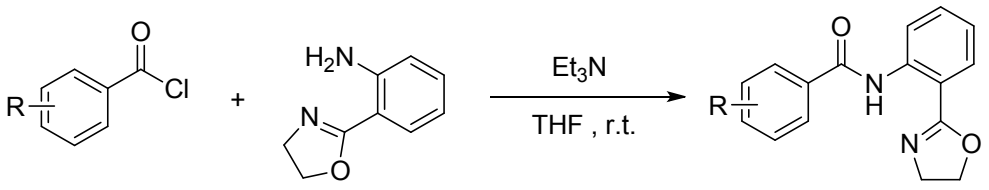
2.1 General procedure for the synthesis of 1a-1m and 4.[1]

2.1.1 Synthesis of 2-(4, 5-dihydrooxazol-2-yl)aniline.



2-aminobenzonitrile (19 g, 250 mmol) and $ZnCl_2$ (3.34 g, 25 mmol) was added to a 500 mL three-necked flask, and then suspended in chlorobenzene (350 mL) under nitrogen. 2-aminoethanol (45 mL, 750 mmol) was added to the suspension via a syringe. The mixture was slowly heated to reflux until no gas was produced. After refluxing for 36 hours, the reaction mixture was cooled down to room temperature and the solvent was removed in a rotary evaporator. CH_2Cl_2 (250 mL) was added to the residue and washed with saturated $NaHCO_3$ (150 mL) and H_2O (150 mL). The aqueous fraction was extracted with CH_2Cl_2 (250 mL × 3). The combined organic phase was dried over Na_2SO_4, filtered and the solvent was removed in a rotary evaporator. The crude product was recrystallized from EtOAc/Hexane to give colorless crystals of the compound 2-(4,5-dihydrooxazol-2-yl)aniline 29 g (72%).

2.1.2 Preparation of Substrates 1a-1m and 4

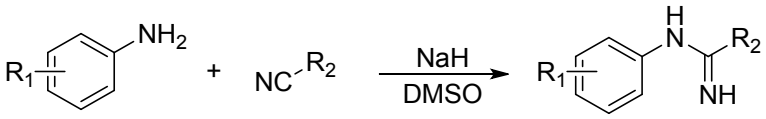


An acid chloride (5 mmol), prepared from the corresponding carboxylic acid and oxalyl chloride and 2-(4,5-dihydrooxazol-2-yl)aniline (5 mmol) were added to a 50 mL flask and then dissolved with THF (10 mL). Et_3N (7.5 mmol) was taken to the vigorously stirred solution via a syringe. The reaction mixture was stirred at room temperature for 6 h and quenched with saturated $NaHCO_3 \cdot H_2O$ (100 mL) was added to the mixture and extracted with EtOAc (150 mL × 3). Combined organic phase was washed with

saturated NaCl (aq) and dried over Na_2SO_4, and then filtered, the solvent was removed in a rotary evaporator. The crude product was recrystallized from EtOAc/Hexane to give colorless crystals of the product

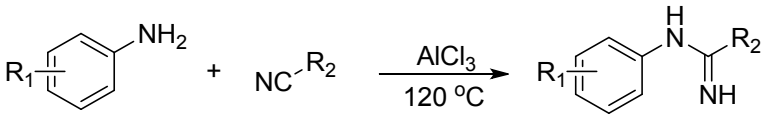
2.2 General Procedures for the Synthesis of Amidines.[2]

Procedure A:



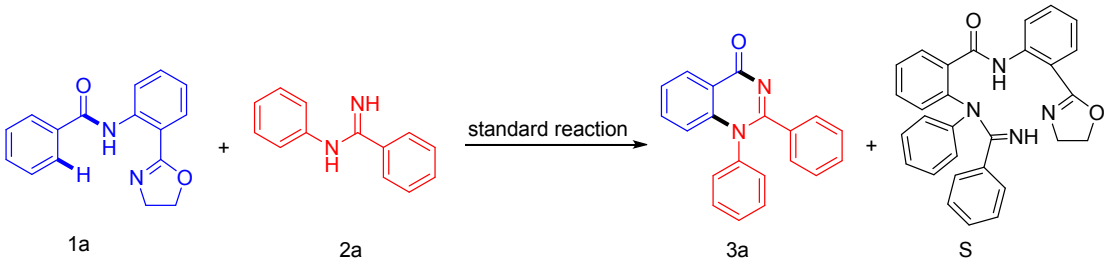
A round bottom flask (25 mL in volume) was charged with NaH (60% in mineraloil) (360 mg, 15.0 mmol, 60%, 1.5 equiv). Under a stream of Ar, DMSO (5 mL) was added, and the resulting suspension was cooled with an ice-water bath prior to the addition of the aniline (11.0 mmol, 1.1 equiv) and the carbonitrile (10.0 mmol). The mixture was kept at 0 ℃ for 30-60 min 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. In the cases when the amidine precipitated upon addition of water, the solid was filtered off and dissolved in EtOAc (20 mL). In all other cases, the aqueous layer was extracted with EtOAc (3 × 20 mL). The extracts were combined and washed with water (2 × 50 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified either by silica gel chromatography or upon recrystallization.

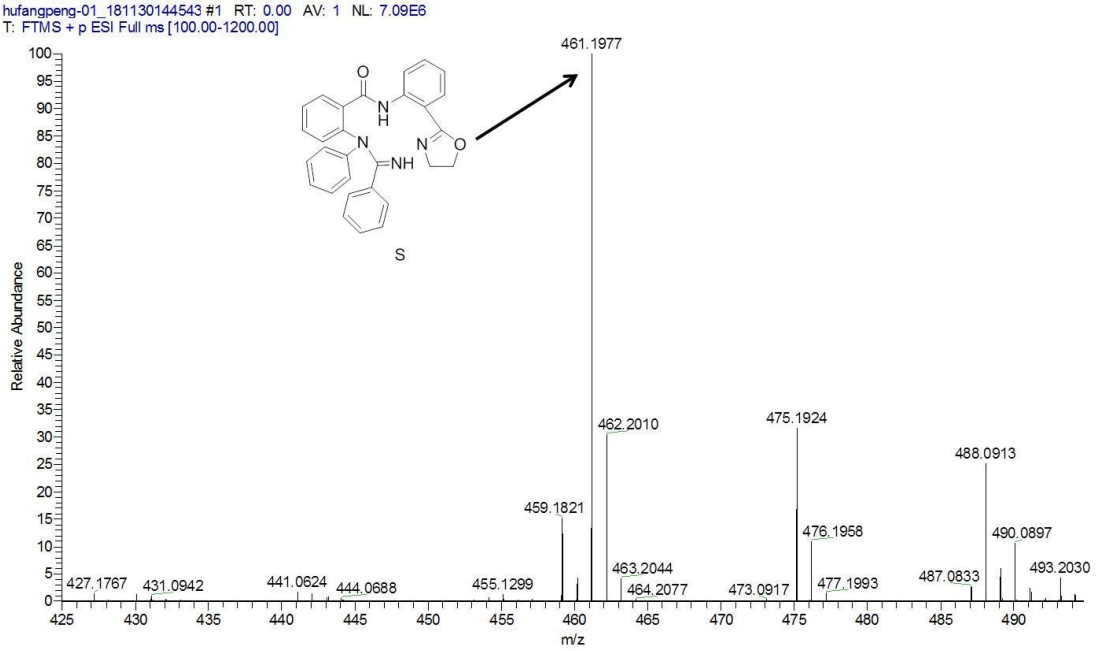
Procedure B:



A pressure flask (75 mL in volume) equipped with a stirrer bar was charged with the aniline (11.0 mmol, 1.1 equiv) and the carbonitrile (10.0 mmol) under air. $AlCl_3$(1.33 g, 10.0 mmol, 1.0 equiv) was added in one portion. The flask was tightly sealed with a screw cap and lowered into a preheated oil bath at 120 ℃. The reaction mixture was stirred for the indicated time, and taken out of the oil bath. Ice-water (50 mL) was then added to the hot mixture while maintaining vigorous stirring. If necessary, the mixture was warmed with a heat gun to obtain a homogenous aqueous solution, before it was transferred into a separatory funnel. Concentrated aqueous NaOH was added until a pH of 14 was reached, and the aqueous layer was extracted with EtOAc (3 × 30 mL). The combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was either purified by silica gel chromatography.

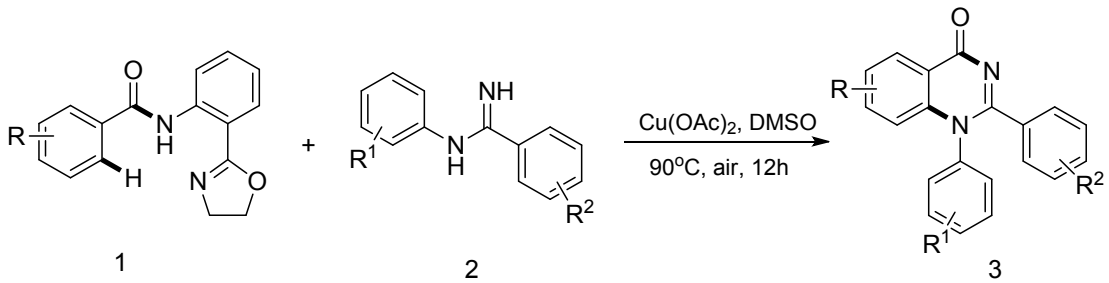
2.3 General Procedures for trapping S by HRMS-ESI





1a (0.1 mmol), **2a** (0.16 mmol), $Cu(OAc)_2$ (0.1 mmol), DMSO (1.0 mL), 90 ℃ under air for 0.5 h. Upon completion of the reaction, the mixture obtained were dried over anhydrous Na_2SO_4 and filtered. The resulting mixture was analyzed by HRMS-ESI.

2.4 General procedure to Produce quinazolin-4(1*H*)-ones

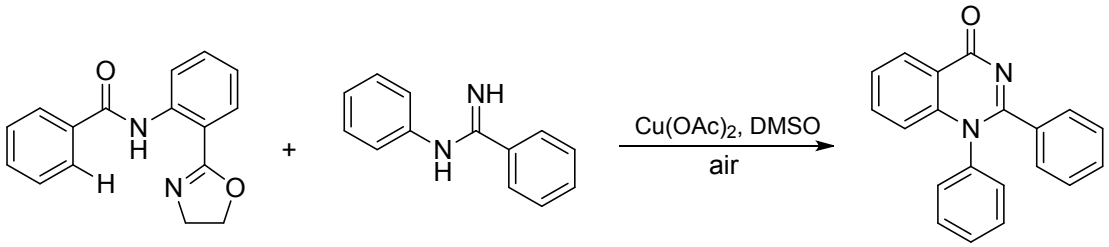


A mixture of benzamide **1** (1.0 equiv, 0.1 mmol), amidine **2** (0.16 mmol), $Cu(OAc)_2$ (0.1 mmol), DMSO (1.0 mL), were stirred at 90 ℃ under air for 12 h (TLC monitored).

Upon completion of the reaction, the reaction mixture was then extracted with ethyl acetate and saturated brine. The combined organic phase was dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum *n*-Hexane/ethyl acetate (2:1) to afford the desired **3**.

2.5 Optimization of reaction conditions

Table 1 Screening of temperature.[a]

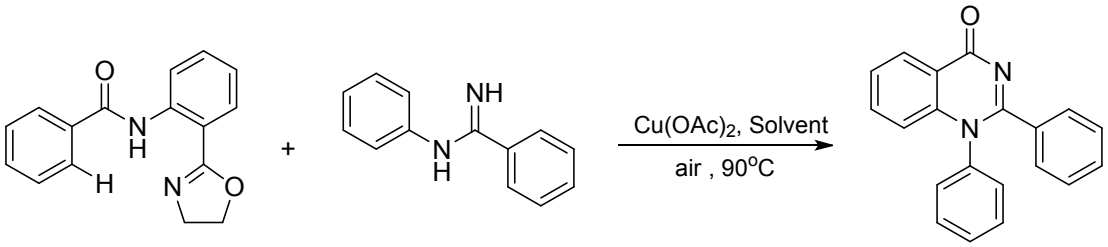


1a 2a 3a

Entry	Temp(℃)	Yield [b](%)
1	50	44
2	70	69
3	90	75
4	110	72
5	120	64

[a] Reaction conditions: amide **1a** (0.1 mmol), **2a** (0.16mmol), $Cu(OAc)_2$ (0.1 mmol), DMSO (1.0 mL), under air for 12 h. [b] Isolated yield.

Table 2 Screening of Solvent.[a]

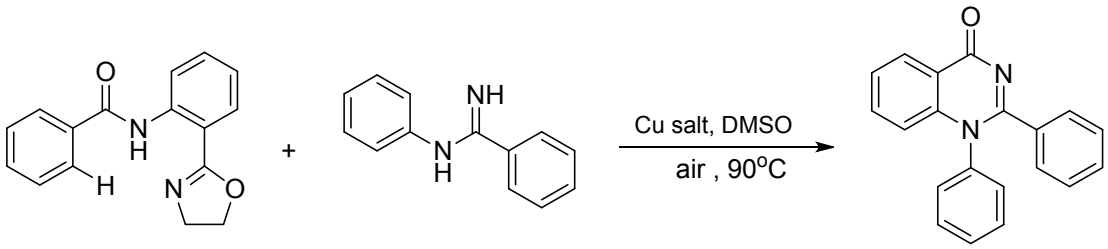


1a 2a 3a

Entry	Solvent	Yield [b](%)
1	DMSO	75
2	DMF	Trace
3	MeOH	17
4	THF	23
5	Toluene	20
6	CH_3CN	26
7	1,4-Dioxane	19
8	DCE	9

[a] Reaction conditions: amide **1a** (0.1 mmol), **2a** (0.16 mmol), $Cu(OAc)_2$ (0.1 mmol), solvent (1.0 mL), 90℃ under air for 12 h. [b] Isolated yield.

Table 3 Screening of Cu salt.[a]



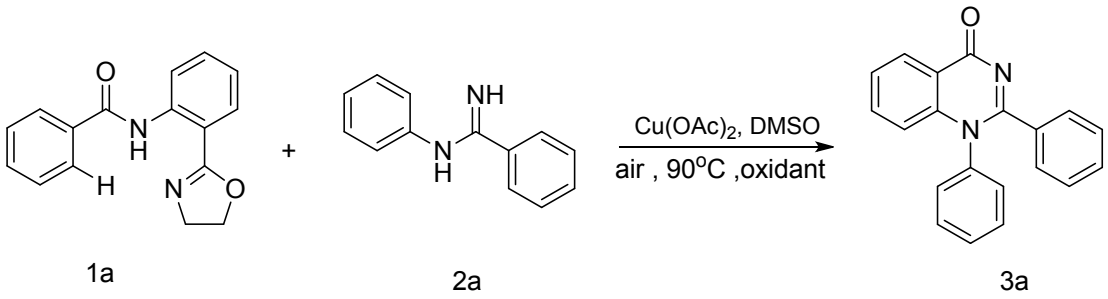
1a 2a 3a

Entry	Cu salt	Yield [b] (%)
1	$Cu(OAc)_2$	75
2	$Cu(OAc)_2 \cdot H_2O$	69
3	$CuSO_4$	0
4	$Cu(OTf)_2$	47
5	CuO	0

6	CuBr	Trace
7	CuI	60
8	CuCl	63
9	-	0

[a] Reaction conditions: amide **1a** (0.1 mmol), **2a** (0.16mmol), Cu salt (0.1 mmol), DMSO (1.0 mL), 90 ℃ under air for 12 h. [b] Isolated yield.

Table 4 Screening of Oxidant.[a]

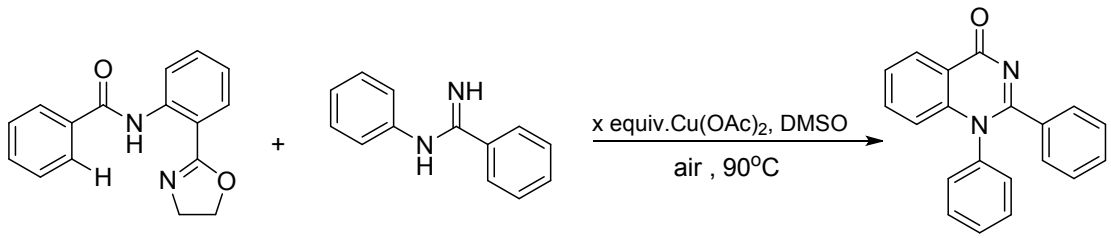


1a 2a 3a

Entry	Oxidant	Yield [b] (%)
1	O_2	25
2	$K_2S_2O_8$	23
3	Ag_2O	72
4	$AgNO_3$	65
5	BQ	Trace
6	$PhI(OAc)_2$	61
7	NFSI	74
8	BPO	60
9	-	75

[a] Reaction conditions: amide **1a** (0.1 mmol), **2a** (0.16mmol), $Cu(OAc)_2$ (0.1 mmol), DMSO (1.0 mL), oxidant (0.1 mmol), 90℃ under air for 12 h. [b] Isolated yield.

Table 5 Screening of the amount of $Cu(OAc)_2$.[a]



1a 2a 3a

Entry	$Cu(OAc)_2$ (equiv.)	Yield [b](%)
1	0.2	44
2	0.4	57
3	0.7	69
4	1.0	75
5	1.2	70
6	1.5	69

[a] Reaction conditions: amide **1a** (0.1 mmol), **2a** (0.16mmol), $Cu(OAc)_2$ (x mmol), DMSO (1.0 mL), 90℃ under air for 12 h. [b] Isolated yield.

2.6 The X-ray data of 3a (CCDC 1881814)

An amount of 20 mg **3a** were dissolved in acetonitrile/petroleum ether (1:1) on the brown small reagent bottle (5 mL), which acted as good solvent, and a layer of ether was injected on the surface of acetonitrile, and the cap is covered with a thin film, white crystals will be presented after ten days.

The data were collected at 296.15 K using a Bruker APEX II area detectordiffractometer equipped with a graphite monochromated Mo Kα radiation source (λ = 0.71073 Å) operation at 50 kV and 0.8 mA. Using Olex2[3], the structure was solved with the ShelXS-1997[4] structure solution program using Direct Methods and refined with the olex2.refine[5] refinement package using Gauss-Newton minimisation. Nonhydrogen atoms were refined with anisotropic displacement parameters during the final cycles. All hydrogen atoms were placed by geometrical

considerations and were added to the structure factor calculations.

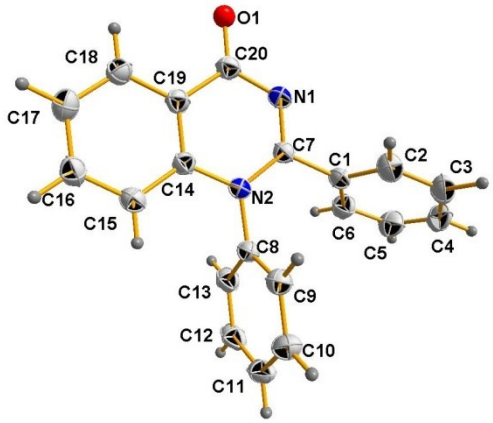


Figure S1. X-ray crystal structure of compound **3a,** thermal ellipsoids are drawn at 30% probability level

Table S1.The crystal data and structure refinement for 3a

Identification code	3a
Empirical formula	$C_{22}H_{17}N_3O$
Formula weight	339.38
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	8.624(3)
b/Å	8.992(3)
c/Å	13.312(4)
α/°	92.425(5)
β/°	103.464(5)
γ/°	118.016(4)
Volume/Å^3	872.4(5)
Z	2
ρ_{calc}g/cm^3	1.292
μ/mm^{-1}	0.081
F(000)	356.0
Crystal size/mm^3	0.3 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.196 to 62.32
Index ranges	$-12 \le h \le 5$, $-9 \le k \le 12$, $-17 \le l \le 18$
Reflections collected	6083
Independent reflections	4564 [R_{int} = 0.0147, R_{sigma} = 0.0295]
Data/restraints/parameters	4564/0/236
Goodness-of-fit on F^2	1.000
Final R indexes [I>=2σ (I)]	R_1 = 0.0484, wR_2 = 0.1301

Final R indexes [all data] $R_1 = 0.0684$, $wR_2 = 0.1463$
Largest diff. peak/hole / e $Å^{-3}$ 0.24/-0.22

[1] M. Shang, S.-Z. Sun, H.-X. Dai and J.-Q. Yu, *J. Am. Chem. Soc.,* 2014, **136**, 3354

[2] Y. Wang, H. Wang, J. Peng and Q. Zhu, *Org. Lett.,* 2011, **13**, 4604.

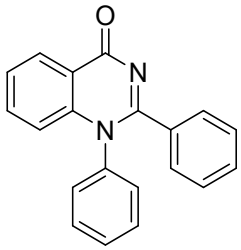
[3] O. V. Dolomanov，L. J. Bourhis, R. J. Gildea，J. A. K. Howard，H. Puschmann and J. Appl, *Cryst.,* 2009, **42**, 339.

[4] G. M. Sheldrick, *Acta Cryst*., 2008, **A64**, 112.

[5] L. J. Bourhis, O. V. Dolomanov, R. J. Gildea, J. A. K. Howard and H. Puschmann, *Acta Cryst*., 2015, **A71**, 59.

3. Characterization data of products.

1,2-diphenylquinazolin-4(1*H*)-one（3a）



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 75% yield;

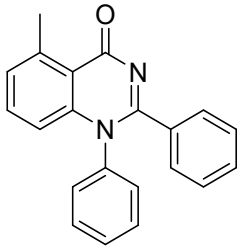
M.p. = 286-289 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.97, 161.42, 142.49, 138.09, 135.00, 133.63, 130.06, 129.64, 129.61, 129.36, 128.27, 127.78, 126.38, 119.48, 117.20.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.72 – 8.02 (m, 1H), 7.56 (m, *J* = 16.2, 9.1, 5.3 Hz, 1H), 7.51 – 7.38 (m, 4H), 7.37 – 7.30 (m, 2H), 7.26 – 7.09 (m, 5H), 6.99 – 6.60 (m, 1H).

HRMS (ESI) calcd for $C_{20}H_{14}N_2OH^+$: $[M+H]^+$ 299.1179, found: 299.1181.

5-methyl-1,2-diphenylquinazolin-4(1*H*)-one（3b）



3b

Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 66% yield;

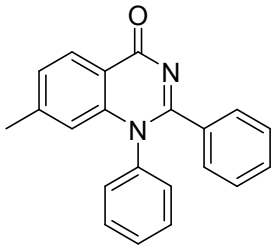
M.p. = 242-245 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.64, 160.33, 143.95, 142.49, 138.53, 132.46, 130.02, 129.74, 129.47, 129.11, 128.99, 128.57, 127.80, 127.56, 118.34, 115.15, 23.39.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.49 (m, *J* = 6.8, 4.4, 1.2 Hz, 1H), 7.40 (m, *J* = 7.7, 7.1, 2.9 Hz, 4H), 7.33 – 7.28 (m, 2H), 7.22 – 7.14 (m, 4H), 6.66 (d, *J* = 8.5 Hz, 1H), 2.96 (s, 3H).

HRMS (ESI) calcd for $C_{21}H_{16}N_2OH^+$: $[M+H]^+$ 313.1336, found: 313.1331.

7-methyl-1, 2-diphenylquinazolin-4(1*H*)-one (3c)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 55% yield;

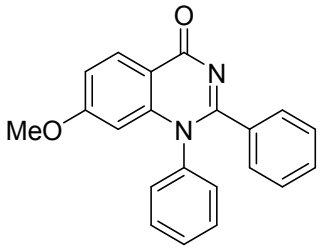
M.p. = 291-294 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.96, 161.27, 144.80, 142.58, 138.13, 135.12, 130.01, 129.64, 129.59, 129.50, 129.32, 128.20, 127.84, 127.73, 117.29, 116.93, 22.30.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (d, *J* = 8.1 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.35 – 7.31 (m, 2H), 7.30 – 7.26 (m, 1H), 7.25 – 7.21 (m, 2H), 7.17 (m, *J* = 16.0, 7.1, 2.0 Hz, 3H), 6.62 (s, 1H), 2.34 (s, 3H).

HRMS (ESI) calcd for $C_{21}H_{16}N_2OH^+$: $[M+H]^+$ 313.1336, found: 313.1332.

7-methoxy-1,2 diphenylquinazolin-4(1*H*)-one（3d）



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 27% yield;

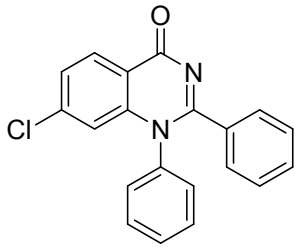
M.p. = 215-218 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.59, 163.74, 161.34, 144.30, 138.21, 135.10, 130.45, 130.05, 129.64, 129.55, 129.32, 127.76, 113.91, 113.39, 100.90, 55.63.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, *J* = 8.8 Hz, 1H), 7.45 – 7.38 (m, 3H), 7.36 – 7.31 (m, 2H), 7.22 (m, *J* = 8.2, 4.4, 1.5 Hz, 3H), 7.20 – 7.13 (m, 2H), 7.04 (dd, *J* = 8.9, 2.3 Hz, 1H), 6.23 (d, *J* = 2.3 Hz, 1H), 3.72 (s, 3H).

HRMS (ESI) calcd for $C_{21}H_{16}N_2O_2H^+$: $[M+H]^+$ 329.1285, found: 329.1291.

7-chloro-1, 2-diphenylquinazolin-4(1*H*)-one (3e)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 80% yield;

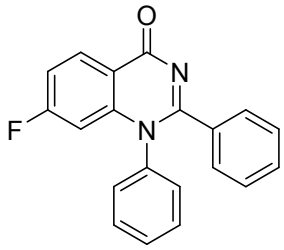
M.p. = 301-304 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.18, 161.92, 143.30, 140.10, 137.65, 134.64, 130.31, 130.02, 129.99, 129.84, 129.45, 129.31, 127.85, 127.05, 117.82, 117.04.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (d, J = 8.5 Hz, 1H), 7.49 – 7.39 (m, 4H), 7.34 (dd, J = 7.1, 1.4 Hz, 2H), 7.27 – 7.20 (m, 3H), 7.20 – 7.14 (m, 2H), 6.85 (d, J = 1.8 Hz, 1H).

HRMS (ESI) calcd for $C_{20}H_{13}ClN_2OH^+$: $[M+H]^+$ 333.0789, found: 333.0794.

7-fluoro-1, 2-diphenylquinazolin-4(1*H*)-one (3f)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 74% yield;

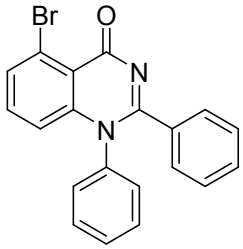
M.p. = 242-246 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.09, 165.72 (d, J = 253.8 Hz), 161.93, 144.21, 137.87, 134.67, 130.29, 129.95, 129.86, 129.34 (d, J = 6.3 Hz), 128.68, 127.88, 127.49 (d, J = 4.1 Hz), 116.13, 114.88 (d, J = 23.9 Hz), 103.86 (d, J = 28.0 Hz).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51 – 8.32 (m, 1H), 7.83 (dd, J = 5.2, 3.4 Hz, 1H), 7.45 (d, J = 5.6 Hz, 3H), 7.37 – 7.29 (m, 2H), 7.26 – 7.14 (m, 5H), 6.52 (m, J = 8.6, 4.3 Hz, 1H).

