

Electronic Supporting Information

Visible Light induced Cascade *N*-Alkylation/Amidation Reaction of Quinazolin-4(3*H*)-ones and Related *N*-Heterocycles

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General remarks

All reagents were obtained from commercial sources and used as received. Ethanol (anhydrous) were used as received. Technical grade petroleum ether (40-60°C bp.) and ethyl acetate were used for chromatography column.

¹H NMR spectra were recorded in CDCl₃ at ambient temperature on Bruker AVANCE I 500 spectrometers at 500.1 MHz, using the solvent as internal standard (7.26 ppm). ¹³C NMR spectra were obtained at 125 MHz and referenced to the internal solvent signals (central peak is 77.2 ppm). Chemical shift (δ) and coupling constants (J) are given in ppm and in Hz, respectively. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet, and br. for broad.

GC analyses were performed with GC-7890A (Agilent) equipped with a 30-m capillary column (HP-5ms, fused silica capillary column, 30 M*0.25 mm*0.25 mm film thickness), was used with N₂/air as vector gas. GCMS were measured by GCMS-7890A-5975C (Agilent) with GC-7890A equipped with a 30-m capillary column (HP-5ms, fused silica capillary column, 30 M*0.25 mm*0.25 mm film thickness), was used with helium as vector gas. HRMS were measured by MAT 95XP (Termol) (LCMS-IT-TOF).

Compounds **3i** were collected at 100 K on a Rigaku Oxford Diffraction Supernova Dual Source, Cu at Zero equipped with an AtlasS2 CCD using Cu K α radiation. Data reduction was carried out with the diffractometer's software.

General procedure for I₂/K₂CO₃ promoted oxidative N-alkylation/amidation of quinazolinone derivatives with alkyl bromides or chlorides

Quinazolinone derivative (0.25 mmol), alkyl bromide or chloride (0.375 mmol), I₂ (0.25 mmol), K₂CO₃ (0.375 mmol), and DMC (0.5 mL) were introduced in Schlenck tube under 36W white LEDs under air atmosphere, equipped with magnetic stirring bar and was stirred at 100 °C. After 6 h, the solvent was then evaporated under vacuum and the desired product was purified by using a silica gel chromatography column and a mixture of petrol ether/ethyl acetate as eluent.



Figure S1. A photo for the reaction set-up.

General procedure for I₂/K₂CO₃ promoted oxidative *N*-alkylation/amidation of *N*-heterocycles with benzyl bromide

N-heterocycle (0.25 mmol), benzyl bromide (0.375 mmol), I₂ (0.25 mmol), K₂CO₃ (0.375 mmol), and DMC (0.5 mL) were introduced in Schlenk tube under 36W white LEDs under air atmosphere, equipped with magnetic stirring bar and was stirred at 100 °C. After 6 h, the solvent was then evaporated under vacuum and the desired product was purified by using a silica gel chromatography column and a mixture of petrol ether/ethyl acetate as eluent.

Procedure for the synthesis of 1,3-dibenzyl-4-oxo-3,4-dihydroquinazolin-1-ium bromide (compound 8)

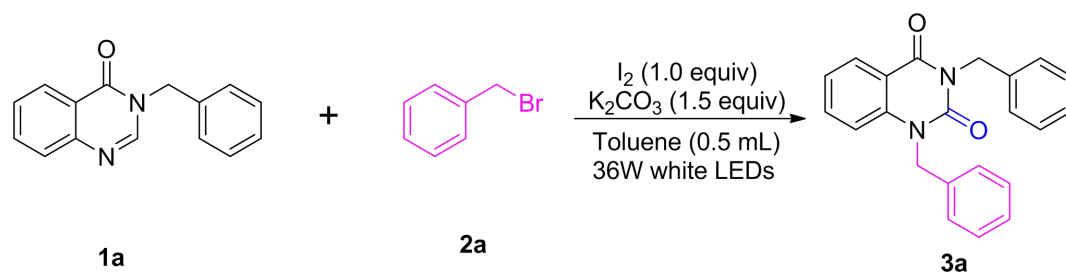
3-Benzylquinazolin-4(3H)-one (0.5 mmol), benzyl bromide (0.75 mmol), acetone (2.0 mL) were introduced in Schlenk tube, equipped with magnetic stirring bar and was stirred at 100 °C. After 12 h, the reaction mixture was filtered, and the residue of the product was washed with diethyl ether (20 mL × 3), and dried under vacuum.

Procedure for the synthesis of 3-benzyl-2-(benzyloxy)quinazolin-4(3H)-one (compound 9)

3-Benzyl-2-chloroquinazolin-4(3H)-one (0.5 mmol), benzyl alcohol (0.75 mmol), KO^tBu (0.75 mmol), 1,4-dioxane (2.0 mL) were introduced in Schlenk tube, equipped with magnetic stirring bar and was stirred at 100 °C. After 18 h, the solvent was then evaporated under vacuum and the desired product was purified by using a silica gel chromatography column and a mixture of petrol ether/ethyl acetate as eluent.

The data of reaction optimization

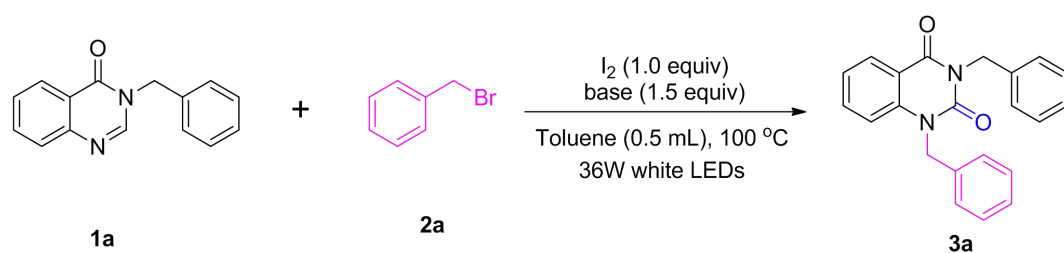
Table S1. Screening of different temperature^a



Entry	Temp. (°C)	Yield (%)
1	R.T	6
2	50	47
3	90	75
4	95	83
5	100	95
6	105	94

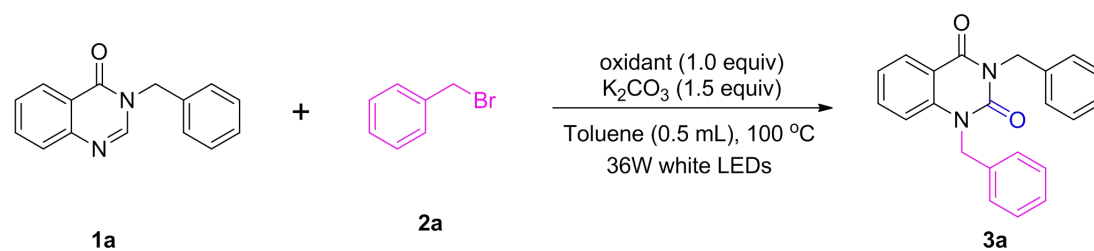
^aReaction conditions: quinazolin-4(3*H*)-one (0.25 mmol), benzyl bromide (1.5 equiv), I₂ (1.0 equiv), K₂CO₃ (1.5 equiv), toluene (0.5 mL) under 36W white LEDs for 6 h, air atmosphere.

Table S2. Screening of different bases^a



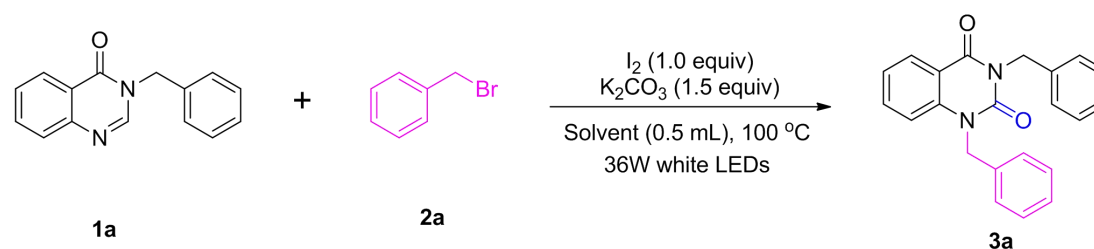
Entry	Base	Yield(%)
1	K ₂ CO ₃	95
2	KOAc	84
3	<i>t</i> -BuOK	43
4	C ₆ H ₅ COOK	68
5	K ₃ PO ₄	88
6	CF ₃ COOK	8
7	KOTf	---
8	KOH	trace
9	Cs ₂ CO ₃	18
10	NaOH	72
11	CaHCO ₃	82

^aReaction conditions: quinazolin-4(3*H*)-one (0.25 mmol), benzyl bromide (1.5 equiv), I₂ (1.0 equiv), base (1.5 equiv), toluene (0.5 mL) at 100°C under 36W white LEDs for 6 h, air atmosphere.

Table S3. Screening of different oxidants^a

Entry	Oxidant	Yield(%)
1	I ₂	95
2	C ₆ Cl ₄ O ₂	trace
3	CuSO ₄	trace
4	TBHP	8
5	CuO	25

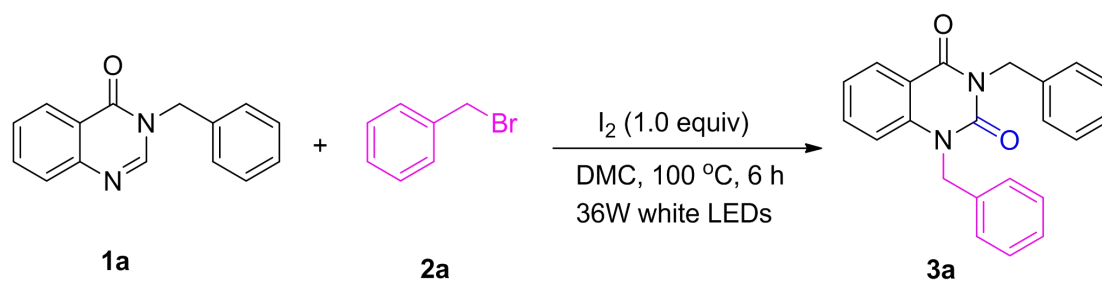
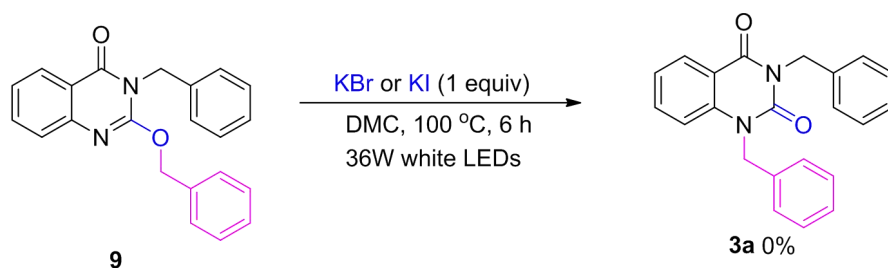
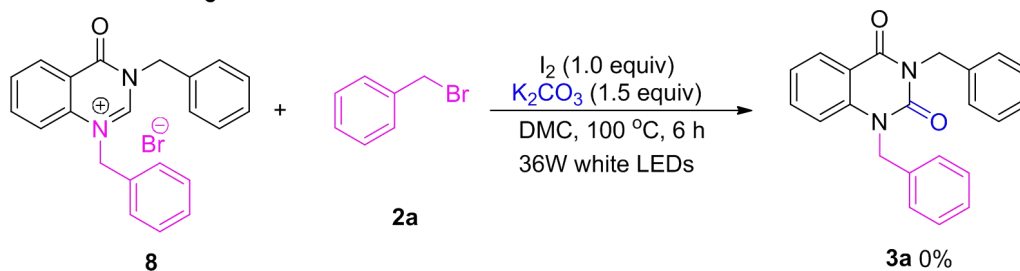
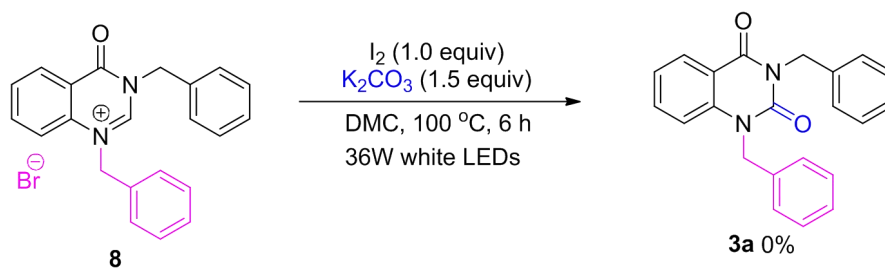
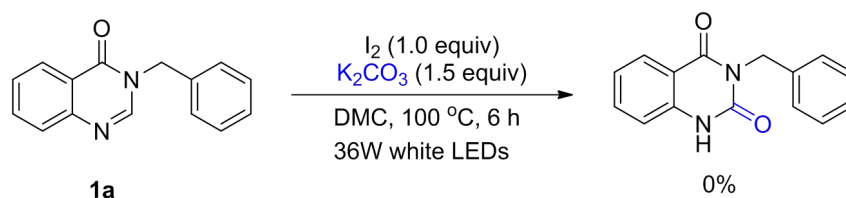
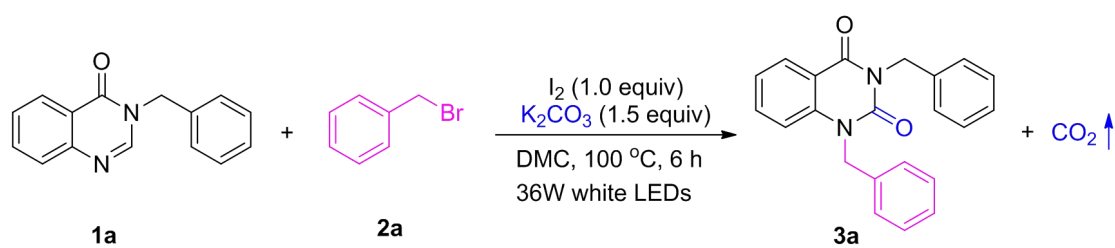
^aReaction conditions: quinazolin-4(3*H*)-one (0.25 mmol), benzyl bromide (1.5 equiv), oxidant (1.0 equiv), K₂CO₃ (1.5 equiv), toluene (0.5 mL) at 100 °C under 36W white LEDs for 6 h, air atmosphere.

Table S3. Screening of different solvents^a

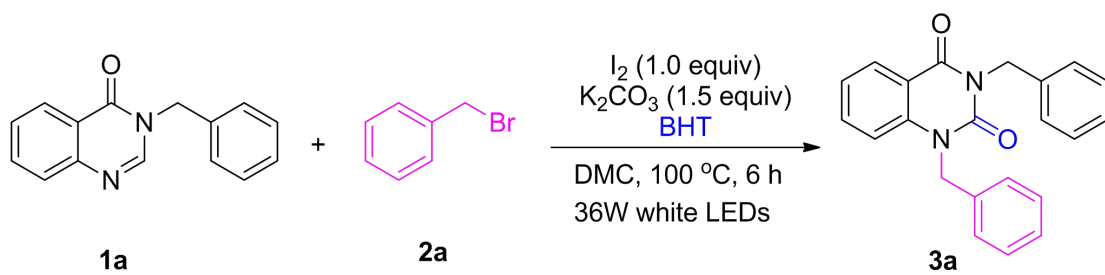
Entry	Solvent	Yield(%)
1	1,4-dioxane	87
2	Toluene	95
3	DMF	36
4	DMC	99
5	THF	55
6	Ethanol	51
7	1,2-Dichloroethane	41

^aReaction conditions: quinazolin-4(3*H*)-one (0.25 mmol), benzyl bromide (1.5 equiv), I₂ (1.0 equiv), K₂CO₃ (1.5 equiv), solvent (0.5 mL) at 100 °C under 36W white LEDs for 6 h, air atmosphere.

Scheme S1 Control experiments.



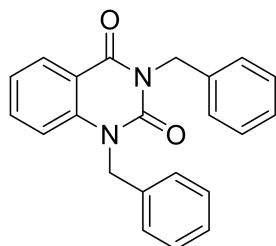
Without K_2CO_3 : 0%
 O_2 instead of K_2CO_3 : 0%
 Under N_2 atmosphere : 95%



Without BHT : 99%
With 1.0 equiv. of BHT : 43%
With 2.2 equiv. of BHT : 0%

Characterization data of substrates

1,3-dibenzylquinazoline-2,4(1H,3H)-dione^[1] (3a)

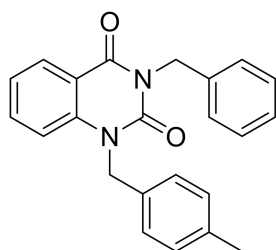


White solid, yield = 76%, 65 mg.

¹H NMR (500 MHz, CDCl₃): δ (ppm) = 8.27 (dd, 1H, *J* = 8.0, 1.5 Hz), 7.60-7.54 (m, 3H), 7.37-7.34 (m, 4H), 7.31-7.29 (m, 2H), 7.28-7.22 (m, 3H), 7.13-7.12 (m, 1H), 5.40 (s, 2H), 5.37 (s, 2H).

¹³C NMR (125 MHz, CDCl₃): δ (ppm) = 161.8, 151.5, 140.0, 137.0, 135.6, 135.1, 139.2, 139.03, 129.00, 128.5, 127.67, 127.66, 126.4, 123.1, 115.8, 114.4, 47.4, 45.2.

3-benzyl-1-(4-methylbenzyl)quinazoline-2,4(1H,3H)-dione (3b)

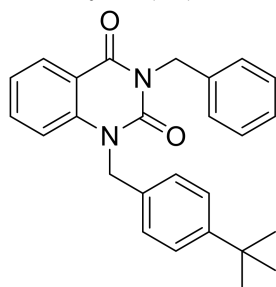


White solid, yield = 57%, 51 mg.

¹H NMR (500 MHz, CDCl₃): δ (ppm) = 8.27 (dd, 1H, *J* = 7.5, 1.5 Hz), 7.59-7.53 (m, 3H), 7.37-7.34 (m, 2H), 7.31-7.28 (m, 1H), 7.24-7.21 (m, 1H), 7.18-7.14 (m, 5H), 5.37 (s, 2H), 5.36 (s, 2H), 2.24 (s, 3H).

¹³C NMR (125 MHz, CDCl₃): δ (ppm) = 161.9, 151.6, 140.1, 137.5, 137.2, 135.2, 132.7, 129.8, 129.2, 129.1, 128.6, 127.8, 126.6, 123.2, 115.9, 114.6, 47.3, 45.3, 21.2.

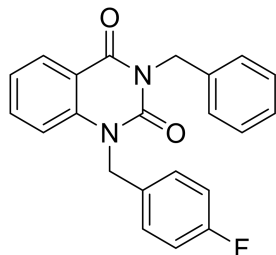
3-benzyl-1-(4-(tert-butyl)benzyl)quinazoline-2,4(1H,3H)-dione (3c)



Yellow solid, yield = 61%, 61 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.27 (dd, 1H, $J = 7.5, 1.5$ Hz), 7.60-7.55 (m, 3H), 7.38-7.34 (m, 4H), 7.31-7.30 (m, 1H), 7.25-7.17 (m, 4H), 5.37 (s, 4H), 1.32 (s, 9H).
 ^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 162.0, 151.6, 150.7, 140.2, 137.2, 135.2, 132.7, 129.2, 129.1, 128.6, 127.8, 126.3, 126.0, 123.2, 115.8, 114.6, 47.2, 45.3, 34.6, 31.4.
HRMS (EI): m/z calcd for $\text{C}_{26}\text{H}_{27}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 399.2067, found 399.2068.

3-benzyl-1-(4-fluorobenzyl)quinazoline-2,4(1H,3H)-dione (3d)



Yellow solid, yield = 70%, 63 mg.

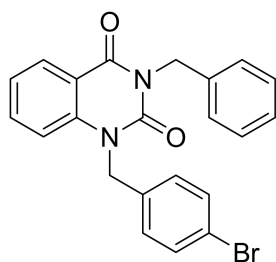
^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.28 (dd, 1H, $J = 8.0, 2.0$ Hz), 7.59-7.56 (m, 3H), 7.37-7.34 (m, 2H), 7.31-7.30 (m, 1H), 7.27-7.23 (m, 3H), 7.11 (d, 1H, $J = 8.5$ Hz), 7.06-7.02 (m, 2H), 5.36 (s, 4H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 163.3 (d, $J_{\text{CF}} = 244.75$ Hz), 161.9, 151.6, 139.9, 137.1, 135.3, 131.5 (d, $J_{\text{CF}} = 3.25$ Hz), 129.4, 129.2, 128.6, 128.4 (d, $J_{\text{CF}} = 8.0$ Hz), 127.8, 123.4, 116.2 (d, $J_{\text{CF}} = 21.5$ Hz), 115.9, 114.3, 46.9, 45.3.

^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -114.5.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{FN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 361.1346, found 361.1346.

3-benzyl-1-(4-bromobenzyl)quinazoline-2,4(1H,3H)-dione (3e)



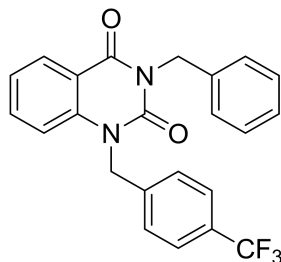
White solid, yield = 53%, 56 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.28 (dd, 1H, $J = 8.0, 1.5$ Hz), 7.58-7.55 (m, 3H), 7.48-7.46 (m, 2H), 7.37-7.33 (m, 2H), 7.31-7.28 (m, 1H), 7.27-7.24 (m, 1H), 7.14 (d, 2H, $J = 8.0$ Hz), 7.06 (d, 1H, $J = 8.0$ Hz), 5.36 (s, 2H), 5.33 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.8, 151.5, 139.8, 137.0, 135.3, 134.8, 132.3, 129.4, 129.2, 128.6, 128.4, 127.9, 123.4, 121.7, 115.9, 114.3, 47.0, 45.3.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{BrN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 421.0546, found 421.0547.

3-benzyl-1-(4-(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (3f)



White solid, yield = 56%, 57 mg.

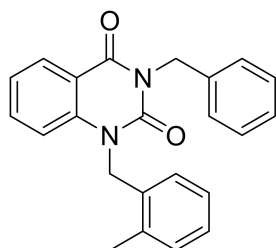
^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.29 (dd, 1H, J = 8.0, 1.5 Hz), 7.62-7.56 (m, 5H), 7.38-7.30 (m, 5H), 7.26 (d, 1H, J = 7.5 Hz), 7.03 (d, 1H, J = 8.5 Hz), 5.44 (s, 2H), 5.36 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.8, 151.6, 139.9, 139.8, 137.0, 135.4, 130.3 (q, J_{CF} = 32.5 Hz), 129.6, 129.2, 128.7, 127.9, 126.9, 126.2 (q, J_{CF} = 3.6 Hz), 125.1 (q, J_{CF} = 270.3 Hz), 123.6, 116.0, 114.2, 47.2, 45.4.

^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -62.6.

HRMS (EI): m/z calcd for $\text{C}_{23}\text{H}_{18}\text{F}_3\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 411.1314, found 411.1313.

3-benzyl-1-(2-methylbenzyl)quinazoline-2,4(1H,3H)-dione (3g)

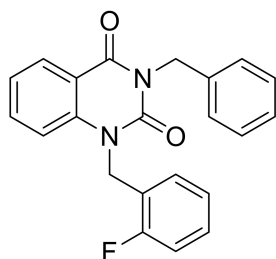


White solid, yield = 73%, 65 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.30 (dd, 1H, J = 8.0, 2.0 Hz), 7.59-7.58 (m, 2H), 7.55-7.51 (m, 1H), 7.36-7.33 (m, 2H), 7.31-7.18 (m, 4H), 7.10-7.07 (m, 1H), 6.90 (d, 1H, J = 8.0 Hz), 6.80-6.78 (m, 1H), 5.37 (s, 2H), 5.34 (s, 2H), 2.46 (s, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 151.4, 140.2, 137.2, 135.3, 134.9, 133.0, 130.8, 129.23, 129.20, 128.6, 127.8, 127.4, 126.6, 124.4, 123.3, 115.8, 114.6, 45.7, 45.3, 19.3.

3-benzyl-1-(2-fluorobenzyl)quinazoline-2,4(1H,3H)-dione (3h)



Yellow solid, yield = 93%, 84 mg.

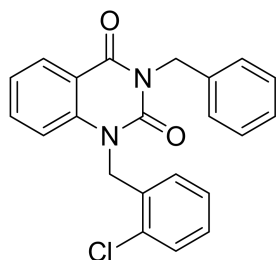
^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.27 (dd, 1H, J = 8.0, 2.0 Hz), 7.60-7.56 (m, 3H), 7.37-7.34 (m, 2H), 7.32-7.29 (m, 1H), 7.28-7.23 (m, 2H), 7.15-7.04 (m, 4H), 5.46 (s, 2H), 5.37 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.8, 161.4 (d, $J_{\text{CF}} = 243.75$ Hz), 151.6, 139.7, 137.1, 135.4, 129.6 (d, $J_{\text{CF}} = 7.5$ Hz), 129.3, 129.1, 128.6, 128.2 (d, $J_{\text{CF}} = 3.75$ Hz), 127.8, 124.9 (d, $J_{\text{CF}} = 3.75$ Hz), 123.4, 122.9 (d, $J_{\text{CF}} = 12.5$ Hz), 115.9 (d, $J_{\text{CF}} = 6.25$ Hz), 115.7, 114.1 (d, $J_{\text{CF}} = 1.25$ Hz), 45.3, 41.2 (d, $J_{\text{CF}} = 5.0$ Hz).

^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -118.5.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{FN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 361.1346, found 361.1350.

3-benzyl-1-(2-chlorobenzyl)quinazoline-2,4(1H,3H)-dione (3i)

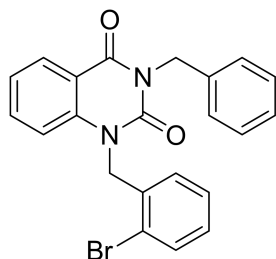


White solid, yield = 73%, 69 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.30 (dd, 1H, $J = 8.0, 1.5$ Hz), 7.60-7.54 (m, 3H), 7.46 (dd, 1H, $J = 8.0, 1.5$ Hz), 7.37-7.34 (m, 2H), 7.32-7.29 (m, 1H), 7.27-7.23 (m, 2H), 7.17-7.14 (m, 1H), 6.94-6.90 (m, 2H), 5.48 (s, 2H), 5.38 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.8, 151.4, 139.7, 137.0, 135.4, 132.8, 132.6, 129.9, 129.3, 129.2, 128.9, 128.6, 127.8, 127.5, 126.7, 123.4, 115.8, 114.5, 45.33, 45.30.

3-benzyl-1-(2-bromobenzyl)quinazoline-2,4(1H,3H)-dione (3j)



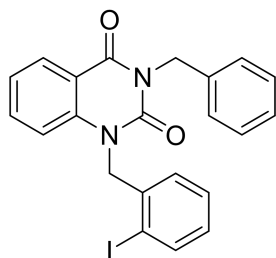
Yellow solid, yield = 83%, 87 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.29 (dd, 1H, $J = 8.0, 1.5$ Hz), 7.65 (dd, 1H, $J = 7.5, 1.5$ Hz), 7.59-7.54 (m, 3H), 7.37-7.33 (m, 2H), 7.31-7.30 (m, 1H), 7.28-7.24 (m, 1H), 7.21-7.15 (m, 2H), 6.91-6.86 (m, 2H), 5.43 (s, 2H), 5.37 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.9, 151.5, 139.8, 137.0, 135.5, 134.2, 133.3, 129.3, 129.24, 129.21, 128.6, 128.1, 127.8, 126.8, 123.5, 122.4, 115.9, 114.5, 48.0, 45.3.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{BrN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 421.0546, found 421.0546.

3-benzyl-1-(2-iodobenzyl)quinazoline-2,4(1H,3H)-dione (3k)



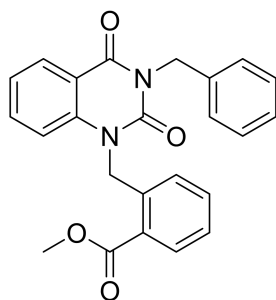
White solid, yield = 73%, 85 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.30 (dd, 1H, J = 8.0, 2.0 Hz), 7.93 (dd, 1H, J = 8.0, 1.0 Hz), 7.60-7.54 (m, 3H), 7.37-7.34 (m, 2H), 7.31-7.21 (m, 3H), 7.02-6.99 (m, 1H), 6.85-6.80 (m, 2H), 5.37 (s, 2H), 5.33 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.8, 151.4, 139.9, 139.7, 137.0, 136.8, 135.5, 129.4, 129.3, 129.2, 128.9, 128.6, 127.8, 126.2, 123.5, 115.8, 114.6, 97.2, 53.1, 45.3.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{IN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 469.0407, found 469.0408.

methyl 2-((3-benzyl-2,4-dioxo-3,4-dihydroquinazolin-1(2H)-yl)methyl)benzoate (3l)



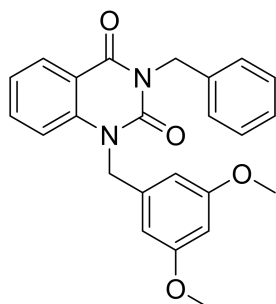
Yellow solid, yield = 65%, 65 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.30 (dd, 1H, J = 8.0, 1.5 Hz), 8.13 (dd, 1H, J = 8.0, 1.5 Hz), 7.58-7.56 (m, 2H), 7.55-7.51 (m, 1H), 7.42-7.32 (m, 4H), 7.30-7.28 (m, 1H), 7.27-7.23 (m, 1H), 6.98-6.94 (m, 2H), 5.84 (s, 2H), 5.36 (s, 2H), 4.00 (s, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 167.5, 162.0, 151.5, 140.2, 137.7, 137.2, 135.4, 133.2, 131.8, 129.3, 129.2, 128.6, 128.0, 127.8, 127.4, 125.6, 123.4, 115.9, 114.6, 52.4, 56.8, 45.3.

HRMS (EI): m/z calcd for $\text{C}_{24}\text{H}_{21}\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$ 401.1495, found 401.1496.

3-benzyl-1-(3,5-dimethoxybenzyl)quinazoline-2,4(1H,3H)-dione (3m)



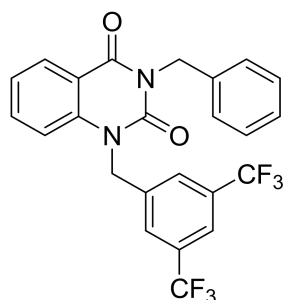
White solid, yield = 51%, 51 mg.

¹H NMR (500 MHz, CDCl₃): δ (ppm) = 8.26 (dd, 1H, *J* = 7.5, 1.5 Hz), 7.58-7.54 (m, 3H), 7.34-7.31 (m, 2H), 7.28-7.22 (m, 2H), 7.14 (d, 1H, *J* = 8.5 Hz), 6.38-6.35 (m, 3H), 5.36 (s, 2H), 5.32 (s, 2H), 3.72 (s, 6H).

¹³C NMR (125 MHz, CDCl₃): δ (ppm) = 161.9, 161.4, 151.6, 140.1, 138.3, 137.2, 135.3, 129.3, 129.1, 128.6, 127.8, 123.3, 115.9, 114.6, 104.6, 99.3, 55.4, 47.6, 45.2.

HRMS (EI): *m/z* calcd for C₂₄H₂₃N₂O₄ [M+H]⁺ 403.1652, found 403.1652.

3-benzyl-1-(3,5-bis(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (3n)



White solid, yield = 63%, 75 mg.

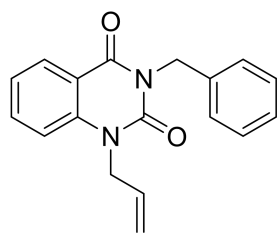
¹H NMR (500 MHz, CDCl₃): δ (ppm) = 8.32 (dd, 1H, *J* = 8.0, 2.0 Hz), 7.84 (s, 1H), 7.73 (s, 2H), 7.64-7.60 (m, 1H), 7.55 (d, 2H, *J* = 7.5 Hz), 7.36-7.28 (m, 4H), 7.03 (d, 1H, *J* = 8.5 Hz), 5.48 (s, 2H), 5.37 (s, 2H).

¹³C NMR (125 MHz, CDCl₃): δ (ppm) = 161.6, 151.6, 139.5, 138.8, 136.8, 135.6, 132.7 (q, *J*_{CF} = 33.3 Hz), 129.9, 129.0, 128.7, 128.0, 126.9, 124.2 (q, *J*_{CF} = 271.1 Hz), 123.9, 122.2 (q, *J*_{CF} = 4.0 Hz), 116.1, 113.6, 46.9, 45.4.

¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -62.9.