HRMS (ESI) calcd for $C_{20}H_{13}FN_2OH^+$: $[M+H]^+$ 317.1085, found: 317.1082.

5-bromo-1, 2-diphenylquinazolin-4(1*H*)-one (3g)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 45% yield;

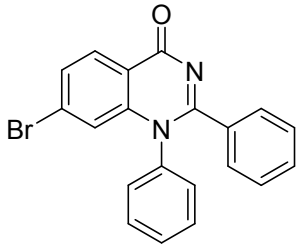
M.p. = 281-284℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.97, 161.42, 142.49, 138.09, 135.00, 133.64, 130.06, 129.60, 129.35, 128.31, 127.78, 126.37, 119.49, 117.20.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.62 – 7.51 (m, 1H), 7.48 – 7.39 (m, 3H), 7.37 – 7.32 (m, 2H), 7.27 – 7.12 (m, 5H), 6.87 (d, *J* = 8.5 Hz, 1H).

HRMS (ESI) calcd for $C_{20}H_{13}BrN_2OH^+$: $[M+H]^+$ 377.0284, found: 377.0288.

7-bromo-1, 2-diphenylquinazolin-4(1*H*)-one (3h)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 71% yield;

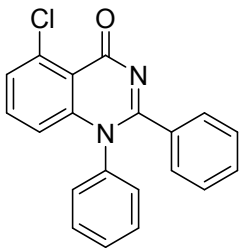
M.p. = 319-322 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.29, 161.83, 143.34, 137.63, 134.67, 130.32, 130.08, 130.00, 129.92, 129.87, 129.46, 129.30, 128.59, 127.88, 119.99, 118.23.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (d, *J* = 8.5 Hz, 1H), 7.59 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.50 – 7.40 (m, 3H), 7.33 (dd, *J* = 5.2, 3.3 Hz, 2H), 7.26 – 7.21 (m, 3H), 7.21 – 7.15 (m, 2H), 7.01 (d, *J* = 1.6 Hz, 1H).

HRMS (ESI) calcd for $C_{20}H_{13}BrN_2OH^+$: $[M+H]^+$ 377.0284, found: 377.0279.

5-chloro-1, 2-diphenylquinazolin-4(1*H*)-one (3i)



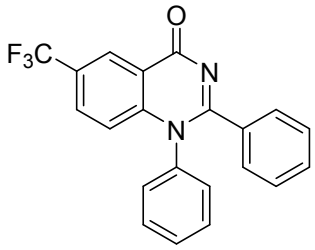
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 37% yield;

M.p. = 252-256 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 166.60, 160.51, 144.75, 138.14, 135.65, 134.50, 132.71, 130.20, 129.81, 129.68, 129.19, 128.98, 127.83, 127.54, 116.85, 116.16.

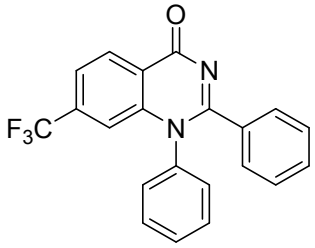
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 – 7.37 (m, 5H), 7.33 – 7.28 (m, 2H), 7.25 – 7.19 (m, 3H), 7.19 – 7.12 (m, 2H), 6.76 (dd, *J* = 8.4, 1.2 Hz, 1H).
HRMS (ESI) calcd for $C_{20}H_{13}ClN_2OH^+$: $[M+H]^+$ 333.0789, found: 333.0785.

1, 2-diphenyl-6-(trifluoromethyl)quinazolin-4(1*H*)-one (3j)



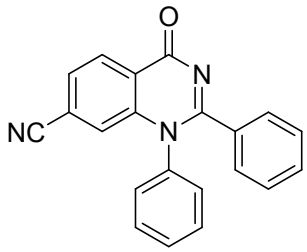
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 55% yield;
^{13}C NMR (101 MHz, $CDCl_3$): δ 168.04, 162.43, 144.50, 137.64, 134.40, 130.33, 130.06, 129.98, 129.42, 129.32, 128.40 (d, *J* = 33.7 Hz), 127.85, 126.10, 124.83, 122.13, 119.14, 118.31.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (d, *J* = 0.7 Hz, 1H), 7.75 (dd, *J* = 8.9, 1.9 Hz, 1H), 7.51 – 7.44 (m, 3H), 7.39 – 7.33 (m, 2H), 7.32 – 7.27 (m, 2H), 7.26 – 7.21 (m, 1H), 7.20 – 7.13 (m, 2H), 7.01 (d, *J* = 8.9 Hz, 1H).
HRMS (ESI) calcd for $C_{21}H_{13}F_3N_2OH^+$: $[M+H]^+$ 367.1053, found: 367.1054.

1, 2-diphenyl-7-(trifluoromethyl)quinazolin-4(1*H*)-one (3k)



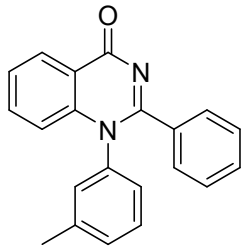
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 57% yield;
M.p. = 324-327℃;
^{13}C NMR (101 MHz, $CDCl_3$): δ 167.92, 162.41, 142.49, 137.44, 135.22 (d, *J* = 33.2 Hz), 134.51, 132.02, 130.44, 130.19, 129.86 (d, *J* = 30.4 Hz), 129.35 (d, *J* = 9.1 Hz), 128.66, 127.94, 127.48, 122.65 (d, *J* = 3.4 Hz), 121.53, 114.60 (d, *J* = 4.0 Hz).
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (d, *J* = 8.2 Hz, 1H), 7.69 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.54 – 7.41 (m, 3H), 7.39 – 7.32 (m, 2H), 7.30 – 7.23 (m, 3H), 7.23 – 7.16 (m, 2H), 7.12 (s, 1H).
HRMS (ESI) calcd for $C_{21}H_{13}F_3N_2OH^+$: $[M+H]^+$ 367.1053, found:367.1057.

4-oxo-1, 2-diphenyl-1,4-dihydroquinazoline-7-carbonitrile (3m)



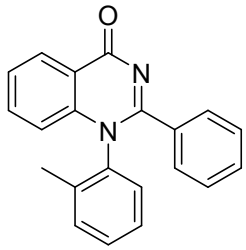
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/n-hexane =1/2) as yellow solid in 58% yield;
M.p. = 256-259℃;
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (d, *J* = 8.1 Hz, 1H), 7.67 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.53 – 7.44 (m, 3H), 7.40 – 7.31 (m, 2H), 7.30 – 7.25 (m, 3H), 7.18 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 167.52, 162.53, 142.56, 137.20, 134.23, 130.60, 130.35, 130.16, 129.63, 129.33, 129.30, 128.58, 127.95, 121.77, 117.50, 116.97.
HRMS (ESI) calcd for $C_{21}H_{13}N_3OH^+$: $[M+H]^+$ 324.1663, found:324.1668.

2-phenyl-1-(*m*-tolyl)quinazolin-4(1*H*)-one (3aa)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 66% yield;
M.p. = 214-217℃;
^{13}C NMR (101 MHz, $CDCl_3$): δ 169.03, 161.40, 142.56, 140.35, 137.98, 135.07, 133.60, 130.36, 129.95, 129.75, 129.61, 129.32, 127.75, 126.60, 126.33, 119.50, 117.32, 21.30.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (dd, *J* = 17.7, 7.9 Hz, 1H), 7.60 – 7.51 (m, 1H), 7.47 (dd, *J* = 14.1, 7.2 Hz, 1H), 7.39 – 7.28 (m, 3H), 7.26 – 7.12 (m, 4H), 7.03 (d, *J* = 9.0 Hz, 2H), 6.92 – 6.80 (m, 1H), 2.79 – 2.07 (m, 3H).
HRMS (ESI) calcd for $C_{21}H_{16}N_2OH^+$: $[M+H]^+$ 313.1336, found: 313.1332.

2-phenyl-1-(*o*-tolyl)quinazolin-4(1*H*)-one (3ab)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 70% yield;

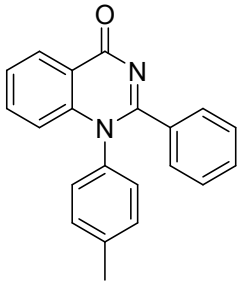
M.p. = 263-266 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.10, 161.36, 141.87, 136.87, 136.17, 134.72, 133.88, 132.00, 130.16, 129.91, 129.12, 128.49, 127.72, 127.51, 126.51, 119.61, 116.79, 17.61.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 – 8.36 (m, 1H), 7.60 – 7.43 (m, 2H), 7.39 (dd, *J* = 6.9, 1.6 Hz, 2H), 7.34 – 7.13 (m, 7H), 6.71 (d, *J* = 6.9 Hz, 1H), 2.01 – 1.92 (m, 3H).

HRMS (ESI) calcd for $C_{21}H_{16}N_2OH^+$: $[M+H]^+$ 313.1336, found: 313.1330.

2-phenyl-1-(*p*-tolyl)quinazolin-4(1*H*)-one (3ac)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 72% yield;

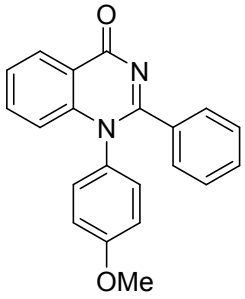
M.p. = 236-238 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.03, 161.53, 142.67, 139.80, 135.42, 135.12, 133.57, 130.64, 129.55, 129.37, 129.23, 128.22, 127.76, 126.29, 119.53, 117.30, 21.31.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.38 (m, *J* = 10.8 Hz, 1H), 7.58 – 7.50 (m, 1H), 7.49 – 7.39 (m, 1H), 7.36 (dd, *J* = 10.8, 4.1 Hz, 2H), 7.26 – 7.13 (m, 5H), 7.10 (dd, *J* = 7.4, 5.6 Hz, 2H), 6.87 (dd, *J* = 8.1, 5.7 Hz, 1H), 2.41 – 2.30 (m, 3H).

HRMS (ESI) calcd for $C_{21}H_{16}N_2OH^+$: $[M+H]^+$ 313.1336, found: 313.1331.

1-(4-methoxyphenyl)-2-phenylquinazolin-4(1*H*)-one (3ad)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 65% yield;

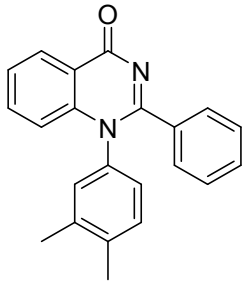
M.p. = 244-247℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.02, 161.77, 159.97, 142.89, 135.17, 133.58, 130.58, 129.53, 129.34, 128.24, 127.81, 126.29, 119.57, 117.27, 115.10, 55.63.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.39 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.60 – 7.52 (m, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.39 – 7.33 (m, 2H), 7.25 – 7.10 (m, 5H), 6.90 (dd, *J* = 12.0, 5.2 Hz, 3H), 3.81 (s, 3H).

HRMS (ESI) calcd for $C_{21}H_{16}N_2O_2H^+$: $[M+H]^+$ 329.1285, found: 329.1293.

1-(3, 4-dimethylphenyl)-2-phenylquinazolin-4(1*H*)-one (3ae)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 64% yield;

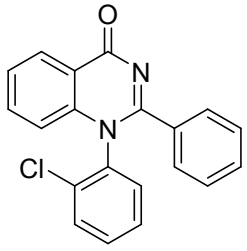
M.p. = 251-254℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.07, 161.51, 142.77, 138.74, 138.40, 135.60, 135.23, 133.51, 130.96, 130.12, 129.53, 129.36, 128.24, 127.73, 126.72, 126.24, 119.57, 117.40, 19.87, 19.65.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.42 (dd, *J* = 7.5, 6.1 Hz, 1H), 7.58 – 7.49 (m, 1H), 7.46 (dd, *J* = 13.4, 6.7 Hz, 1H), 7.42 – 7.34 (m, 2H), 7.26 – 7.11 (m, 4H), 6.99 – 6.91 (m, 2H), 6.88 (d, *J* = 8.4 Hz, 1H), 2.26 (d, *J* = 2.5 Hz, 3H), 2.21 (s, 3H).

HRMS (ESI) calcd for $C_{22}H_{18}N_2OH^+$: $[M+H]^+$ 327.1492, found: 327.1496.

1-(2-chlorophenyl)-2-phenylquinazolin-4(1*H*)-one（3af）



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 60% yield;

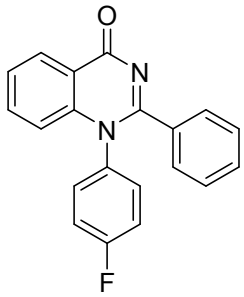
M.p. = 232-236℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.86, 161.51, 141.46, 135.79, 134.53, 133.93, 133.54, 131.74, 131.36, 131.08, 130.03, 128.71, 128.58, 128.37, 127.82, 126.59, 119.43 116.47.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (d, *J* = 7.8 Hz, 1H), 7.59 (t, *J* = 7.7 Hz, 1H), 7.53 – 7.31 (m, 7H), 7.30 – 7.15 (m, 3H), 6.69 (d, *J* = 8.3 Hz, 1H).

HRMS (ESI) calcd for $C_{20}H_{13}ClN_2OH^+$: $[M+H]^+$ 333.0789, found: 333.0793.

1-(4-fluorophenyl)-2-phenylquinazolin-4(1*H*)-one (3ag)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 65% yield;

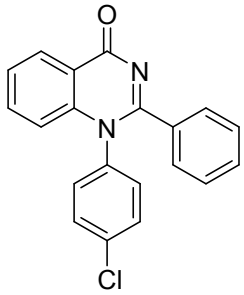
M.p. = 295-297 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.78, 163.81, 161.43 (d, *J* = 23.3 Hz), 142.43, 134.81, 134.05, 133.73, 131.52 (d, *J* = 8.7 Hz), 129.69, 129.28, 128.31, 127.89, 126.47, 119.43, 117.30, 117.03 (d, *J* = 8.6 Hz).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.31 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.57 (m, *J* = 8.6, 7.3, 1.5 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.28 (m, *J* = 10.4, 5.2, 2.8 Hz, 2H), 7.24 – 7.20 (m, 1H), 7.14 (m, *J* = 14.7, 11.6, 4.9 Hz, 4H), 6.84 (d, *J* = 8.5 Hz, 1H).

HRMS (ESI) calcd for $C_{20}H_{13}FN_2OH^+$: $[M+H]^+$ 317.1085, found: 317.1088.

1-(4-chlorophenyl)-2-phenylquinazolin-4(1*H*)-one (3ah)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 63% yield;

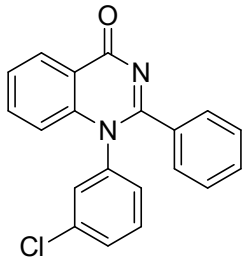
M.p. = 256-259 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.73, 161.29, 142.27, 136.64, 135.71, 134.71, 133.77, 130.97, 130.36, 129.85, 129.30, 128.46, 128.02, 126.55, 119.46, 116.88.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 – 8.21 (m, 1H), 7.61 – 7.54 (m, 1H), 7.48 (m, *J* = 14.3, 7.2 Hz, 1H), 7.44 – 7.38 (m, 2H), 7.36 – 7.31 (m, 2H), 7.28 – 7.16 (m, 5H), 6.84 (d, *J* = 8.4 Hz, 1H).

HRMS (ESI) calcd for $C_{21}H_{16}N_2OH^+$: $[M+H]^+$ 313.1336, found: 313.1331.

1-(3-chlorophenyl)-2-phenylquinazolin-4(1*H*)-one（3ai）



3ai

Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 62% yield;

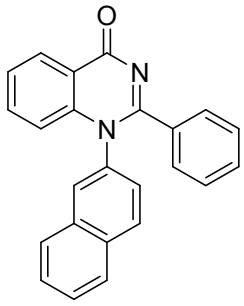
M.p. = 286-289 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.69, 161.15, 142.14, 139.18, 135.68, 134.60, 133.84, 131.04, 130.04, 129.92, 129.87, 129.24, 128.50, 128.05, 128.02, 126.61, 119.41, 116.87.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.39 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.59 (m, *J* = 8.7, 7.3, 1.6 Hz, 1H), 7.52 – 7.44 (m, 1H), 7.38 (dd, *J* = 5.2, 2.9 Hz, 2H), 7.36 – 7.32 (m, 2H), 7.30 – 7.14 (m, 5H), 6.85 (d, *J* = 8.4 Hz, 1H).

HRMS (ESI) calcd for $C_{20}H_{13}ClN_2OH^+$: $[M+H]^+$ 333.0789, found: 333.0783.

1-(naphthalen-2-yl)-2-phenylquinazolin-4(1*H*)-one (3aj)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 67% yield;

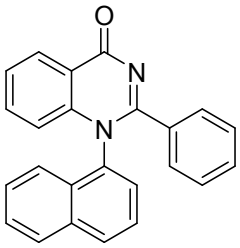
M.p. = 253-256 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.01, 161.61, 142.71, 135.39, 134.98, 133.66, 133.24, 132.93, 130.24, 129.67, 129.32, 128.85, 128.34, 128.23, 128.03, 127.87, 127.85, 127.53, 126.50, 126.42, 119.52, 117.34.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.43 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.90 (dd, *J* = 16.4, 8.3 Hz, 2H), 7.81 – 7.76 (m, 1H), 7.74 – 7.68 (m, 1H), 7.62 – 7.43 (m, 4H), 7.41 (dd, *J* = 7.9, 1.5 Hz, 2H), 7.38 – 7.32 (m, 1H), 7.17 – 7.04 (m, 3H), 6.90 – 6.80 (m, 1H).

HRMS (ESI) calcd for $C_{24}H_{16}N_2OH^+$: $[M+H]^+$ 349.1336, found: 349.1341.

1-(naphthalen-1-yl)-2-phenylquinazolin-4(1*H*)-one (3ak)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 70% yield;

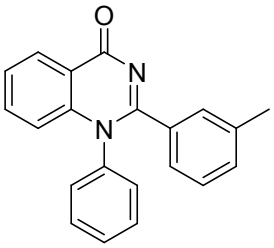
M.p. = 304-307 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.11, 162.34, 142.61, 134.95, 134.47, 134.24, 133.82, 130.57, 130.52, 129.76, 128.97, 128.45, 128.38, 128.33, 127.57, 127.31, 126.51, 125.57, 122.24, 119.49, 117.51.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.49 (dd, *J* = 7.6, 1.9 Hz, 1H), 8.01 – 7.83 (m, 2H), 7.55 (m, *J* = 11.7, 8.2, 4.1 Hz, 3H), 7.49 – 7.40 (m, 3H), 7.40 – 7.34 (m, 1H), 7.26 (dd, *J* = 8.8, 1.4 Hz, 2H), 7.11 (t, *J* = 7.4 Hz, 1H), 7.00 (t, *J* = 7.7 Hz, 2H), 6.72 – 6.49 (m, 1H).

HRMS (ESI) calcd for $C_{24}H_{16}N_2OH^+$: $[M+H]^+$ 349.1336, found: 349.1333.

1-phenyl-2-(*m*-tolyl)quinazolin-4(1*H*)-one (3ba)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 79% yield;

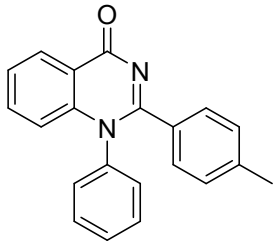
M.p. = 236-239 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.00, 161.54, 142.52, 138.20, 137.70, 134.85, 133.59, 130.41, 130.29, 129.98, 129.60, 128.34, 127.50, 126.40, 126.32, 119.51, 117.17, 21.25.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.42 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.62 – 7.51 (m, 1H), 7.45 (m, *J* = 7.5, 0.9 Hz, 4H), 7.31 – 7.18 (m, 3H), 7.05 (m, *J* = 14.4, 4.5 Hz, 3H), 6.87 (d, *J* = 8.4 Hz, 1H), 2.22 (s, 3H).

HRMS (ESI) calcd for $C_{21}H_{16}N_2OH^+$: $[M+H]^+$ 313.1336, found: 313.1332.

1-phenyl-2-(*p*-tolyl)quinazolin-4(1*H*)-one (3bb)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 71% yield;

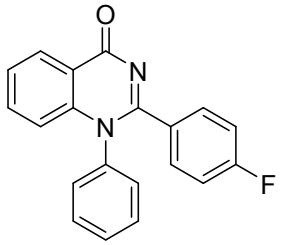
M.p. = 228-231 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.07, 161.46, 142.58, 139.92, 138.32, 133.54, 132.11, 130.05, 129.62, 129.55, 128.46, 128.31, 126.26, 119.48, 117.14, 21.40.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.55 (m, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.49 – 7.40 (m, 4H), 7.27 – 7.20 (m, 4H), 6.97 (d, *J* = 8.1 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 1H), 2.25 (s, 3H).

HRMS (ESI) calcd for $C_{21}H_{16}N_2OH^+$: $[M+H]^+$ 313.1336, found: 313.1331.

2-(4-fluorophenyl)-1-phenylquinazolin-4(1*H*)-one (3bc)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 58% yield;

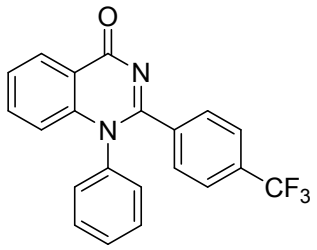
M.p. = 291-294 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.86, 163.17 (d, *J* = 251.1 Hz), 160.39, 142.45, 138.08, 133.71, 131.73 (d, *J* = 8.7 Hz), 131.12, 130.23, 129.81, 129.57, 128.37, 126.51, 119.49, 117.17, 115.03 (d, *J* = 21.9 Hz).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.63 – 7.53 (m, 1H), 7.52 – 7.42 (m, 4H), 7.41 – 7.32 (m, 2H), 7.30 – 7.19 (m, 2H), 6.96 – 6.80 (m, 3H).

HRMS (ESI) calcd for $C_{20}H_{13}FN_2OH^+$: $[M+H]^+$ 317.1085, found: 317.1091.

1-phenyl-2-(4-(trifluoromethyl)phenyl)quinazolin-4(1*H*)-one (3bd)



3bd

Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 65% yield;

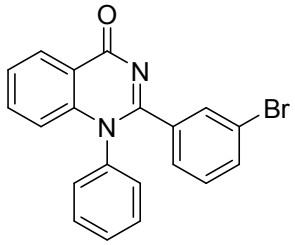
M.p. = 281-284 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.66, 159.98, 142.32, 138.38, 137.62, 133.87, 131.44 (d, *J* = 33.1 Hz), 130.35, 130.10, 129.79, 129.50, 128.37, 126.75, 124.79, 119.51, 117.23.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.38 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.59 (m, *J* = 8.7, 7.3, 1.6 Hz, 1H), 7.46 (m, *J* = 13.7, 12.6, 8.8 Hz, 8H), 7.31 – 7.23 (m, 2H), 6.87 (d, *J* = 8.4 Hz, 1H).

HRMS (ESI) calcd for $C_{21}H_{13}F_3N_2OH^+$: $[M+H]^+$ 367.1053, found: 367.1057.

2-(3-bromophenyl)-1-phenylquinazolin-4(1*H*)-one (3be)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 57% yield;

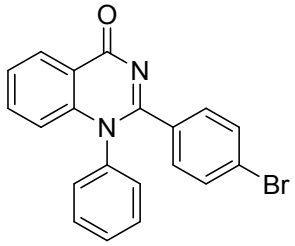
M.p. = 275-279 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.74, 159.77, 142.34, 137.74, 136.70, 133.81, 132.74, 132.50, 130.27, 129.98, 129.52, 129.22, 128.30, 127.91, 126.63, 121.92, 119.47, 117.25.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.64 – 7.54 (m, 2H), 7.52 – 7.43 (m, 4H), 7.39 – 7.32 (m, 1H), 7.30 – 7.25 (m, 2H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.01 (t, *J* = 7.9 Hz, 1H), 6.88 (d, *J* = 8.4 Hz, 1H).

HRMS (ESI) calcd for $C_{20}H_{13}BrN_2OH^+$: $[M+H]^+$ 377.0284, found: 377.0279.

2-(4-bromophenyl)-1-phenylquinazolin-4(1*H*)-one (3bf)



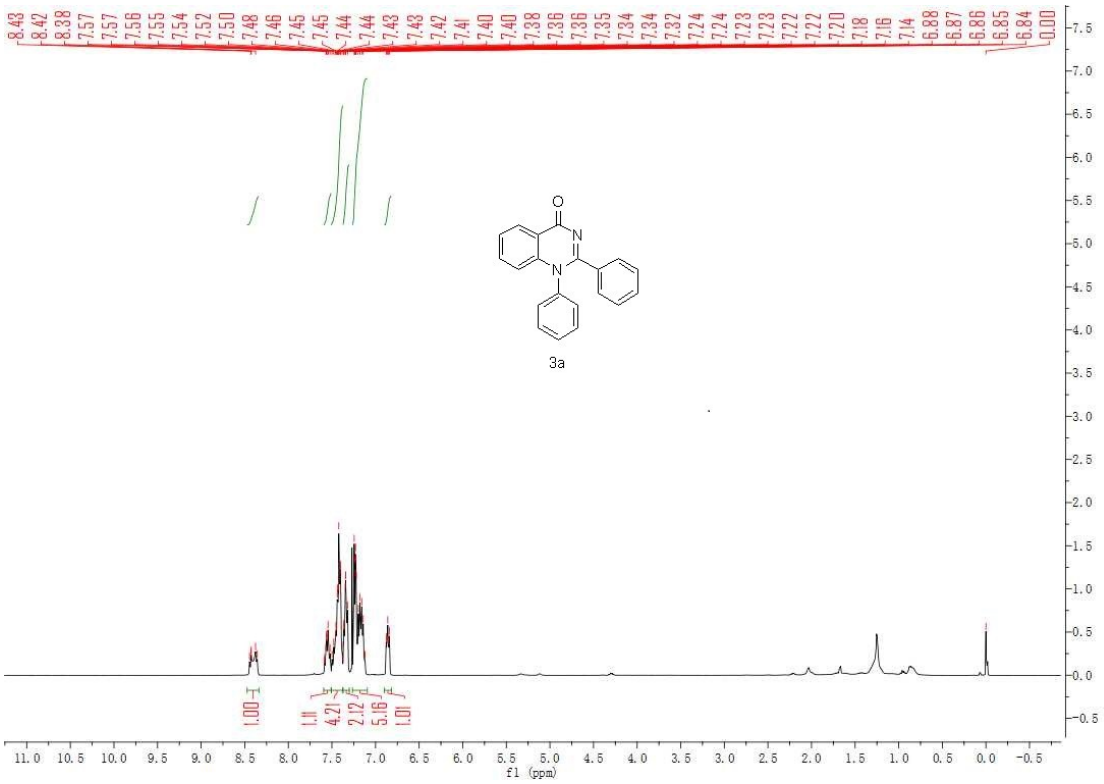
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/*n*-hexane =1/2) as yellow white solid in 80% yield;

M.p. = 252-256 ℃;

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.82, 160.36, 142.37, 137.85, 131.73, 131.07, 131.01, 130.29, 129.93, 129.53, 129.34, 128.19, 126.57, 124.38, 119.37, 117.25.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.31 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.60 – 7.53 (m, 1H), 7.51 – 7.40 (m, 4H), 7.27 (dt, *J* = 23.0, 5.2 Hz, 6H), 6.87 (d, *J* = 8.5 Hz, 1H).