HRMS (EI): *m/z* calcd for C₂₄H₁₇F₆N₂O₂ [M+H]⁺ 479.1188, found 479.1189.

1-allyl-3-benzylquinazoline-2,4(1H,3H)-dione^[2] (3o)

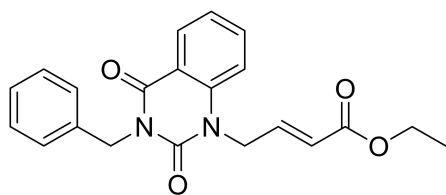


White solid, yield = 63%, 46 mg.

¹H NMR (500 MHz, CDCl₃): δ (ppm) = 8.26 (dd, 1H, *J* = 8.0, 1.5 Hz), 7.66-7.63 (m, 1H), 7.55 (d, 2H, *J* = 7.5 Hz), 7.33 (t, 2H, *J* = 7.0 Hz), 7.29-7.25 (m, 2H), 7.18 (d, 1H, *J* = 8.5 Hz), 5.98-5.90 (m, 1H), 5.32 (s, 2H), 5.30-5.20 (m, 2H), 4.79 (t, 2H, *J* = 2.5 Hz).

¹³C NMR (125 MHz, CDCl₃): δ (ppm) = 161.9, 151.0, 140.0, 137.1, 135.2, 131.3, 129.25, 129.20, 128.6, 127.8, 123.2, 117.8, 115.8, 114.3, 46.2, 45.2.

ethyl (E)-4-(3-benzyl-2,4-dioxo-3,4-dihydroquinazolin-1(2H)-yl)but-2-enoate (3p)



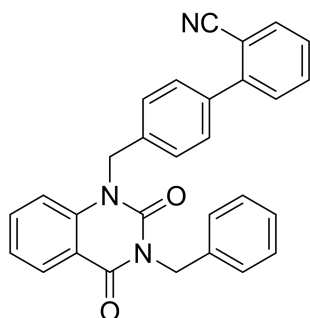
Yellow oil, yield = 86%, 78 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.28 (dd, 1H, J = 7.5, 1.5 Hz), 7.67-7.64 (m, 1H), 7.55-7.53 (m, 2H), 7.35-7.32 (m, 2H), 7.31-7.29 (m, 1H), 7.285-7.280 (m, 1H), 7.06-7.01 (m, 2H), 5.87-5.84 (m, 1H), 5.30 (s, 2H), 4.95-4.94 (m, 2H), 4.19 (q, 2H, J = 7.0 Hz), 1.28 (t, 3H, J = 7.0 Hz).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 165.6, 161.7, 150.9, 140.9, 139.5, 136.9, 135.5, 129.5, 129.2, 128.6, 127.8, 123.6, 123.3, 115.8, 113.9, 60.9, 45.3, 44.6, 14.3.

HRMS (EI): m/z calcd for $\text{C}_{21}\text{H}_{21}\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$ 365.1495, found 365.1494.

4'-((3-benzyl-2,4-dioxo-3,4-dihydroquinazolin-1(2H)-yl)methyl)-[1,1'-biphenyl]-2-carbonitrile (3q)



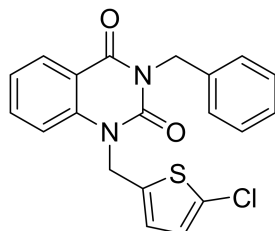
Yellow solid, yield = 86%, 95 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.30 (dd, 1H, J = 7.5, 1.5 Hz), 7.78 (dd, 1H, J = 7.5, 1.0 Hz), 7.67-7.54 (m, 6H), 7.50-7.45 (m, 2H), 7.40-7.34 (m, 4H), 7.31-7.29 (m, 1H), 7.27-7.25 (m, 1H), 7.12 (d, 1H, J = 8.5 Hz), 5.46 (s, 2H), 5.38 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.9, 151.6, 144.9, 140.0, 137.7, 137.1, 136.4, 135.5, 134.0, 133.1, 130.2, 129.5, 129.4, 129.2, 128.6, 127.9, 127.8, 127.0, 123.4, 118.8, 115.9, 114.5, 111.2, 47.3, 45.3.

HRMS (EI): m/z calcd for $\text{C}_{29}\text{H}_{22}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 444.1706, found 444.1706.

3-benzyl-1-((5-chlorothiophen-2-yl)methyl)quinazoline-2,4(1H,3H)-dione (3r)



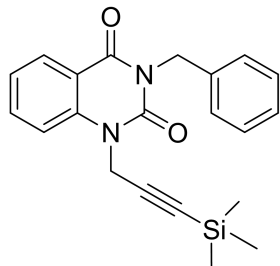
Yellow solid, yield = 76%, 73 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.27 (dd, 1H, J = 8.0, 1.5 Hz), 7.70-7.66 (m, 1H), 7.55 (d, 2H, J = 7.0 Hz), 7.36-7.30 (m, 4H), 7.28-7.27 (m, 1H), 6.90 (d, 1H, J = 3.5 Hz), 6.78 (d, 1H, J = 4.0 Hz), 5.38 (s, 2H), 5.33 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.7, 151.1, 139.4, 136.9, 136.8, 135.4, 130.4, 129.7, 129.1, 128.6, 127.8, 126.4, 125.8, 123.5, 116.0, 113.6, 45.2, 42.8.

HRMS (EI): m/z calcd for $\text{C}_{20}\text{H}_{16}\text{ClN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 383.0615, found 383.0619.

3-benzyl-1-(3-(trimethylsilyl)prop-2-yn-1-yl)quinazoline-2,4(1H,3H)-dione (3t)

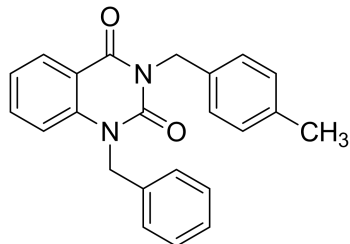


Colorless oil, yield = 51%, 46 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.28 (dd, 1H, J = 8.0, 1.5 Hz), 7.73-7.70 (m, 1H), 7.56 (d, 2H, J = 7.0 Hz), 7.41 (d, 1H, J = 8.5 Hz), 7.35-7.27 (m, 4H), 5.30 (s, 2H), 4.96 (s, 2H), 0.15 (s, 9H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.8, 150.6, 139.3, 137.0, 135.1, 129.3, 129.2, 128.6, 127.8, 123.5, 116.0, 114.5, 98.6, 90.8, 45.3, 34.6, 0.1.

1-benzyl-3-(4-methylbenzyl)quinazoline-2,4(1H,3H)-dione (5a)



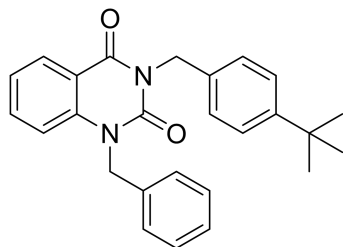
White solid, yield = 65%, 58 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.27 (dd, 1H, J = 8.0, 1.5 Hz), 7.56-7.52 (m, 1H), 7.49 (d, 2H, J = 7.5 Hz), 7.35 (t, 2H, J = 7.0 Hz), 7.30-7.28 (m, 1H), 7.27-7.21 (m, 3H), 7.16 (d, 2H, J = 8.0 Hz), 7.11 (d, 1H, J = 8.5 Hz), 5.39 (s, 2H), 5.33 (s, 2H), 2.34 (s, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.9, 151.6, 140.1, 137.5, 135.8, 135.2, 129.29, 129.27, 129.20, 129.1, 127.8, 126.6, 123.2, 115.9, 114.5, 47.5, 45.1, 21.3.

HRMS (EI): m/z calcd for $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 357.1597, found 357.1598.

1-benzyl-3-(4-(tert-butyl)benzyl)quinazoline-2,4(1H,3H)-dione (5b)



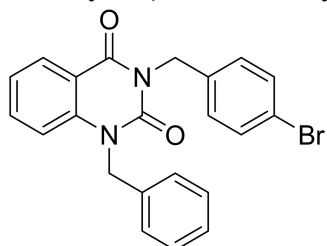
Colorless oil, yield = 75%, 75 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.27 (dd, 1H, J = 8.0, 1.5 Hz), 7.55-7.54 (m, 3H), 7.39-7.34 (m, 4H), 7.31-7.28 (m, 2H), 7.27-7.21 (m, 2H), 7.12 (d, 1H, J = 8.5 Hz), 5.40 (s, 2H), 5.35 (s, 2H), 1.33 (s, 9H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 162.0, 151.6, 150.6, 140.1, 135.8, 135.2, 134.2, 129.3, 129.1, 129.0, 127.8, 126.6, 125.5, 123.2, 116.0, 114.5, 47.6, 45.0, 34.7, 31.5.

HRMS (EI): m/z calcd for $\text{C}_{26}\text{H}_{27}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 399.2067, found 399.2068.

1-benzyl-3-(4-bromobenzyl)quinazoline-2,4(1H,3H)-dione (5c)



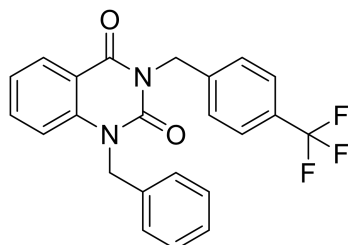
Yellow oil, yield = 83%, 87 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.27-8.25 (m, 1H), 7.58-7.54 (m, 1H), 7.47 (s, 4H), 7.37-7.34 (m, 2H), 7.31-7.28 (m, 1H), 7.26-7.23 (m, 3H), 7.13 (d, 1H, J = 8.5 Hz), 5.39 (s, 2H), 5.30 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.9, 151.5, 140.0, 136.1, 135.6, 131.7, 131.1, 129.3, 129.2, 127.9, 126.5, 123.4, 121.9, 115.8, 114.6, 47.6, 44.7.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{BrN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 421.0546, found 421.0546.

1-benzyl-3-(4-(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (5d)



White solid, yield = 81%, 83 mg.

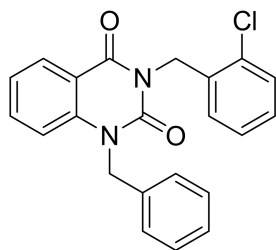
^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.27 (dd, 1H, J = 8.0, 1.5 Hz), 7.68 (d, 2H, J = 8.0 Hz), 7.62-7.56 (m, 3H), 7.36 (t, 2H, J = 7.5 Hz), 7.31 (d, 1H, J = 7.0 Hz), 7.27-7.24 (m, 3H), 7.15 (d, 1H, J = 8.5 Hz), 5.41 (s, 4H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.9, 151.5, 141.0, 140.1, 135.6, 135.5, 130.1 (q, J_{CF} = 32.1 Hz), 129.4, 129.3, 129.2, 127.9, 126.5, 125.7 (q, J_{CF} = 3.9 Hz), 125.4 (q, J_{CF} = 270.4 Hz), 123.5, 115.7, 114.7, 47.6, 44.9.

^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -62.5.

HRMS (EI): m/z calcd for $\text{C}_{23}\text{H}_{18}\text{F}_3\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 411.1314, found 411.1314.

1-benzyl-3-(2-chlorobenzyl)quinazoline-2,4(1H,3H)-dione (5e)



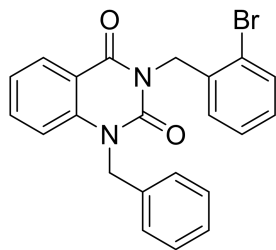
White solid, yield = 66%, 62 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.29 (dd, 1H, J = 8.0, 2.0 Hz), 7.62-7.58 (m, 1H), 7.43-7.41 (m, 1H), 7.36 (t, 2H, J = 7.5 Hz), 7.31-7.28 (m, 2H), 7.27-7.26 (m, 2H), 7.24-7.18 (m, 3H), 7.12-7.10 (m, 1H), 5.51 (s, 2H), 5.43 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 162.0, 151.5, 140.2, 135.7, 135.5, 134.2, 133.2, 129.8, 129.4, 129.2, 128.5, 127.9, 127.09, 127.03, 126.6, 123.4, 115.7, 114.7, 47.6, 43.2.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{ClN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 377.1051, found 377.1052.

1-benzyl-3-(2-bromobenzyl)quinazoline-2,4(1H,3H)-dione (5f)



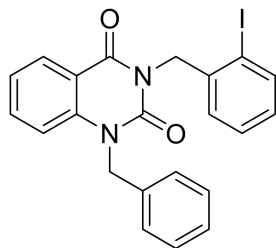
Yellow solid, yield = 61%, 64 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.29 (dd, 1H, J = 8.0, 1.5 Hz), 7.62-7.59 (m, 2H), 7.36 (t, 2H, J = 7.5 Hz), 7.31-7.28 (m, 3H), 7.27 (s, 1H), 7.24 (t, 1H, J = 7.0 Hz), 7.20 (d, 1H, J = 8.5 Hz), 7.15-7.12 (m, 1H), 7.05 (dd, 1H, J = 8.0, 1.5 Hz), 5.48 (s, 2H), 5.43 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.9, 151.4, 140.2, 135.67, 135.66, 135.5, 133.1, 129.4, 129.1, 128.7, 127.9, 127.6, 126.7, 126.6, 123.4, 123.0, 115.7, 114.7, 47.6, 45.6.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{BrN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 421.0546, found 421.0545.

1-benzyl-3-(2-iodobenzyl)quinazoline-2,4(1H,3H)-dione (5g)

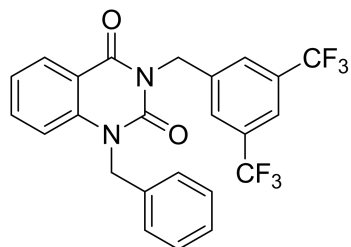


Yellow solid, yield = 39%, 46 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.29 (dd, 1H, J = 8.0, 2.0 Hz), 7.91-7.89 (m, 1H), 7.63-7.59 (m, 1H), 7.38-7.35 (m, 2H), 7.32-7.29 (m, 2H), 7.28-7.26 (m, 3H), 7.20 (d, 1H, J = 8.5 Hz), 6.99-6.95 (m, 2H), 5.43 (s, 2H), 5.39 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.8, 151.4, 140.2, 139.8, 138.5, 135.7, 135.6, 129.5, 129.2, 128.9, 128.5, 127.9, 126.6, 125.9, 123.5, 115.7, 114.7, 98.1, 50.6, 47.6.
HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 469.0407, found 469.0410.

1-benzyl-3-(3,5-bis(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (5h)



White solid, yield = 70%, 84 mg.

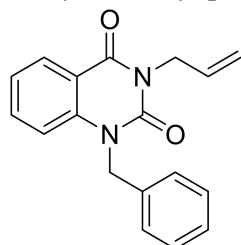
^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.27 (dd, 1H, J = 8.0, 2.0 Hz), 8.05 (s, 2H), 7.83 (s, 1H), 7.62-7.58 (s, 1H), 7.38-7.34 (m, 2H), 7.32-7.29 (m, 1H), 7.28-7.26 (m, 3H), 7.18 (d, 1H, J = 8.5 Hz), 5.46 (s, 2H), 5.42 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.8, 151.5, 140.1, 139.5, 135.7, 135.5, 132.0 (q, J_{CF} = 33.0 Hz), 129.5 (q, J_{CF} = 3.9 Hz), 129.4, 129.2, 128.0, 126.6, 124.5 (q, J_{CF} = 271.0 Hz), 123.6, 122.0 (q, J_{CF} = 3.9 Hz), 115.6, 114.7, 47.6, 44.4.

^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -62.7.

HRMS (EI): m/z calcd for $\text{C}_{24}\text{H}_{17}\text{F}_6\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 479.1188, found 479.1187.

3-allyl-1-benzylquinazoline-2,4(1H,3H)-dione (5i)



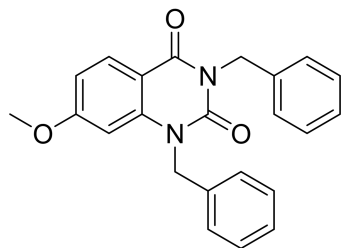
Yellow solid, yield = 90%, 66 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.26 (dd, 1H, J = 8.0, 1.5 Hz), 7.58-7.54 (m, 1H), 7.37-7.34 (m, 2H), 7.31-7.22 (m, 4H), 7.14 (d, 1H, J = 8.5 Hz), 6.06-5.98 (m, 1H), 5.41 (s, 2H), 5.38-5.34 (m, 1H), 5.27-5.25 (m, 1H), 4.80-4.79 (m, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.6, 151.3, 140.1, 135.8, 135.2, 132.0, 129.2, 129.1, 127.8, 126.6, 123.2, 118.0, 115.8, 114.6, 47.4, 44.2.

HRMS (EI): m/z calcd for $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 293.1284, found 293.1284.

1,3-dibenzyl-7-methoxyquinazoline-2,4(1H,3H)-dione (5j)



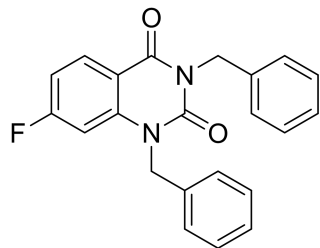
Yellow solid, yield = 80%, 74 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.18 (d, 1H, J = 9.0 Hz), 7.58-7.56 (m, 2H), 7.37-7.33 (m, 4H), 7.30-7.28 (s, 2H), 7.28-7.27 (m, 2H), 6.77 (dd, 1H, J = 9.0, 2.0 Hz), 6.55 (d, 1H, J = 2.0 Hz), 5.36 (s, 2H), 5.34 (s, 2H), 3.77 (s, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 165.2, 161.6, 152.0, 141.8, 137.3, 135.9, 131.2, 129.2, 129.1, 128.6, 127.8, 127.7, 126.6, 109.9, 109.3, 99.5, 55.7, 47.7, 45.1.

HRMS (EI): m/z calcd for $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ 373.1546, found 373.1549.

1,3-dibenzyl-7-fluoroquinazoline-2,4(1H,3H)-dione (5k)



White, solid = 97%, 87 mg.

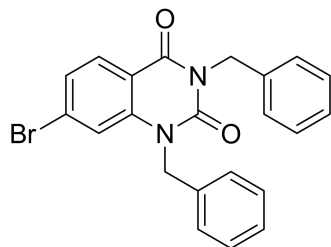
^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.94 (dd, 1H, J = 8.0, 3.0 Hz), 7.59-7.57 (m, 2H), 7.38-7.34 (m, 4H), 7.32-7.28 (m, 2H), 7.28-7.24 (m, 3H), 7.10 (dd, 1H, J = 9.0, 4.0 Hz), 5.39 (s, 2H), 5.36 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.1, 161.0, 159.4, 157.5, 151.3, 136.9, 136.5 (d, J_{CF} = 2.1 Hz), 135.5, 129.2, 128.6, 127.9 (d, J_{CF} = 5.1 Hz), 126.5, 123.0 (d, J_{CF} = 23.8 Hz), 117.2 (d, J_{CF} = 7.6 Hz), 116.6 (d, J_{CF} = 7.6 Hz), 114.8 (d, J_{CF} = 23.9 Hz), 47.9, 45.5.

^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -118.8.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{FN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 361.1346, found 361.1346.

1,3-dibenzyl-7-bromoquinazoline-2,4(1H,3H)-dione (5l)

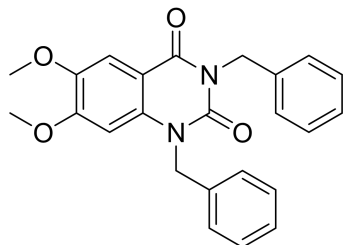


White solid, yield = 73%, 77 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.11 (d, 1H, J = 8.5 Hz), 7.57-7.55 (m, 2H), 7.39-7.30 (m, 8H), 7.28-7.26 (m, 2H), 5.34 (s, 4H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.3, 151.4, 140.9, 136.8, 135.2, 130.7, 130.2, 129.3, 129.2, 128.7, 128.1, 127.9, 126.68, 126.64, 117.6, 114.7, 47.7, 45.4.
HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{18}\text{BrN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 421.0546, found 421.0547.

1,3-dibenzyl-6,7-dimethoxyquinazoline-2,4(1H,3H)-dione (5m)



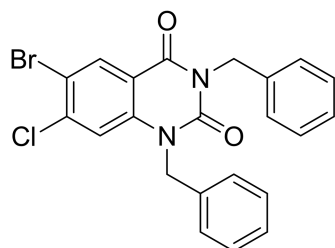
Translucent oil, yield = 73%, 73 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.62 (s, 1H), 7.58-7.56 (m, 2H), 7.36-7.33 (m, 4H), 7.30-7.26 (m, 4H), 6.54 (s, 1H), 5.38 (s, 2H), 5.36 (s, 2H), 3.92 (s, 3H), 3.76 (s, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.5, 155.0, 151.8, 145.7, 137.3, 136.1, 135.7, 129.1, 129.0, 128.5, 127.9, 127.6, 126.6, 109.0, 108.2, 97.7, 56.3, 56.2, 47.9, 45.2.

HRMS (EI): m/z calcd for $\text{C}_{24}\text{H}_{23}\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$ 403.1652, found 403.1653.

1,3-dibenzyl-6-bromo-7-chloroquinazoline-2,4(1H,3H)-dione (5n)



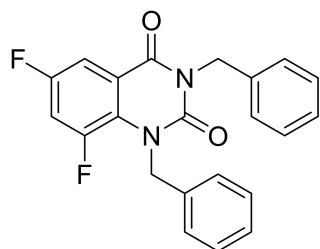
White, solid = 59%, 67 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.29 (s, 1H), 7.56-7.54 (m, 2H), 7.43 (s, 1H), 7.39-7.31 (m, 6H), 7.26-7.24 (m, 2H), 5.33 (s, 4H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 160.4, 151.1, 138.9, 136.6, 134.9, 130.3, 130.1, 129.7, 129.4, 129.2, 128.7, 128.2, 128.0, 126.6, 119.9, 116.2, 47.9, 45.6.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{17}\text{BrClN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 455.0156, found 455.0140.

1,3-dibenzyl-6,8-difluoroquinazoline-2,4(1H,3H)-dione (5o)



Translucent oil, yield = 74%, 70 mg.

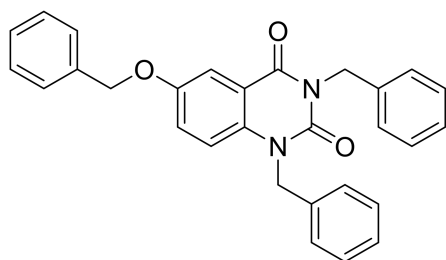
^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.60-7.59 (m, 2H), 7.39-7.31 (m, 6H), 7.25-7.23 (m, 2H), 6.68-6.62 (m, 2H), 5.33 (s, 2H), 5.32 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 167.4 (d, $J_{\text{CF}} = 15.1$ Hz), 165.4 (dd, $J_{\text{CF}} = 4.6$ Hz, $J_{\text{CF}} = 4.6$ Hz), 163.2 (d, $J_{\text{CF}} = 15.4$ Hz), 158.1 (d, $J_{\text{CF}} = 4.5$ Hz), 151.1, 143.1 (dd, $J_{\text{CF}} = 4.3$ Hz, $J_{\text{CF}} = 4.3$ Hz), 136.7, 134.8, 129.5, 129.3, 128.6, 128.2 (d, $J_{\text{CF}} = 23.1$ Hz), 126.5, 102.7 (dd, $J_{\text{CF}} = 2.9$ Hz, $J_{\text{CF}} = 2.9$ Hz), 100.1 (t, $J_{\text{CF}} = 25.4$ Hz), 98.3 (dd, $J_{\text{CF}} = 4.0$ Hz, $J_{\text{CF}} = 4.0$ Hz), 48.4, 45.1.

^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -97.1, -103.4.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{17}\text{F}_2\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 379.1252, found 379.1252.

1,3-dibenzyl-6-(benzyloxy)quinazoline-2,4(1H,3H)-dione (5p)



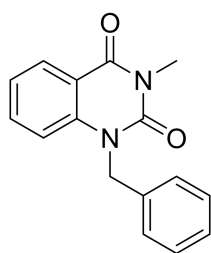
Colorless oil, yield = 31%, 36 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.80 (d, 1H, $J = 3.0$ Hz), 7.59-7.57 (m, 2H), 7.45-7.33 (m, 9H), 7.30-7.28 (m, 2H), 7.26-7.24 (m, 2H), 7.23-7.20 (m, 1H), 7.06 (d, 1H, $J = 9.0$ Hz), 5.37 (s, 4H), 5.11 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 161.8, 154.7, 151.4, 137.2, 136.4, 135.9, 134.4, 129.2, 129.1, 128.8, 128.6, 128.4, 127.81, 127.79, 127.75, 126.6, 124.8, 116.6, 116.2, 111.3, 70.7, 47.7, 45.4.

HRMS (EI): m/z calcd for $\text{C}_{29}\text{H}_{25}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ 449.1859, found 449.1861.

1-benzyl-3-methylquinazoline-2,4(1H,3H)-dione (5q)

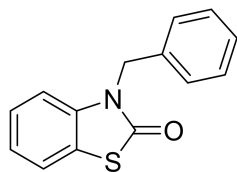


White solid, yield = 95%, 63 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.26 (dd, 1H, $J = 8.0, 1.5$ Hz), 7.57-7.54 (m, 1H), 7.36-7.33 (m, 2H), 7.29-7.21 (m, 4H), 7.14 (d, 1H, $J = 8.5$ Hz), 5.40 (s, 2H), 3.57 (s, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 162.1, 151.7, 139.9, 135.8, 135.1, 129.1, 129.0, 127.8, 126.6, 123.2, 115.7, 114.5, 47.5, 28.8.

3-benzylbenzo[d]thiazol-2(3H)-one^[31] (7a)

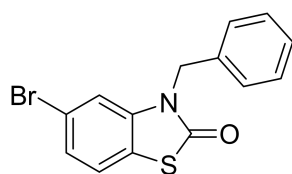


White, solid = 91%, 55 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.46 (dd, 1H, $J = 1.5$ Hz, $J = 1.5$ Hz), 7.37-7.30 (m, 5H), 7.26-7.22 (m, 1H), 7.18-7.14 (m, 1H), 6.99 (dd, 1H, $J = 9.0, 1.0$ Hz), 5.18 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 170.5, 137.1, 135.3, 129.1, 128.1, 127.3, 126.5, 123.4, 122.8, 111.4, 46.4.

3-benzyl-6-bromobenzo[d]thiazol-2(3H)-one (7b)



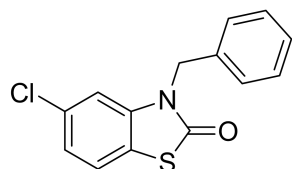
White, solid = 80%, 64 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.40-7.36 (m, 2H), 7.34-7.27 (m, 5H), 7.13 (d, 1H, $J = 2.0$ Hz), 5.14 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 170.2, 138.2, 134.7, 129.2, 128.3, 127.3, 126.4, 123.9, 121.7, 120.0, 114.4, 46.5.

HRMS (EI): m/z calcd for $\text{C}_{14}\text{H}_{11}\text{BrNOS}$ $[\text{M}+\text{H}]^+$ 319.9739, found 319.9739.

3-benzyl-6-chlorobenzo[d]thiazol-2(3H)-one (7c)



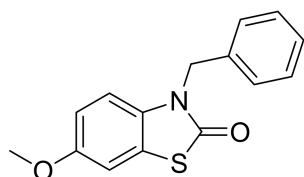
Yellow, solid = 82%, 56 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.39-7.30 (m, 6H), 7.14 (dd, 1H, $J = 2.0$ Hz, $J = 2.0$ Hz), 6.99 (d, 1H, $J = 2.0$ Hz), 5.14 (s, 2H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 170.4, 138.0, 134.7, 132.5, 129.2, 128.3, 127.2, 123.6, 121.0, 111.7, 46.5.

HRMS (EI): m/z calcd for $\text{C}_{14}\text{H}_{11}\text{ClNOS}$ $[\text{M}+\text{H}]^+$ 276.0244, found 276.0247.

3-benzyl-6-methoxybenzo[d]thiazol-2(3H)-one^[4] (7d)

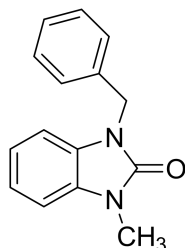


Yellow, solid = 68%, 46 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.36-7.29 (m, 5H), 7.02 (d, 1H, J = 2.5 Hz), 6.87 (d, 1H, J = 9.0 Hz), 6.79 (dd, 1H, J = 9.0, 2.5 Hz), 5.14 (s, 2H), 3.80 (s, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 170.1, 156.3, 135.4, 130.9, 129.0, 128.0, 127.2, 123.8, 113.0, 112.0, 108.1, 56.0, 46.4.

1-benzyl-3-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one^[5] (7e)

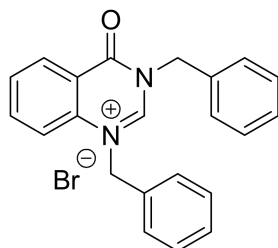


Yellow oil, yield = 60%, 36 mg.

^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.37-7.32 (m, 4H), 7.30-7.27 (m, 1H), 7.12-7.09 (m, 1H), 7.05-7.00 (m, 2H), 6.91-6.89 (m, 1H), 5.10 (s, 2H), 3.49 (s, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ (ppm) = 154.7, 136.53, 136.52, 130.2, 129.3, 128.9, 127.8, 127.6, 121.4, 108.4, 107.6, 45.0, 27.4.

1,3-dibenzyl-4-oxo-3,4-dihydroquinazolin-1-ium bromide (8)



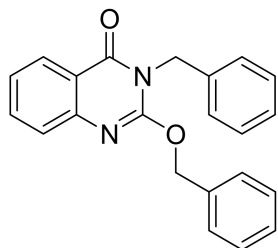
White solid, yield = 73%, 149 mg.

^1H NMR (500 MHz, CD_3OD): δ = 10.08 (s, 1H), 8.48 (dd, 1H, J = 8.0, 1.5 Hz), 8.04-8.00 (m, 1H), 7.93 (d, 1H, J = 9.0 Hz), 7.84 (t, 1H, J = 7.5 Hz), 7.60-7.58 (m, 2H), 7.50-7.40 (m, 8H), 5.87 (s, 2H), 5.48 (s, 2H).

^{13}C NMR (125 MHz, CD_3OD): δ = 158.9, 155.1, 138.0, 134.9, 133.6, 131.5, 130.6, 130.4, 130.26, 130.20, 130.1, 130.0, 128.5, 122.0, 120.1, 58.0, 53.7.

HRMS (EI): m/z calcd for $\text{C}_{22}\text{H}_{19}\text{NO}$ $[\text{M}-\text{Br}]^+$ 327.1491, found 327.1491.

3-benzyl-2-(benzyloxy)quinazolin-4(3H)-one (9)



White solid, yield = 70%, 120 mg.

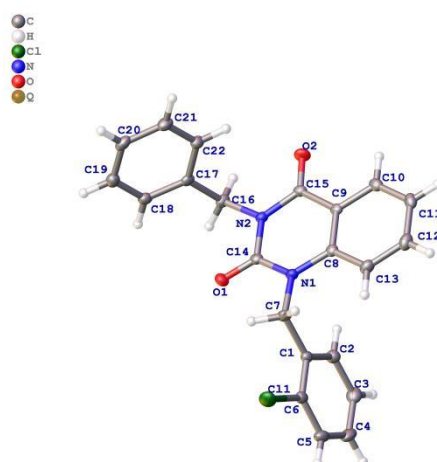
¹H NMR (500 MHz, CDCl₃): δ (ppm) = 8.30-8.28 (m, 1H), 7.72-7.68 (m, 1H), 7.56-7.54 (m, 1H), 7.41-7.34 (m, 8H), 7.30-7.28 (m, 3H), 5.52 (s, 2H), 5.34 (s, 2H).

¹³C NMR (125 MHz, CDCl₃): δ (ppm) = 163.0, 152.3, 147.1, 136.8, 135.3, 134.6, 128.7, 128.66, 128.62, 128.55, 128.49, 127.7, 127.5, 125.7, 124.7, 119.0, 70.3, 44.9.

References

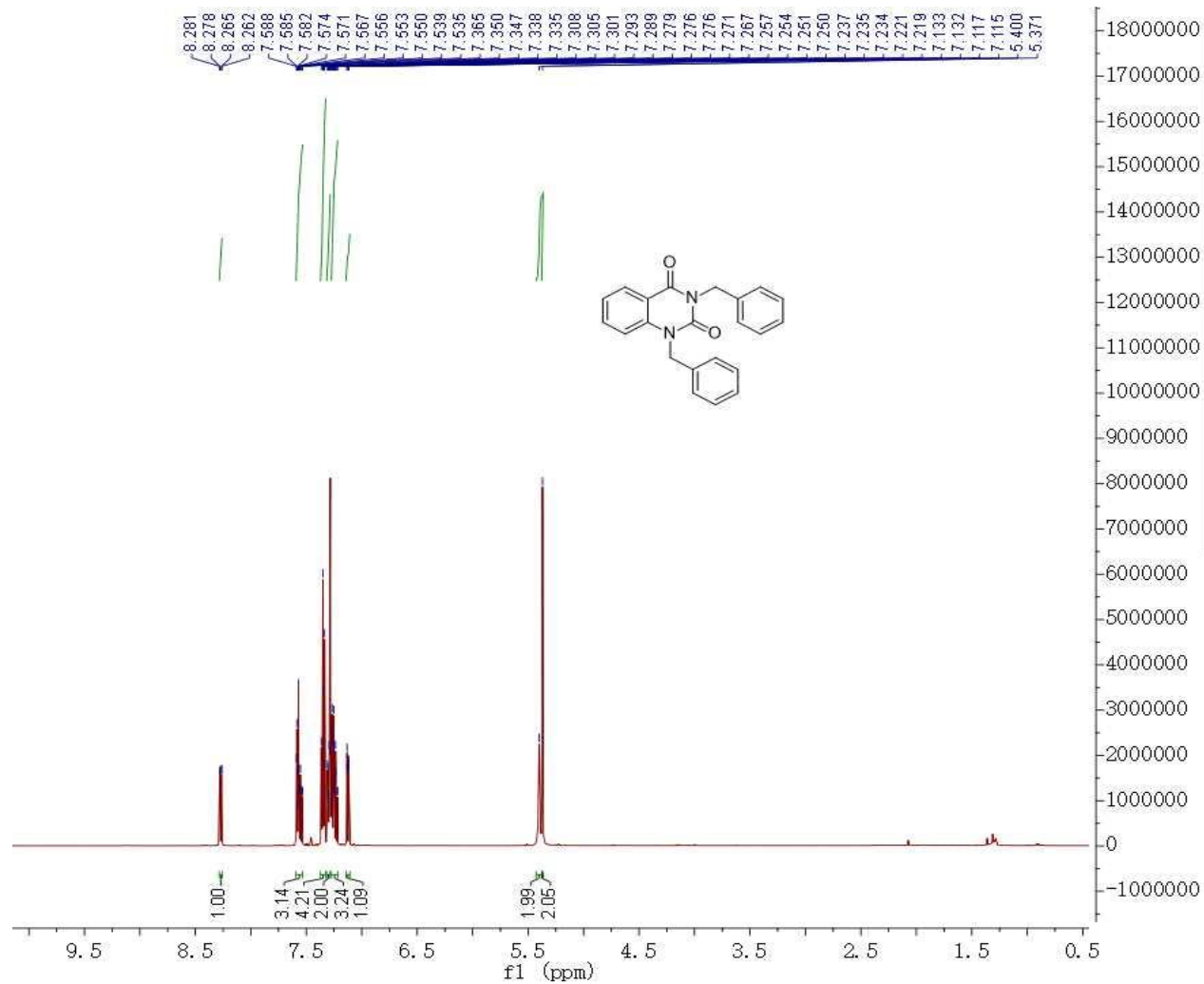
- [1] Shantharjun, B.; Rajeswari, R.; Vani, D.; Unnava, R.; Sridhar, B.; Reddy, K. R. *Asian J. Org. Chem.*, **2019**, *8*, 2162.
- [2] Piotrowska, D. G.; Andrei, G.; Schols, D.; Snoeck, R.; Łysakowska, M. *Eur. J. Med. Chem.*, **2017**, *126*, 84.
- [3] Yang, Y.; Zhang, X.; Zeng, W.; Huang, H.; Liang, Y. *RSC Adv.*, **2014**, *4*, 6090.
- [4] Roy, G.; Das, R.; Banerjee, M.; Rai, R. K.; Karri, R. *Org. Biomol. Chem.*, **2018**, *16*, 4243.
- [5] Zhuge, J.; Jiang, Z.; Jiang, W.; Histan, G.; Lin, D. *Org. Biomol. Chem.*, **2021**, *19*, 5121.

Table of crystallographic data for **3i** (CCDC 2189508)

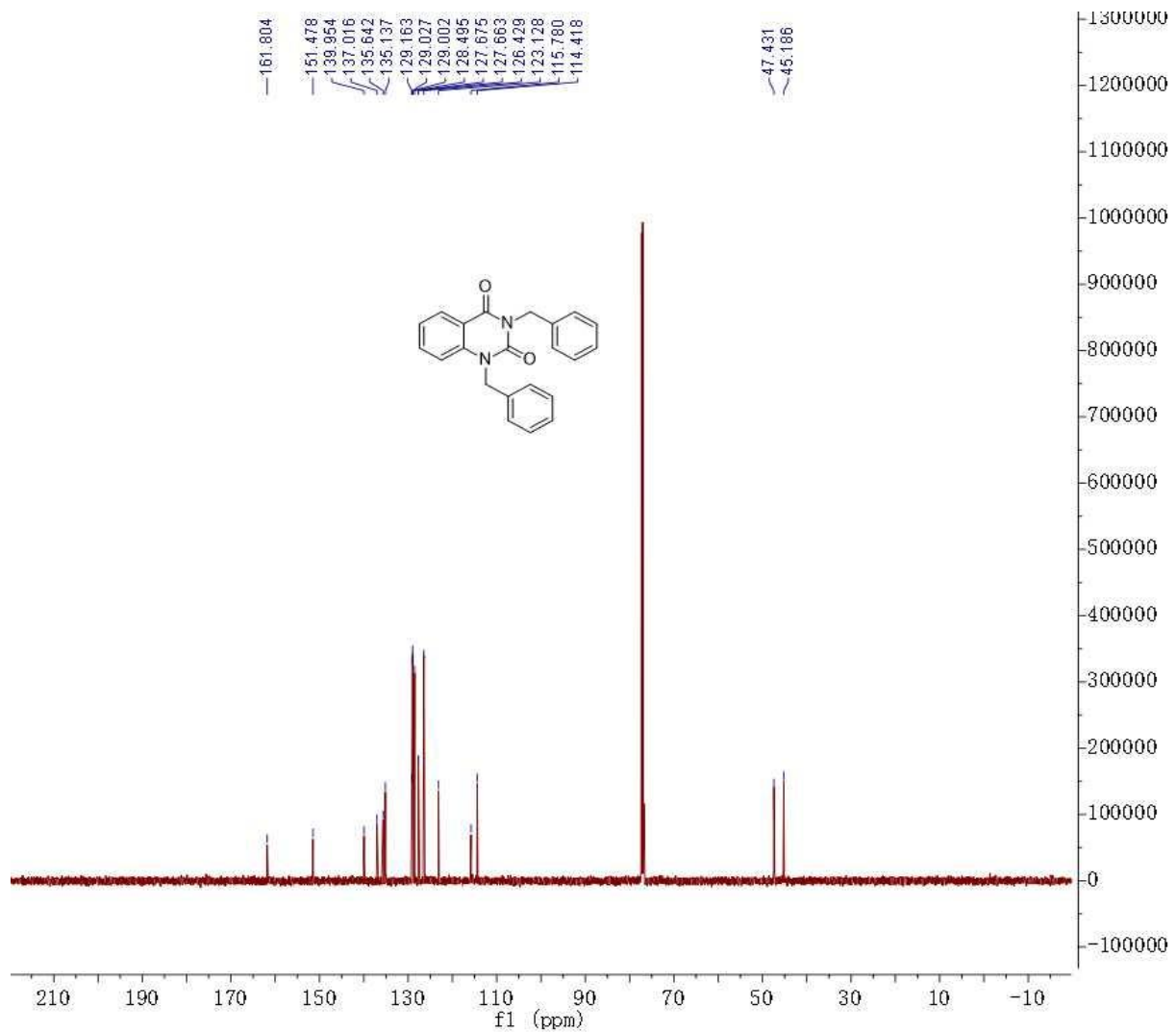


Complex	3i
Empirical formula	C ₂₂ H ₁₇ ClN ₂ O ₂
Formula weight	376.82
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	12.3628(8)
b/Å	8.7568(5)
c/Å	17.4770(12)
α/°	90
β/°	109.330(7)
γ/°	90
Volume/Å ³	1785.4(2)
Z	4
ρ _{calc} /cm ³	1.402
μ/mm ⁻¹	0.234
F(000)	784.0
Crystal size/mm ³	0.15 × 0.13 × 0.12
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.94 to 49.984
Index ranges	-13 ≤ h ≤ 14, -8 ≤ k ≤ 10, -20 ≤ l ≤ 17
Reflections collected	7149
Independent reflections	3149 [R _{int} = 0.0227, R _{sigma} = 0.0318]
Data/restraints/parameters	3149/0/244
Goodness-of-fit on F ²	1.101
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0387, wR ₂ = 0.0875
Final R indexes [all data]	R ₁ = 0.0474, wR ₂ = 0.0930

1,3-dibenzylquinazoline-2,4(1H,3H)-dione (3a)

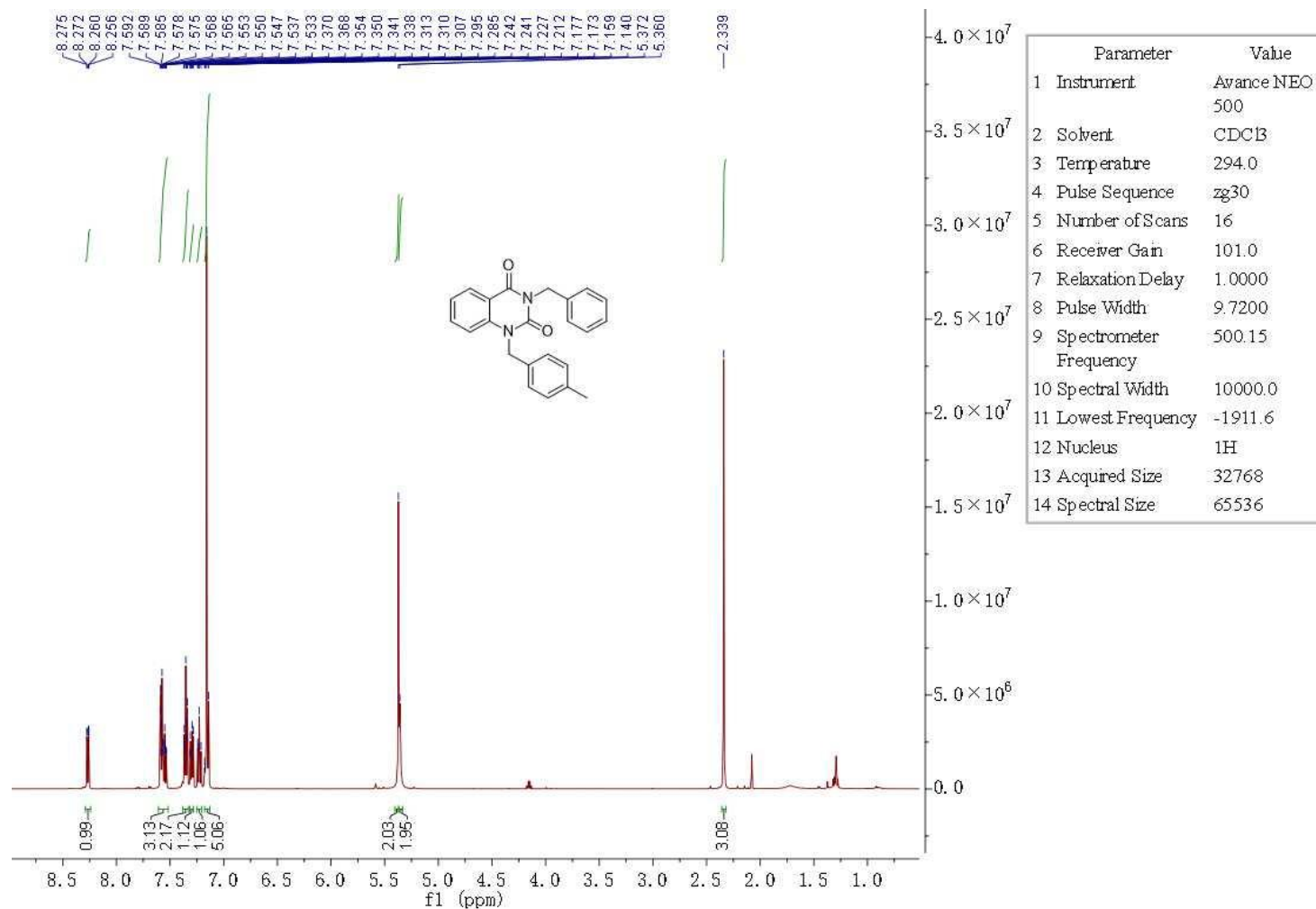


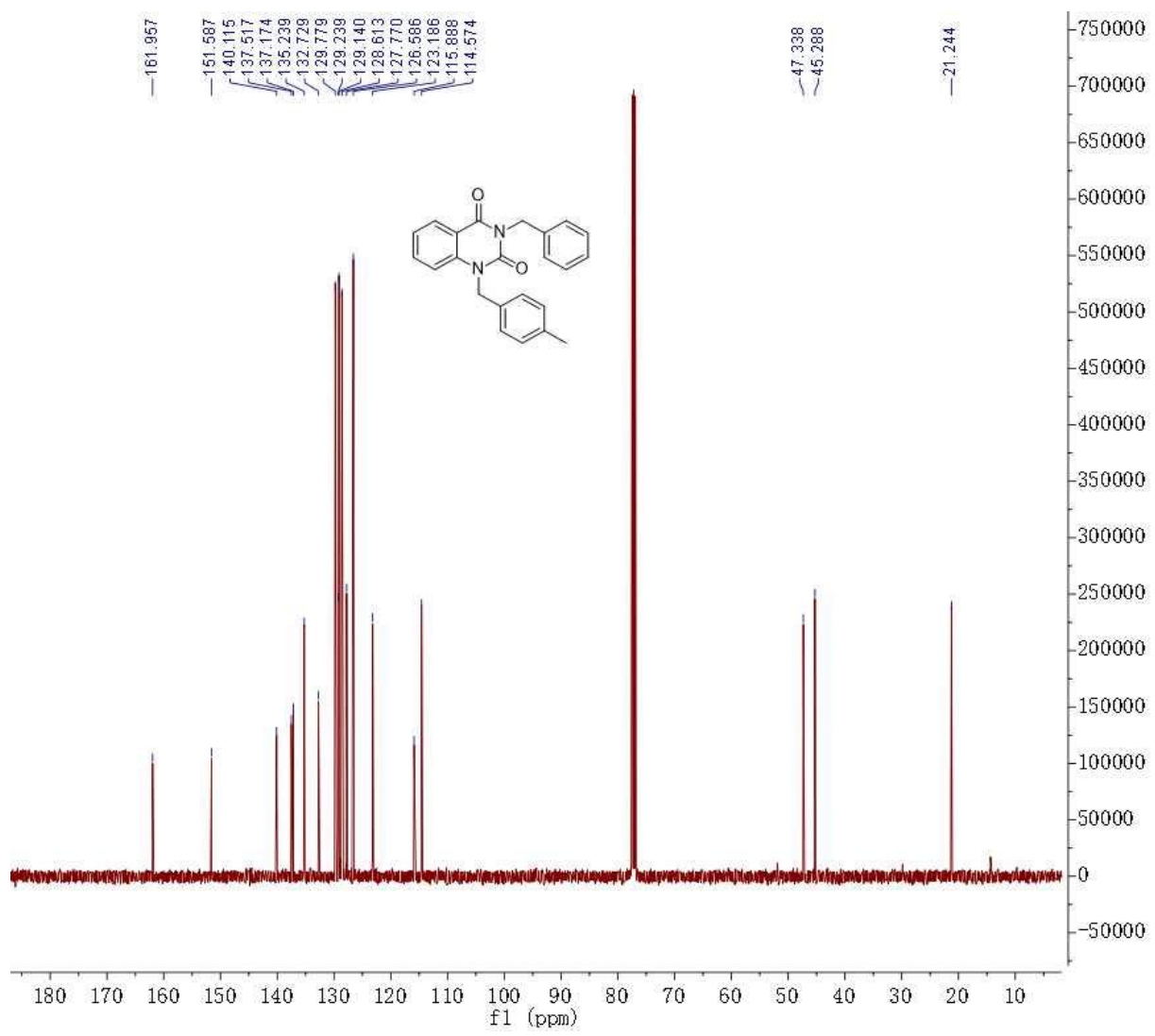
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1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.6
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8 Pulse Width	9.7200
9 Spectrometer	500.15
Frequency	
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



Parameter	Value
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2 Solvent	CDCl ₃
3 Temperature	295.1
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
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10 Spectral Width	30120.5
11 Lowest Frequency	-2484.0
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536

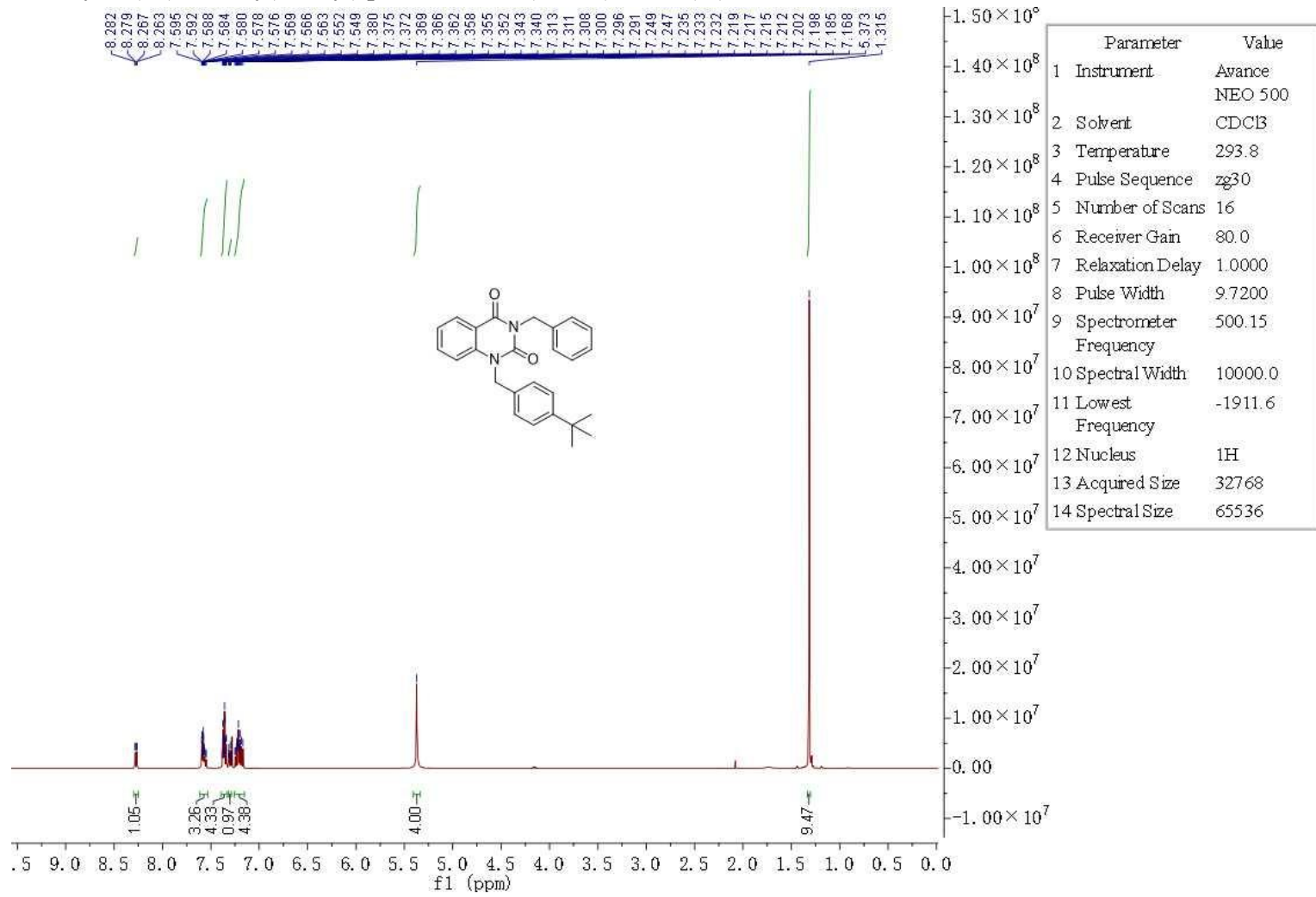
3-benzyl-1-(4-methylbenzyl)quinazoline-2,4(1H,3H)-dione (3b)

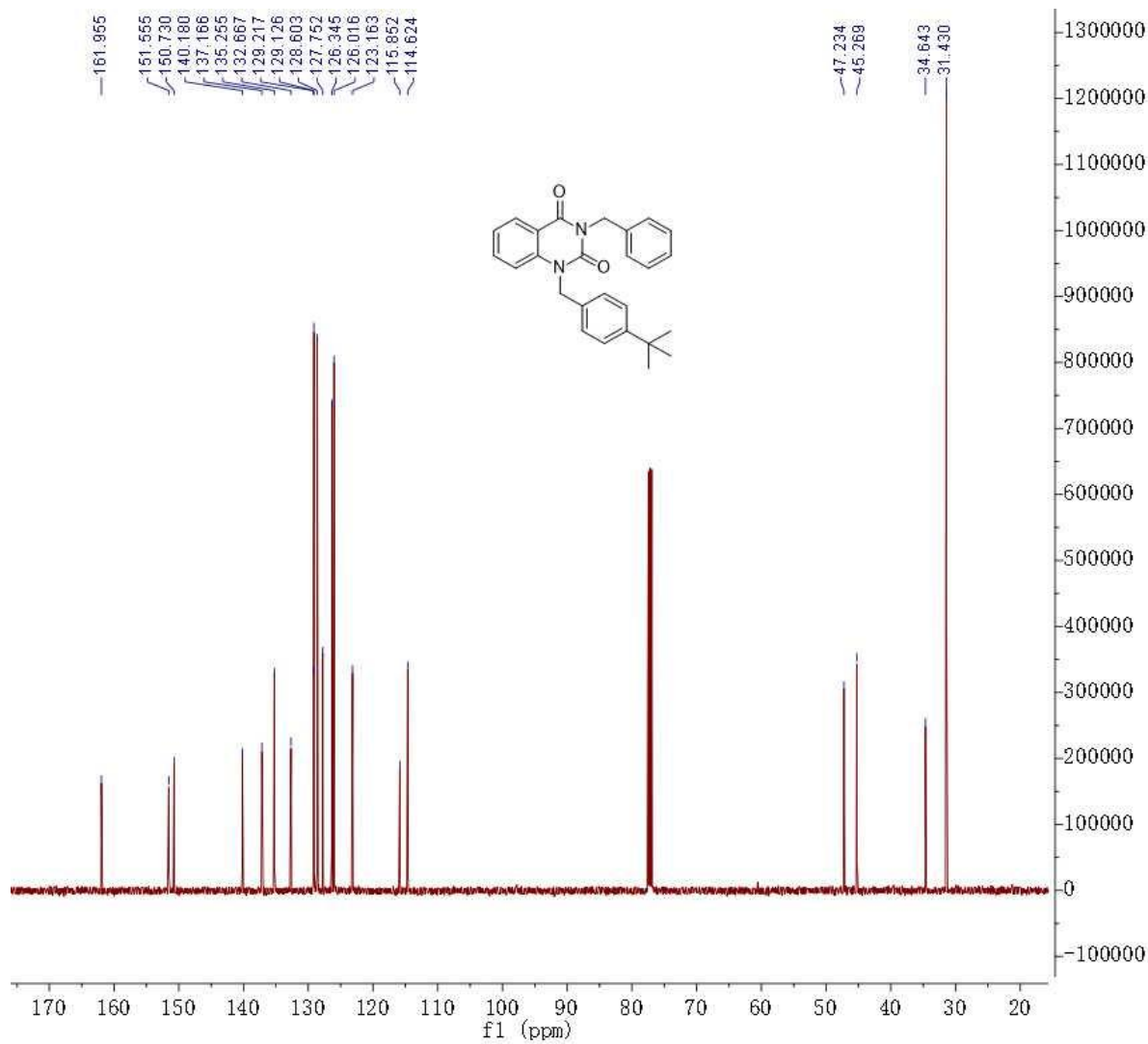




Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.8
4 Pulse Sequence	zgpg30
5 Number of Scans	160
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2468.9
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536

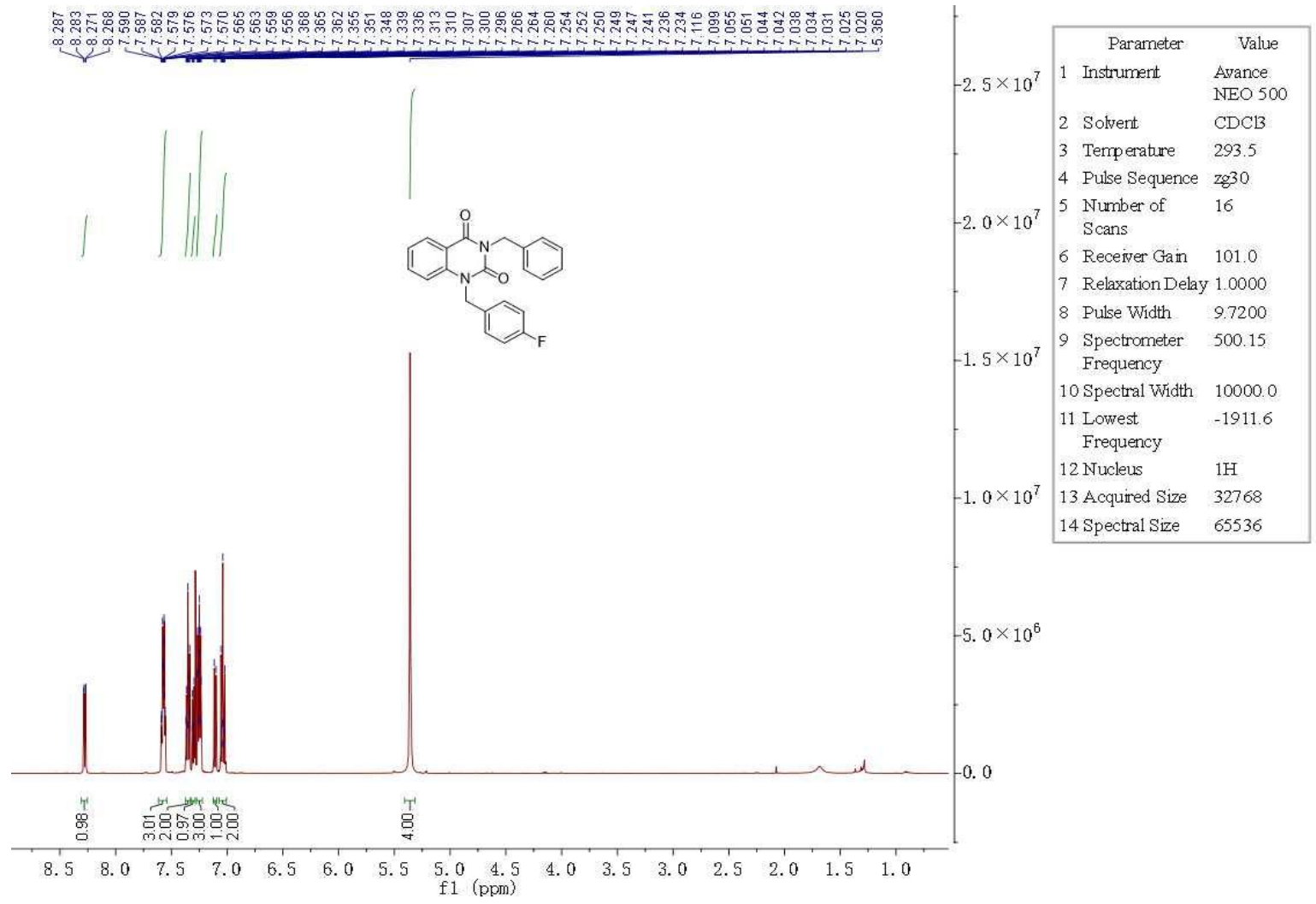
3-benzyl-1-(4-(tert-butyl)benzyl)quinazoline-2,4(1H,3H)-dione (3c)

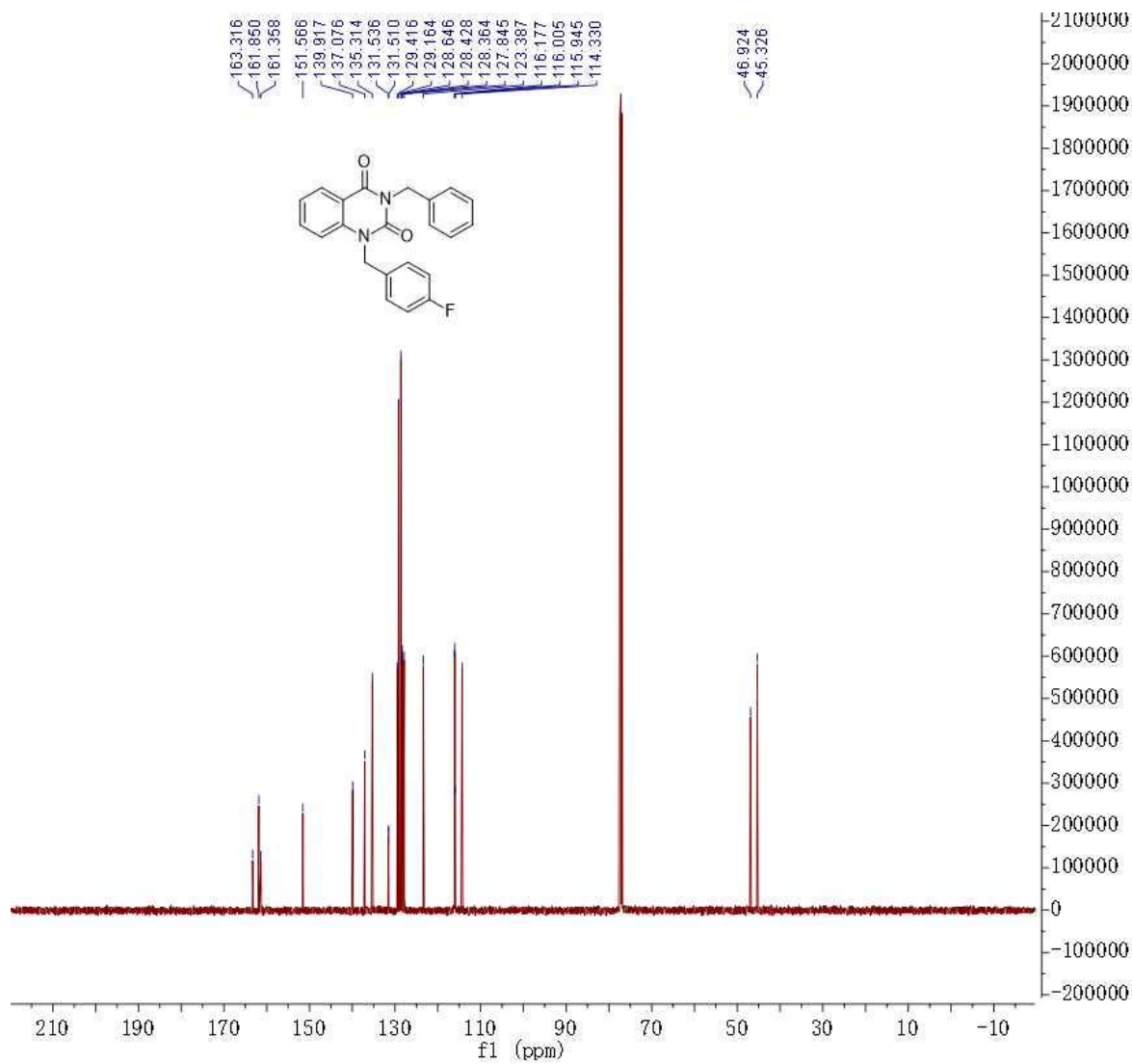




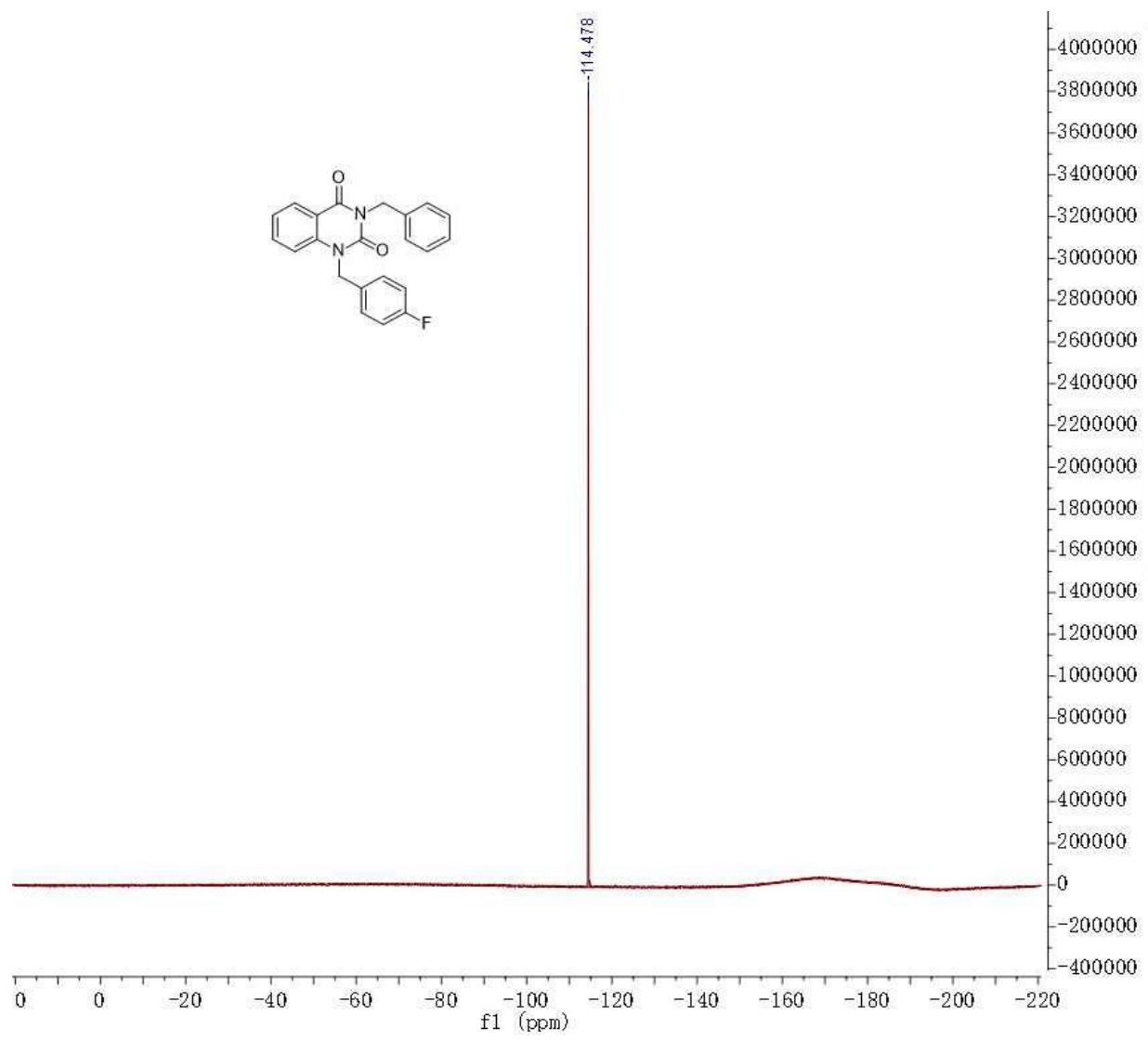
Parameter	Value
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2 Solvent	CDCl3
3 Temperature	294.7
4 Pulse Sequence	zgpg30
5 Number of Scans	160
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest Frequency	-2470.8
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