HRMS (ESI) calcd for $C_{20}H_{13}BrN_2OH^+$: $[M+H]^+$ 377.0284, found:377.0280.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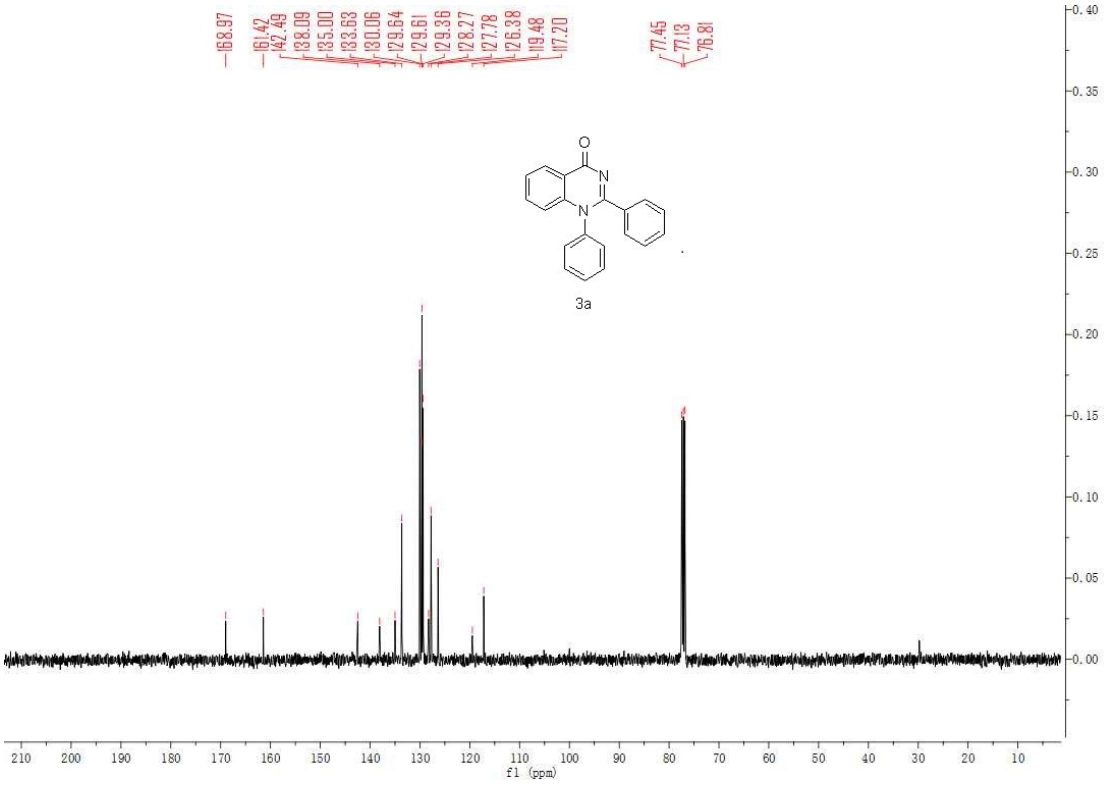
f1 (ppm)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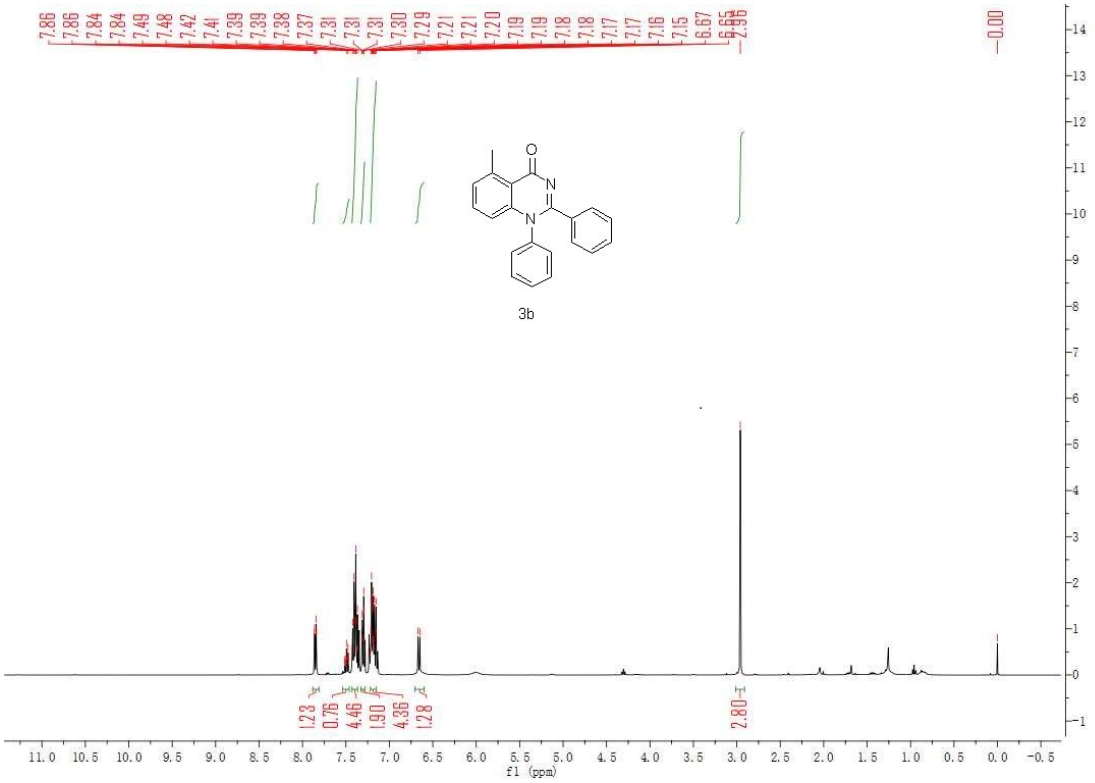
3a
f1 (ppm)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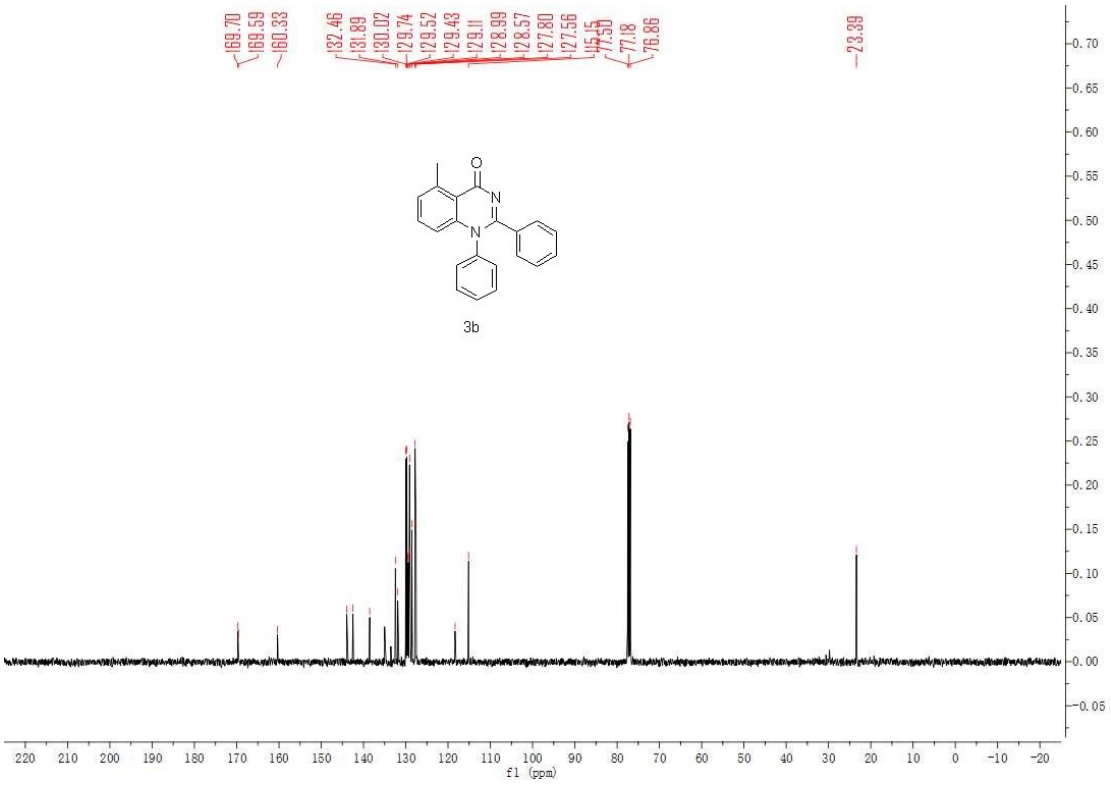
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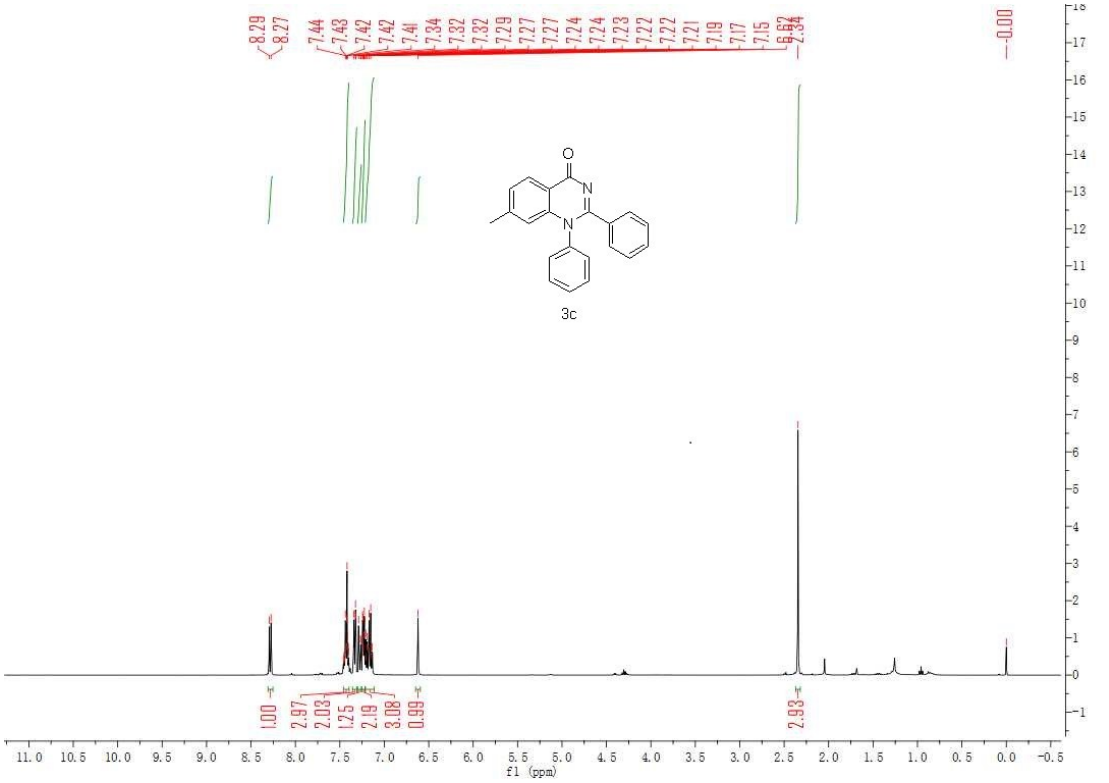
3b
f1 (ppm)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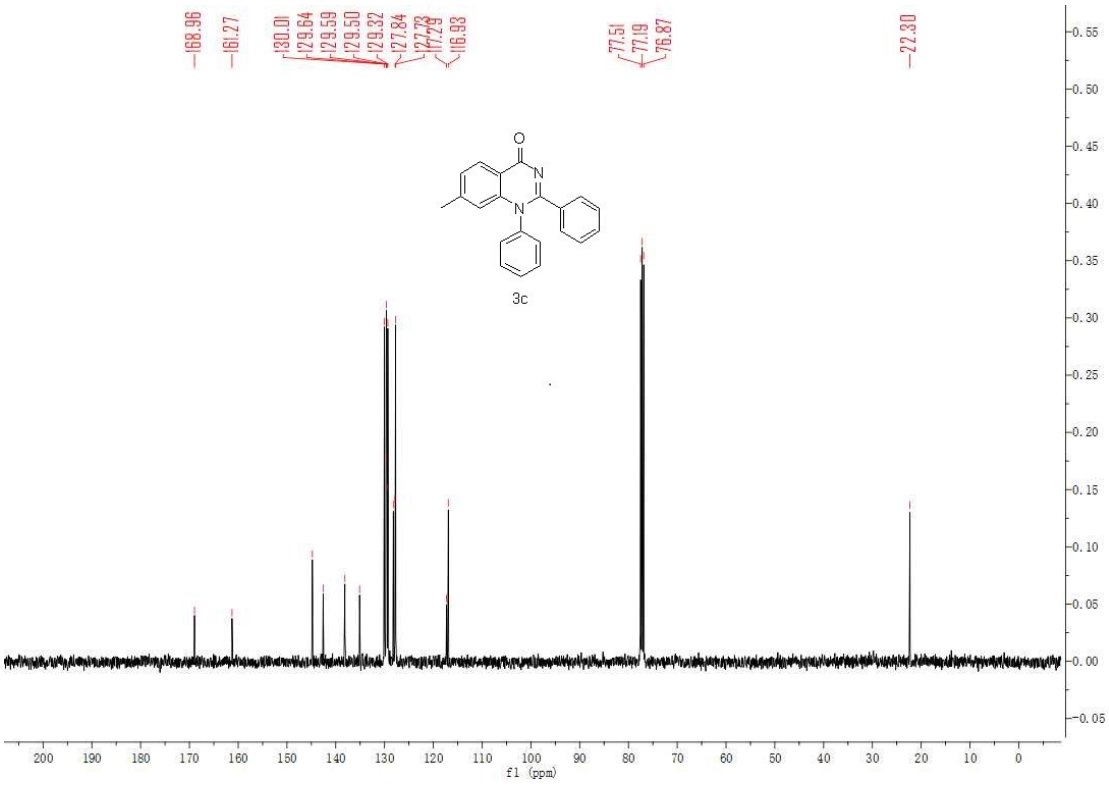
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76.87
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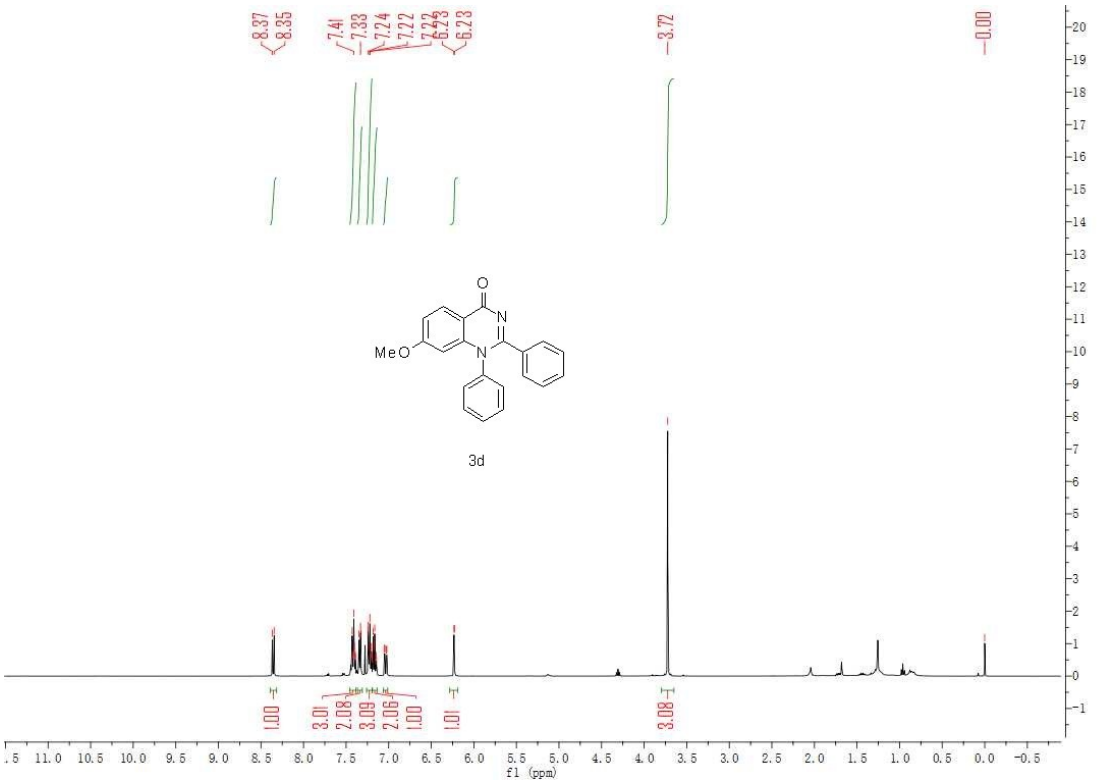
3c
f1 (ppm)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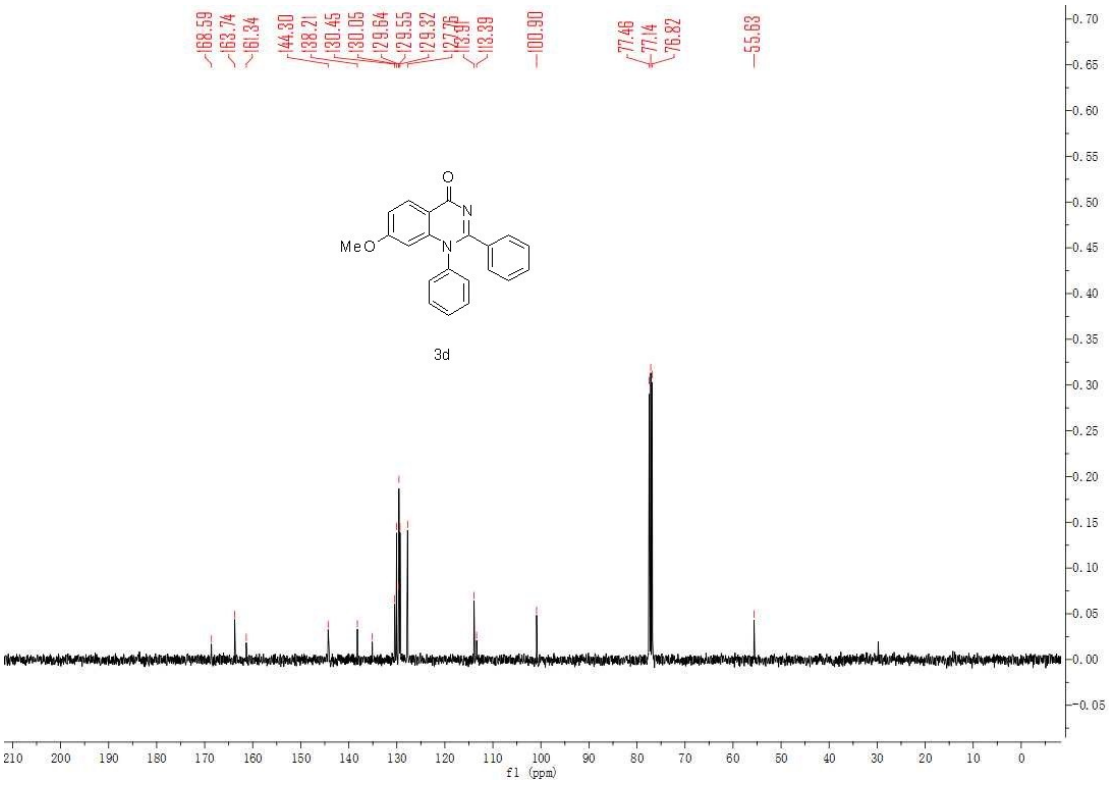
3.08
f1 (ppm)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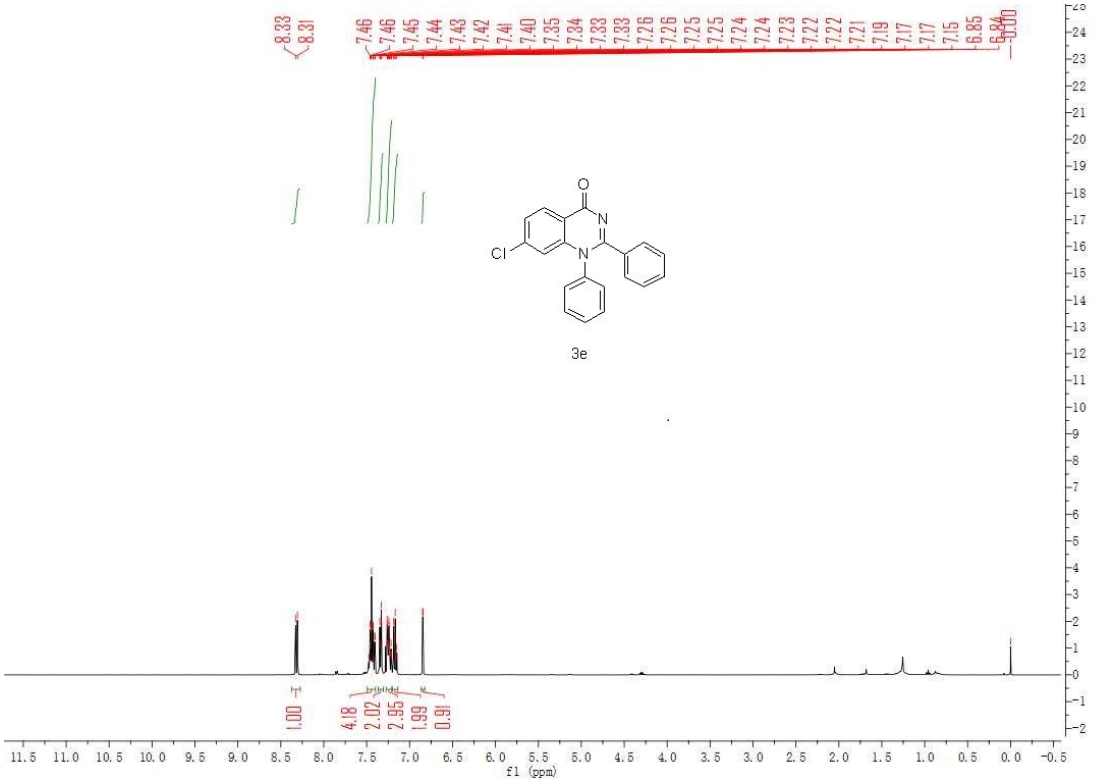
3d
f1 (ppm)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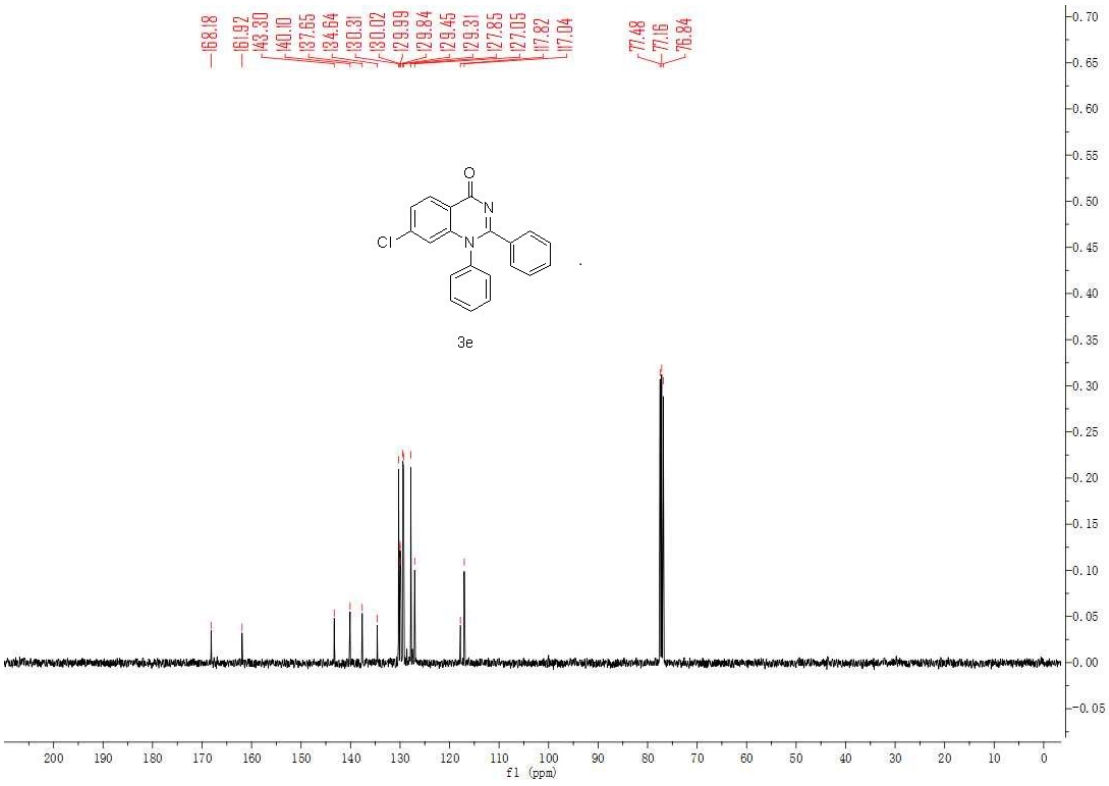
f1 (ppm)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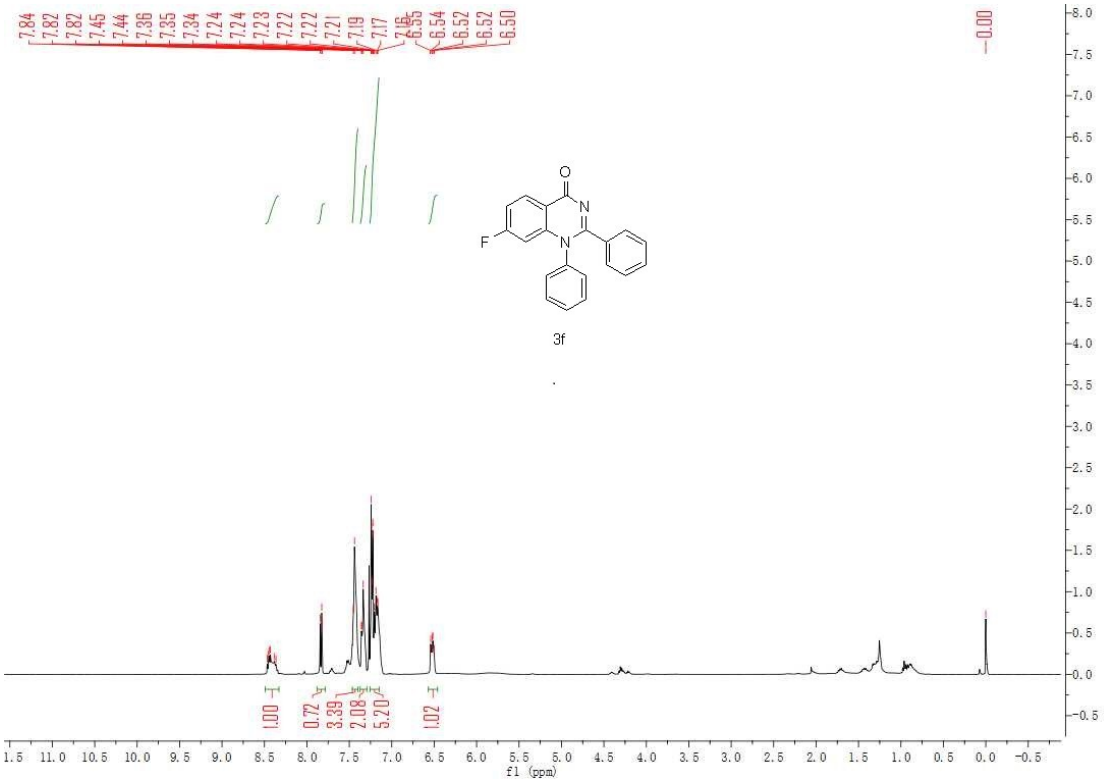
Cl
N
3e
f1 (ppm)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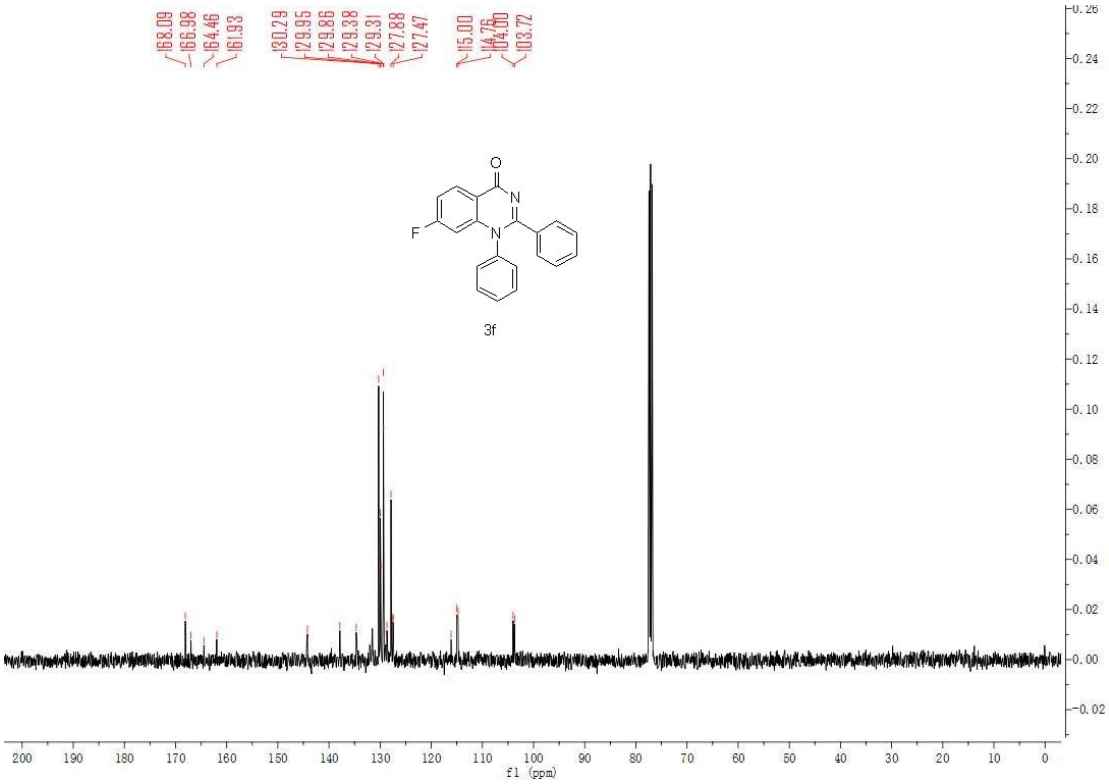
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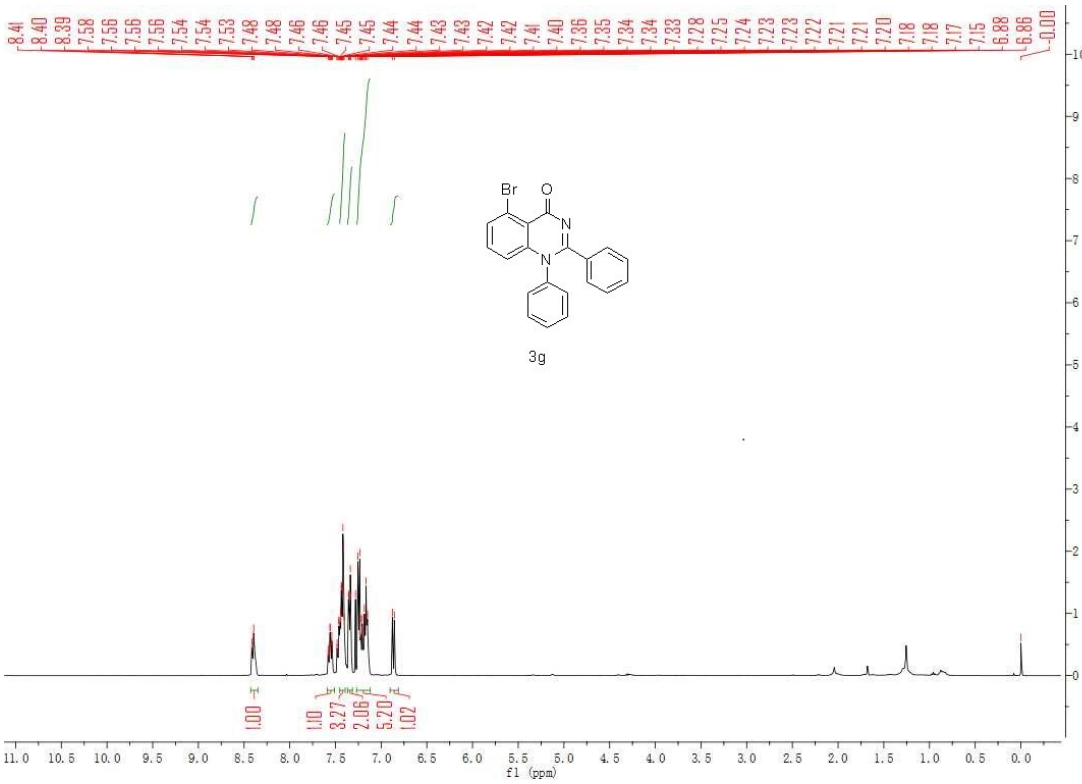
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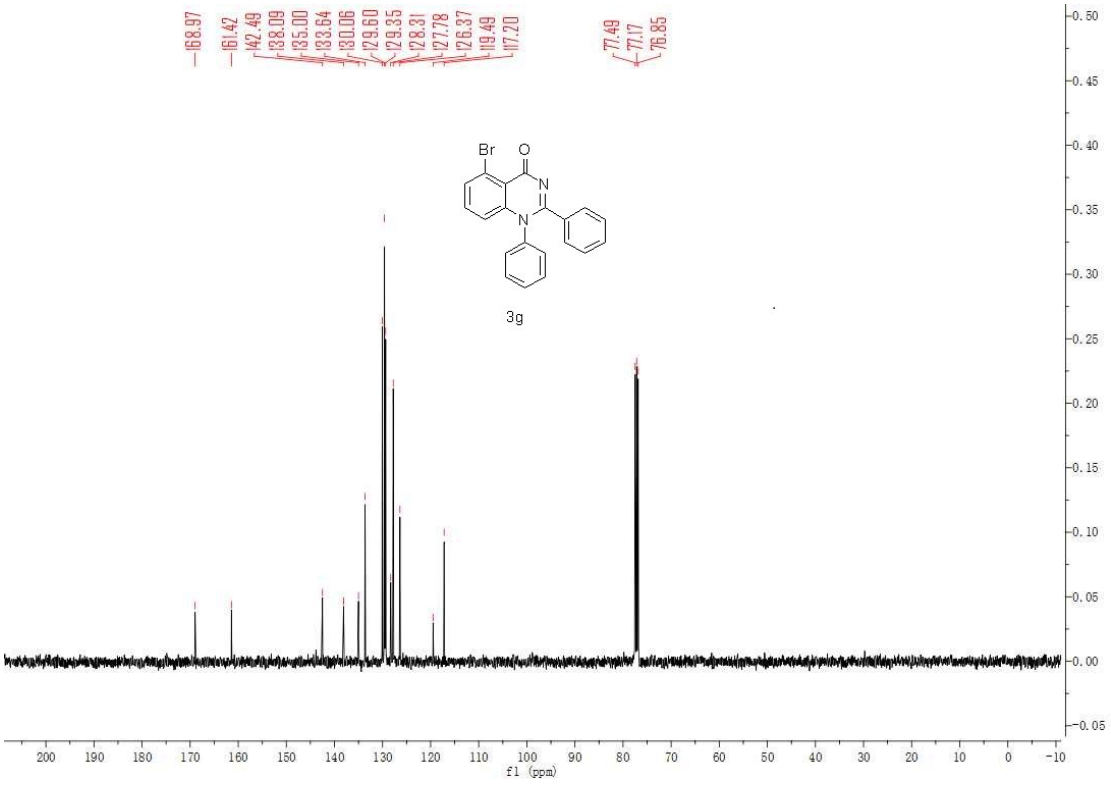
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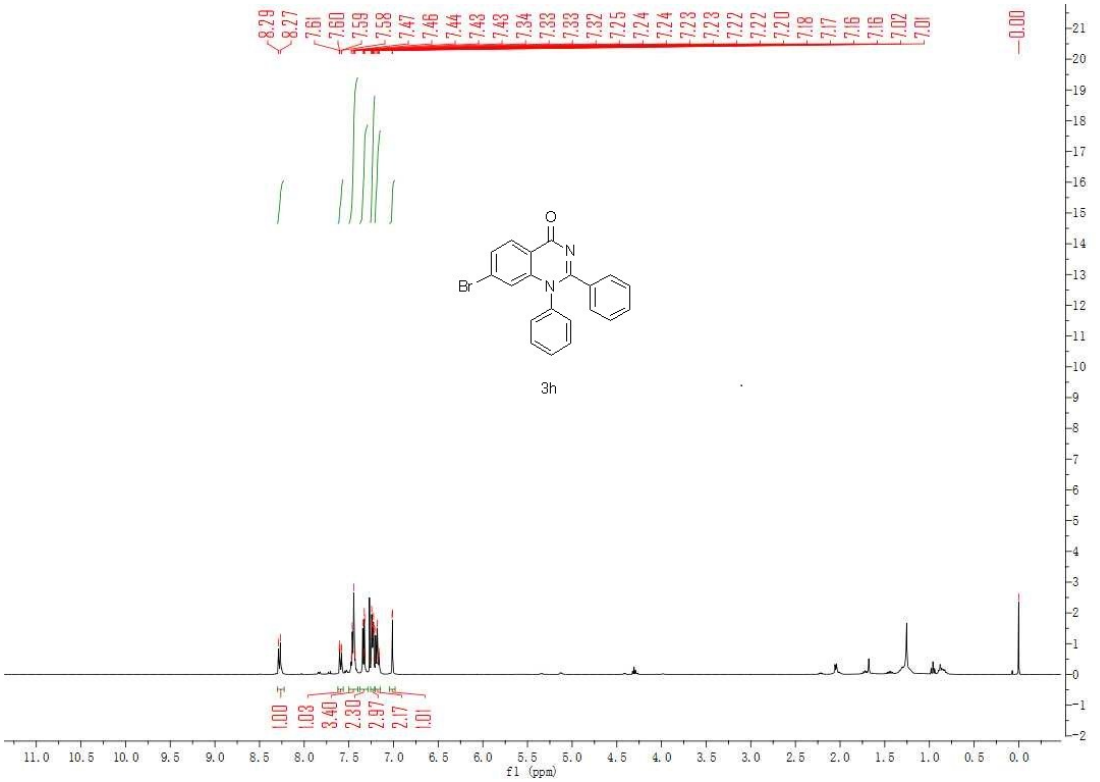
f1 (ppm)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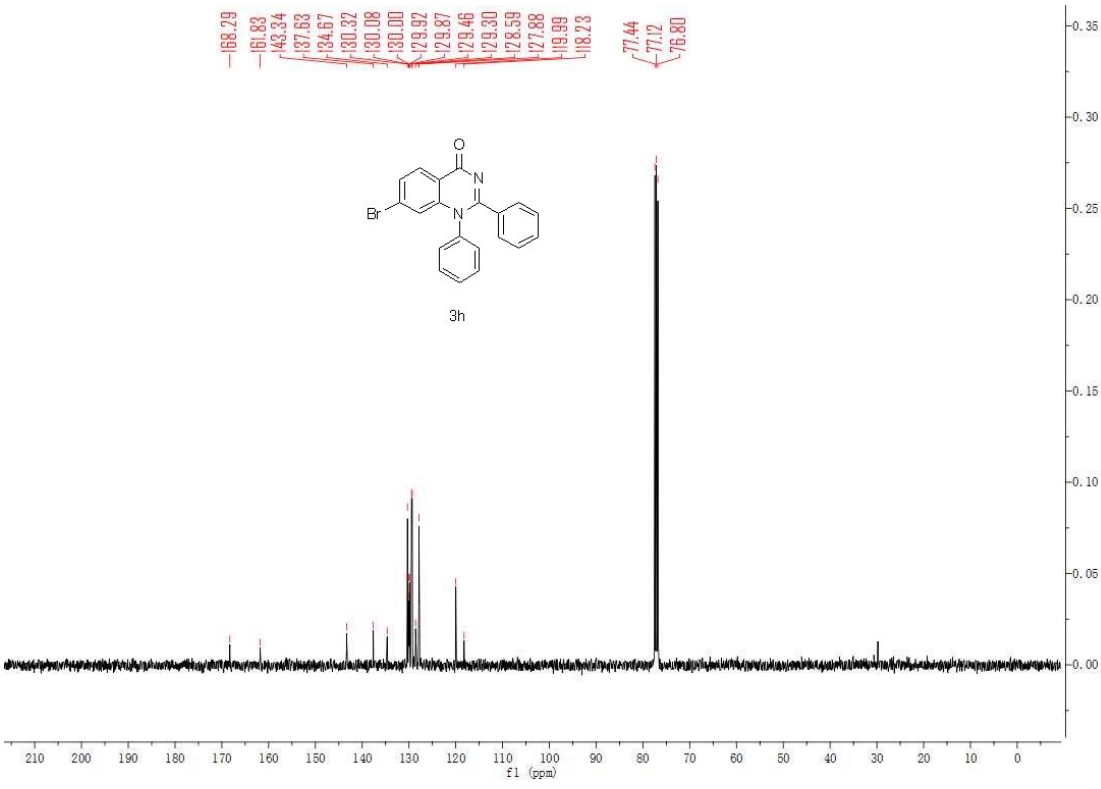
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Br
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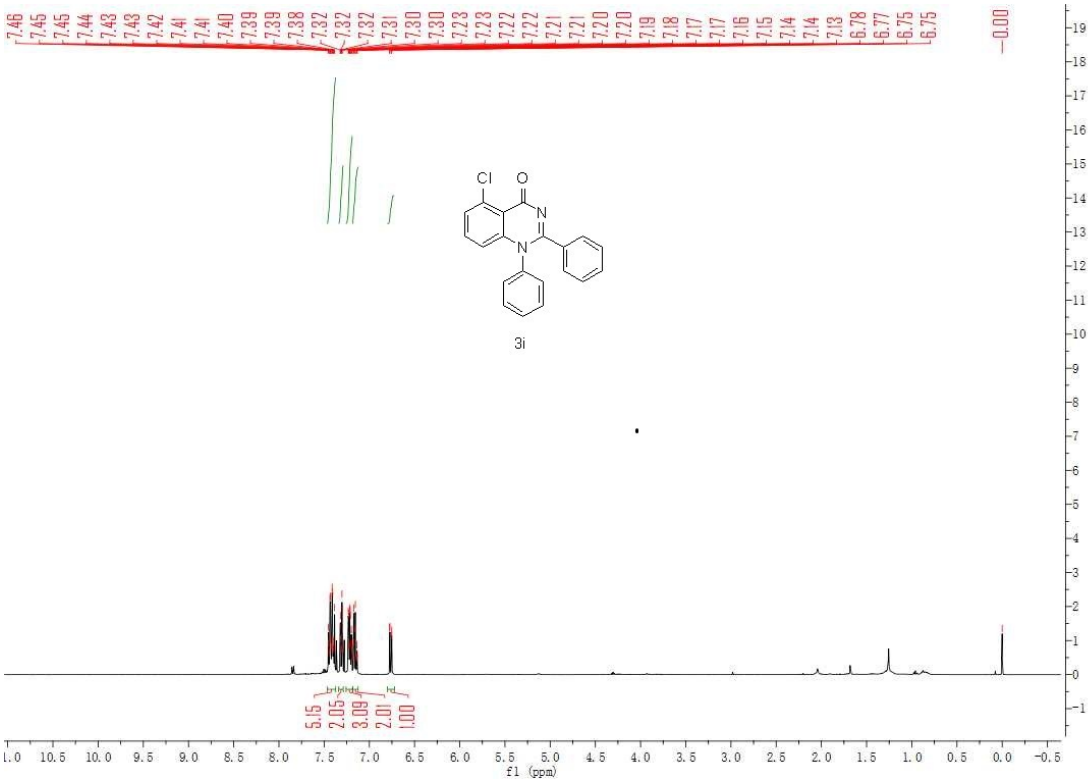
f1 (ppm)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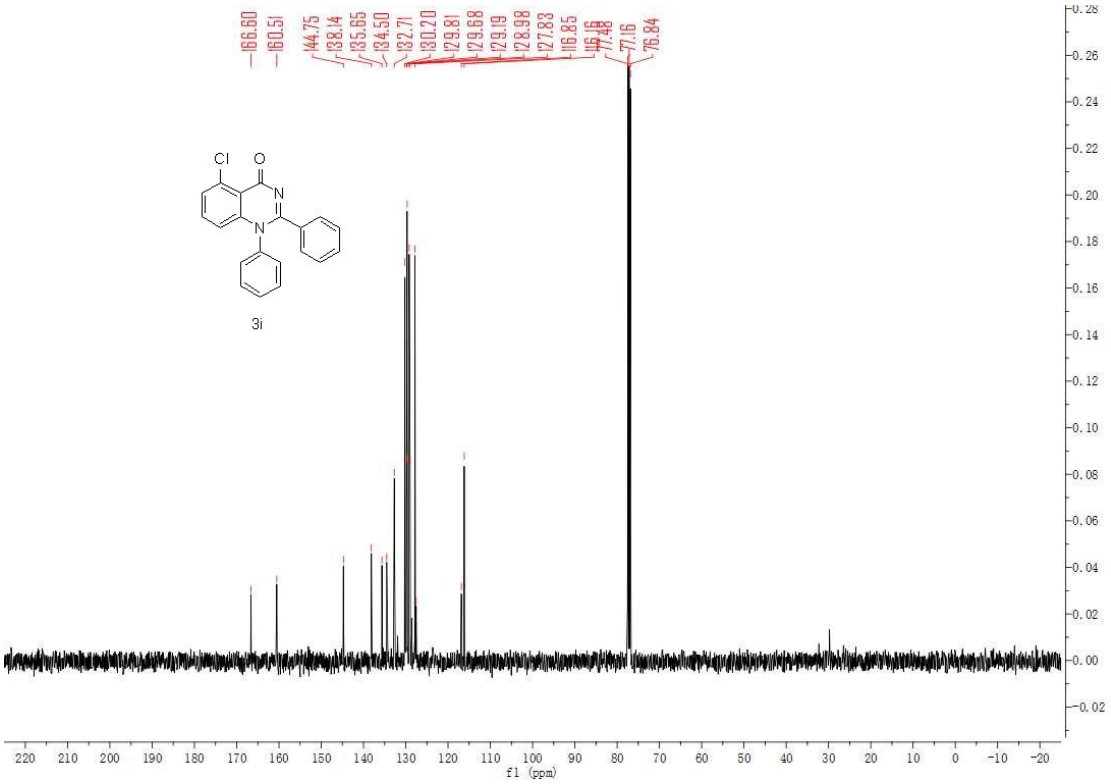
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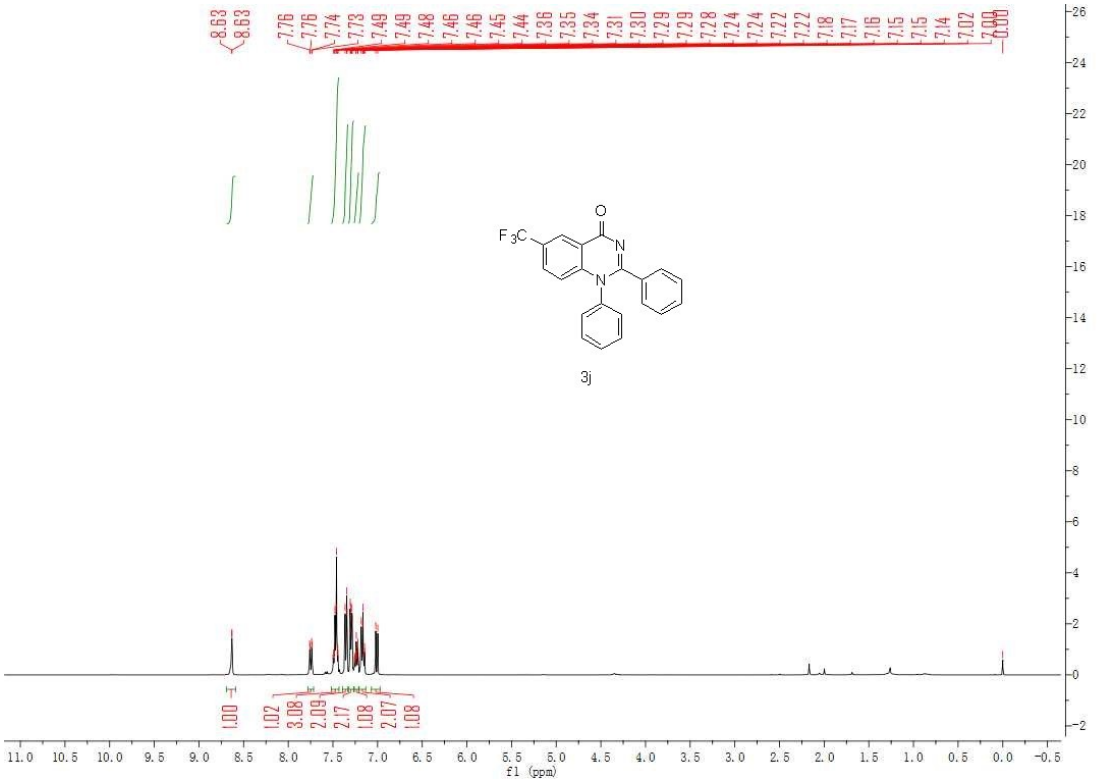
76.84
Cl
O
N
N
3i
f1 (ppm)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7.35
7.34
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7.22
7.18
7.17
7.16
7.15
7.15
7.14
7.02
7.00
0.00
F3C
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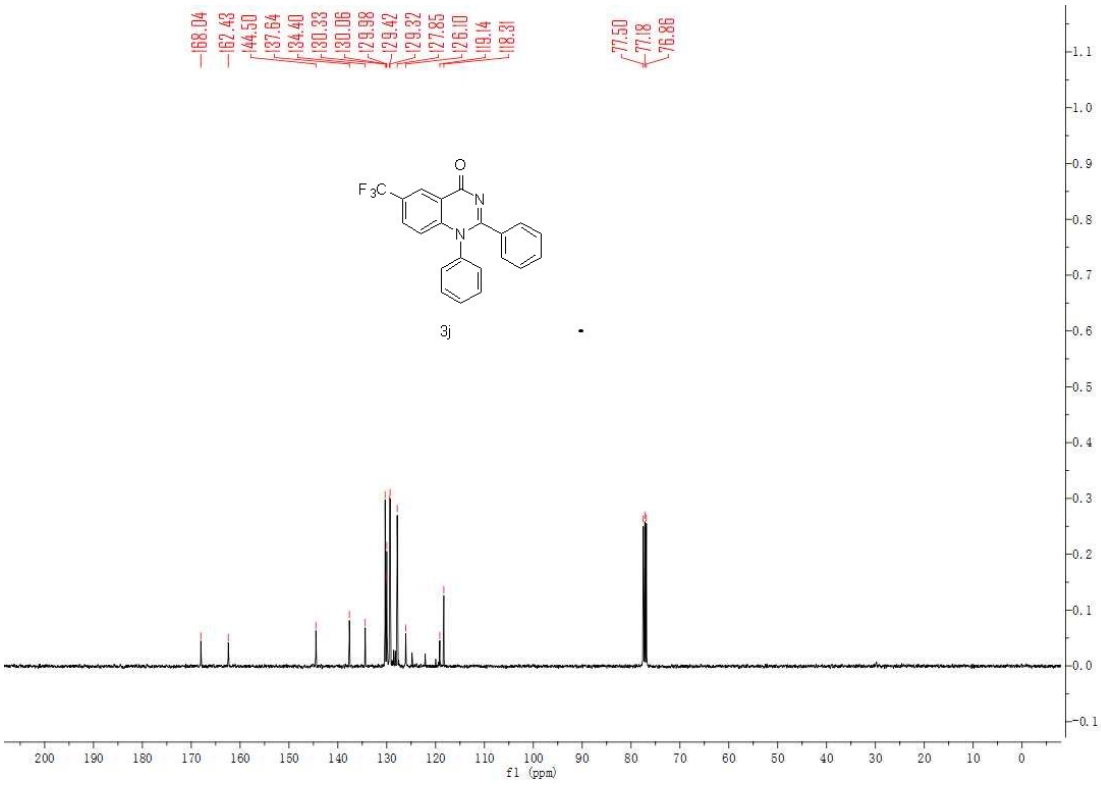
1.08
2.07
1.08