3-benzyl-1-(4-fluorobenzyl)quinazoline-2,4(1H,3H)-dione (3d)



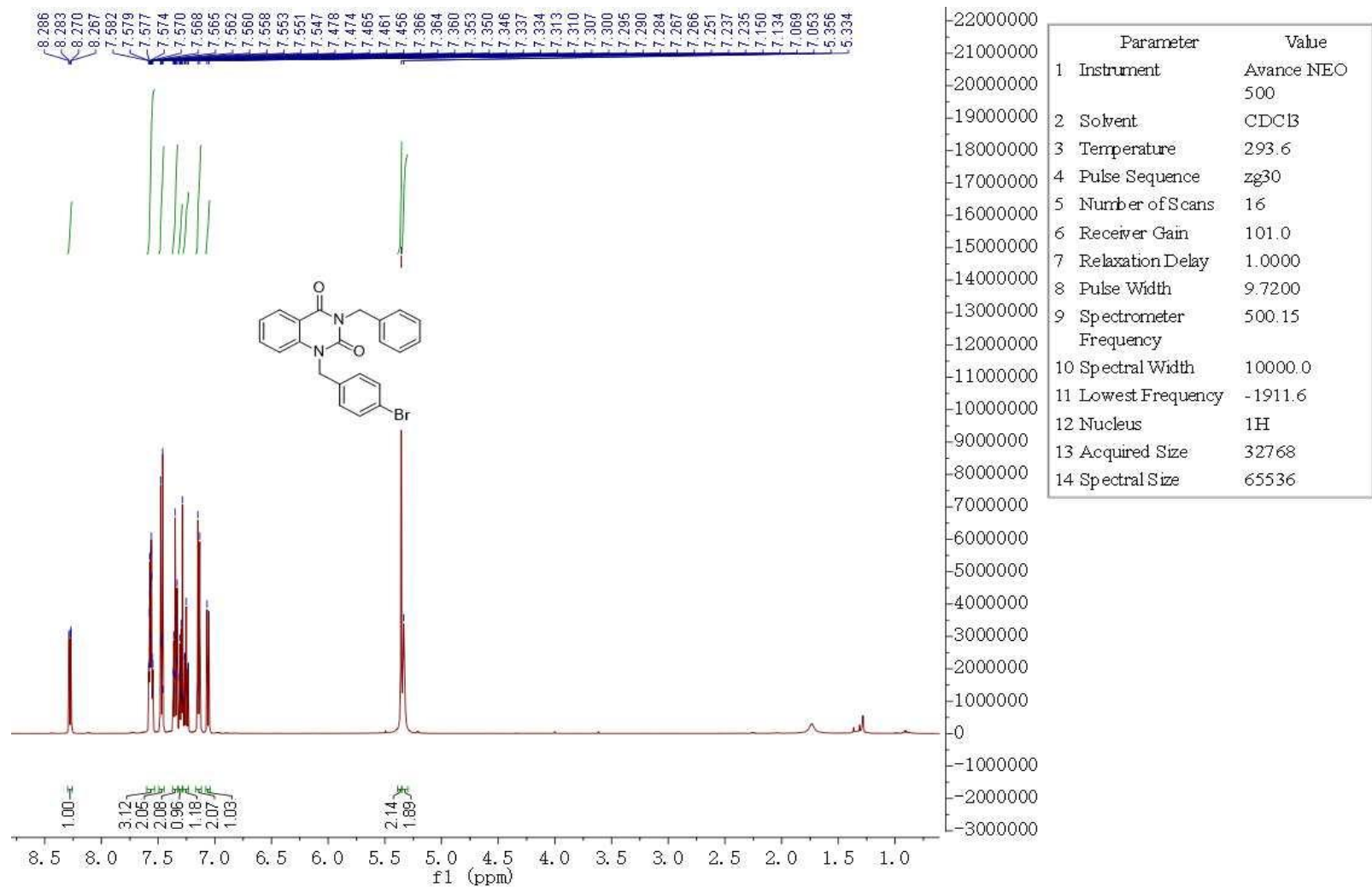


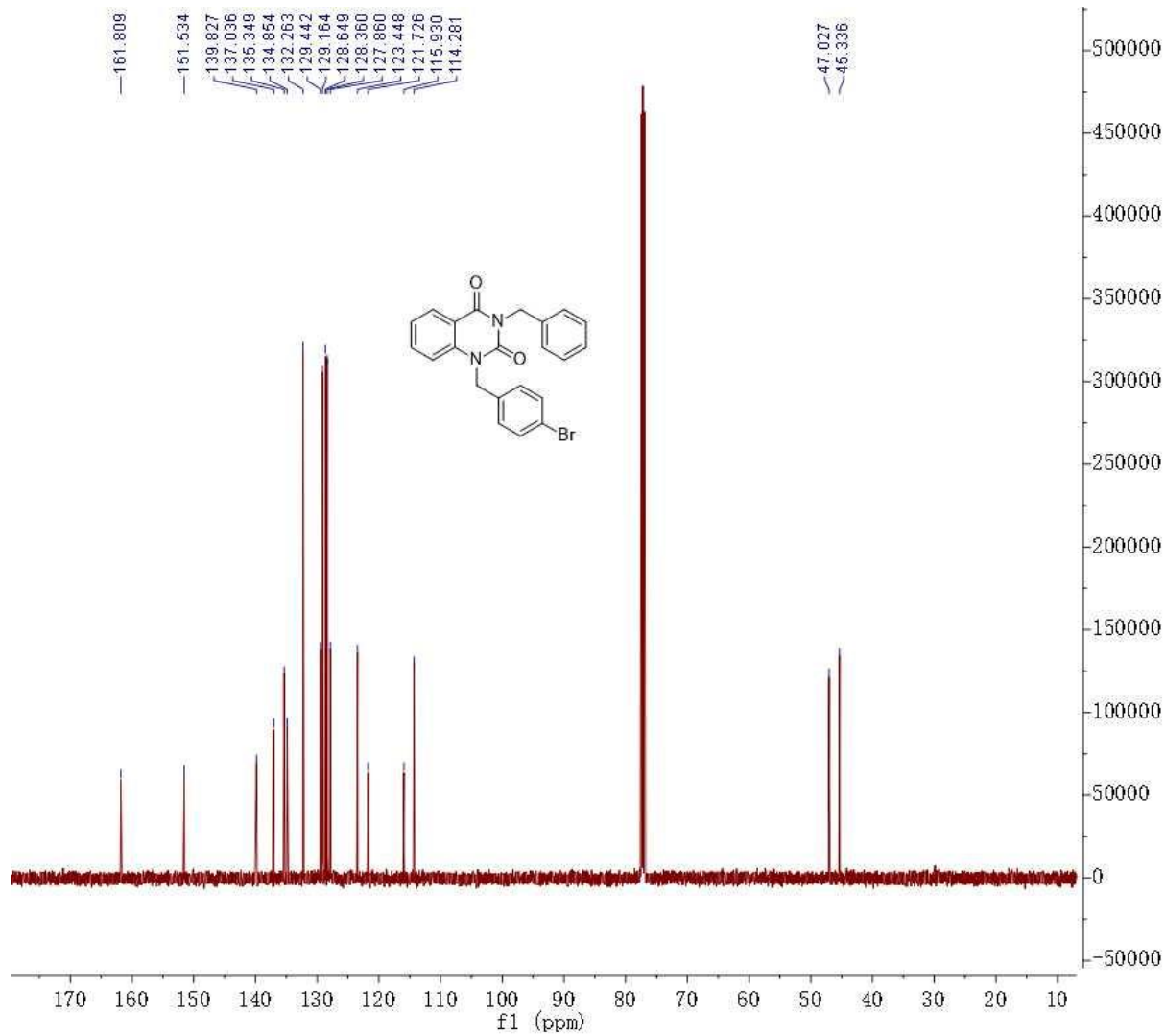
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4 Pulse Sequence	zgpg30
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7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest Frequency	-2484.0
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536



Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.2
4 Pulse Sequence	zg
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	15.0000
9 Spectrometer Frequency	470.56
10 Spectral Width	113636.4
11 Lowest Frequency	-103879.3
12 Nucleus	19F
13 Acquired Size	65536
14 Spectral Size	131072

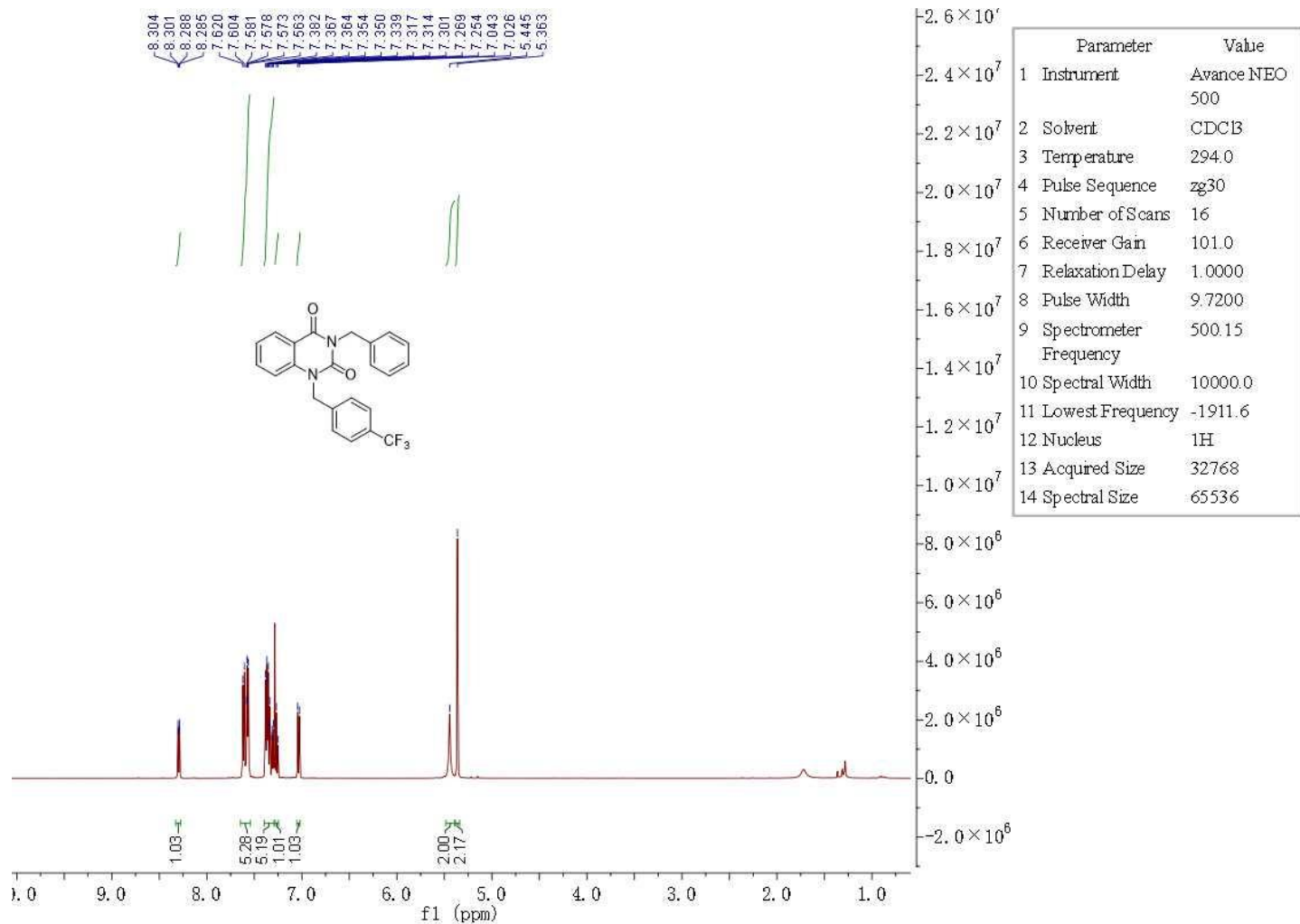
3-benzyl-1-(4-bromobenzyl)quinazoline-2,4(1H,3H)-dione (3e)

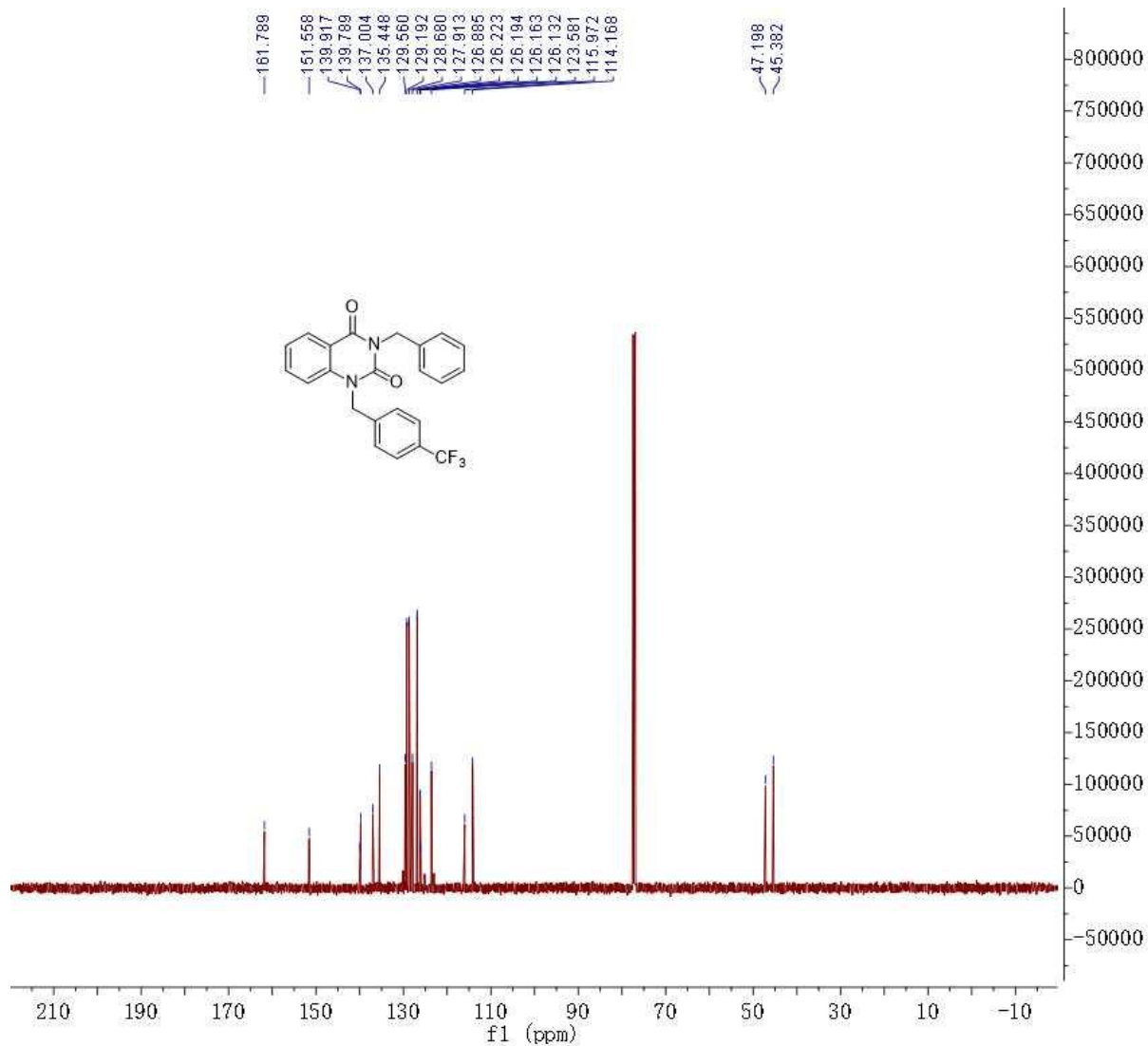




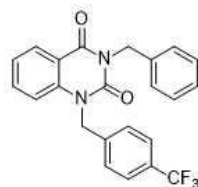
Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	DMSO
3 Temperature	294.3
4 Pulse Sequence	zgpg30
5 Number of Scans	100
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-1870.8
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536

3-benzyl-1-(4-(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (3f)

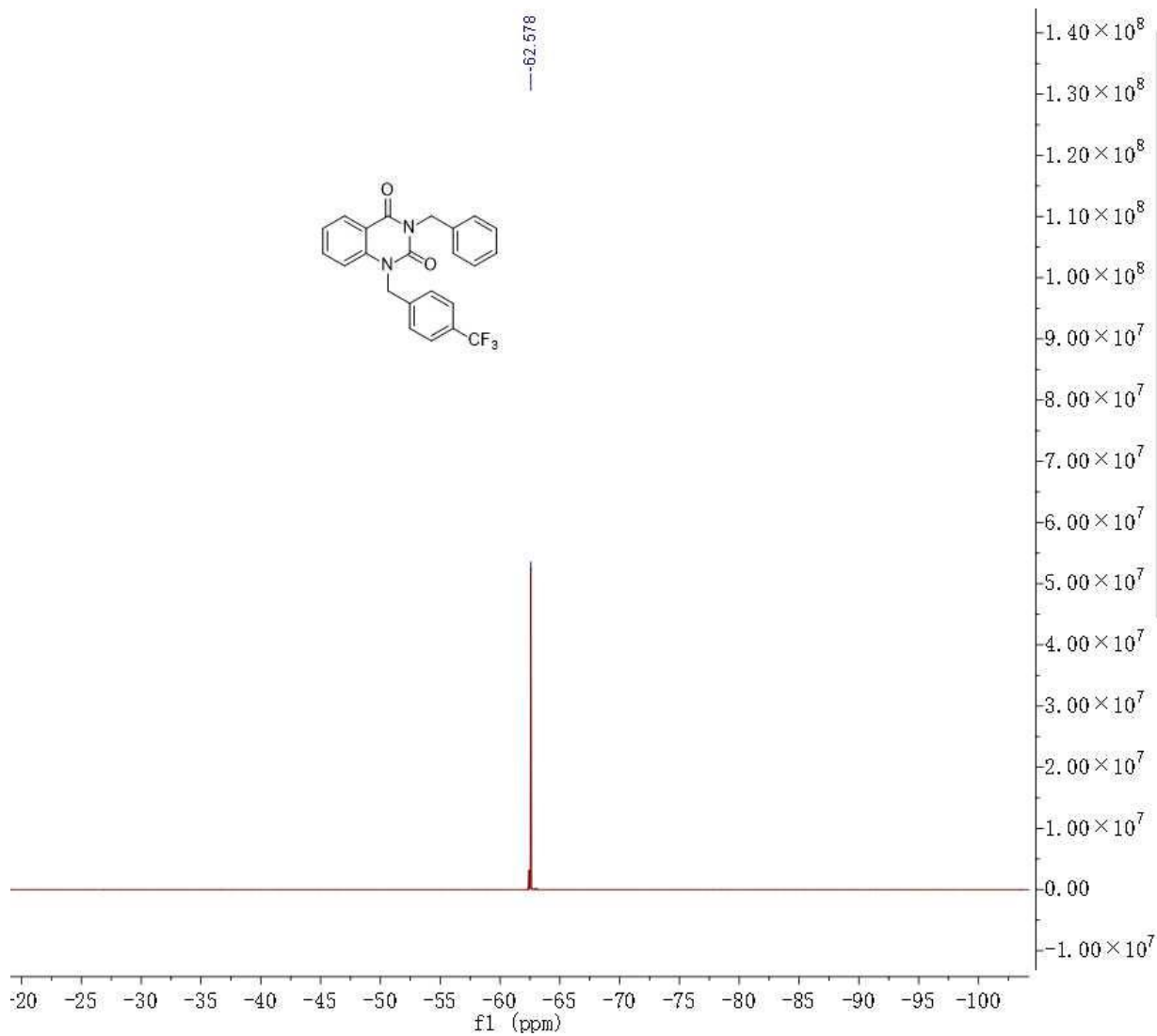




Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.5
4 Pulse Sequence	zgpg30
5 Number of Scans	120
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2465.7
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

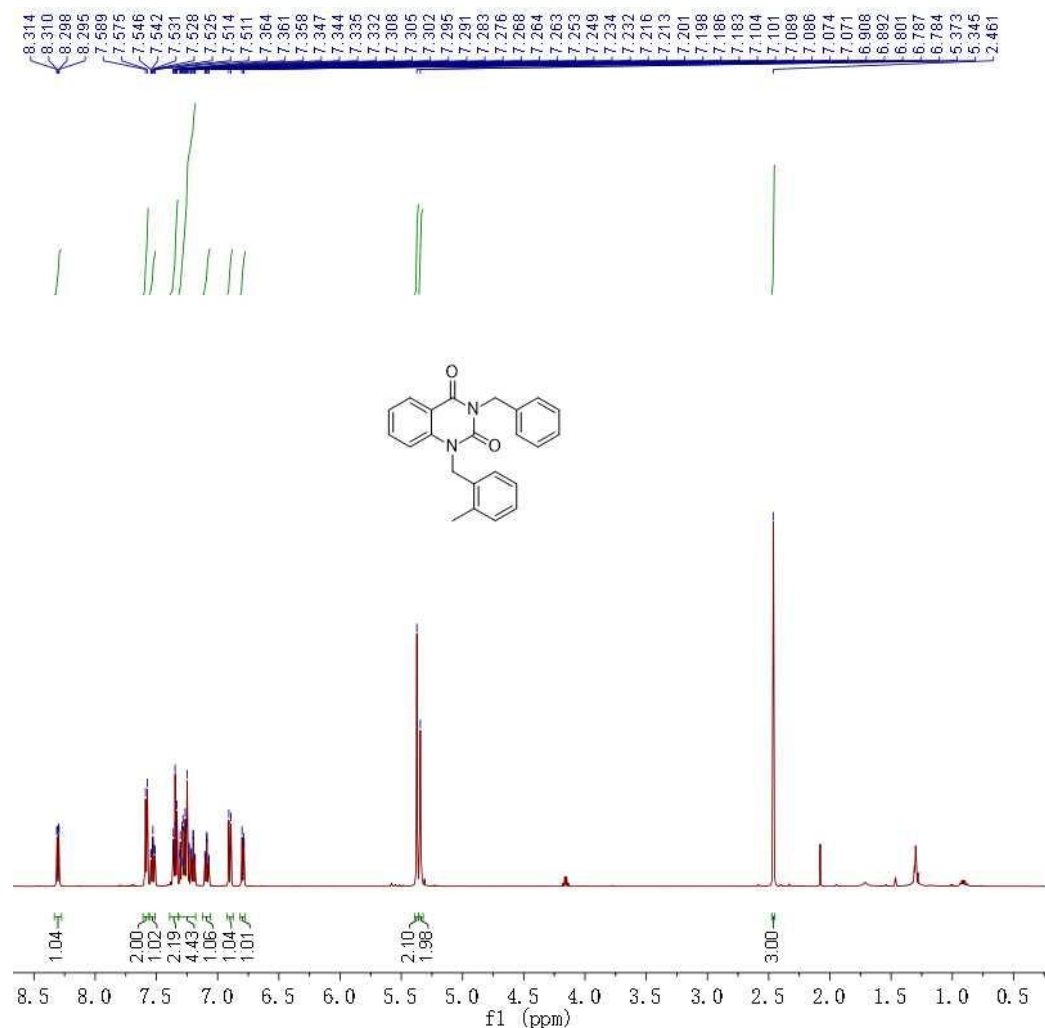


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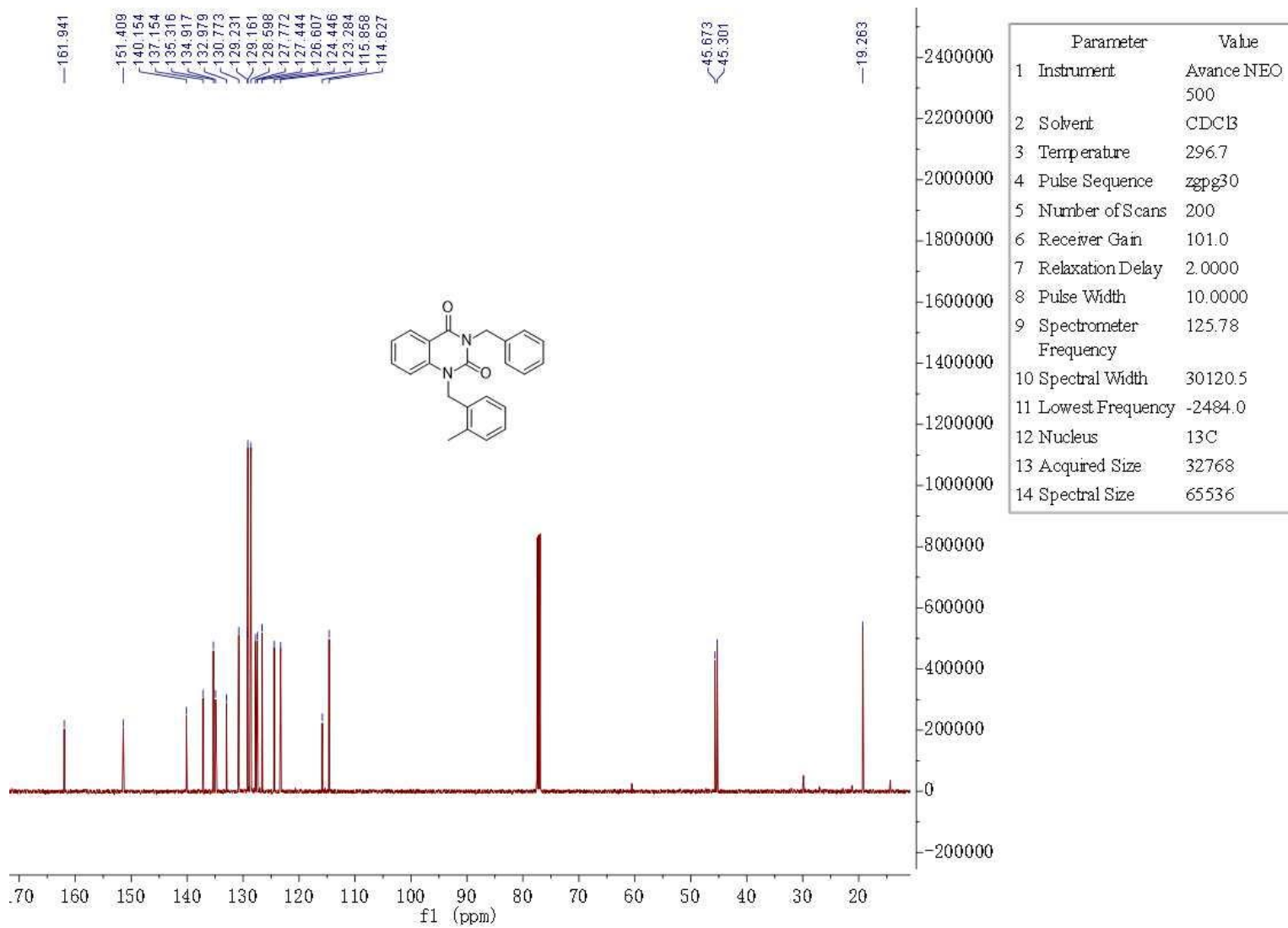


Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	293.7
4 Pulse Sequence	zg
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	15.0000
9 Spectrometer Frequency	470.56
10 Spectral Width	113636.4
11 Lowest Frequency	-103879.3
12 Nucleus	19F
13 Acquired Size	65536
14 Spectral Size	131072

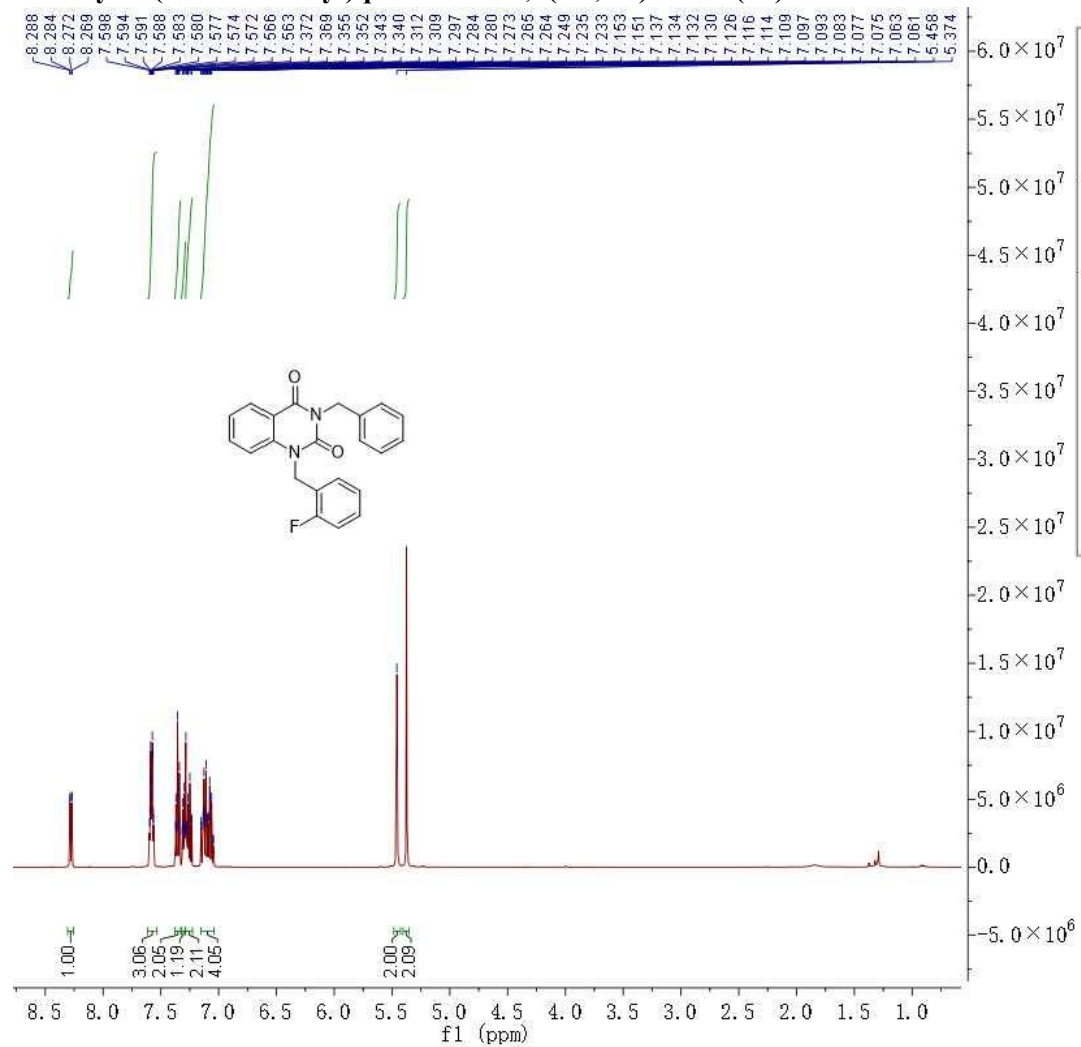
3-benzyl-1-(2-methylbenzyl)quinazoline-2,4(1H,3H)-dione (3g)