f1 (ppm)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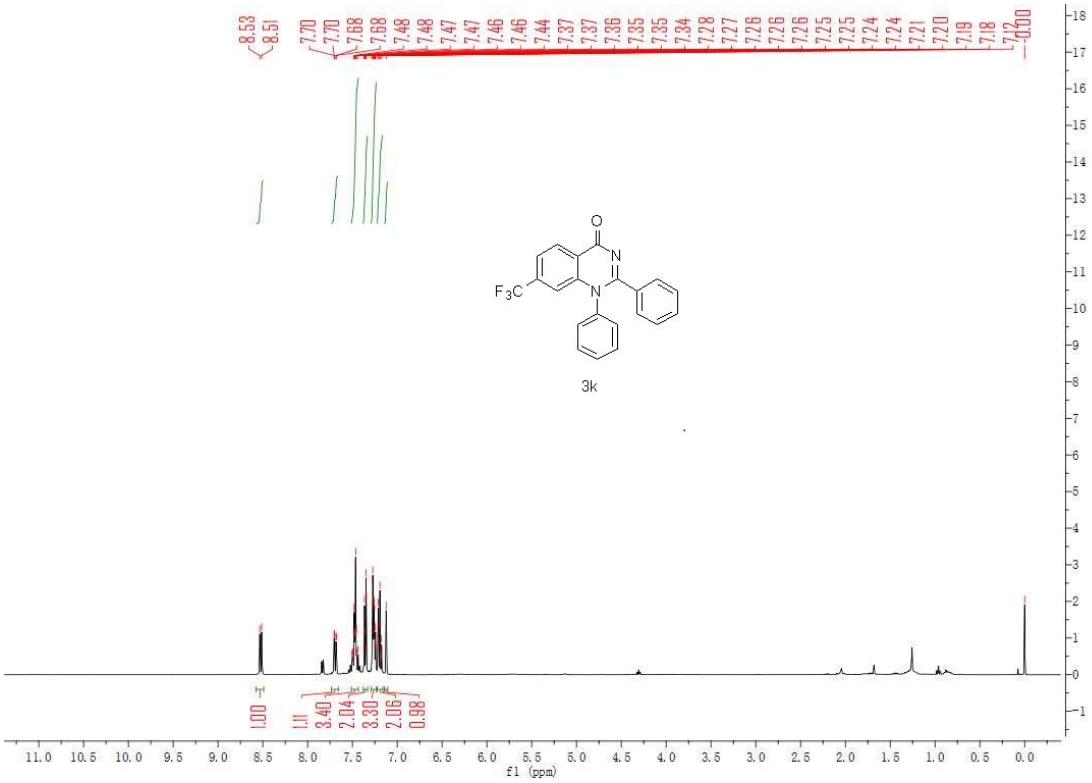
O
N
N
3j
f1 (ppm)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7.24
7.24
7.21
7.20
7.19
7.18
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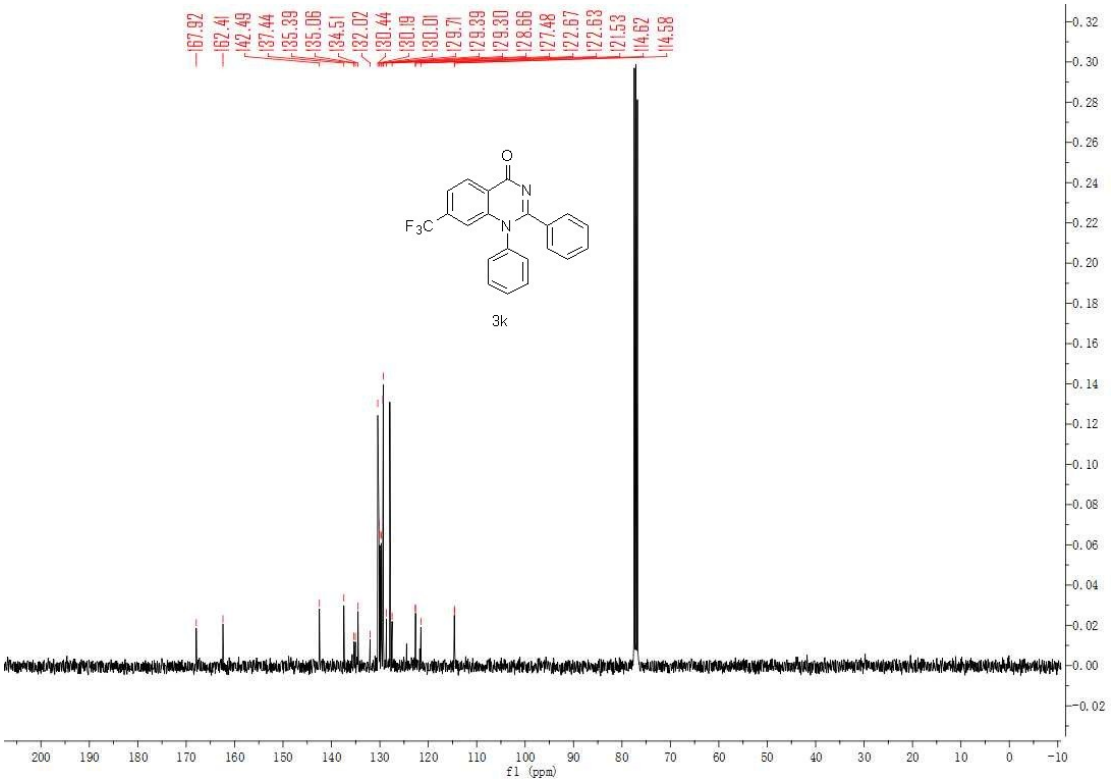
f1 (ppm)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114.58
F3C
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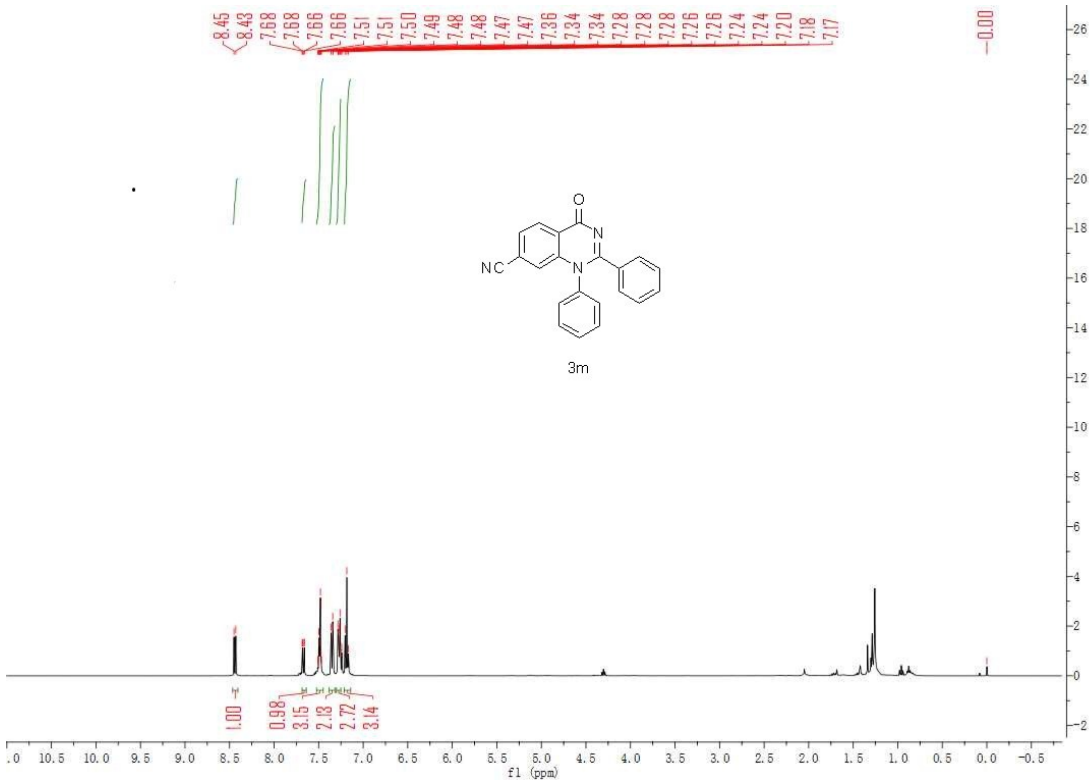
O
3k
f1 (ppm)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7.26
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7.24
7.24
7.20
7.18
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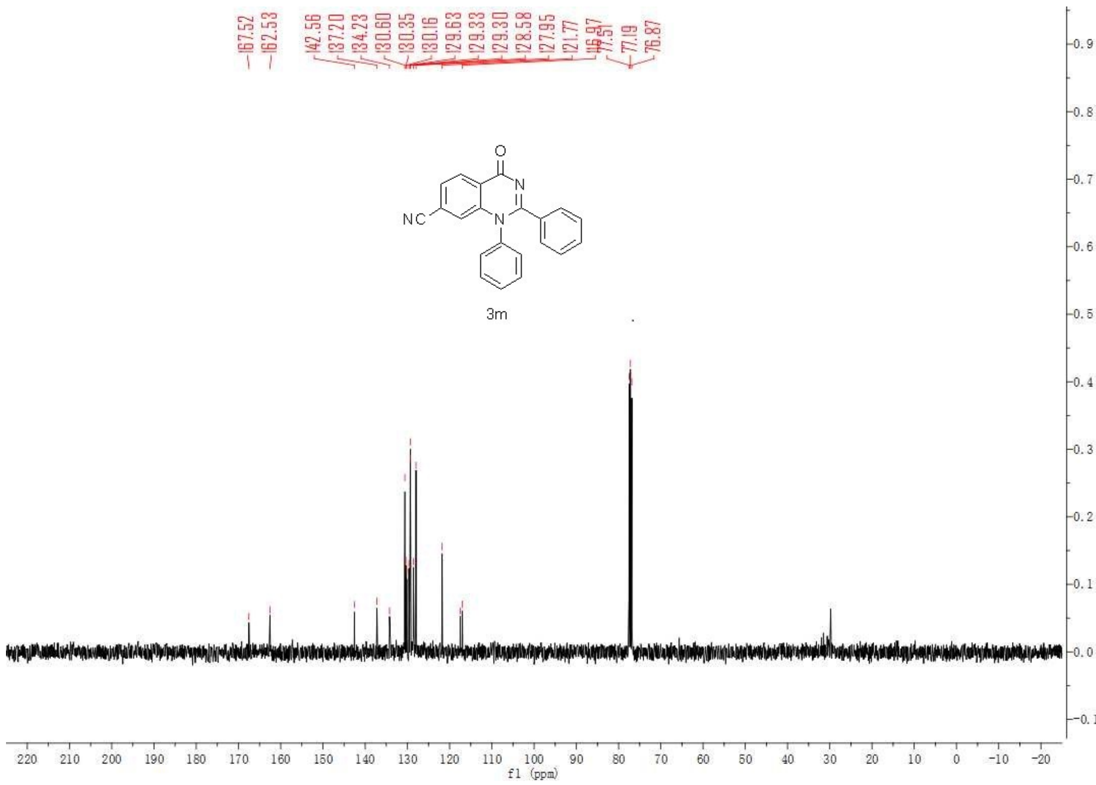
f1 (ppm)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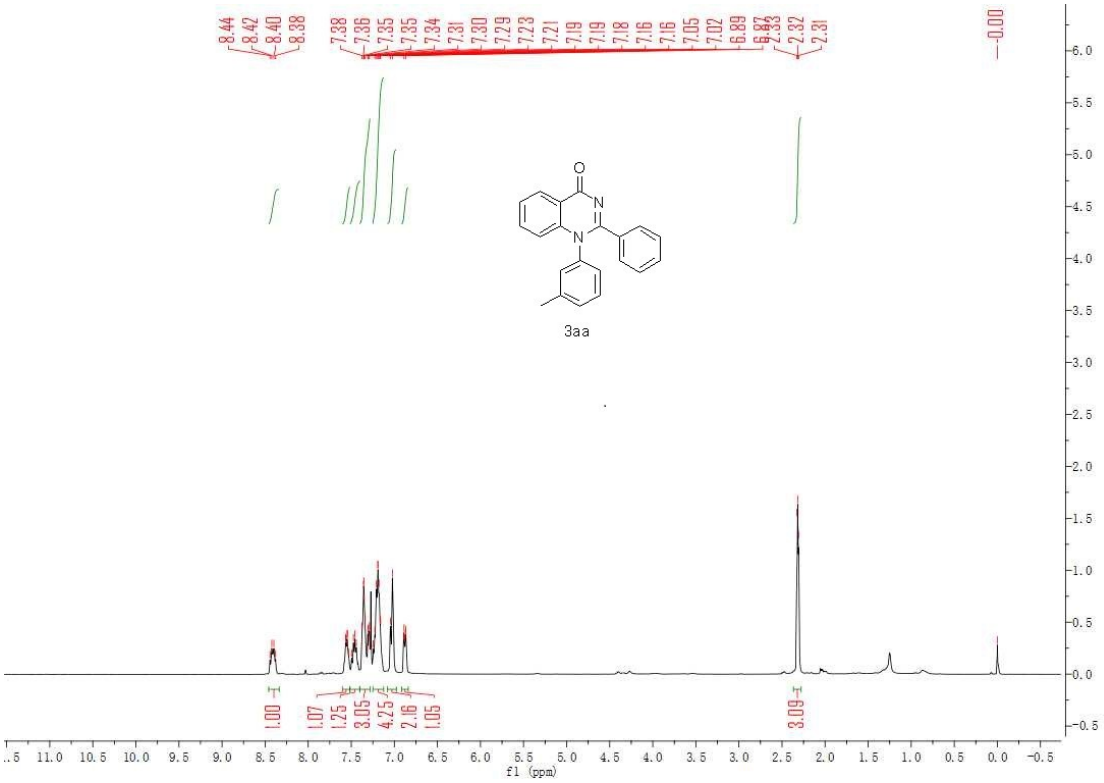
N
3m
f1 (ppm)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7.16
7.16
7.05
7.02
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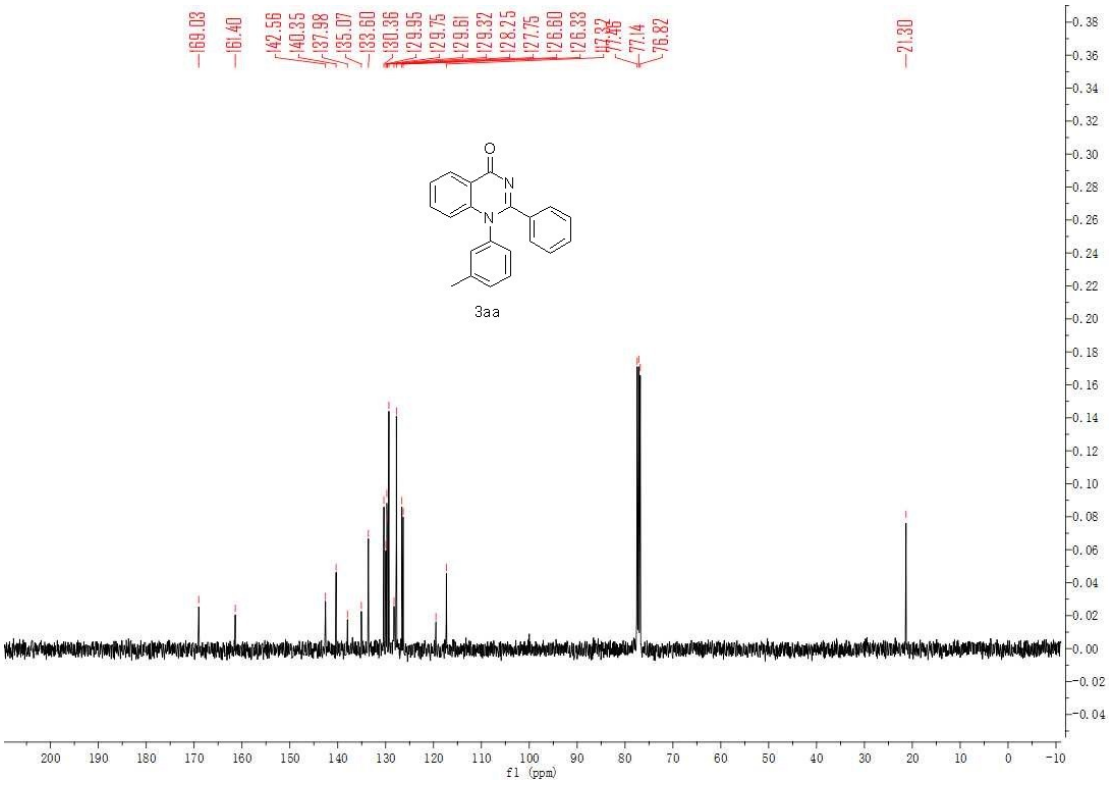
8.09
f1 (ppm)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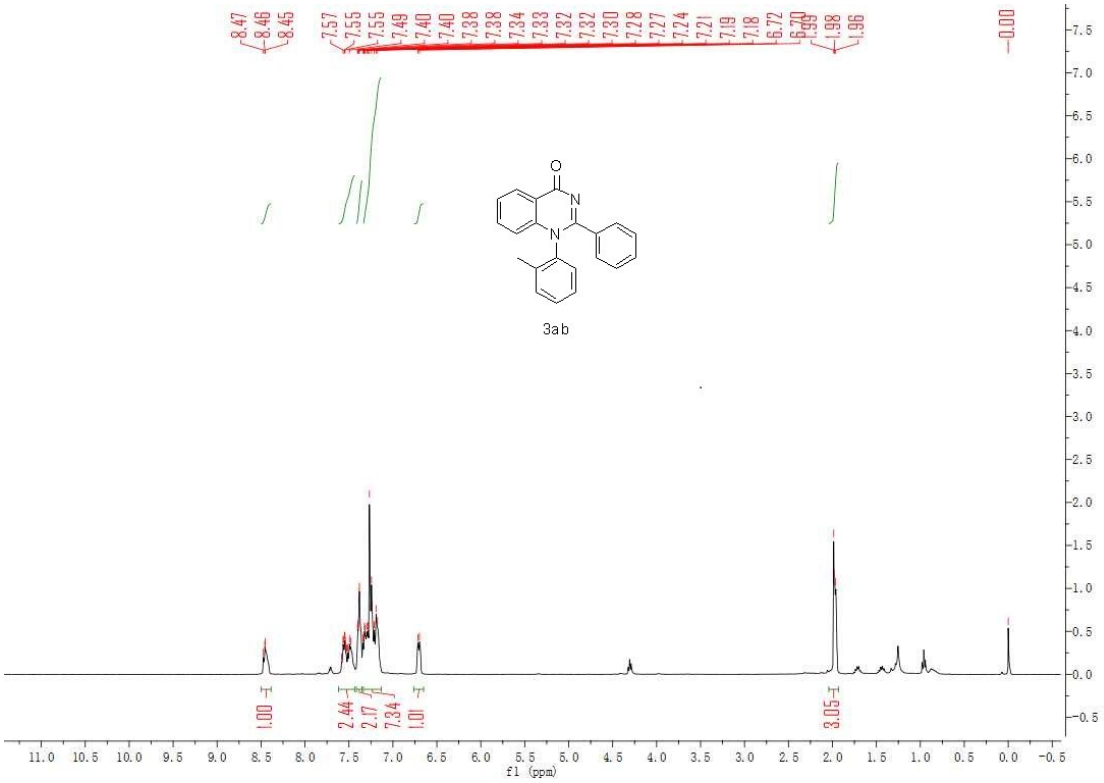
76.82
21.30
3aa
f1 (ppm)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7.24
7.21