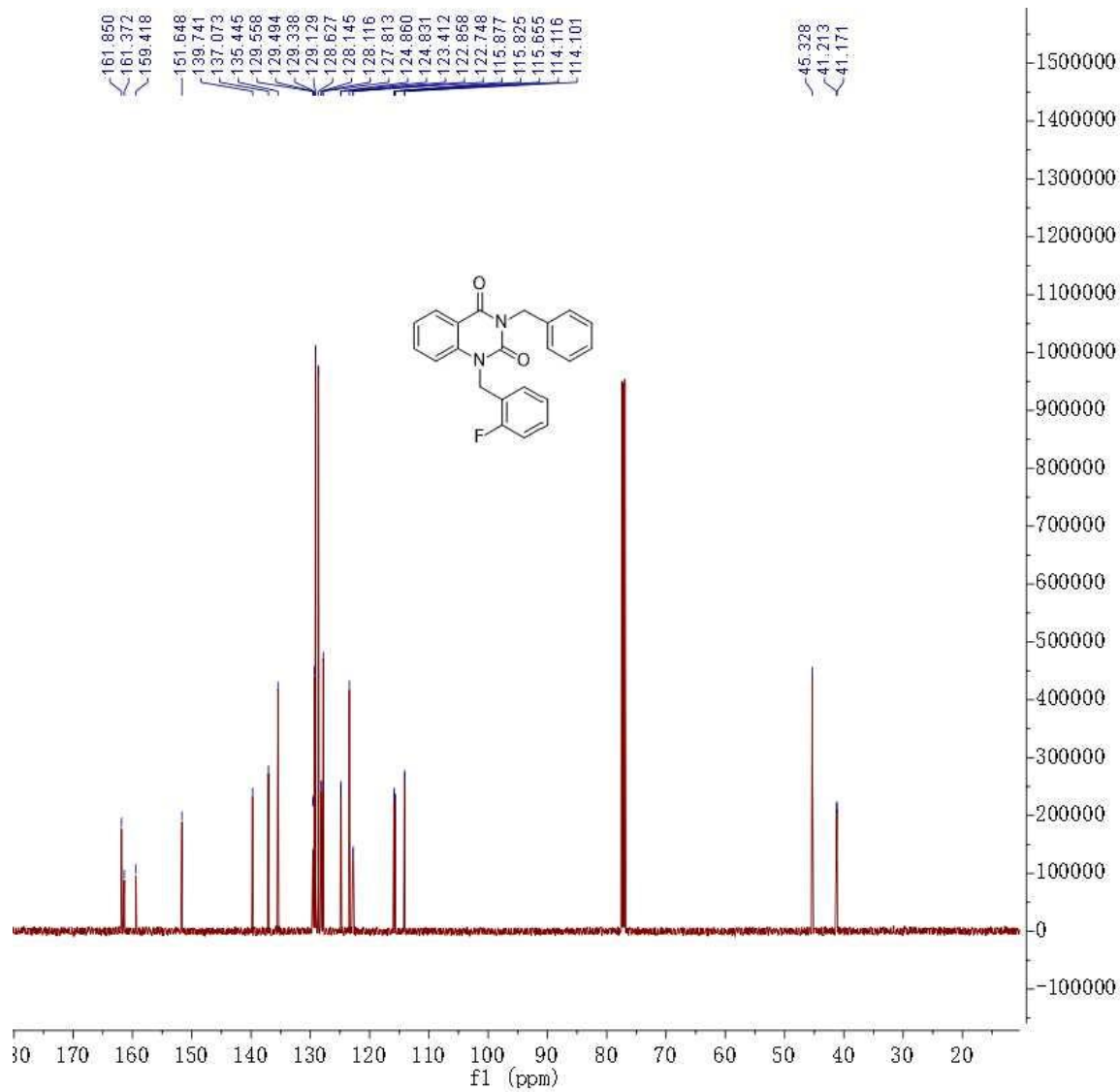
Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	297.2
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	86.7
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer	500.15 Frequency
10 Spectral Width	10000.0
11 Lowest	-1911.6 Frequency
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



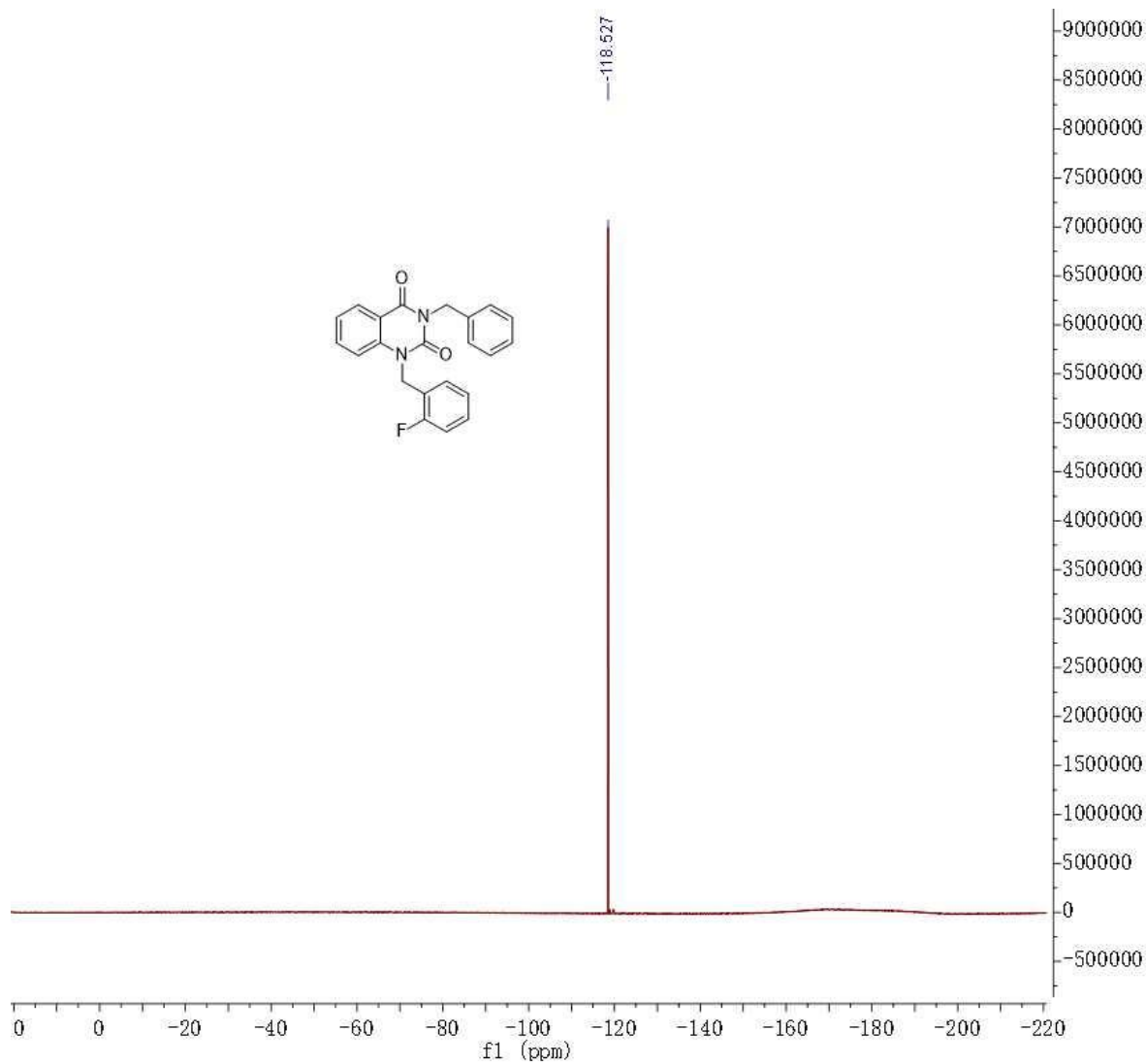
3-benzyl-1-(2-fluorobenzyl)quinazoline-2,4(1H,3H)-dione (3h)



Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	294.0
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer	500.15
Frequency	
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	¹ H
13 Acquired Size	32768
14 Spectral Size	65536

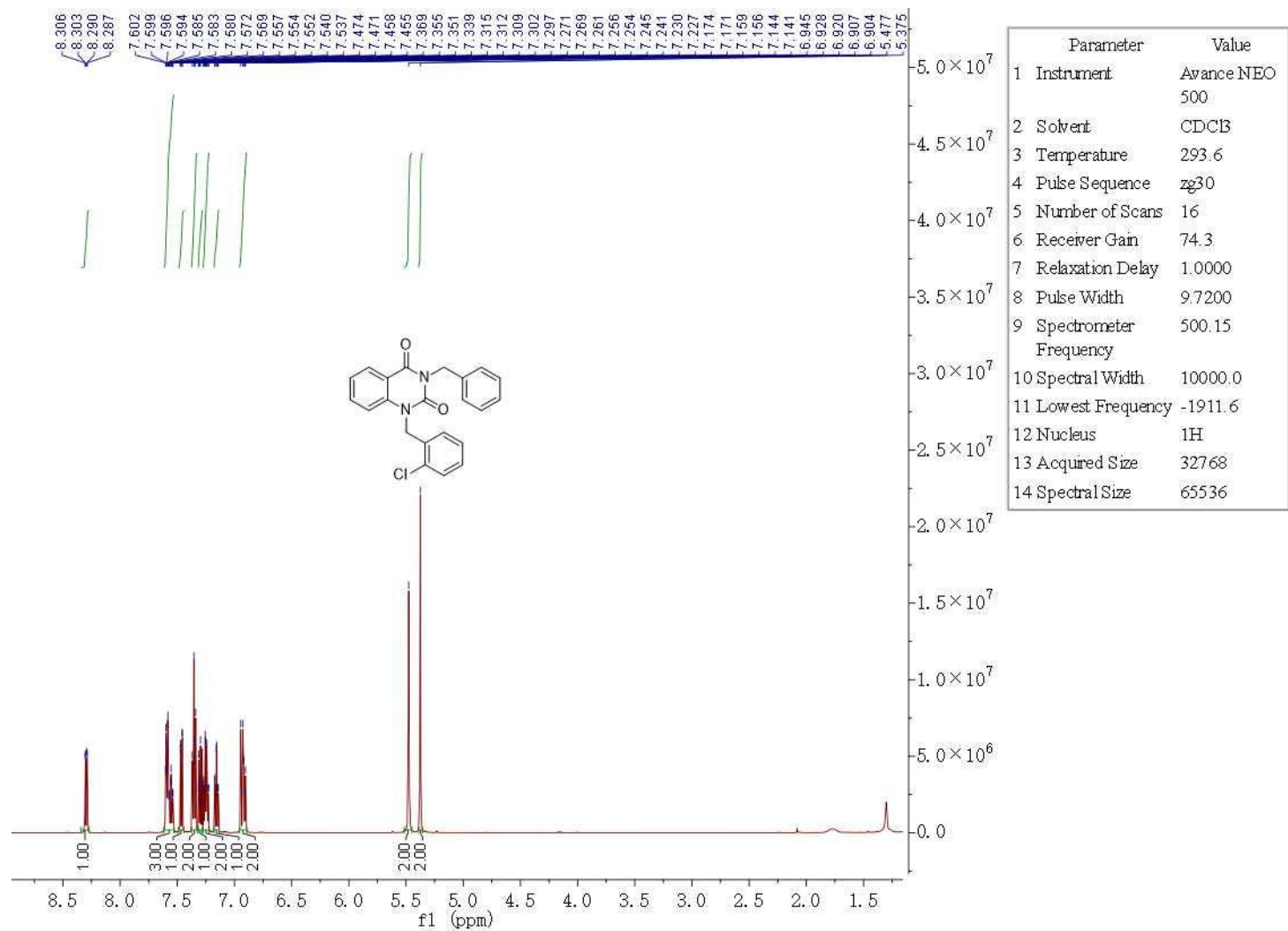


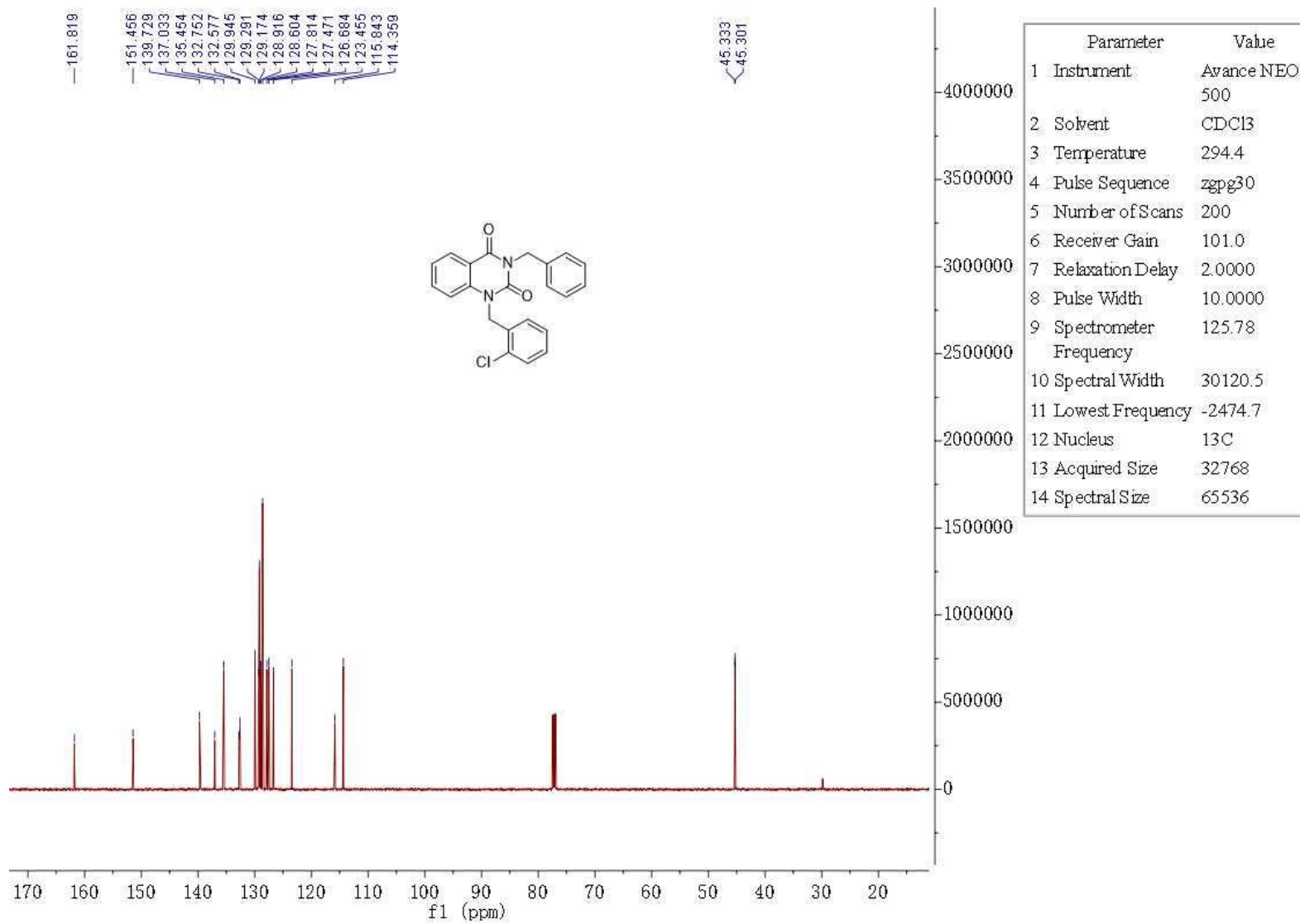
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.7
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2469.9
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536



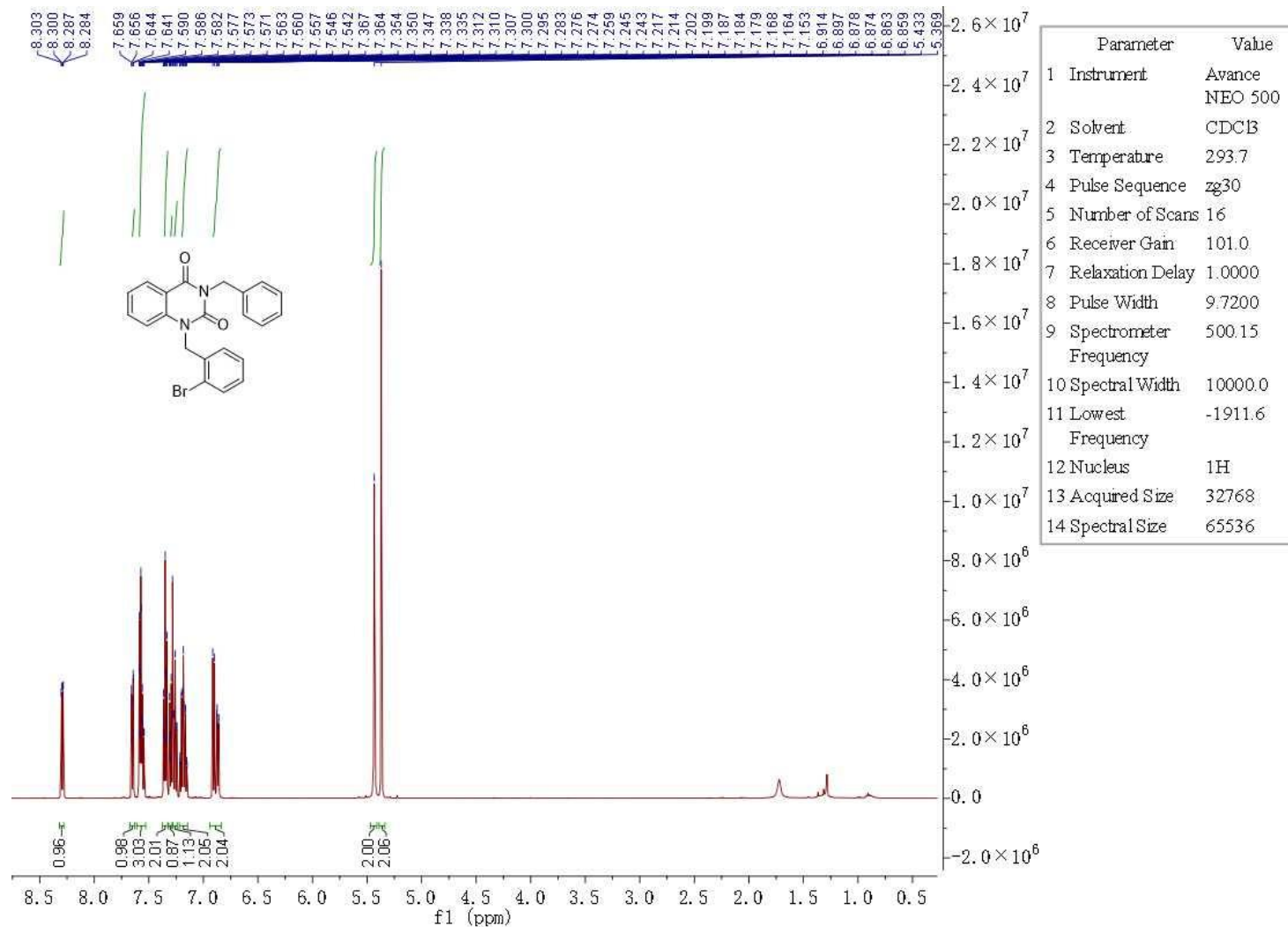
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.0
4 Pulse Sequence	zg
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	15.0000
9 Spectrometer	470.56
Frequency	
10 Spectral Width	113636.4
11 Lowest	-103879.3
Frequency	
12 Nucleus	19F
13 Acquired Size	65536
14 Spectral Size	131072

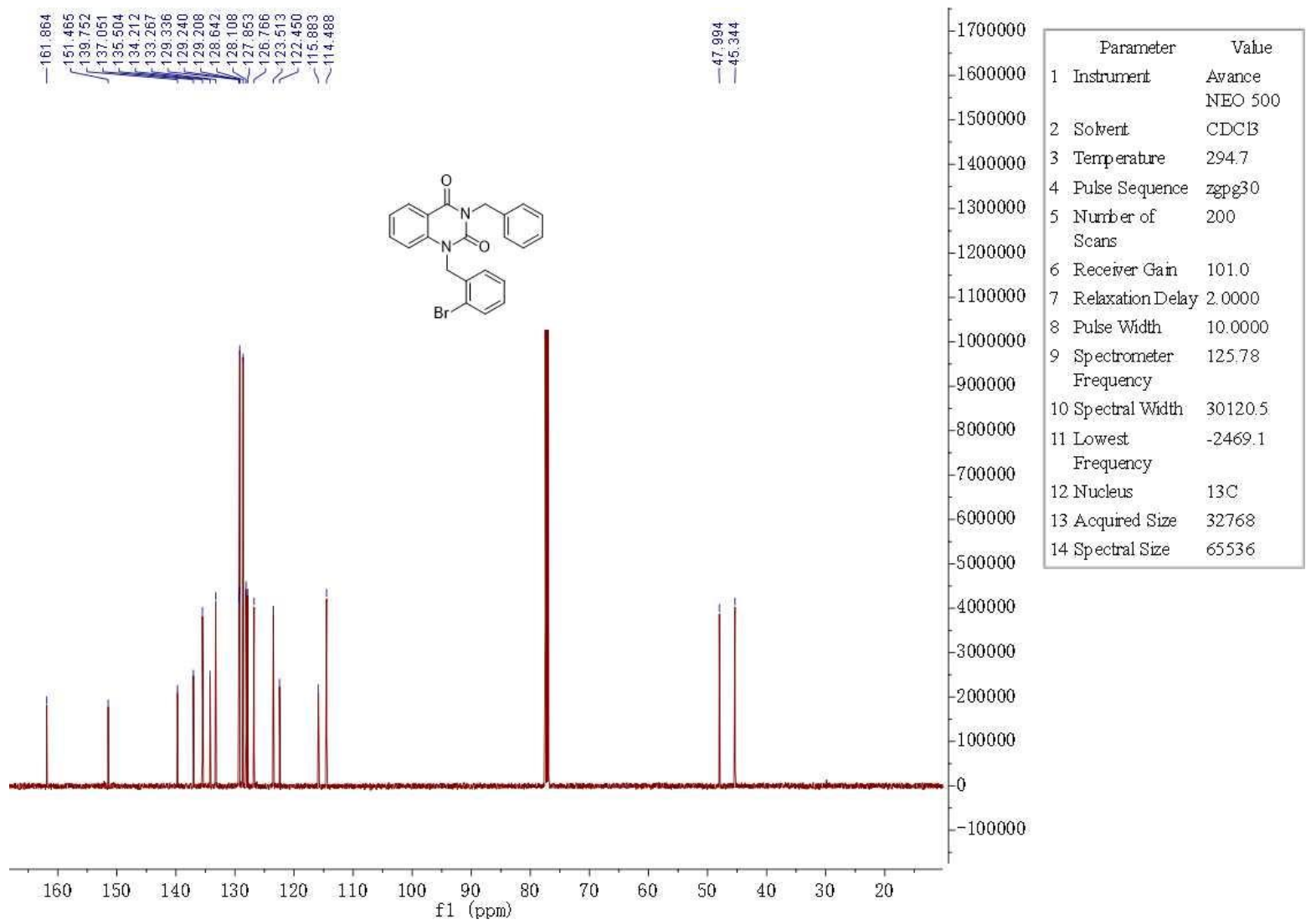
3-benzyl-1-(2-chlorobenzyl)quinazoline-2,4(1H,3H)-dione (3i)



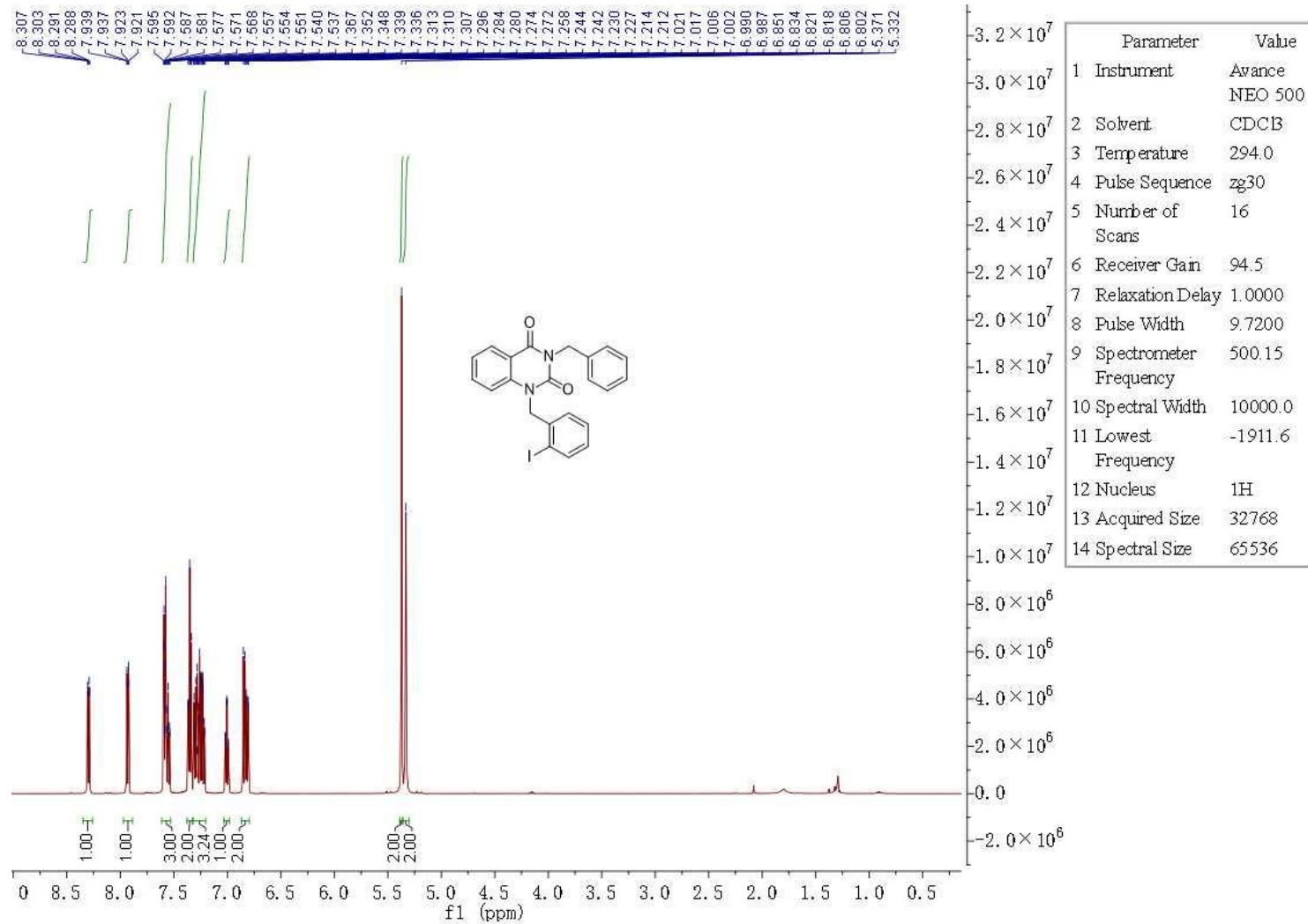


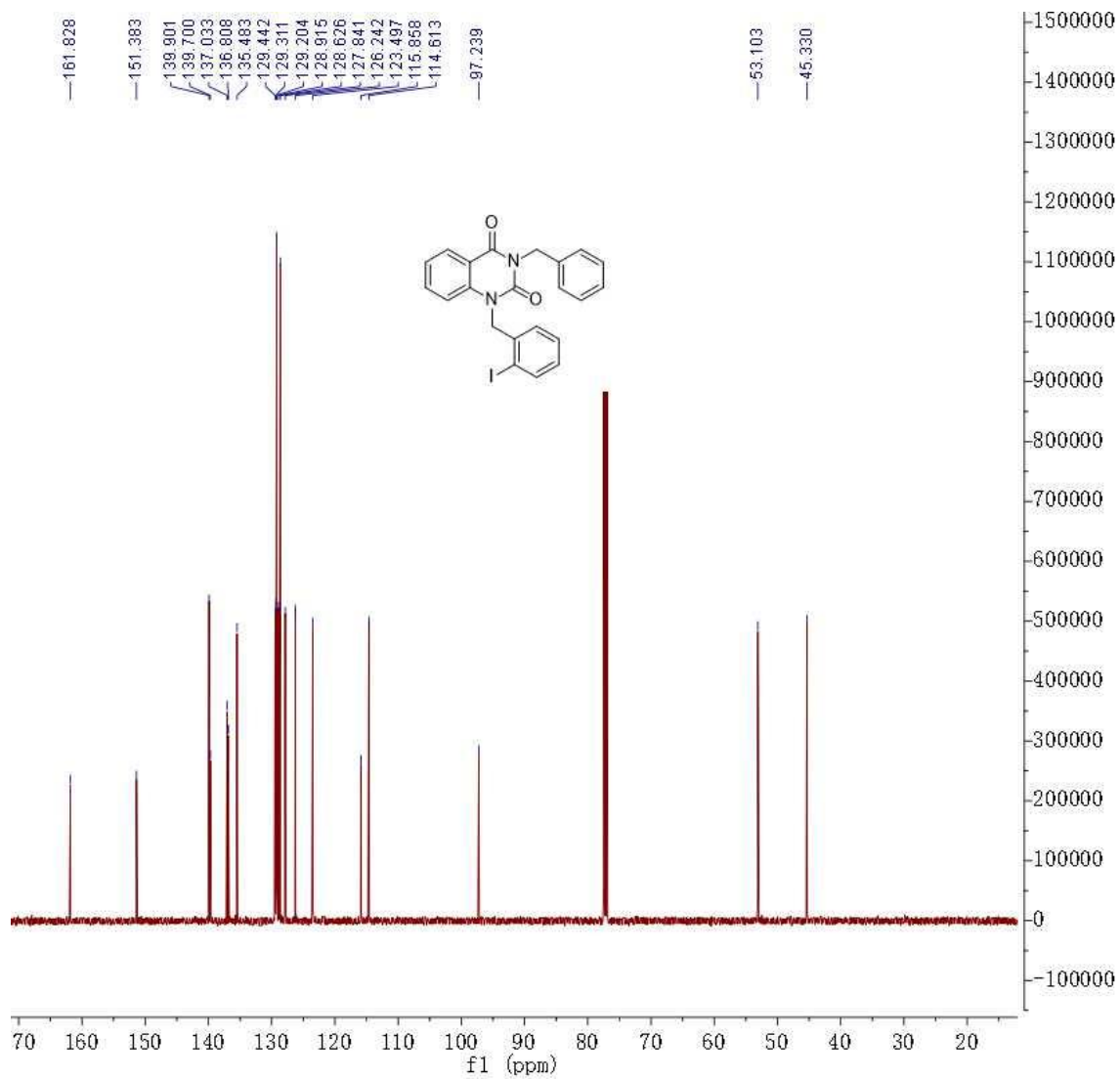
3-benzyl-1-(2-bromobenzyl)quinazoline-2,4(1H,3H)-dione (3j)





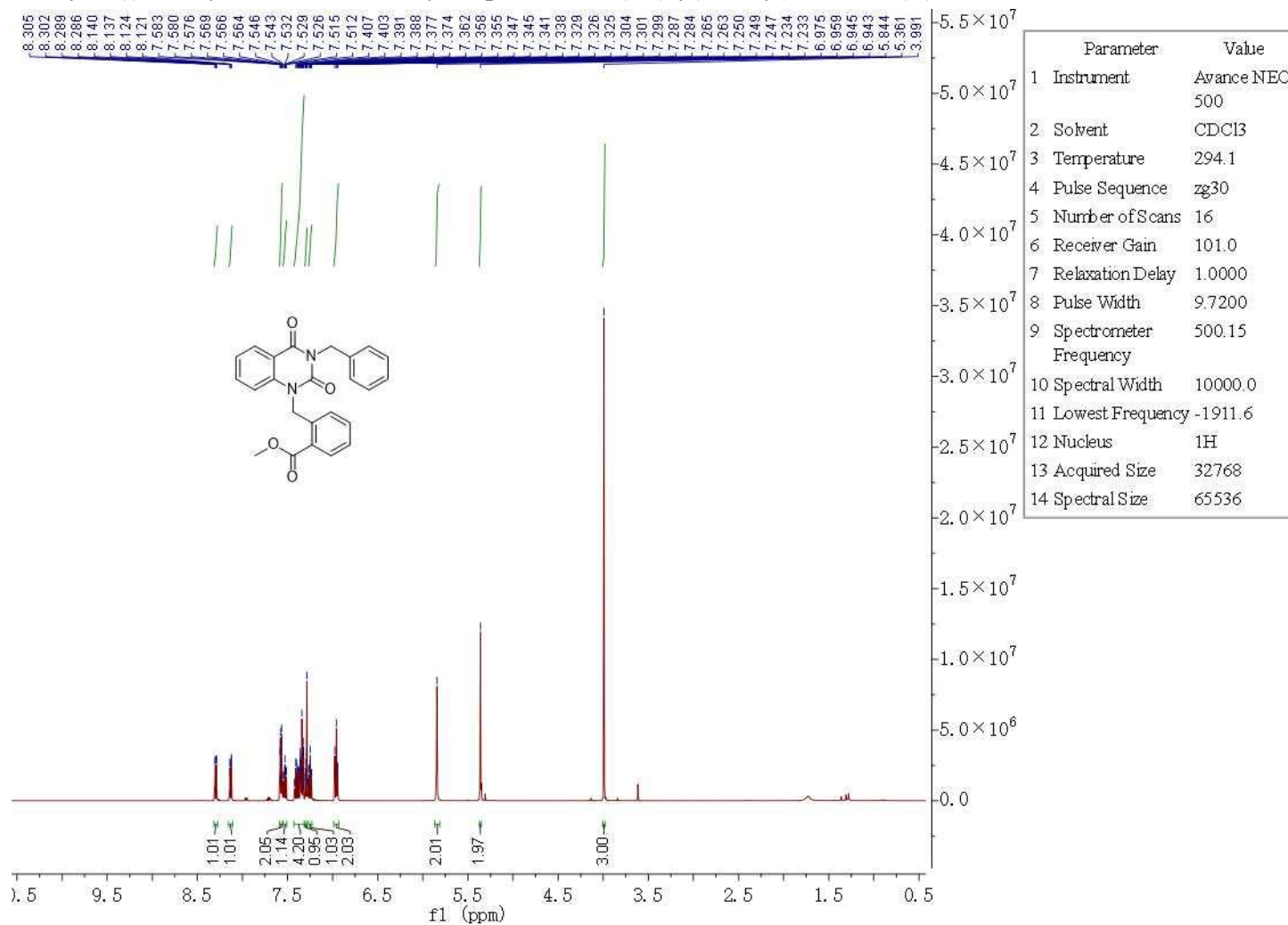
3-benzyl-1-(2-iodobenzyl)quinazoline-2,4(1H,3H)-dione (3k)

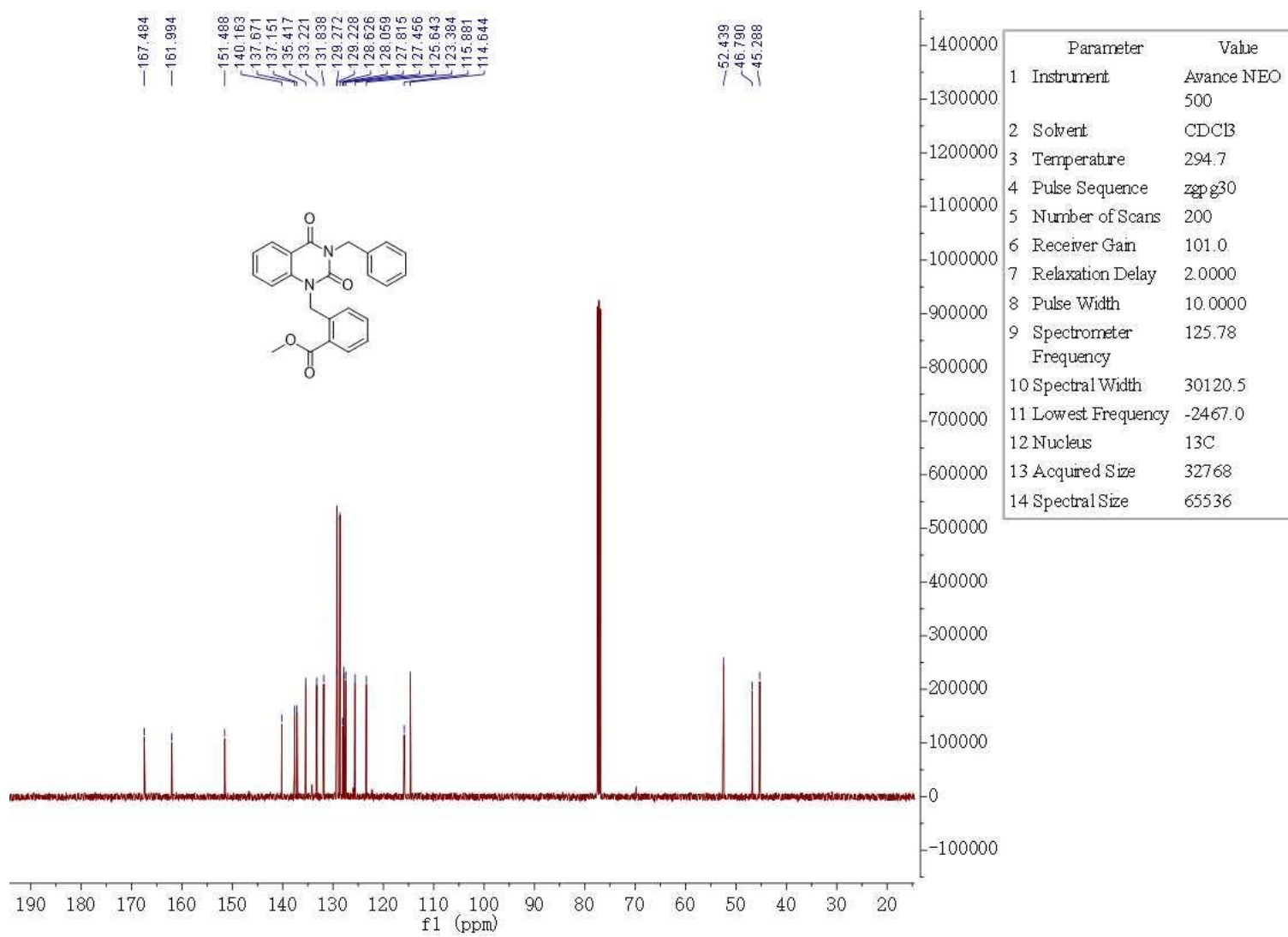




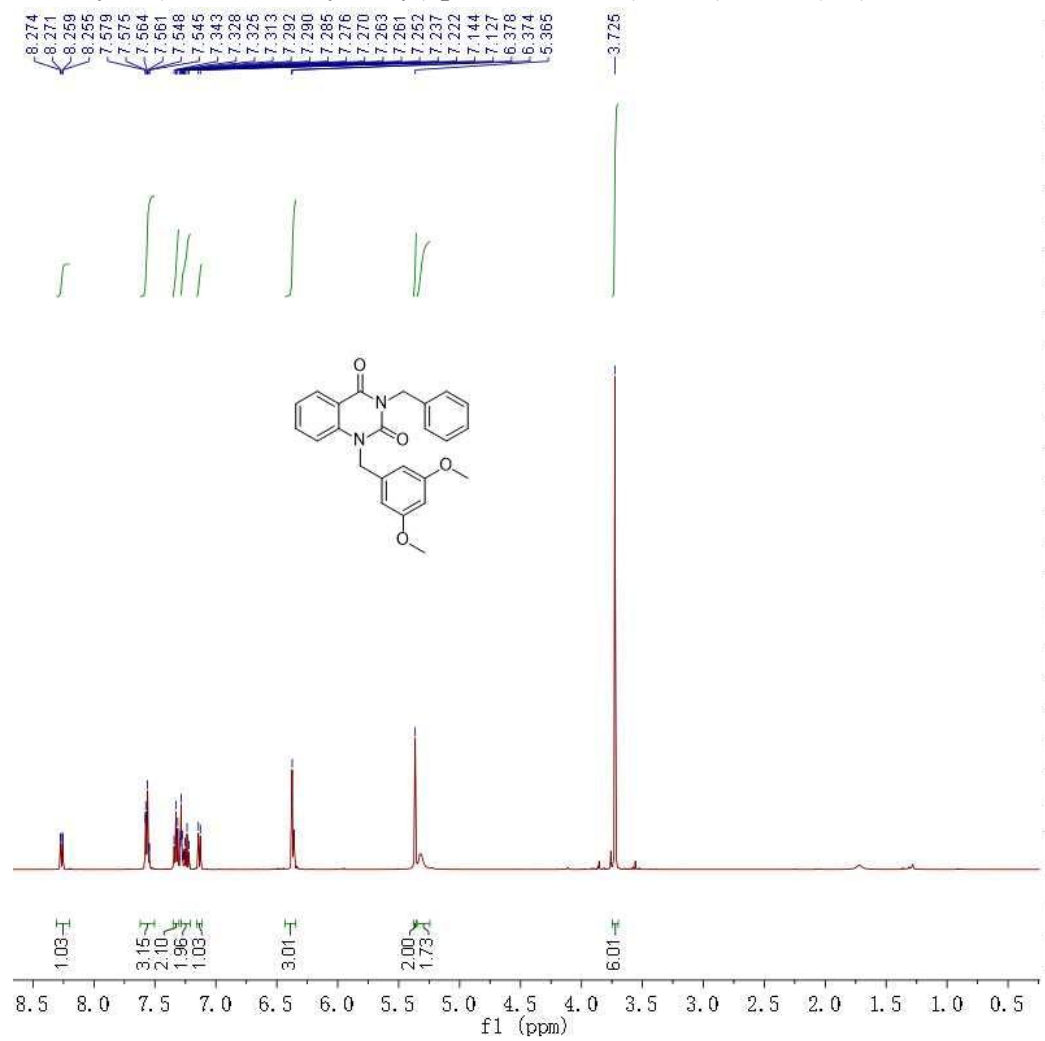
Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	294.6
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2472.3
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

methyl 2-((3-benzyl-2,4-dioxo-3,4-dihydroquinazolin-1(2H)-yl)methyl)benzoate (3l)

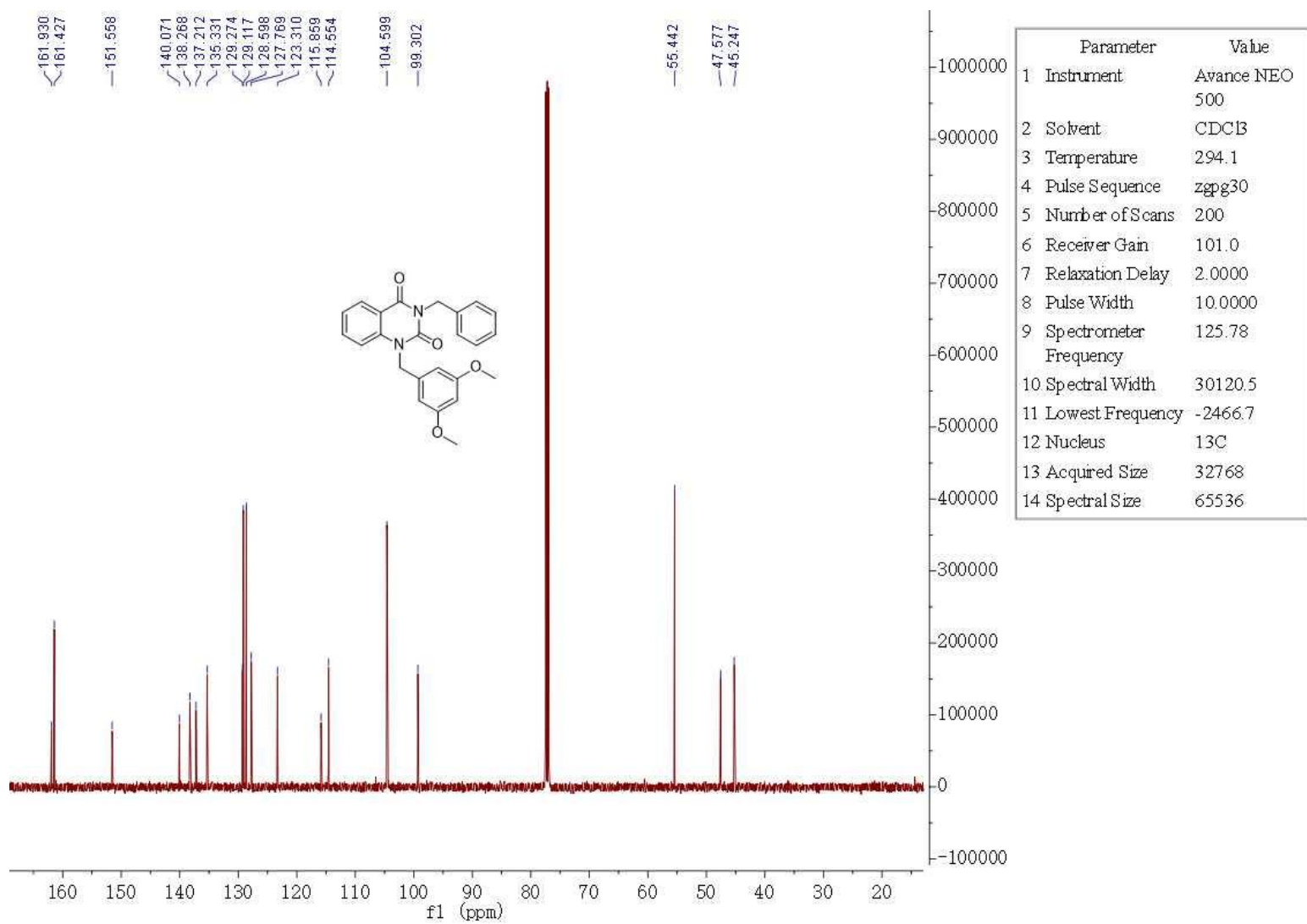




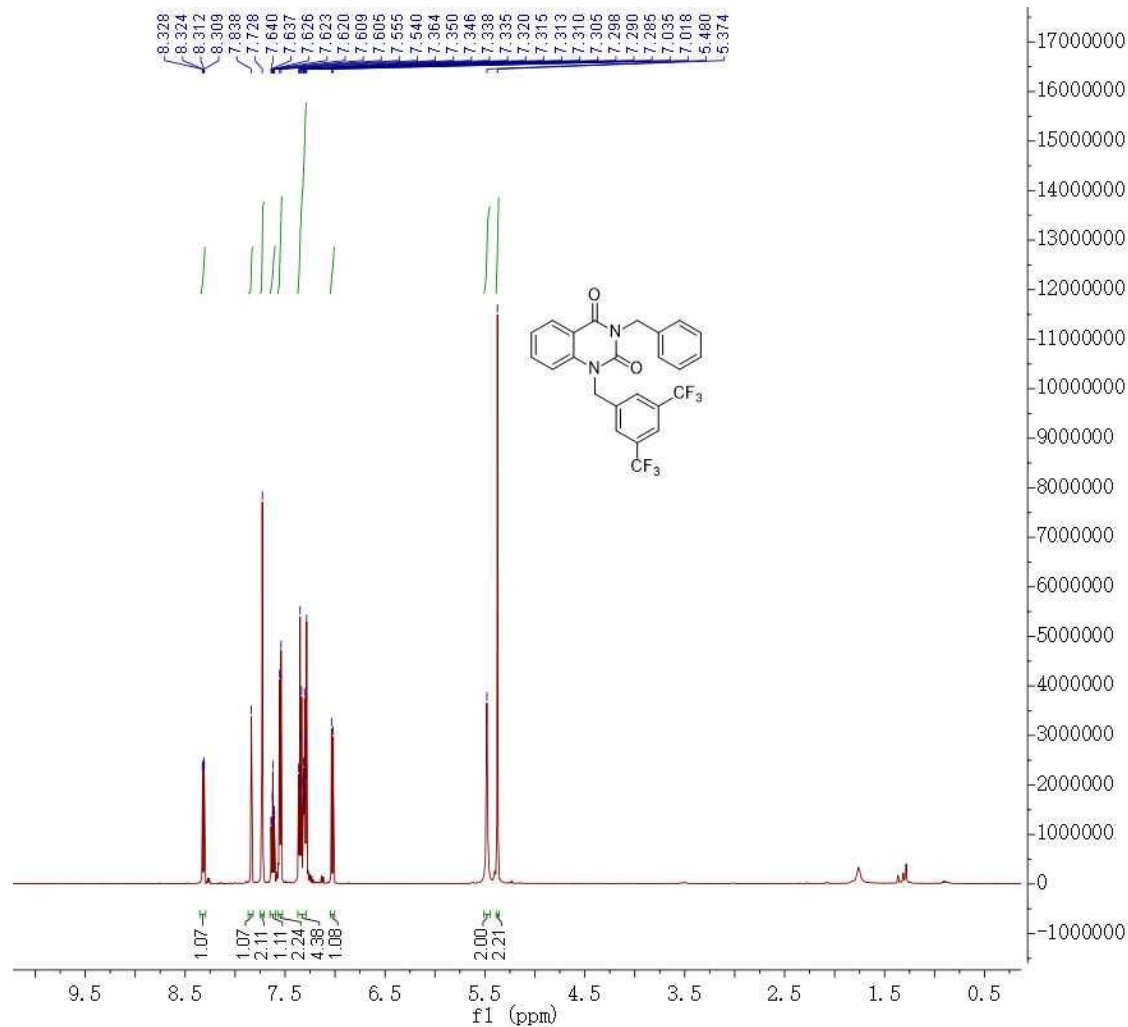
3-benzyl-1-(3,5-dimethoxybenzyl)quinazoline-2,4(1H,3H)-dione (3m)



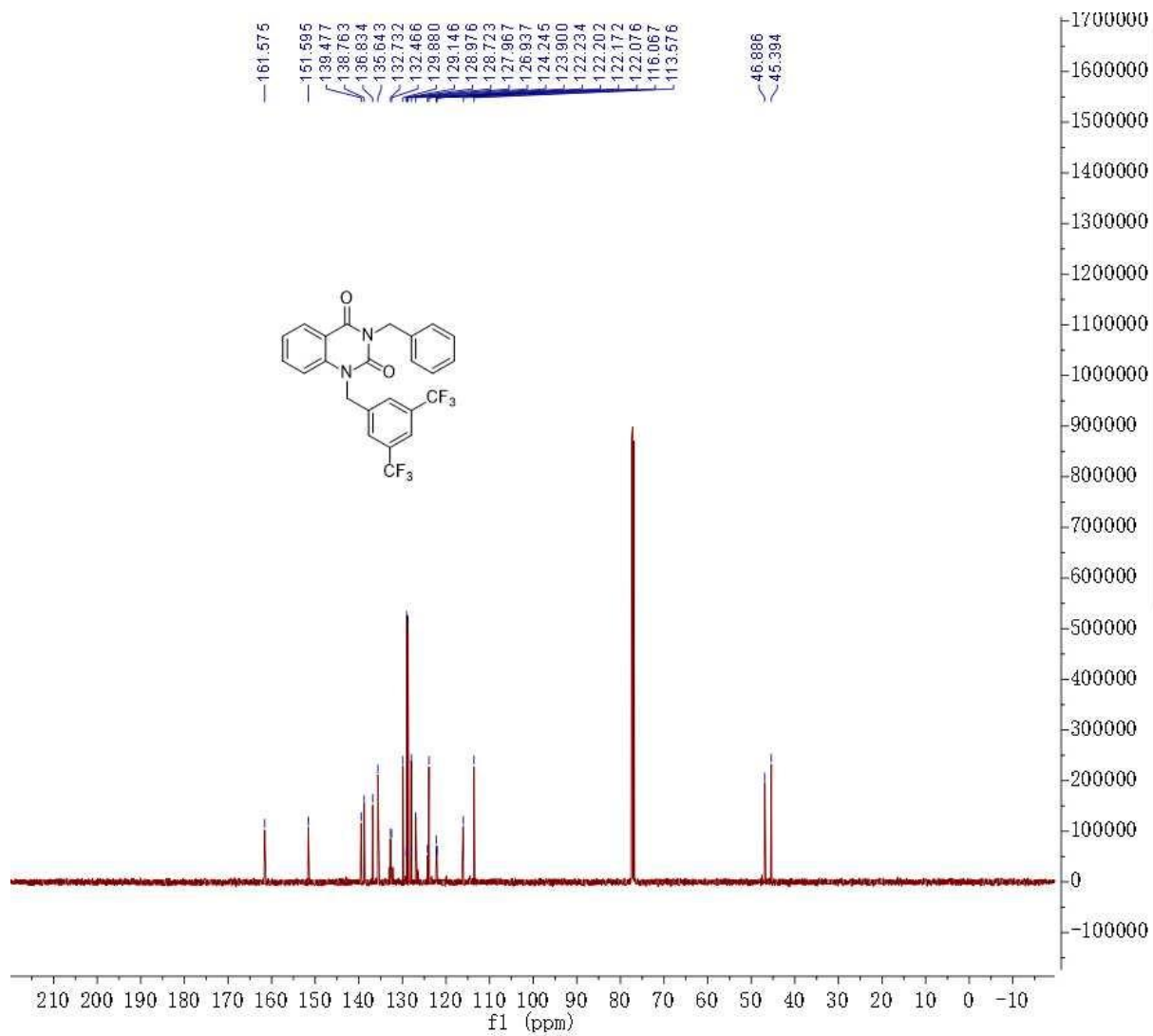
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	293.6
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer	500.15
Frequency	
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



3-benzyl-1-(3,5-bis(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (3n)

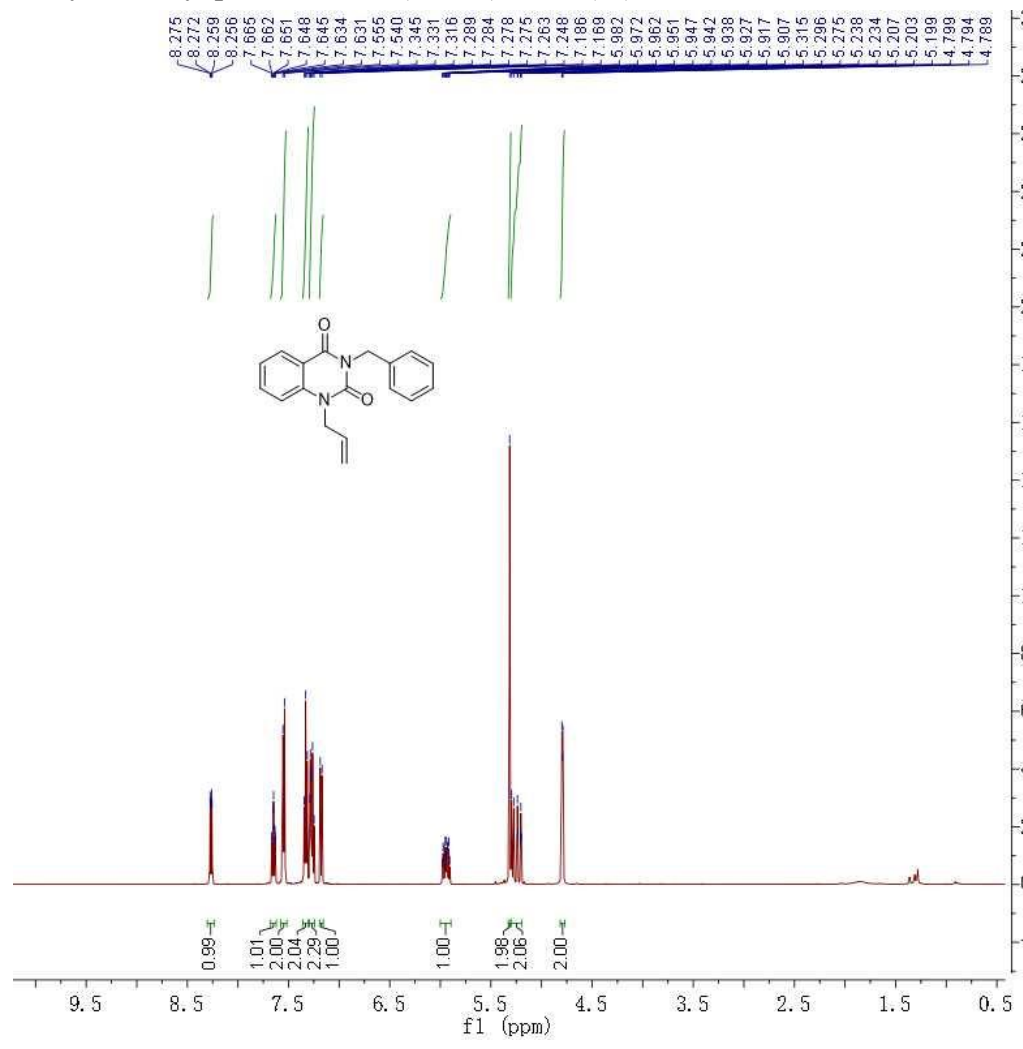


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	293.6
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer	500.15
Frequency	
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536

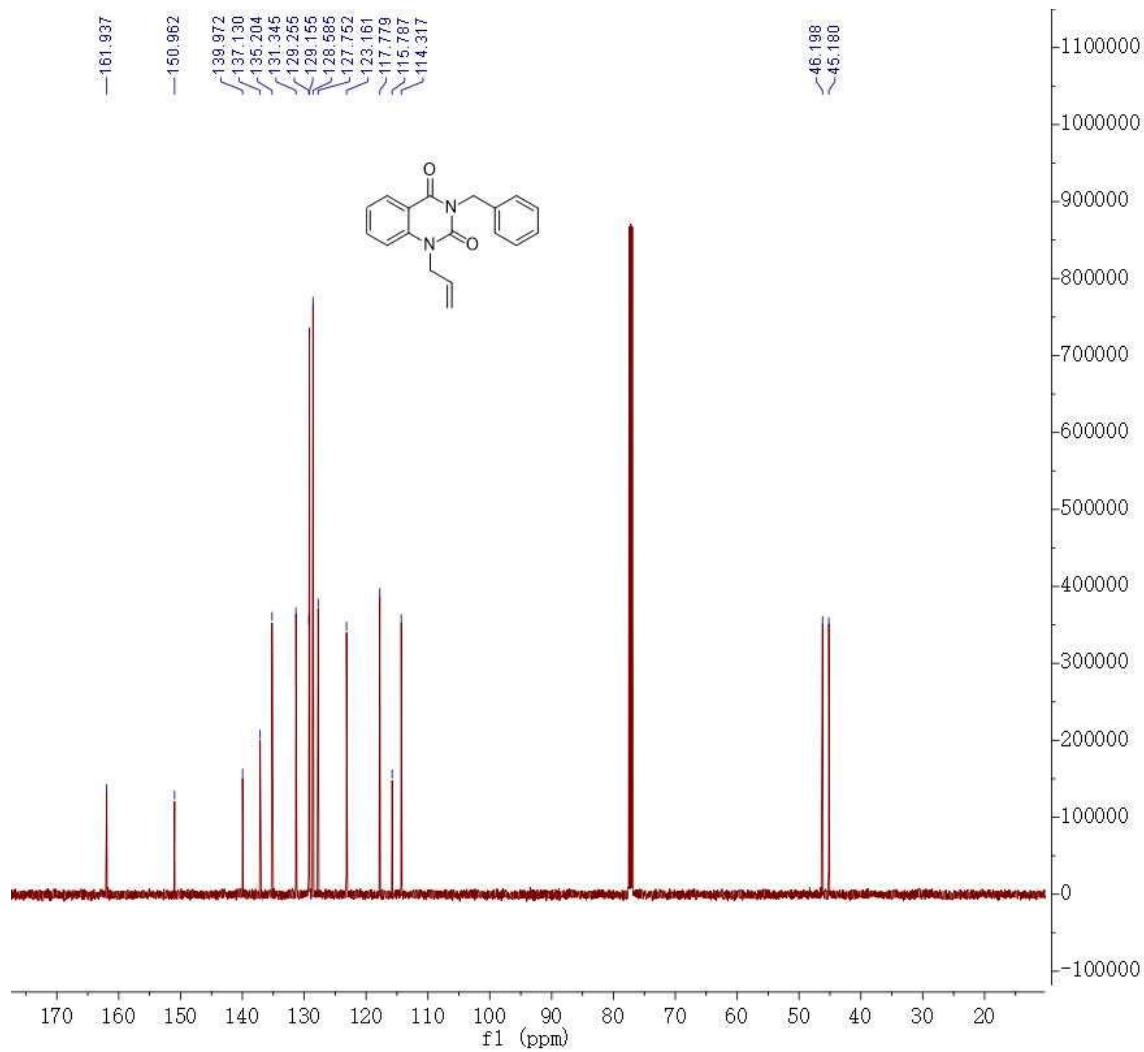


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCB
3 Temperature	294.7
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest	-2465.6
Frequency	
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536

1-allyl-3-benzylquinazoline-2,4(1H,3H)-dione (3o)