7.19
7.18
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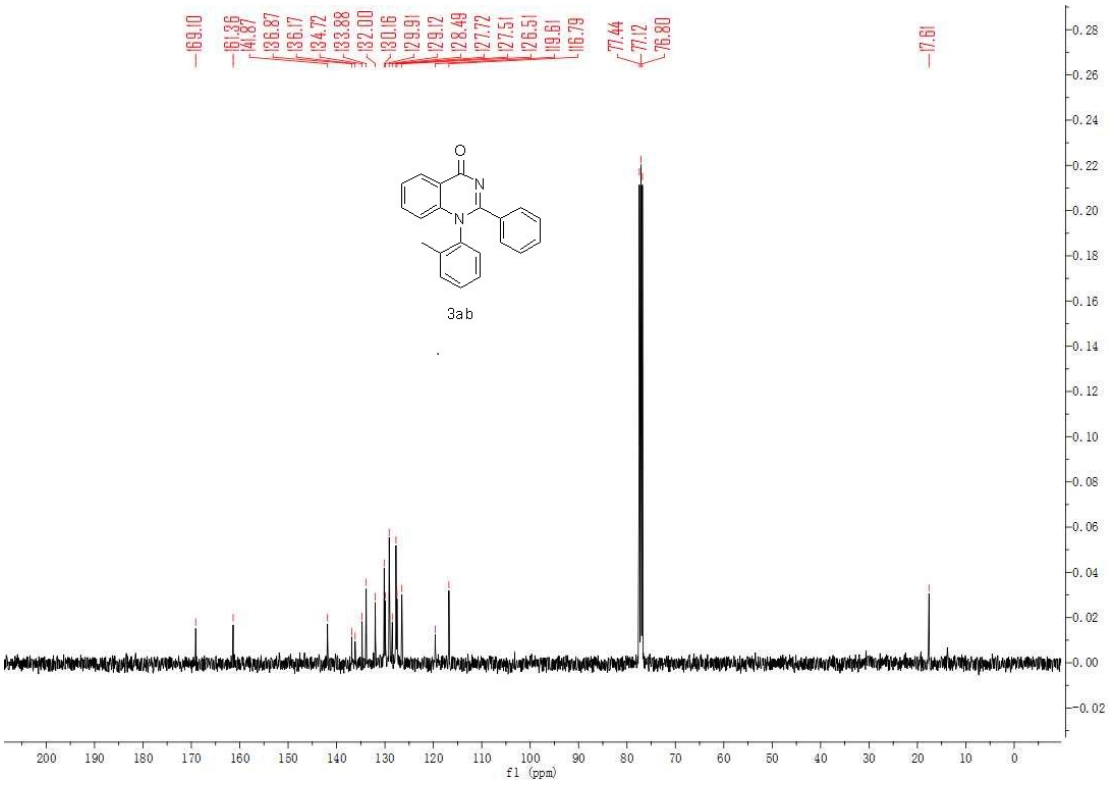
3.05
f1 (ppm)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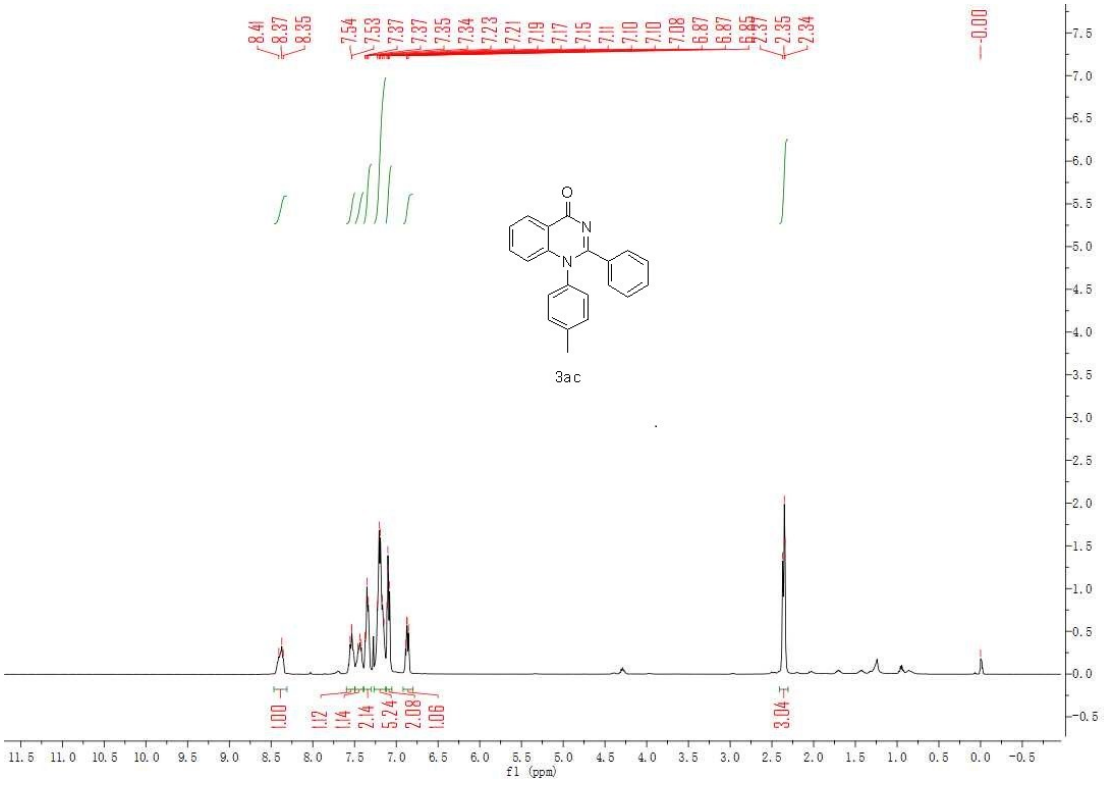
f1 (ppm)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7.08
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3.04
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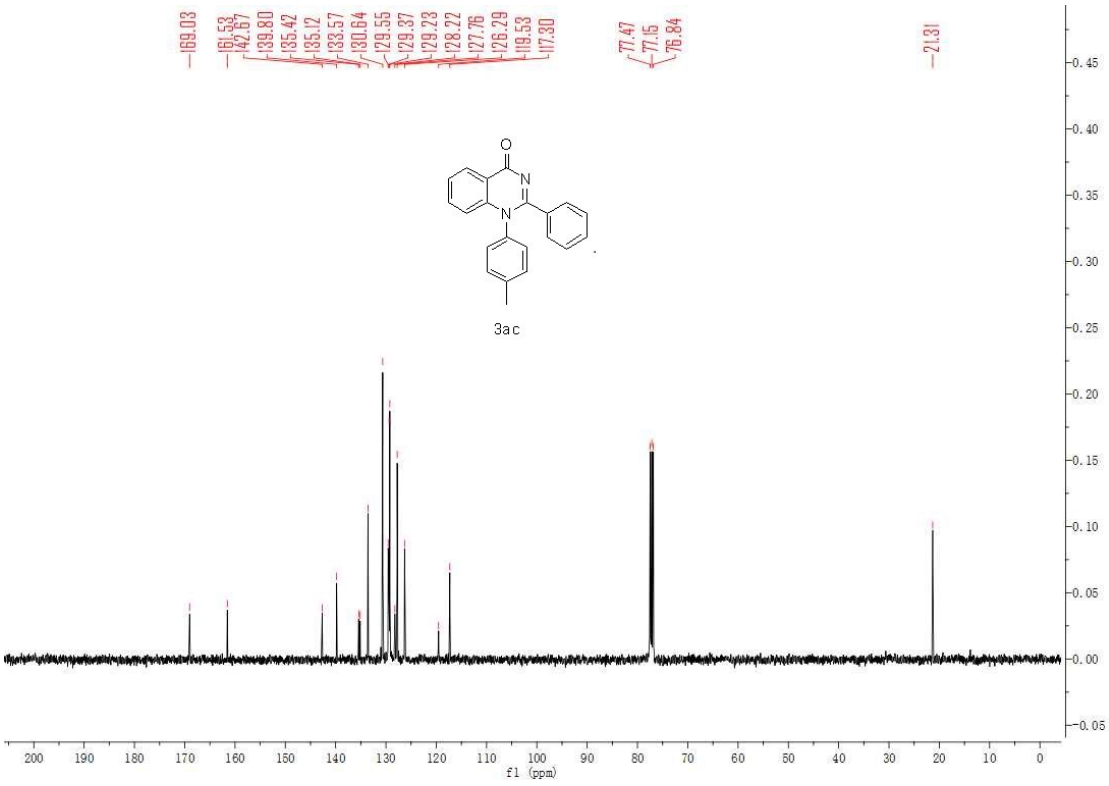
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21.31
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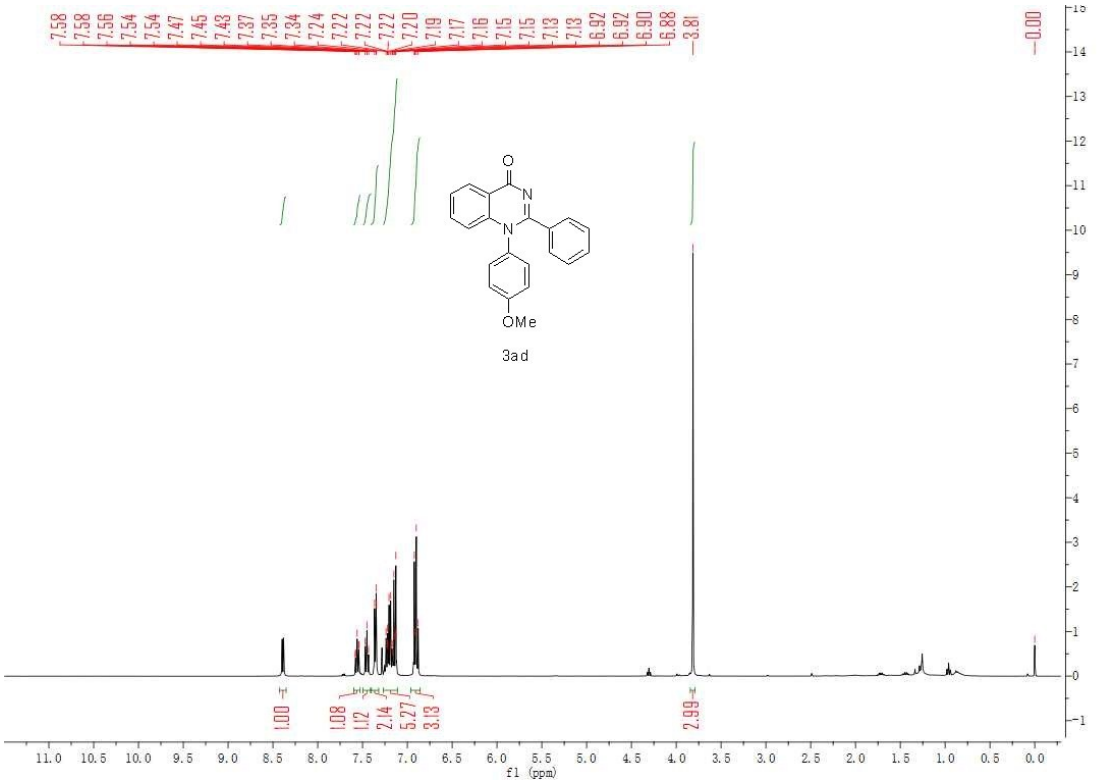
f1 (ppm)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7.15
7.13
7.13
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6.90
6.88
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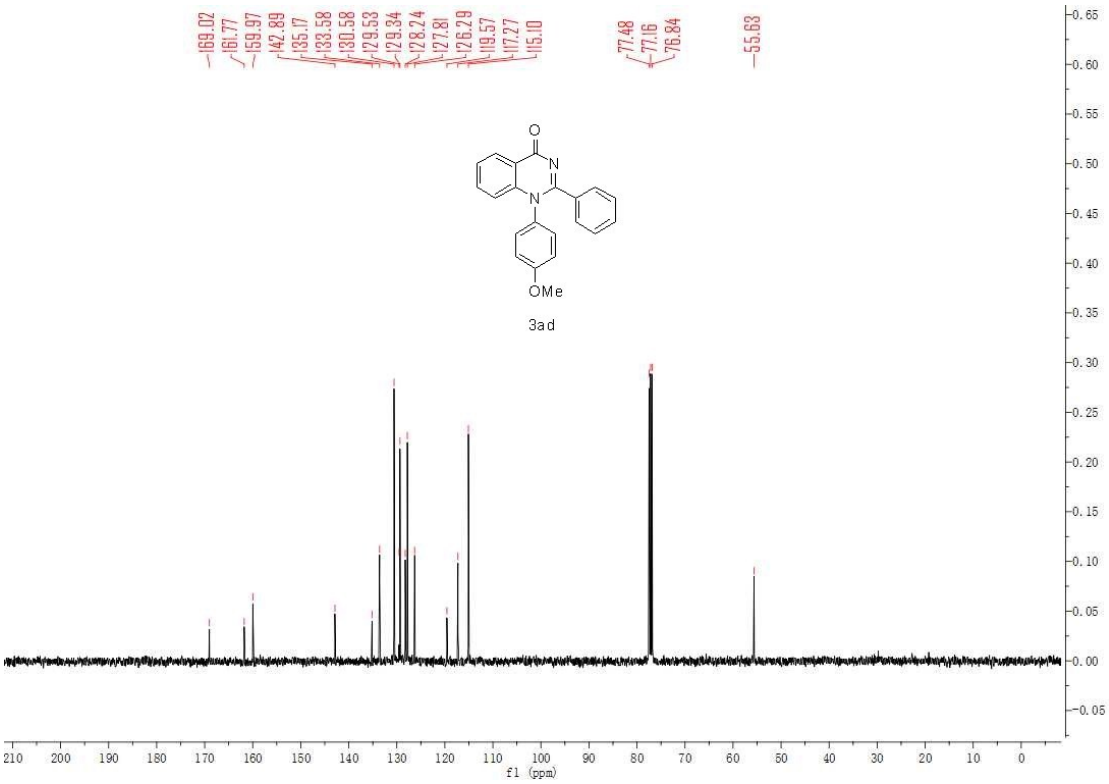
2.99
f1 (ppm)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76.84
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OMe
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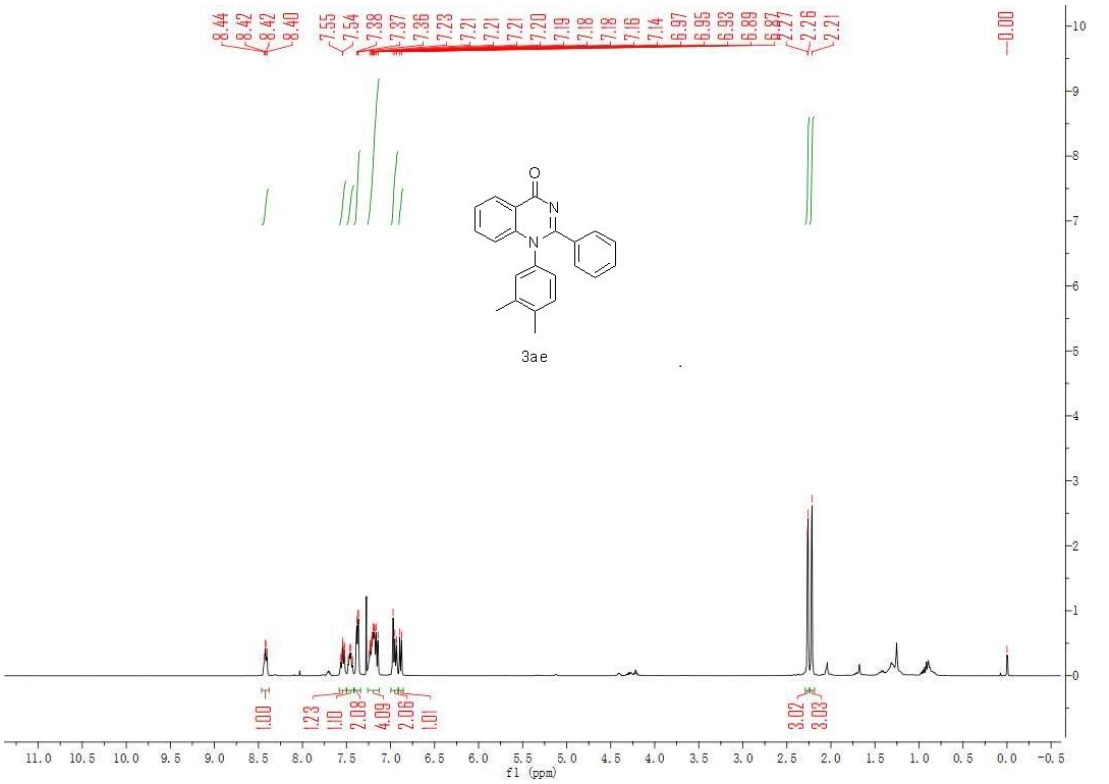
f1 (ppm)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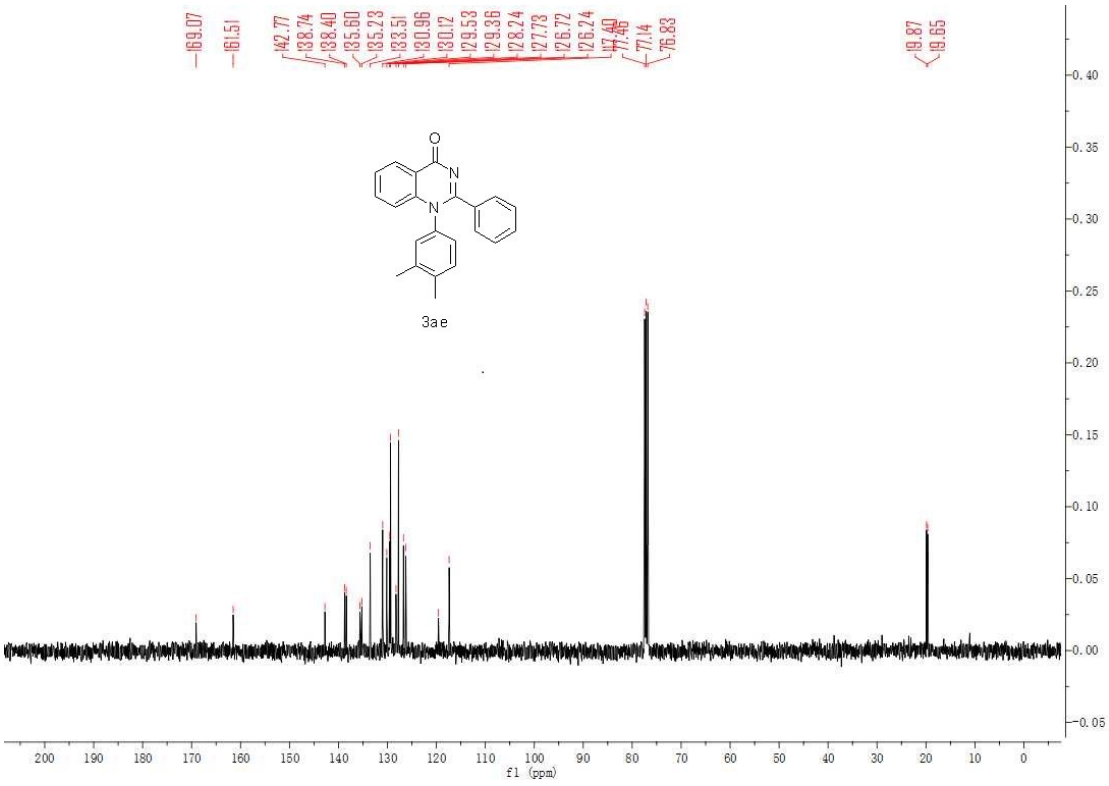
3.03
f1 (ppm)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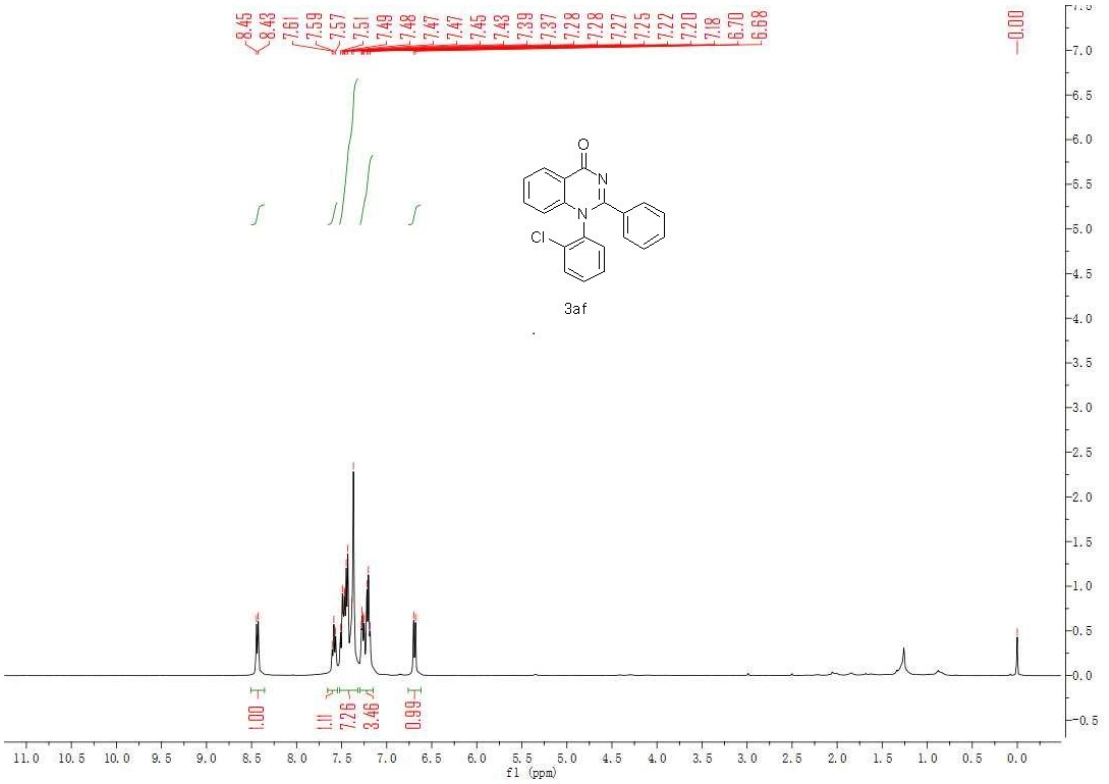
f1 (ppm)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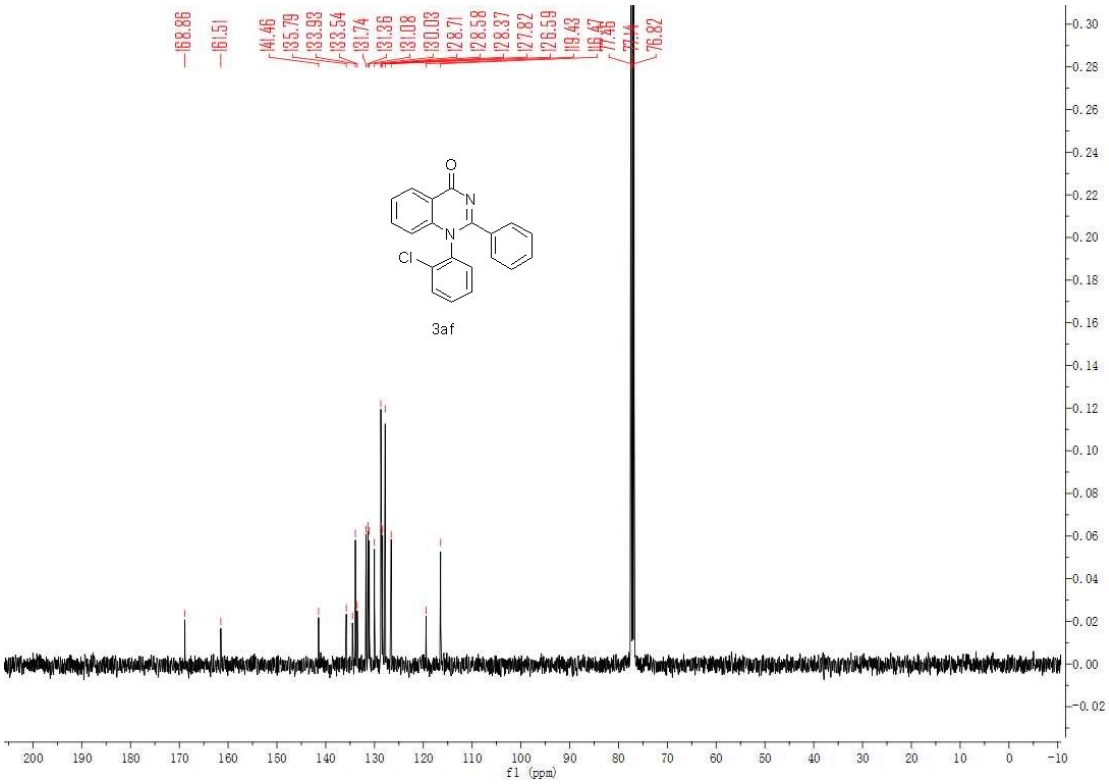
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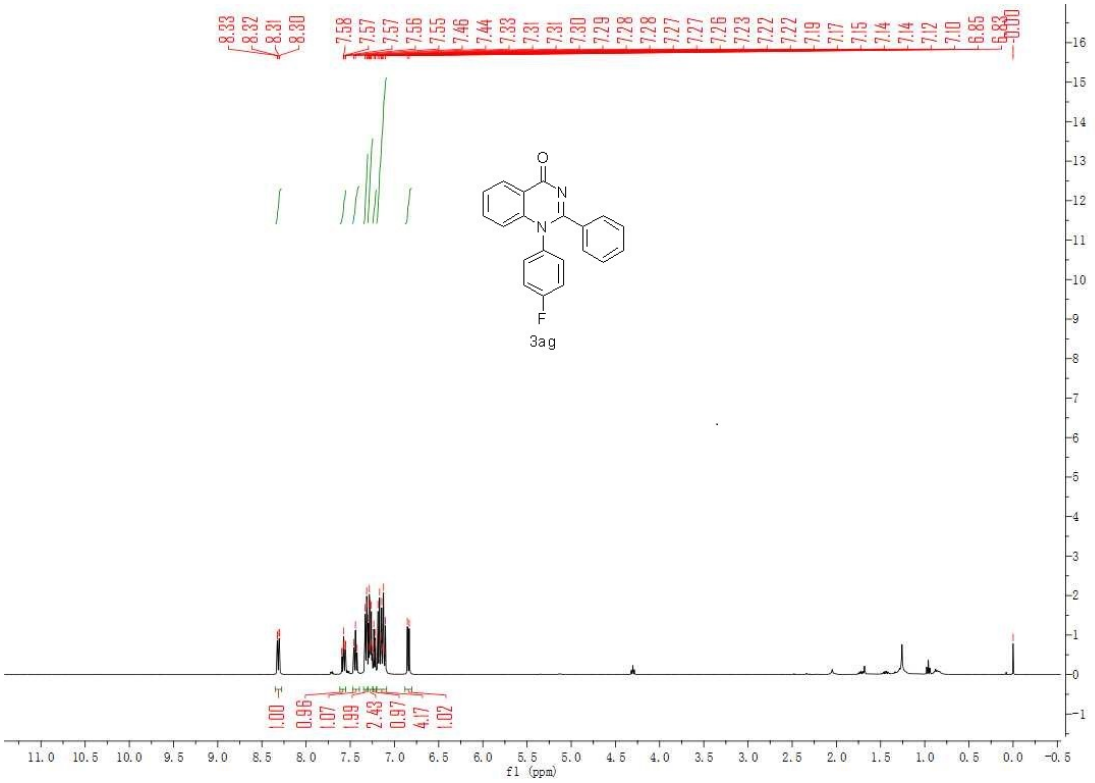
f1 (ppm)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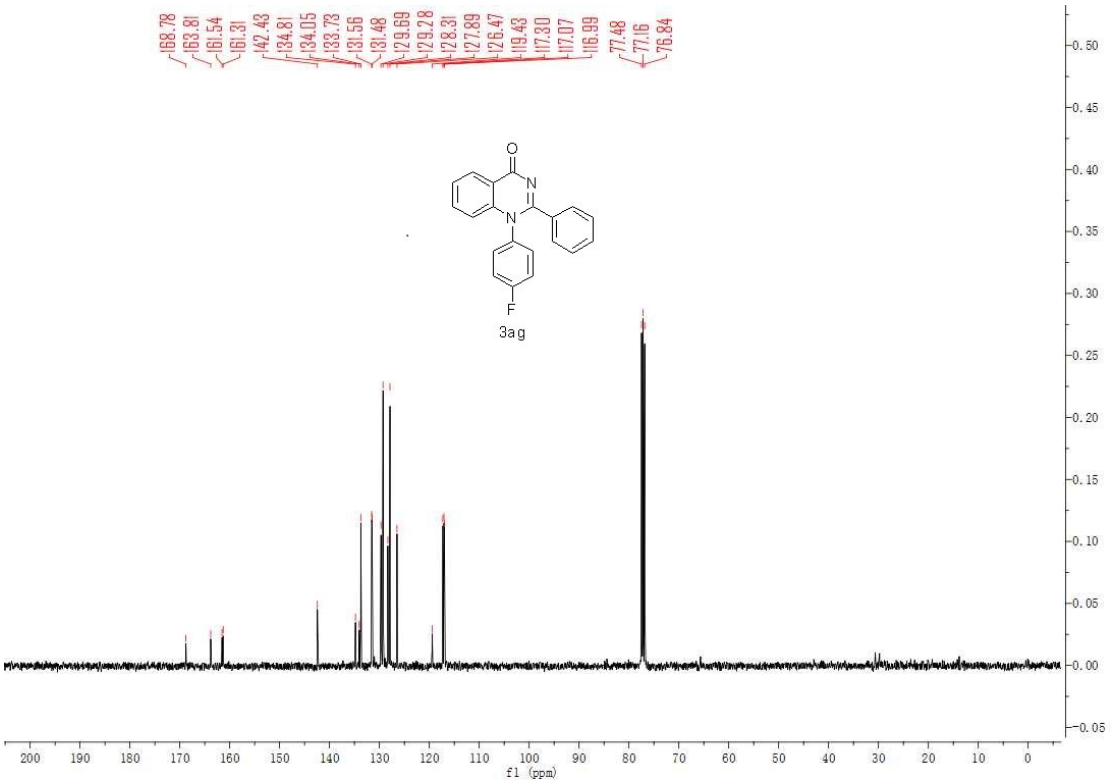
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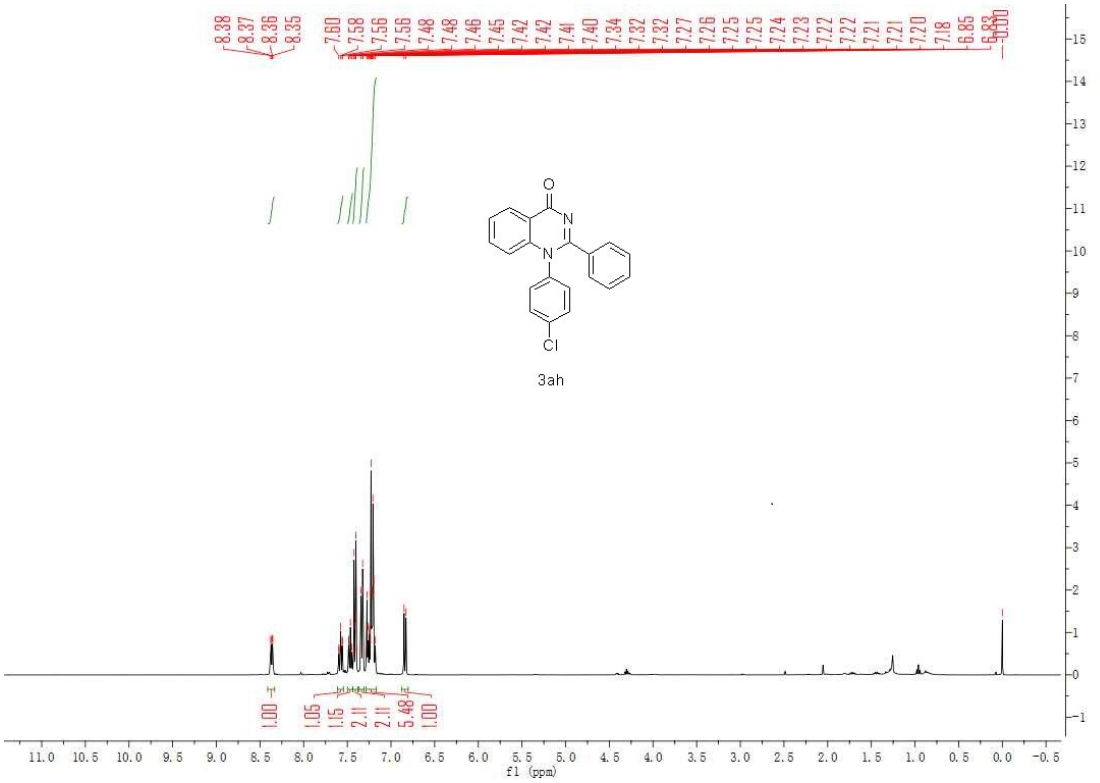
F
3ag
f1 (ppm)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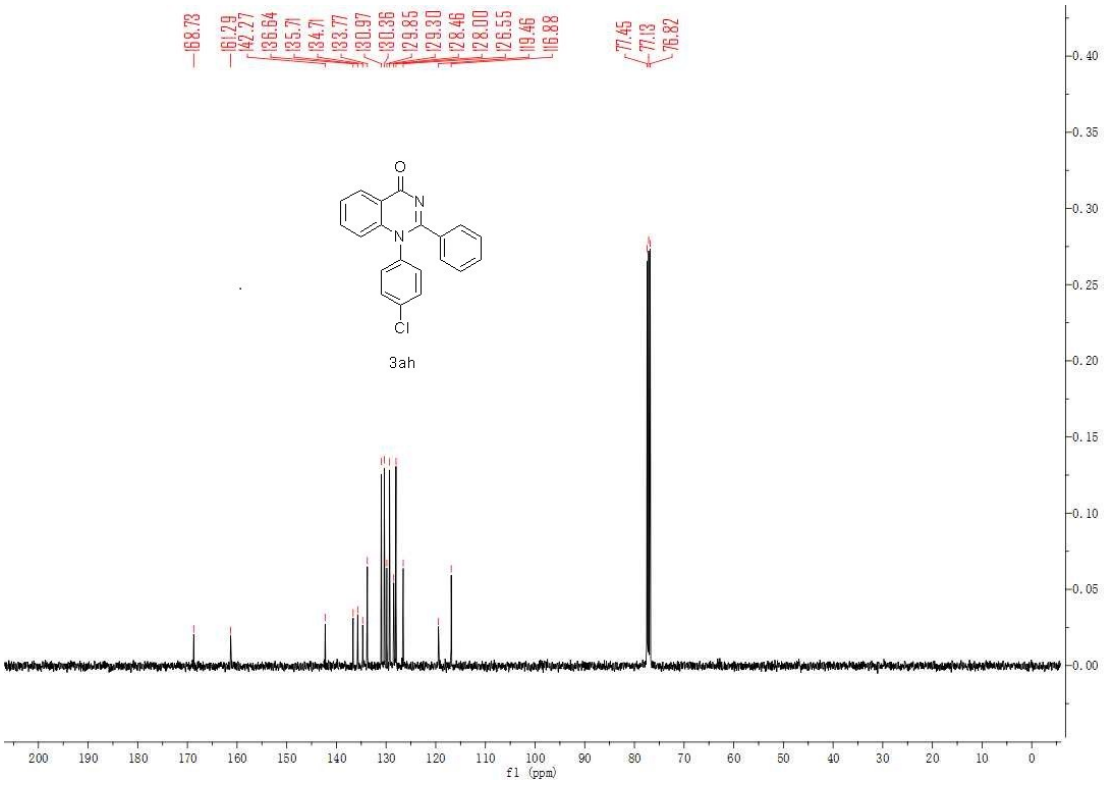
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O
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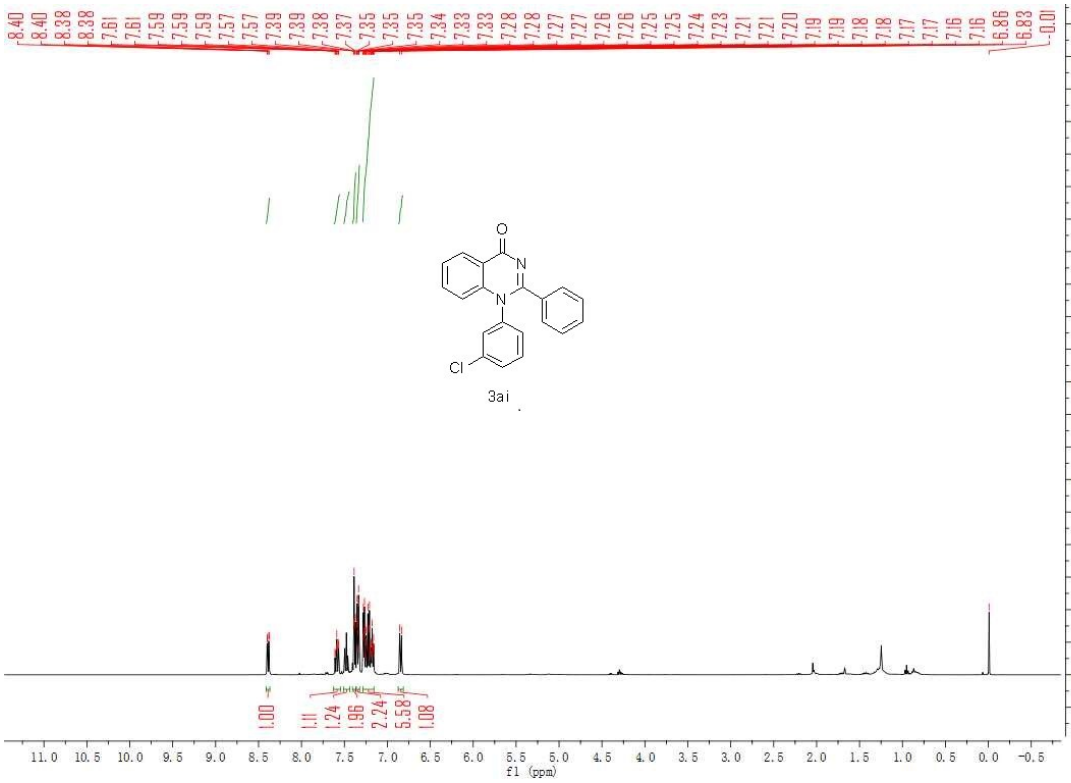
Cl
3ah
f1 (ppm)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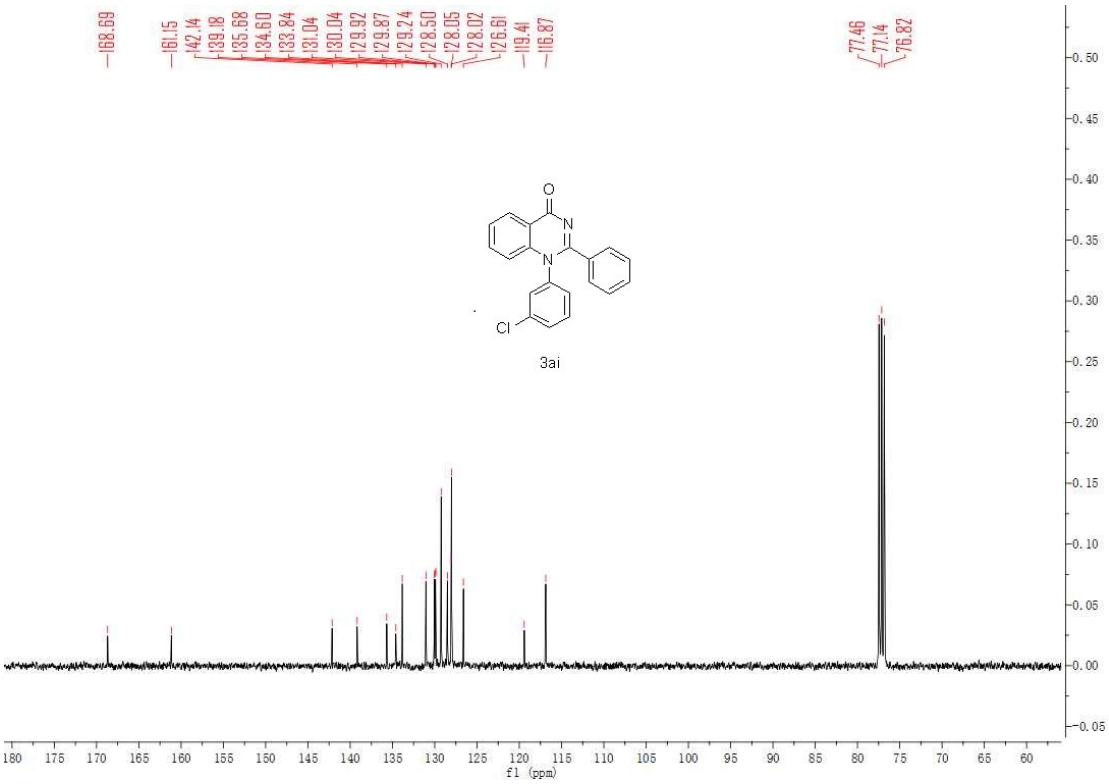
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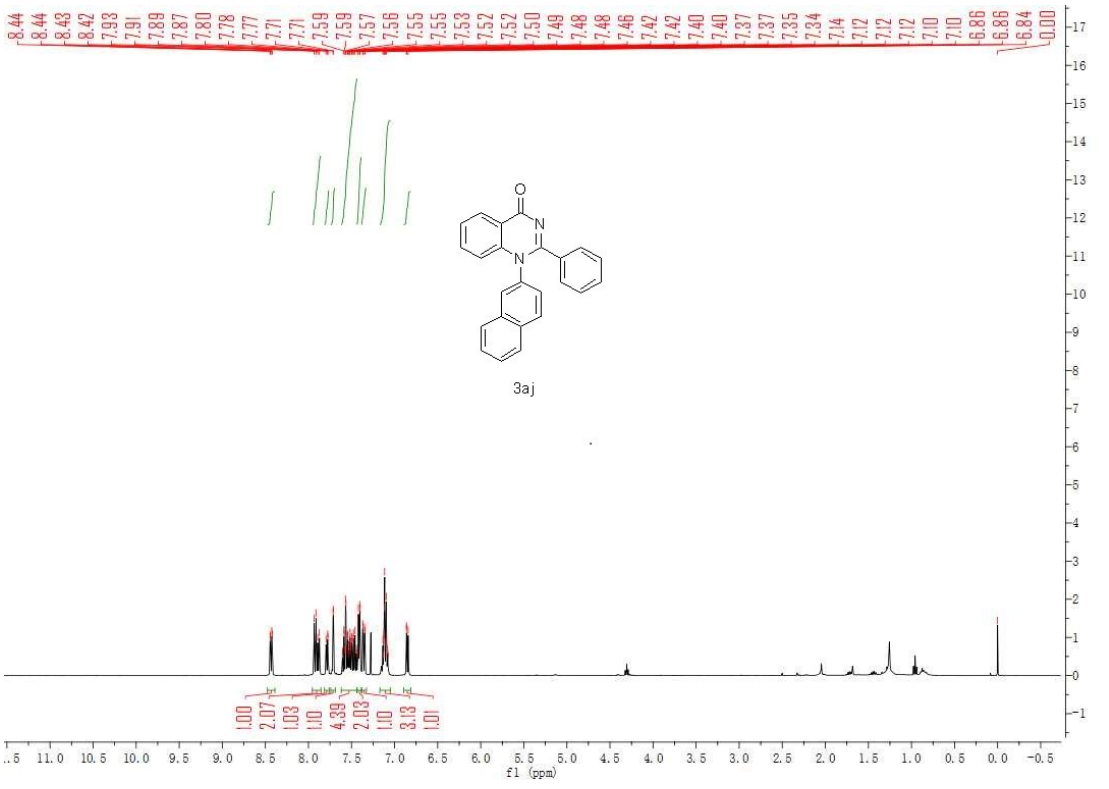
Cl
3ai
f1 (ppm)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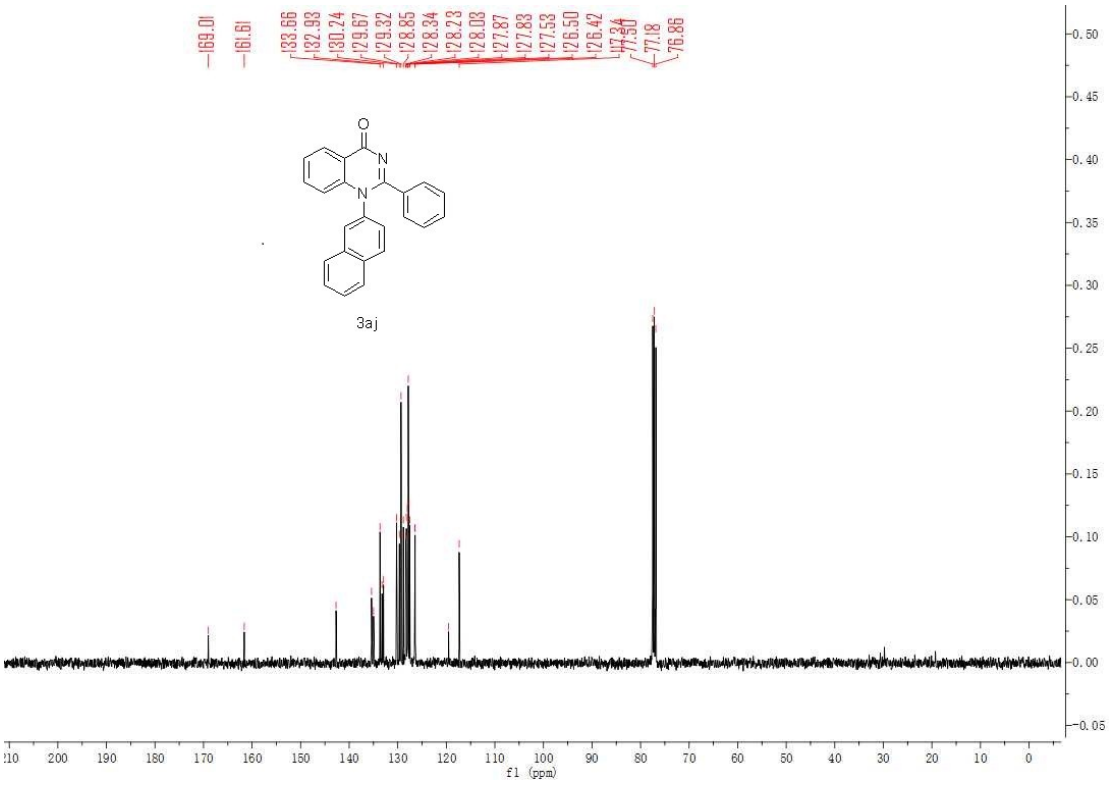
3aj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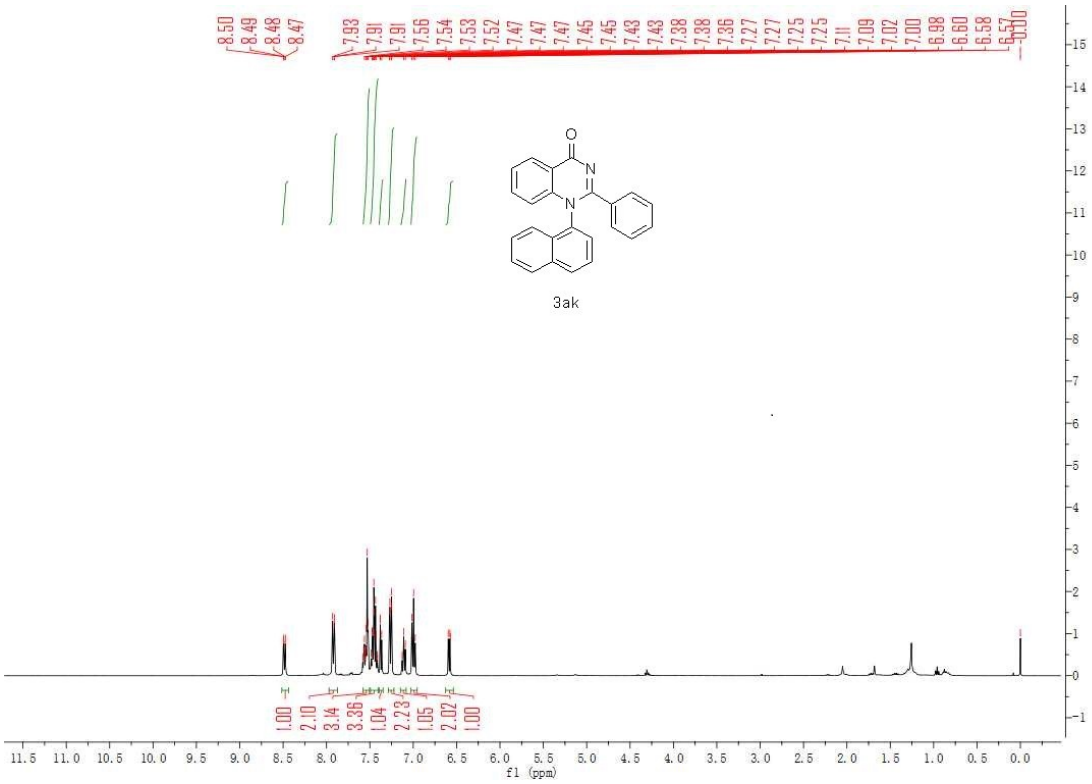
f1 (ppm)