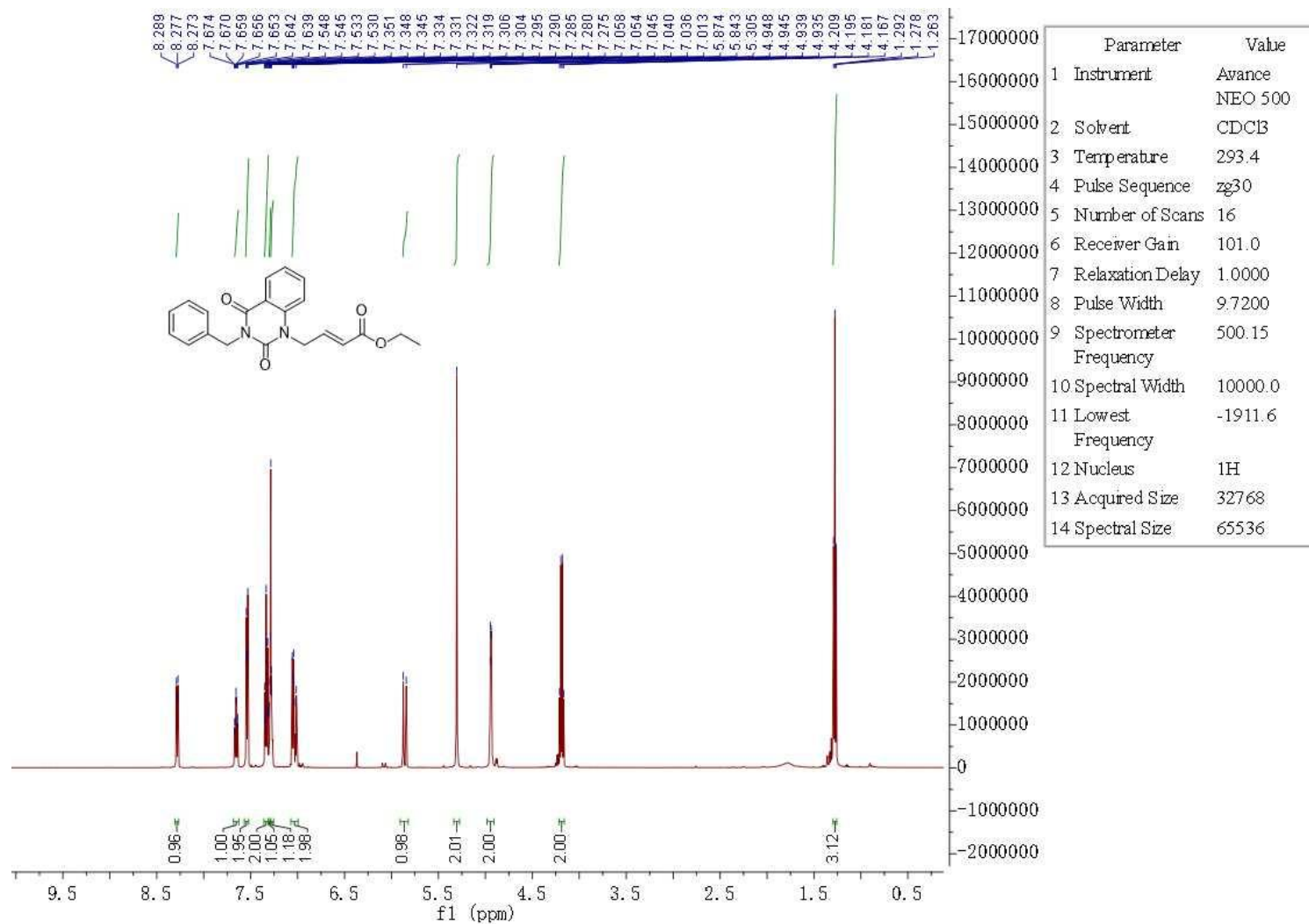


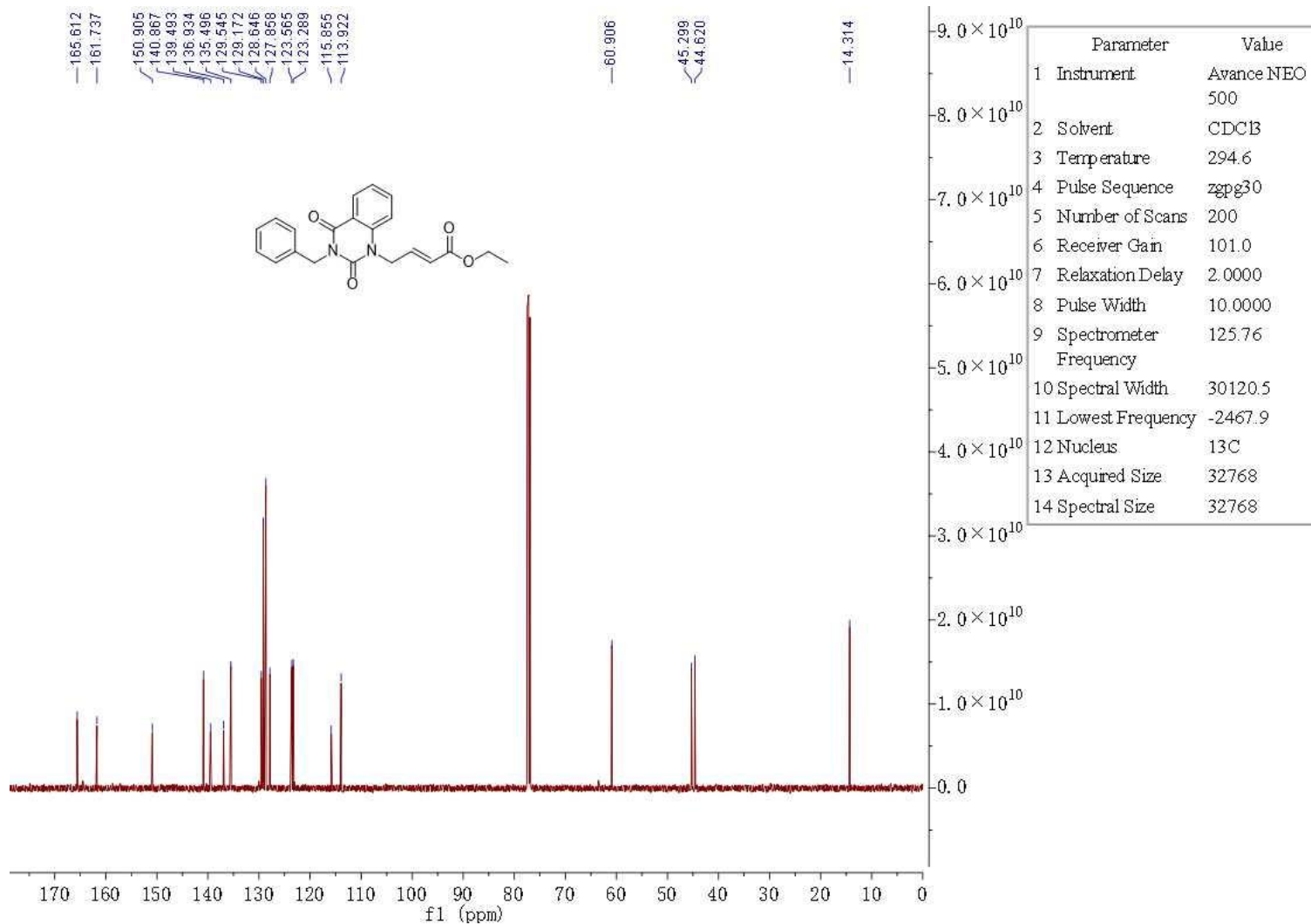
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	293.5
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer Frequency	500.15
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



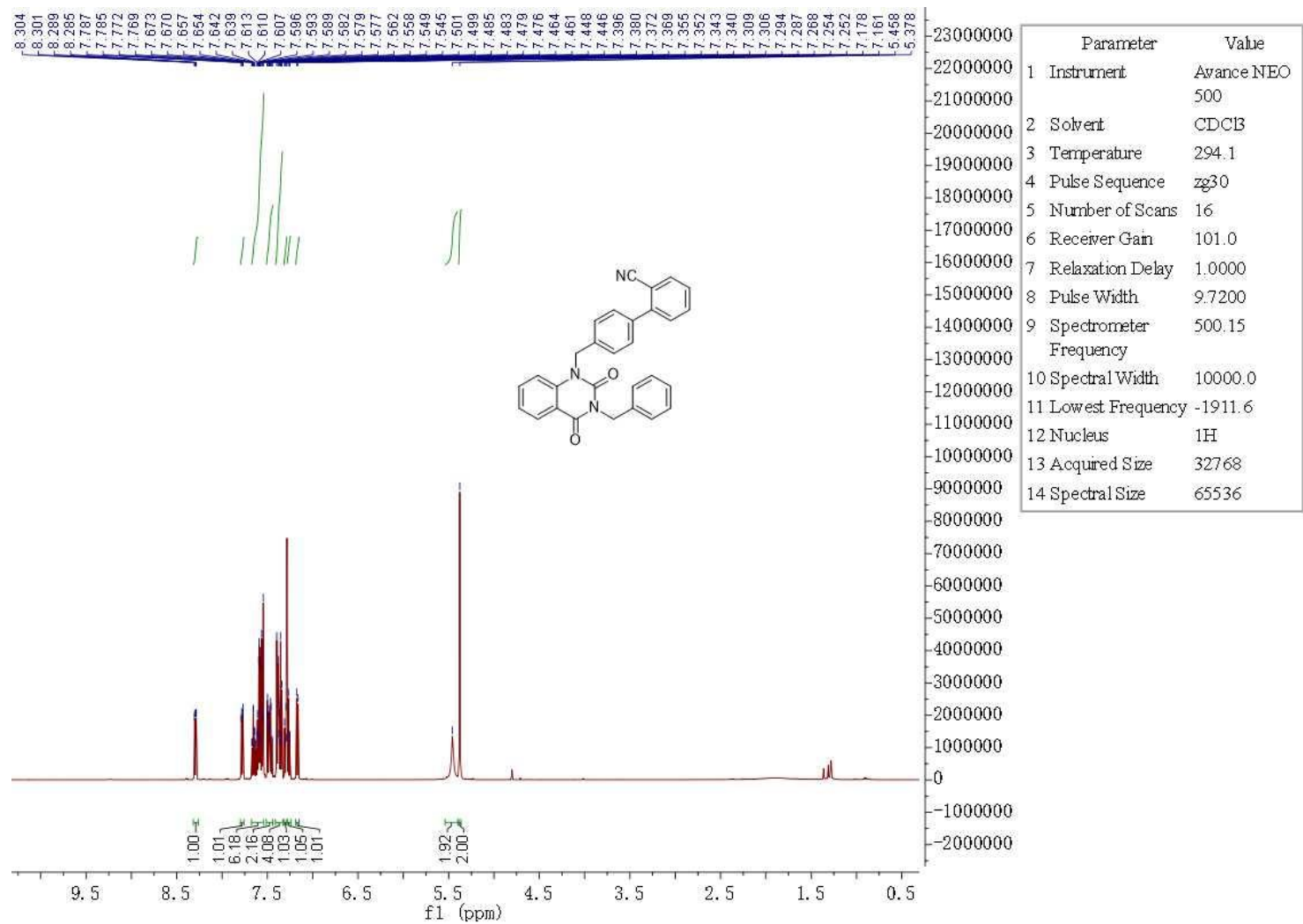
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.2
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest Frequency	-2468.4
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

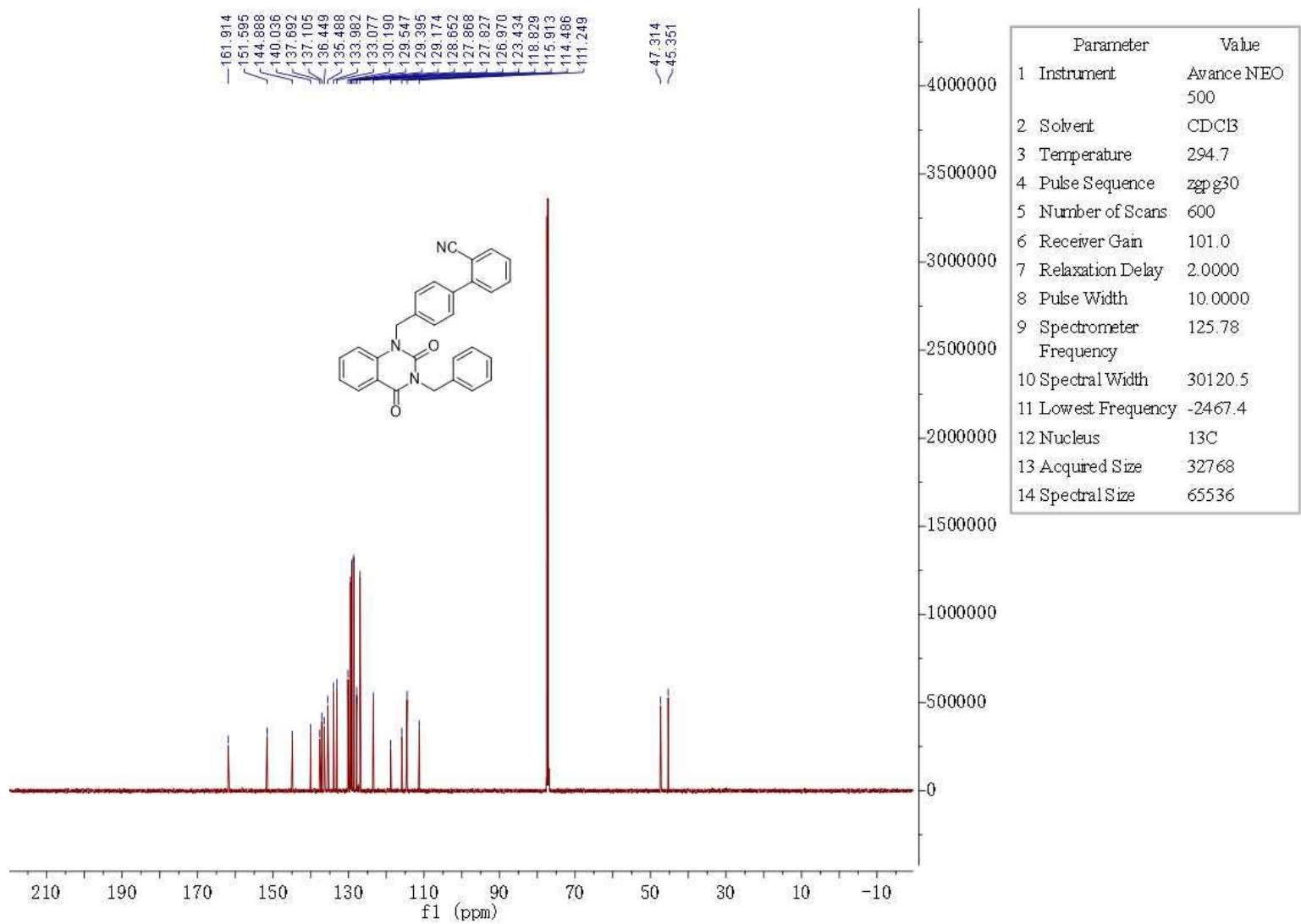
ethyl (E)-4-(3-benzyl-2,4-dioxo-3,4-dihydroquinazolin-1(2H)-yl)but-2-enoate (3p)



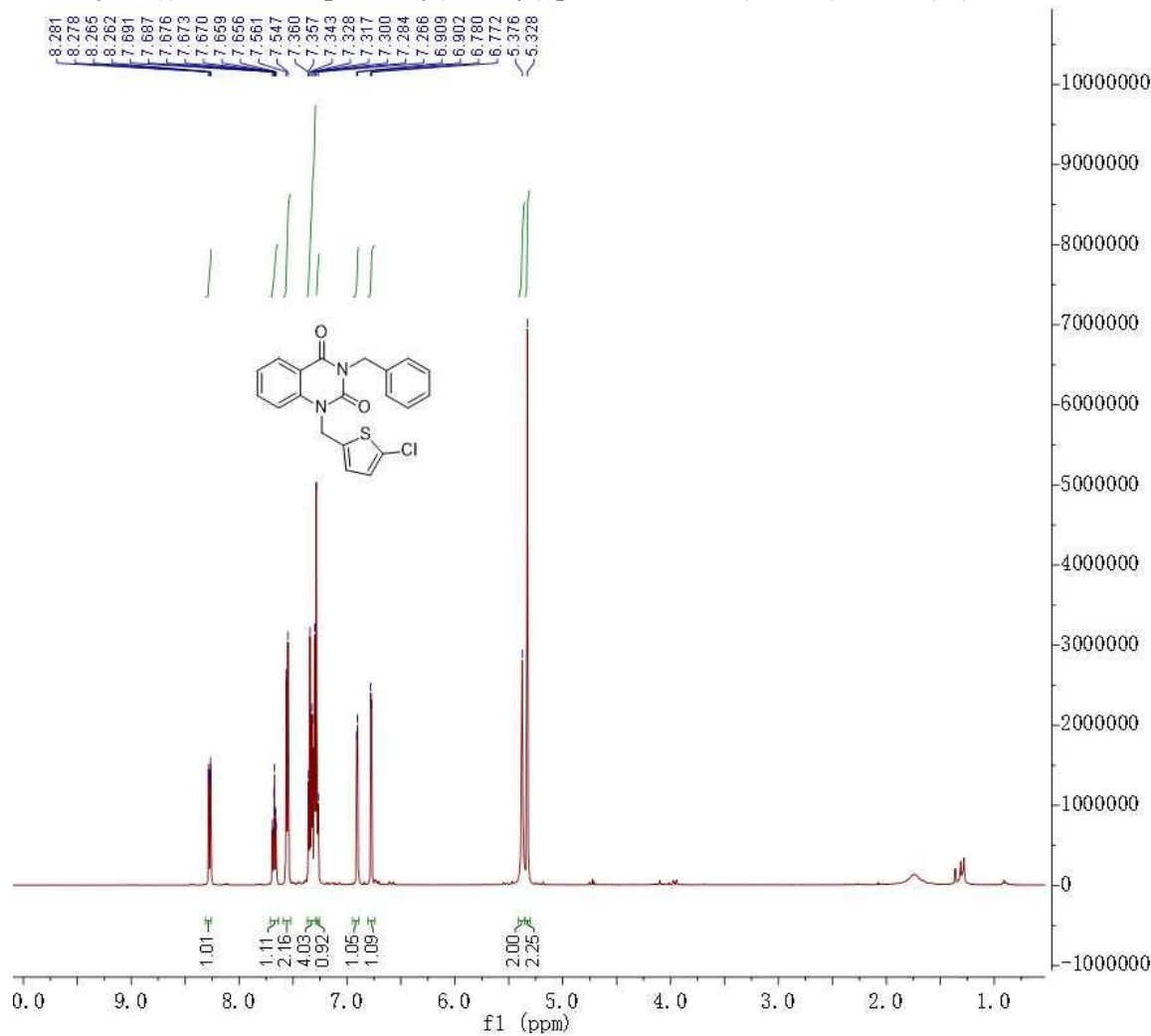


4'-((3-benzyl-2,4-dioxo-3,4-dihydroquinazolin-1(2H)-yl)methyl)-[1,1'-biphenyl]-2-carbonitrile (3q)

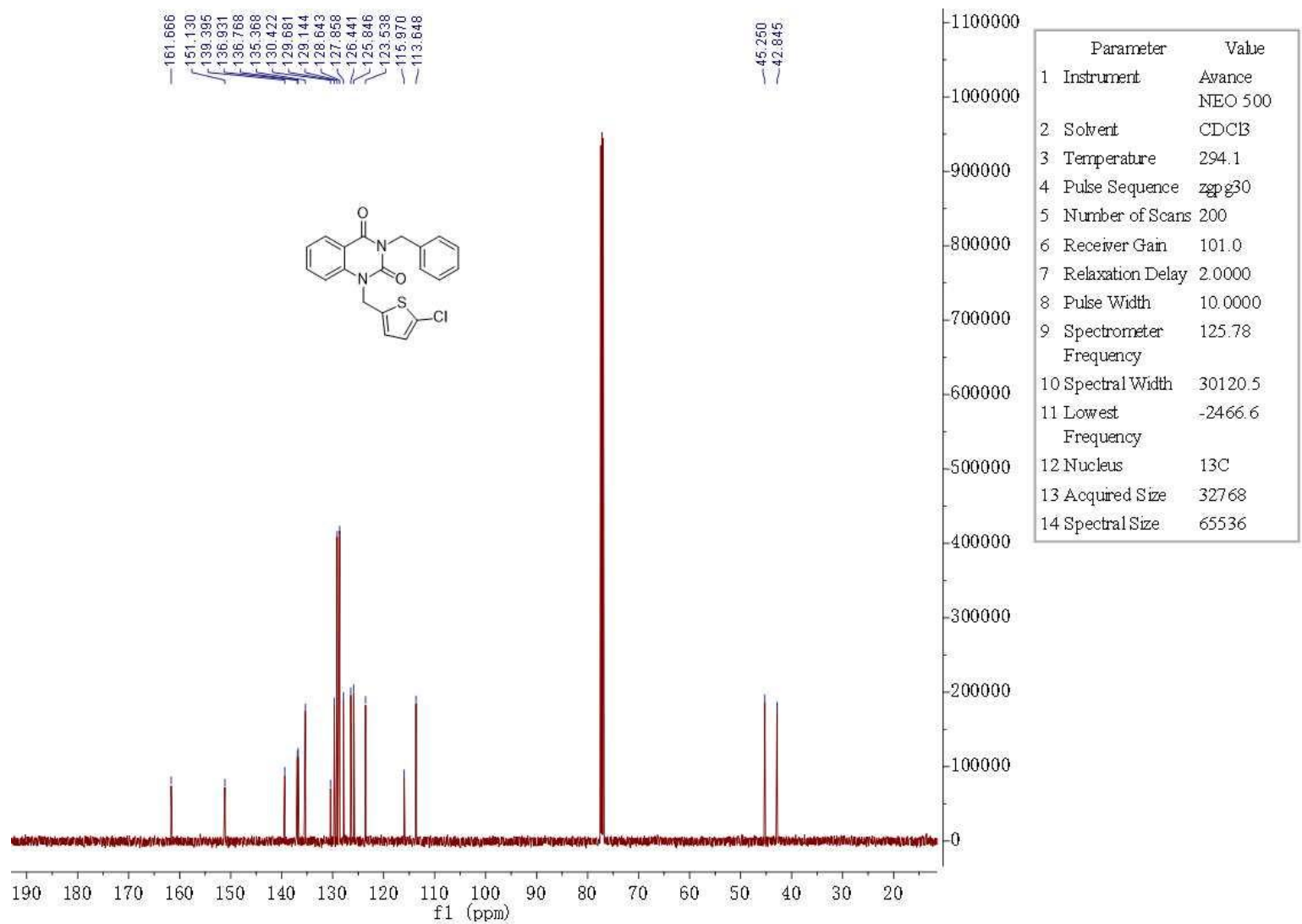




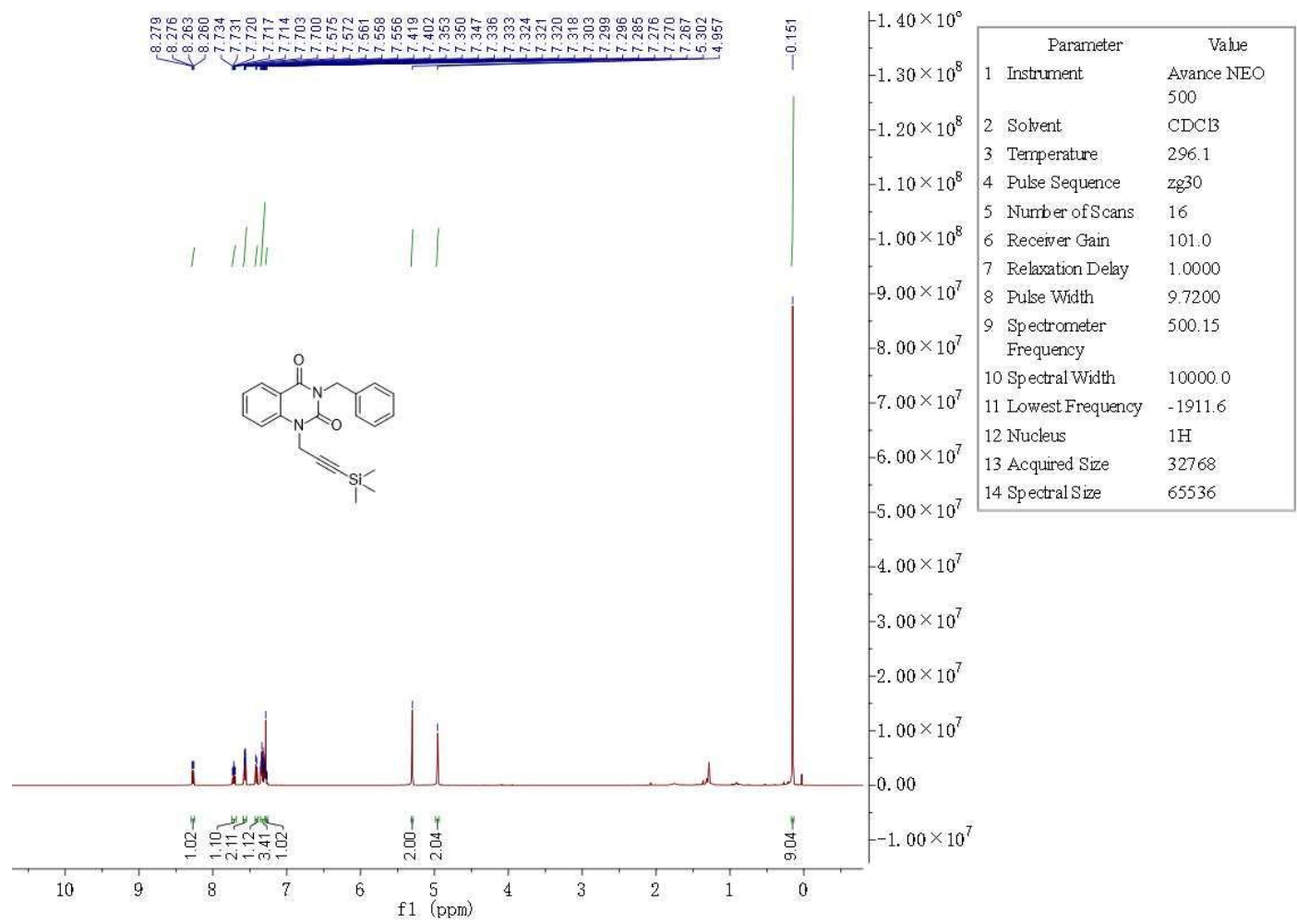
3-benzyl-1-((5-chlorothiophen-2-yl)methyl)quinazoline-2,4(1H,3H)-dione (3r)

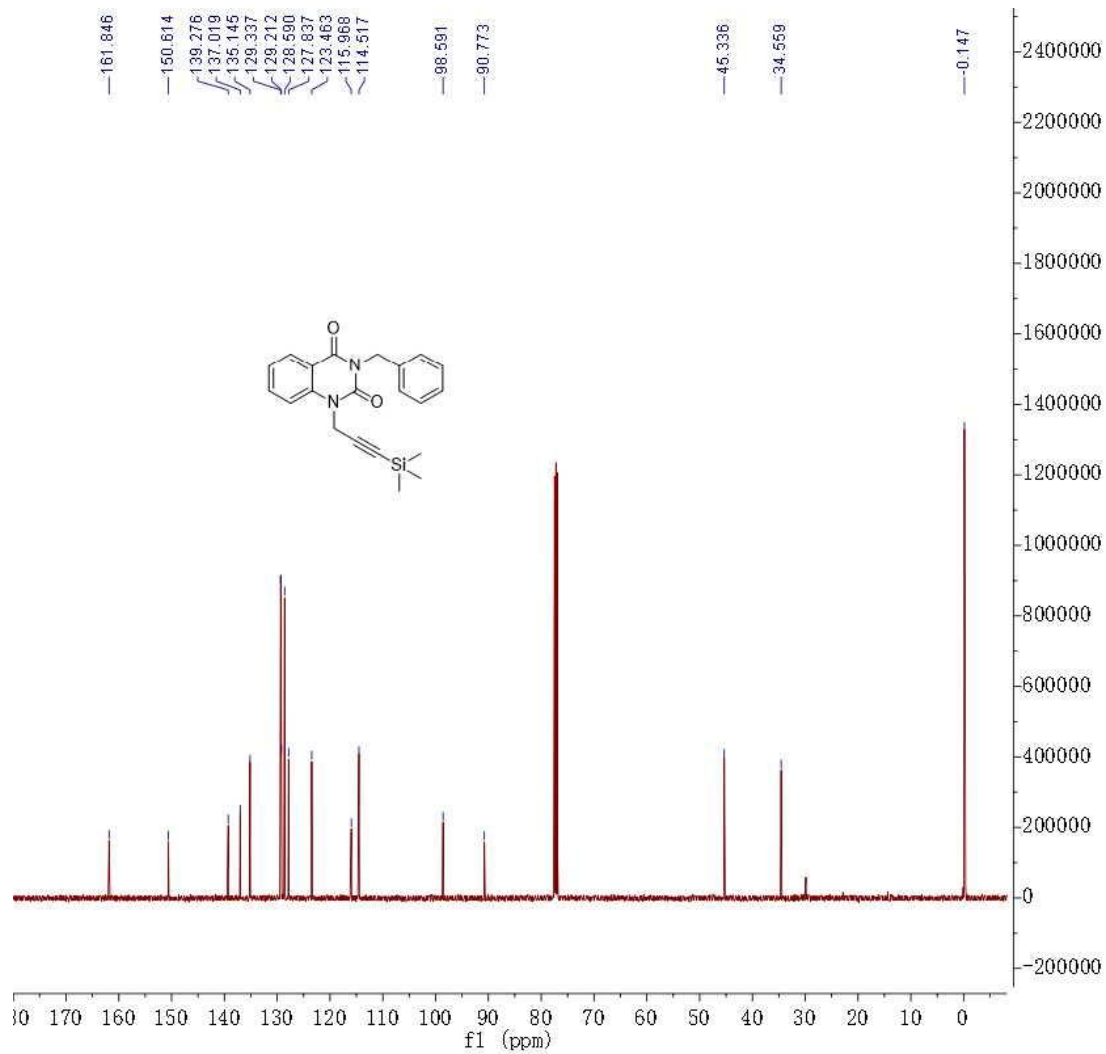


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	293.7
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer Frequency	500.15
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



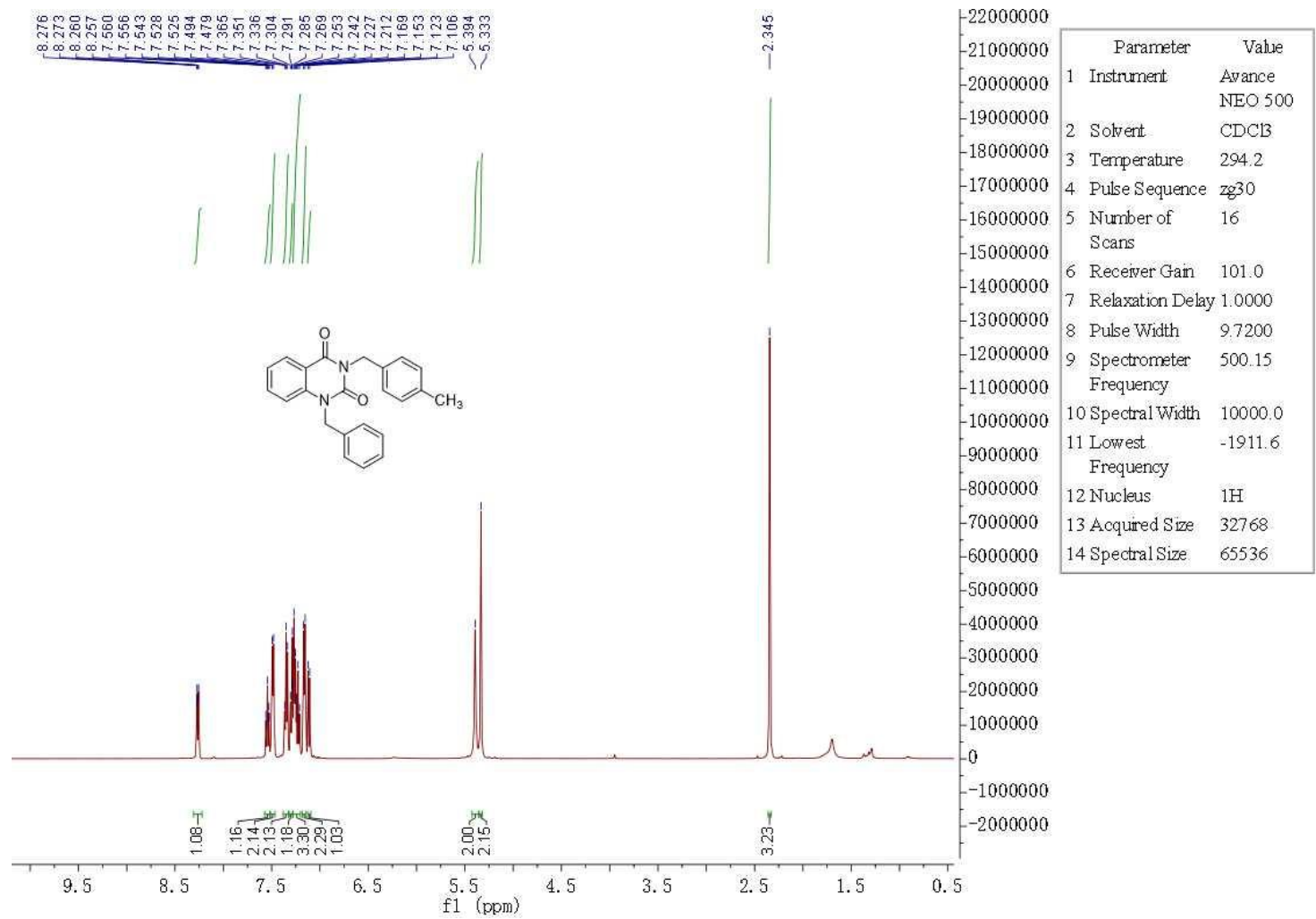
3-benzyl-1-(3-(trimethylsilyl)prop-2-yn-1-yl)quinazoline-2,4(1H,3H)-dione (3t)