3aj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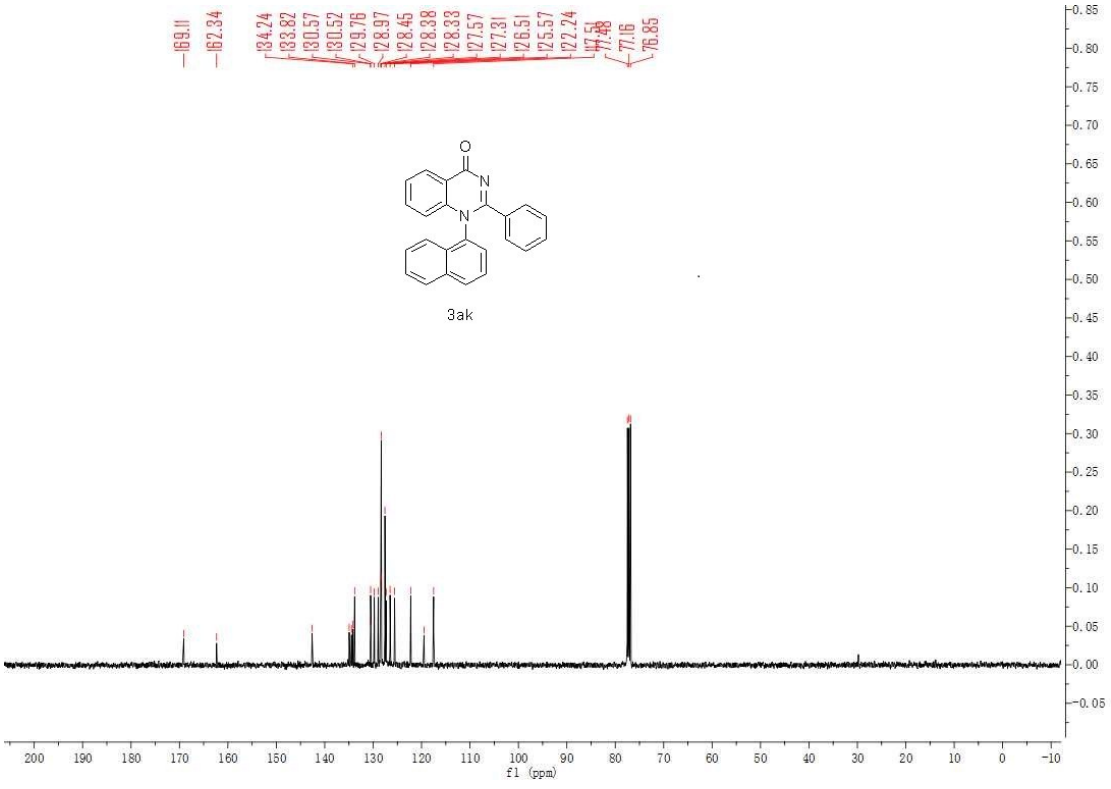
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129.76
128.97
128.45
128.38
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125.57
122.24
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76.85
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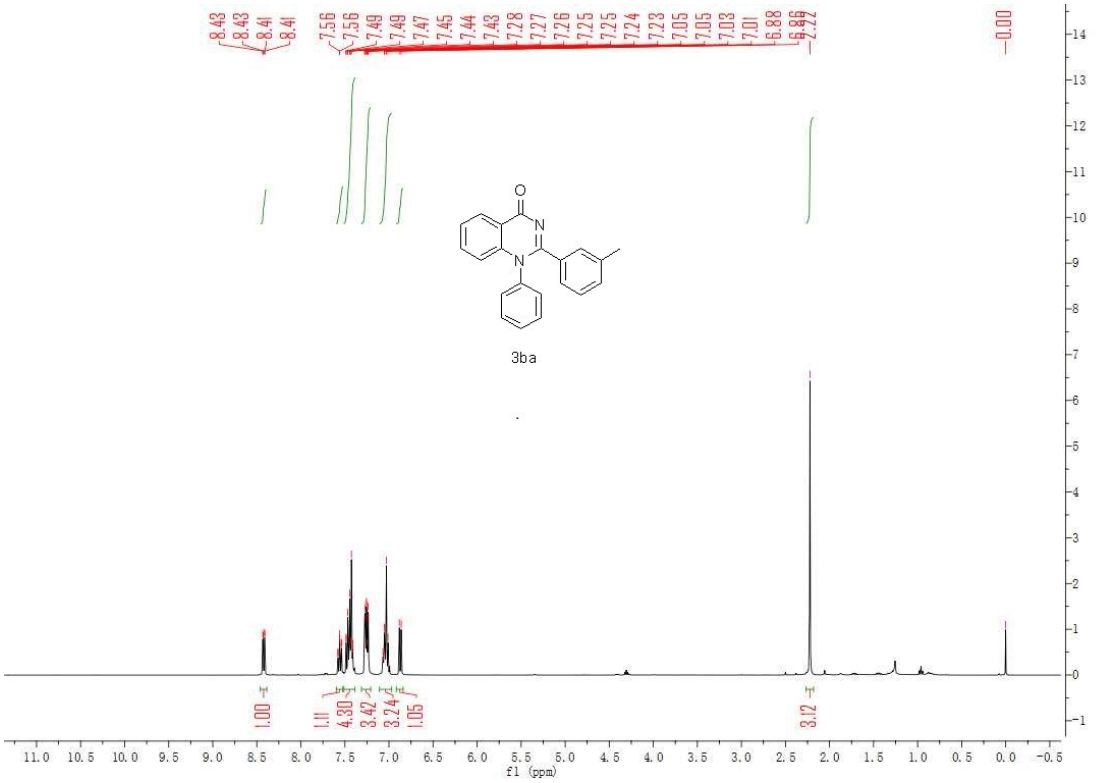
N
3ak
f1 (ppm)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7.26
7.25
7.25
7.24
7.23
7.05
7.05
7.03
7.01
6.88
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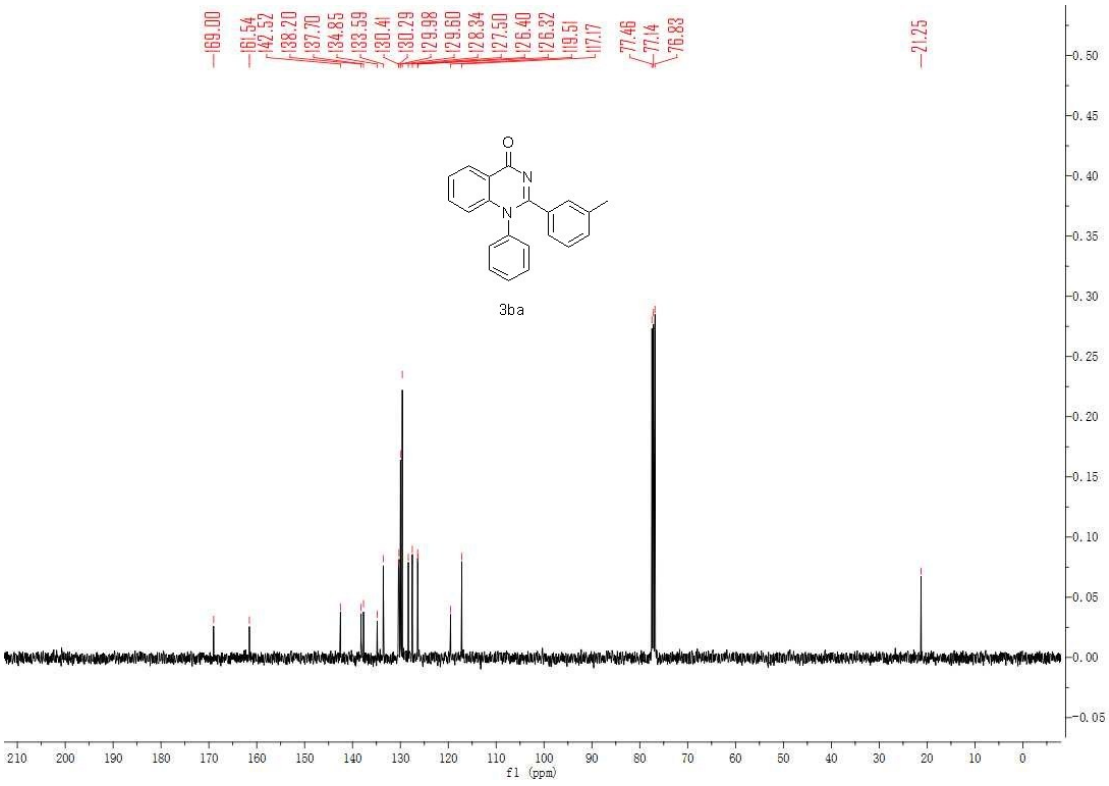
1.11
4.30
3.42
3.24
1.05
3.12
f1 (ppm)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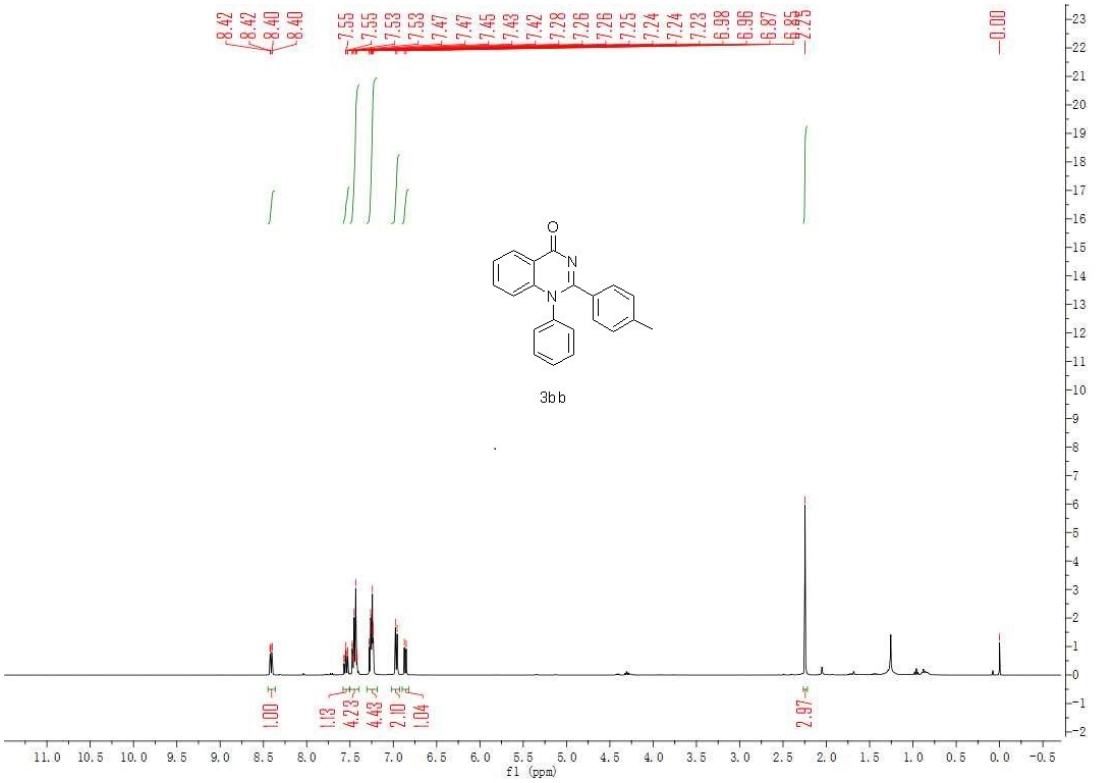
127.50
126.40
126.32
119.51
117.17
77.46
77.14
76.83
21.25
3ba
f1 (ppm)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7.45
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7.42
7.28
7.26
7.26
7.25
7.24
7.24
7.23
6.98
6.96
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4.23
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2.10
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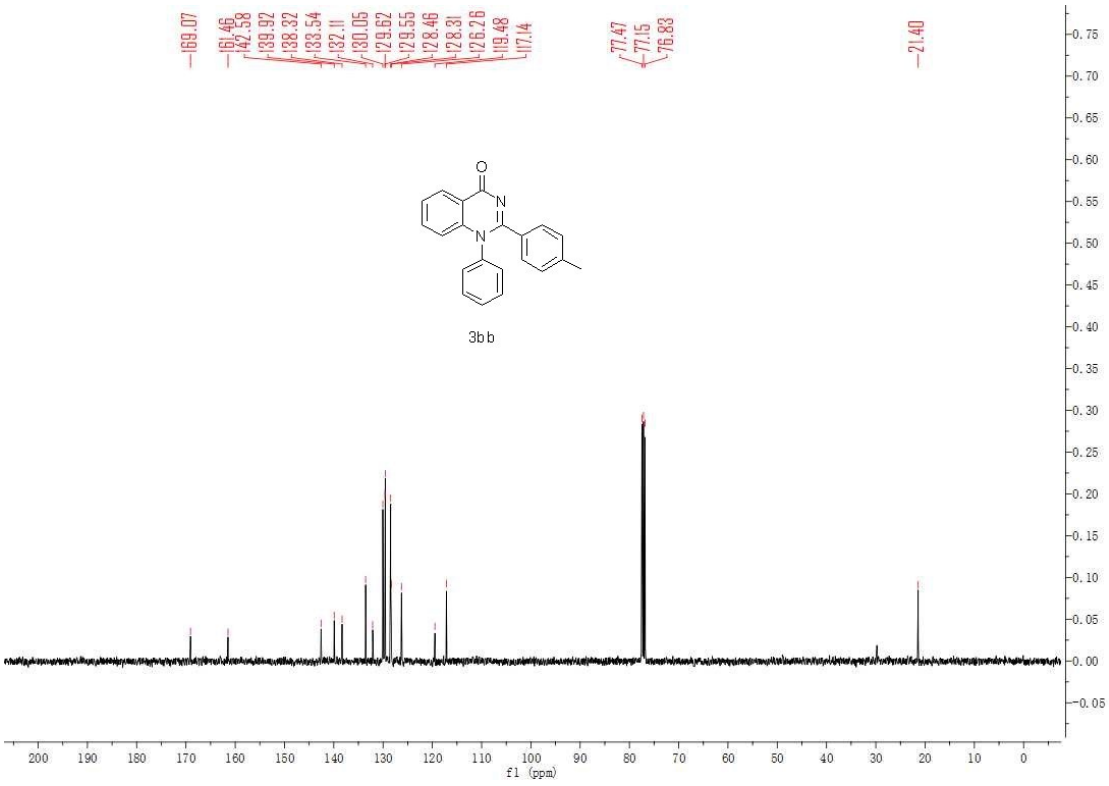
2.97
f1 (ppm)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132.11
130.05
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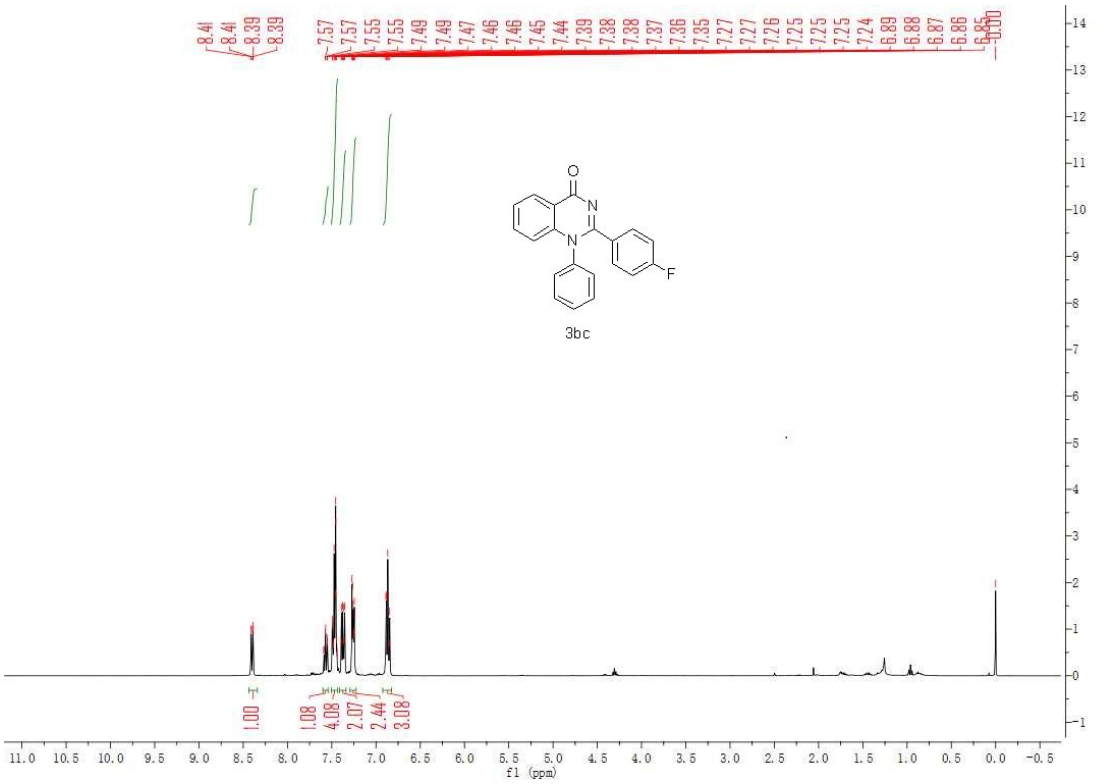
126.26
119.48
117.14
77.47
77.15
76.83
21.40
3bb
f1 (ppm)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7.46
7.45
7.44
7.39
7.38
7.38
7.37
7.36
7.35
7.27
7.27
7.26
7.25
7.25
7.25
7.24
6.89
6.88
6.87
6.86
6.85
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N
F
3bc
1.00
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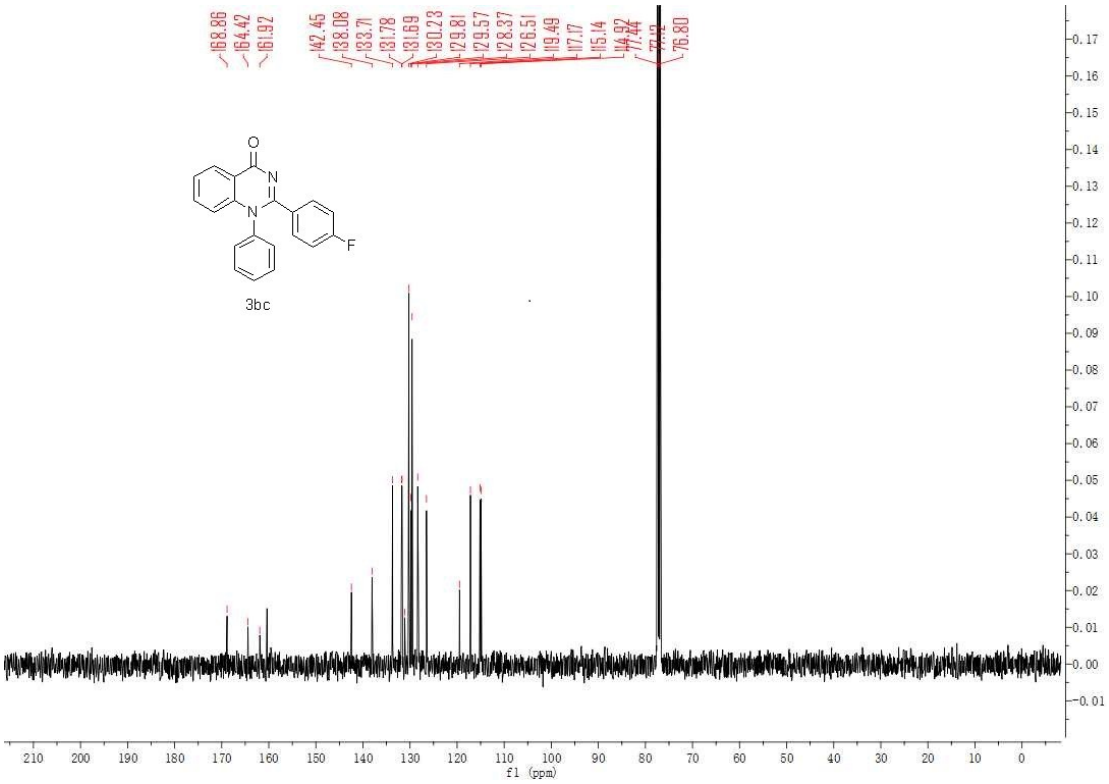
4.08
2.07
2.44
8.08
f1 (ppm)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O
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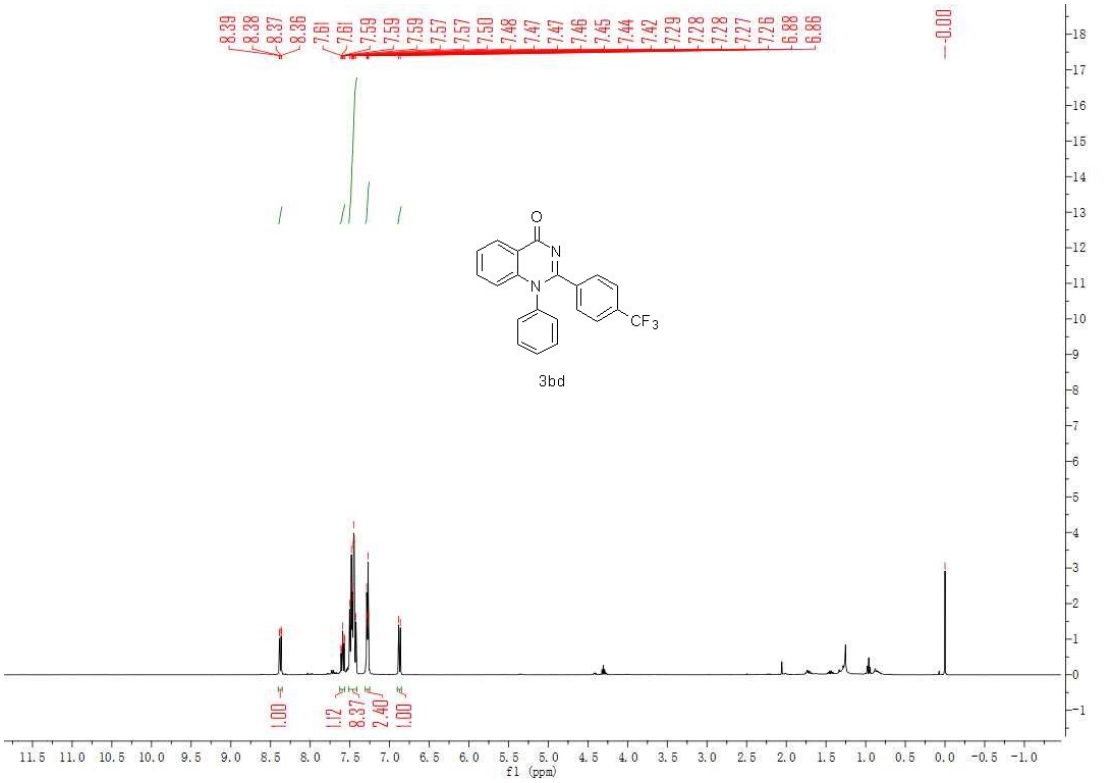
N
F
3bc
f1 (ppm)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7.47
7.46
7.45
7.44
7.42
7.29
7.28
7.28
7.27
7.26
6.88
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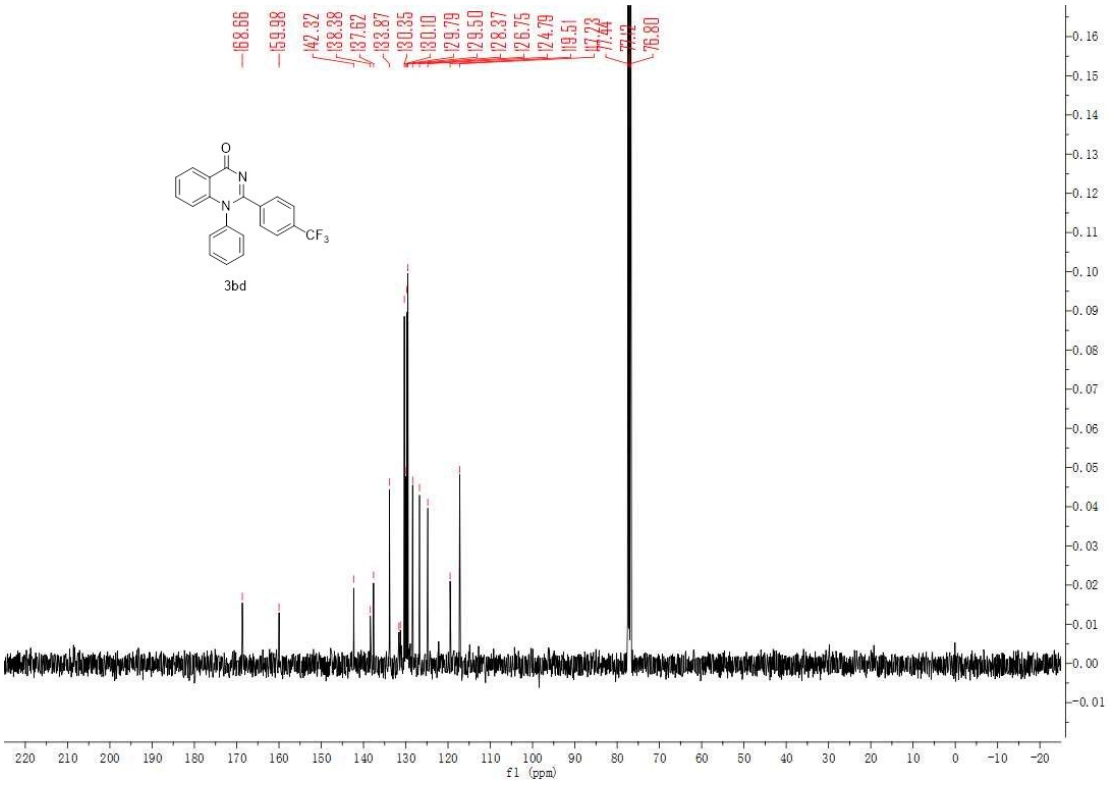
O
N
N
CF3
3bd
1.00
1.12
8.37
2.40
1.00
f1 (ppm)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129.79
129.50
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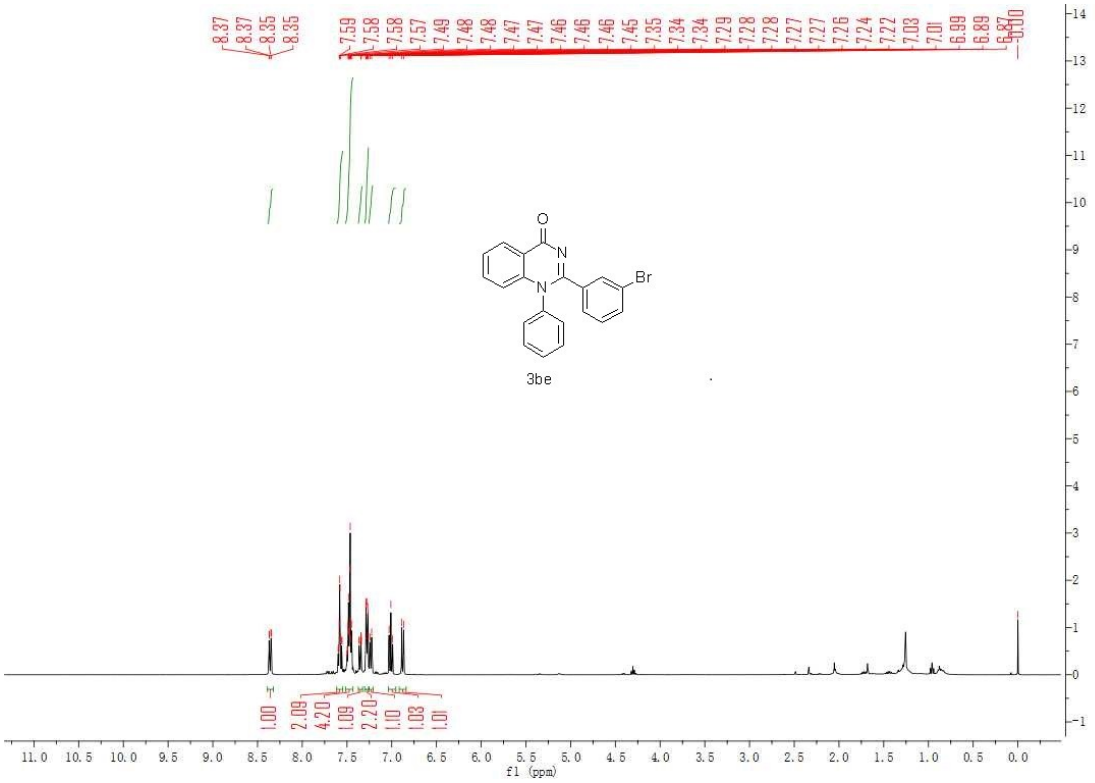
126.75
124.79
119.51
77.44
76.80
O
N
N
CF3
3bd
f1 (ppm)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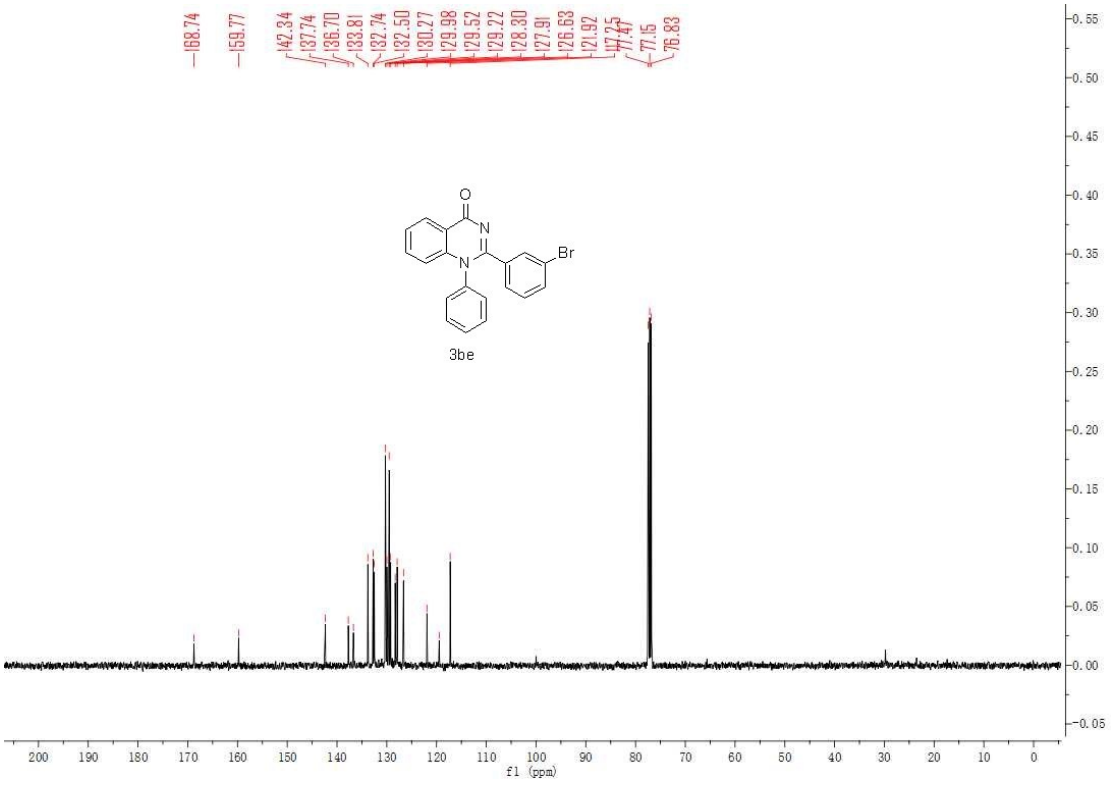
7.28
7.28
7.27
7.27
7.26
7.24
7.22
7.03
7.01
6.99
6.89
6.87
0.00
O
N
N
Br
3be
1.00
2.09
4.20
1.09
2.20
1.10
1.03
1.01
f1 (ppm)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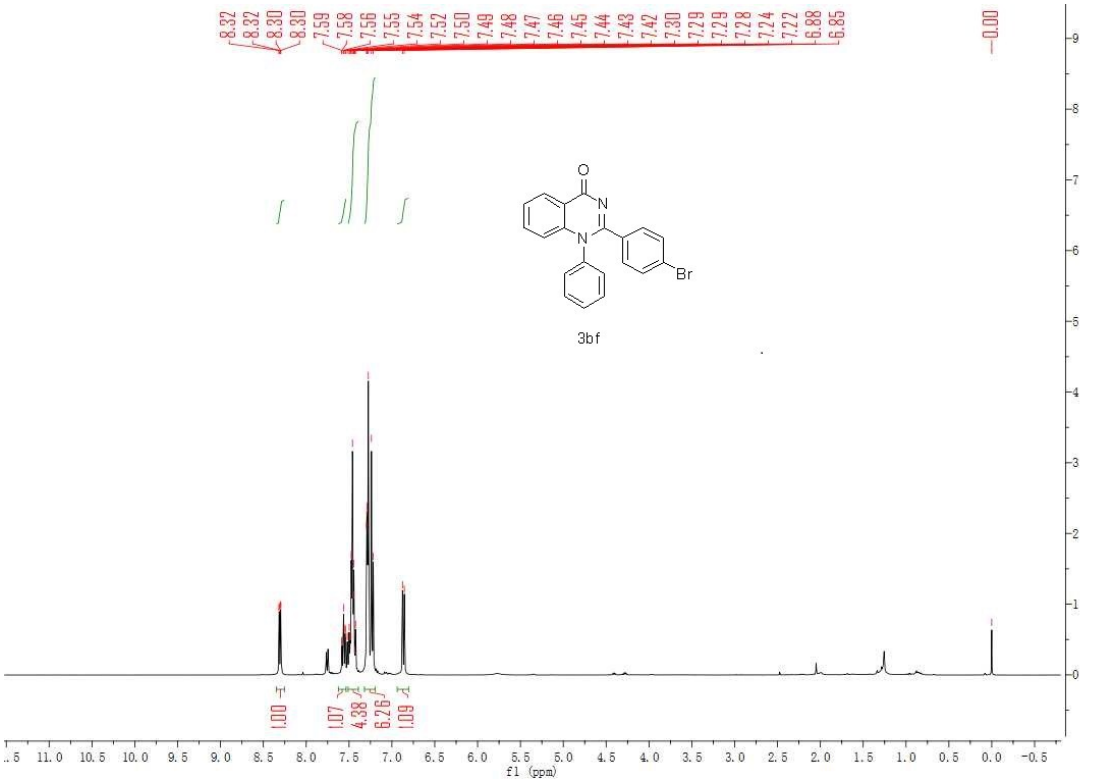
126.63
121.92
77.47
77.15
76.83
O
N
N
Br
3be
f1 (ppm)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7.52
7.50
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7.45
7.44
7.43
7.42
7.30
7.29
7.29
7.28
7.24
7.22
6.88
6.85
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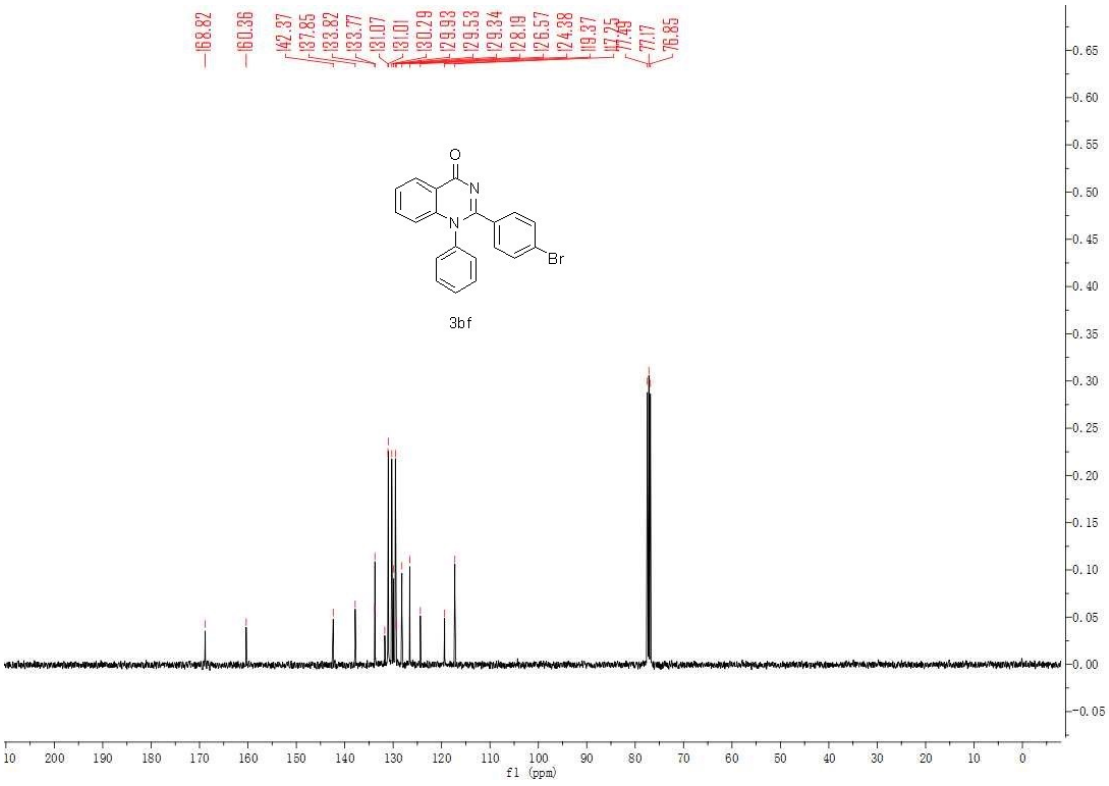
O
N
N
Br
3bf
1.00
1.07
4.38
6.26
1.09
f1 (ppm)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131.01
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129.93
129.53
129.34
128.19
126.57
124.38
119.37
117.25
77.49
77.17
76.85
O
N
N
Br
3bf
f1 (ppm)