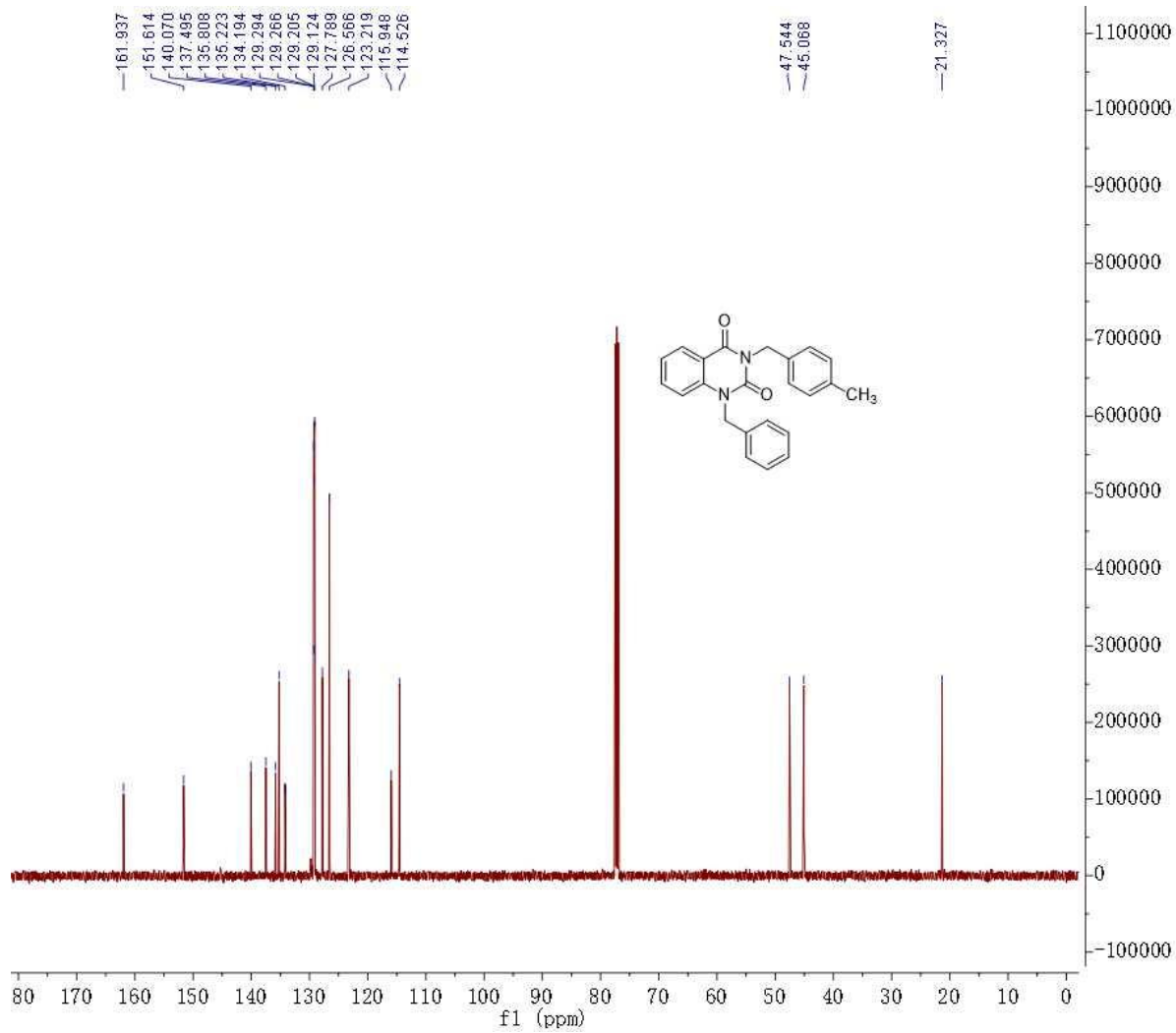




Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	296.1
4 Pulse Sequence	zgpg30
5 Number of Scans	300
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2466.4
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

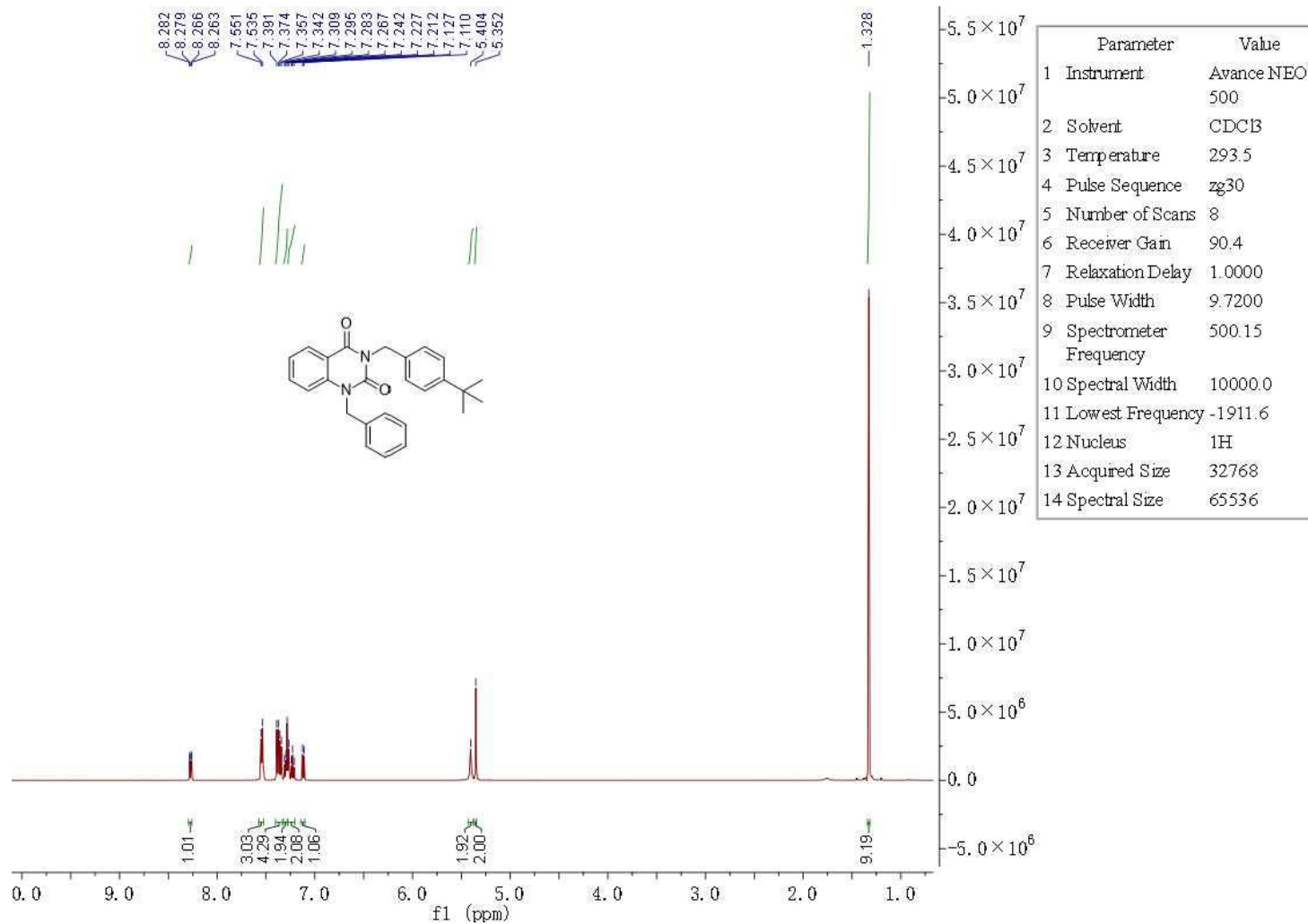
1-benzyl-3-(4-methylbenzyl)quinazoline-2,4(1H,3H)-dione (5a)

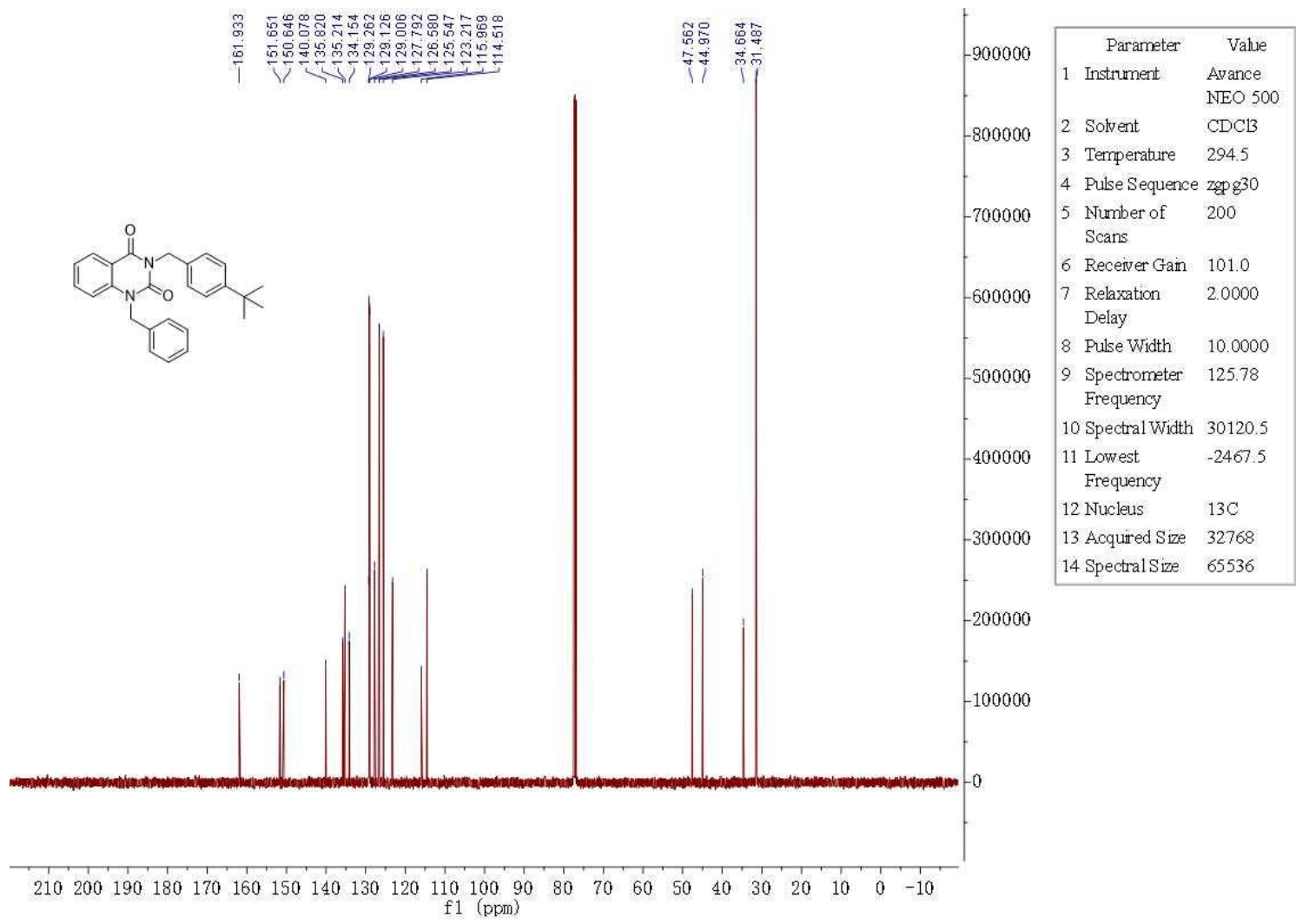




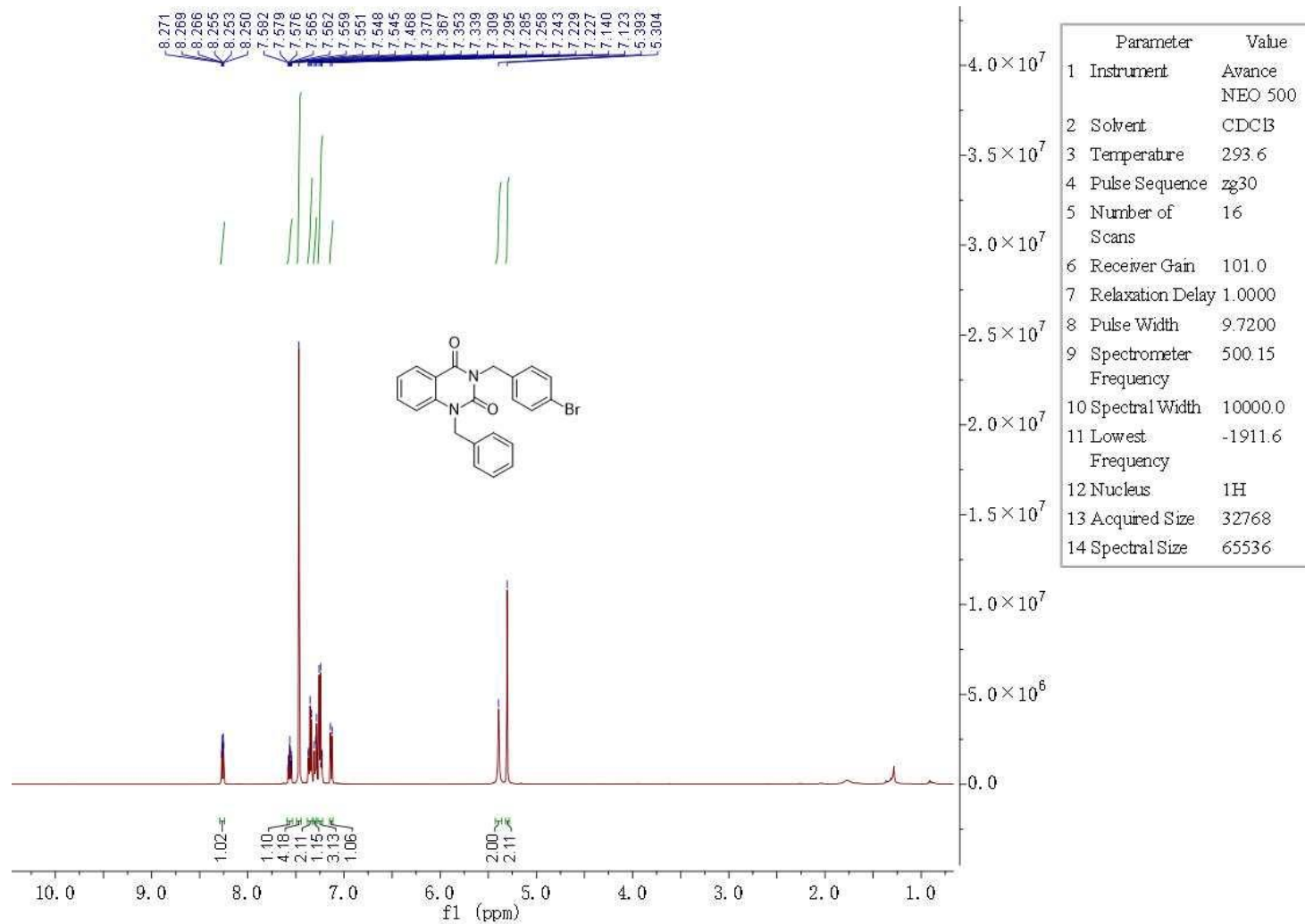
Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	295.2
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2467.7
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

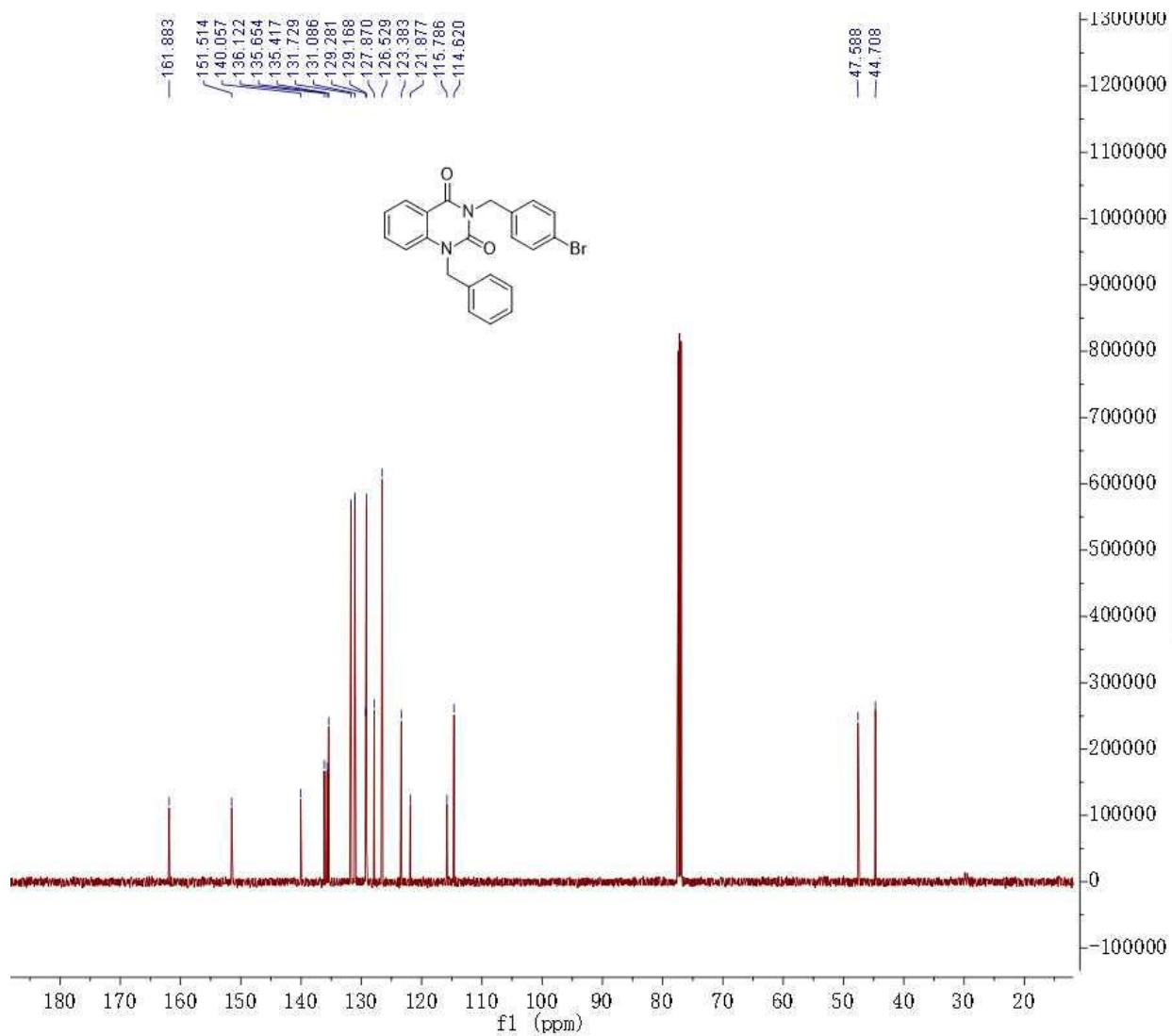
1-benzyl-3-(4-(tert-butyl)benzyl)quinazoline-2,4(1H,3H)-dione (5b)





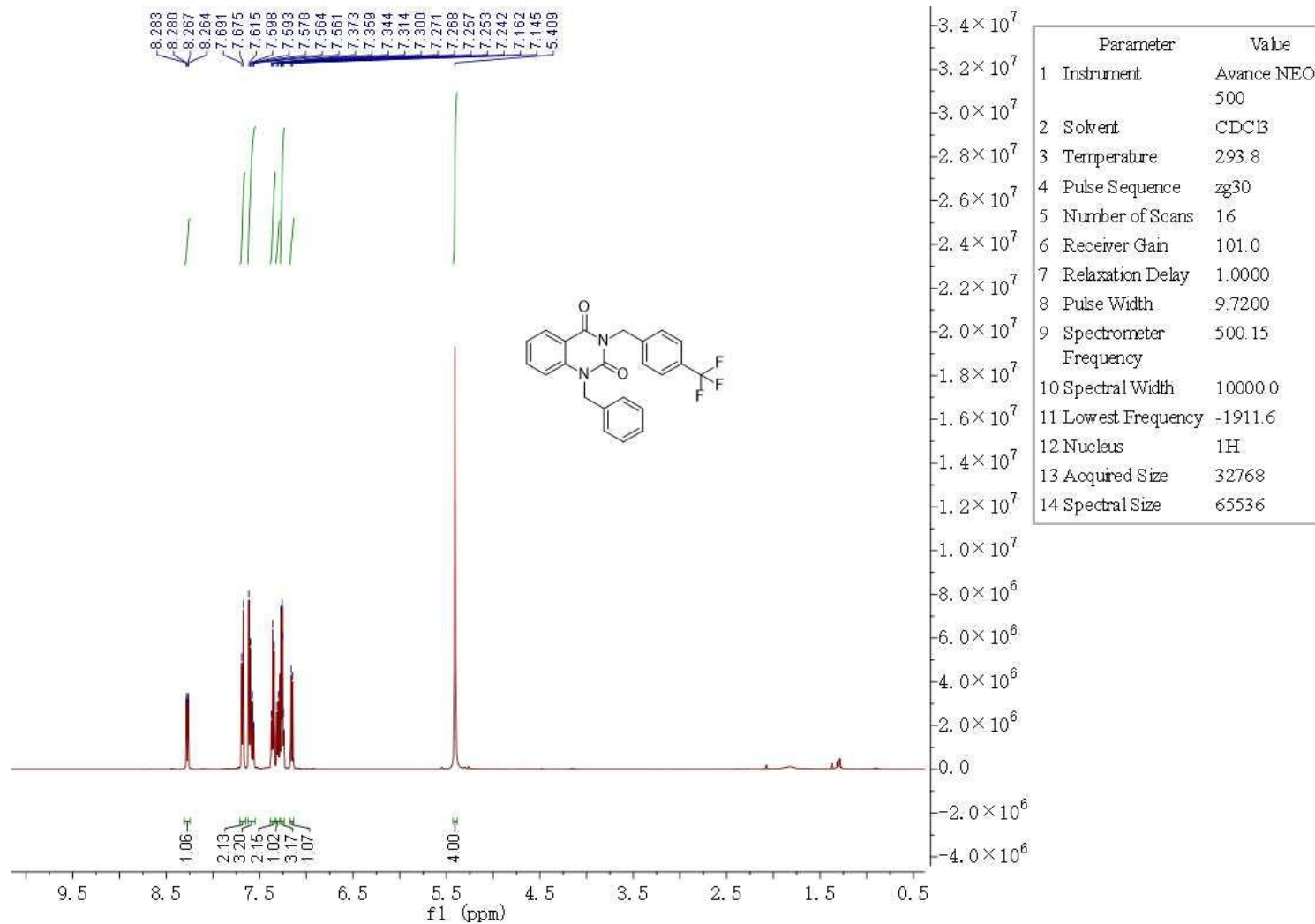
1-benzyl-3-(4-bromobenzyl)quinazoline-2,4(1H,3H)-dione (5c)

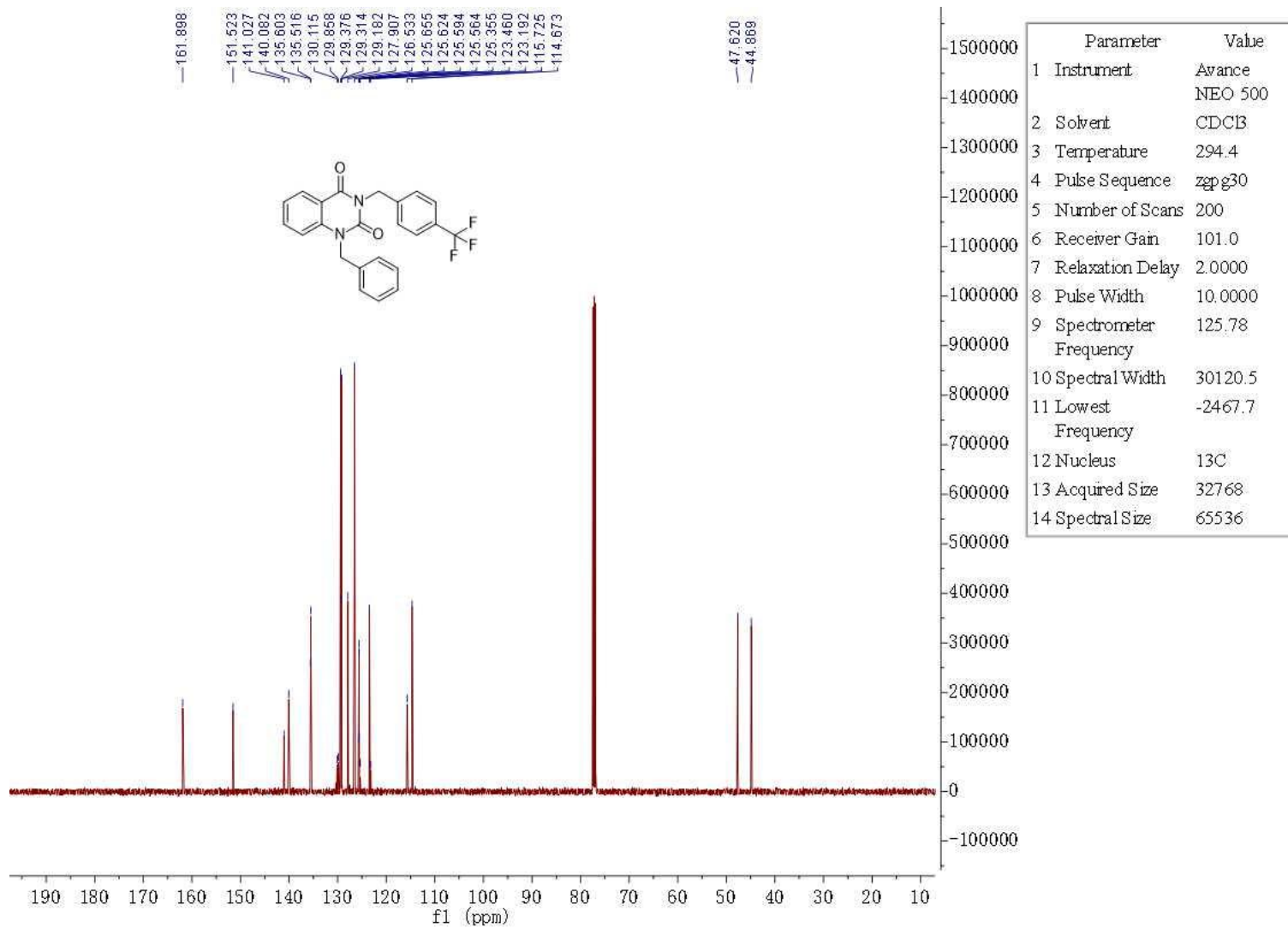




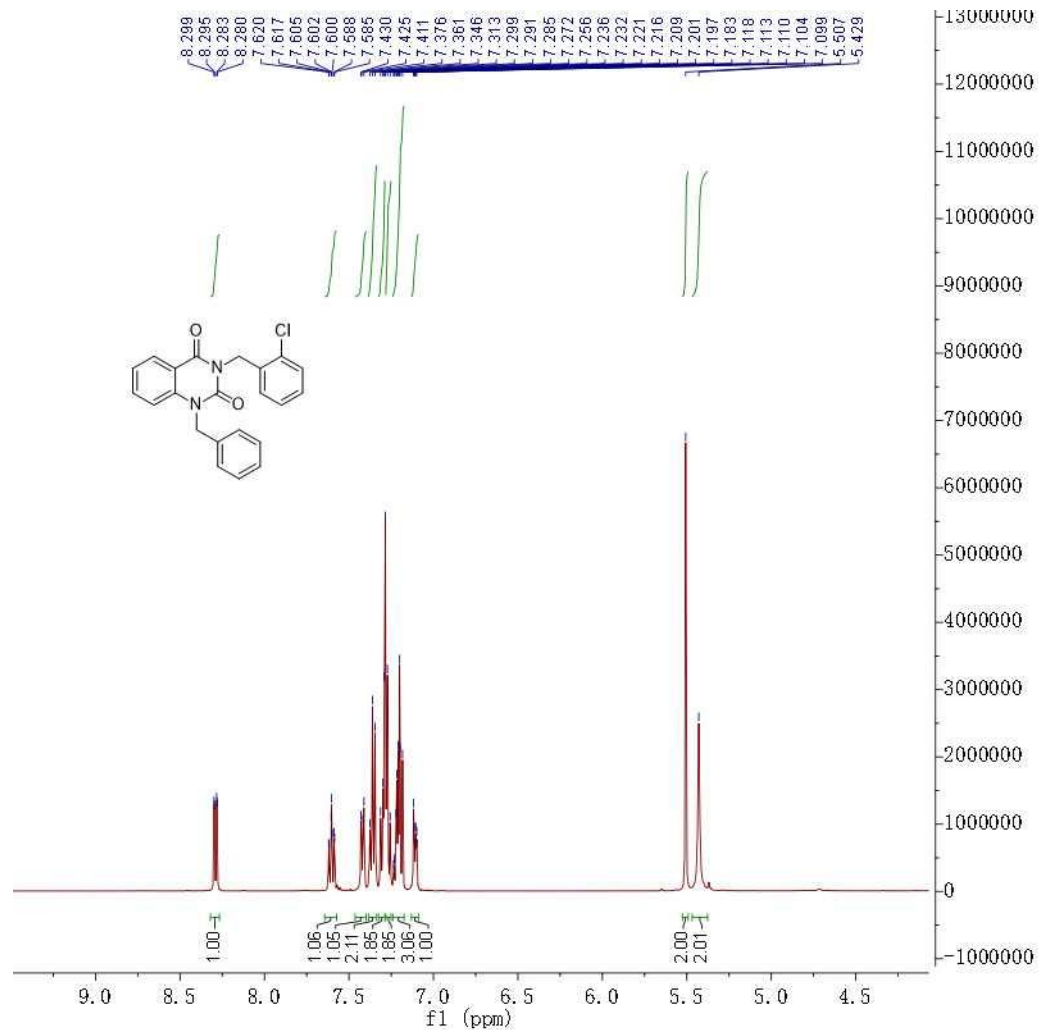
Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	294.8
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2467.7
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

1-benzyl-3-(4-(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (5d)

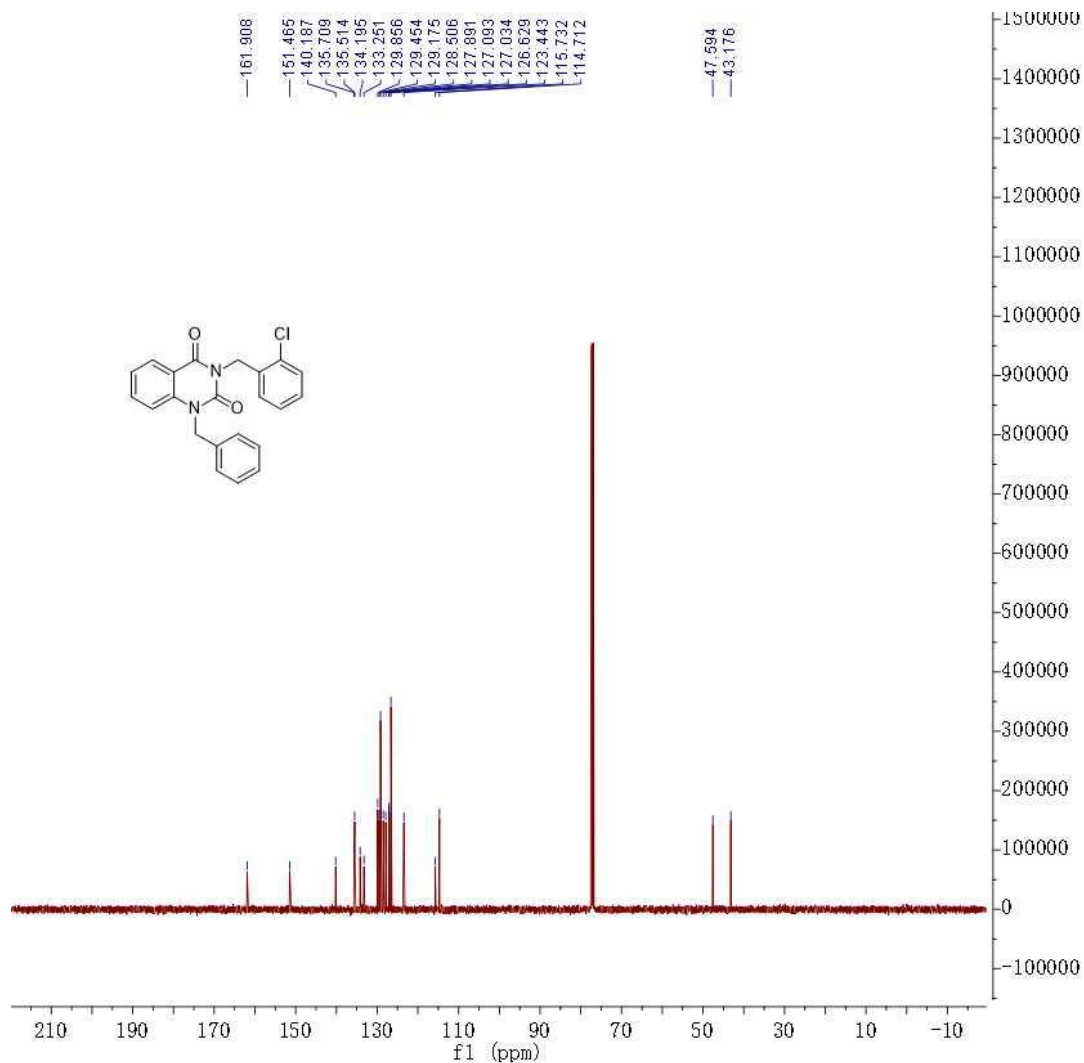




1-benzyl-3-(2-chlorobenzyl)quinazoline-2,4(1H,3H)-dione (5e)

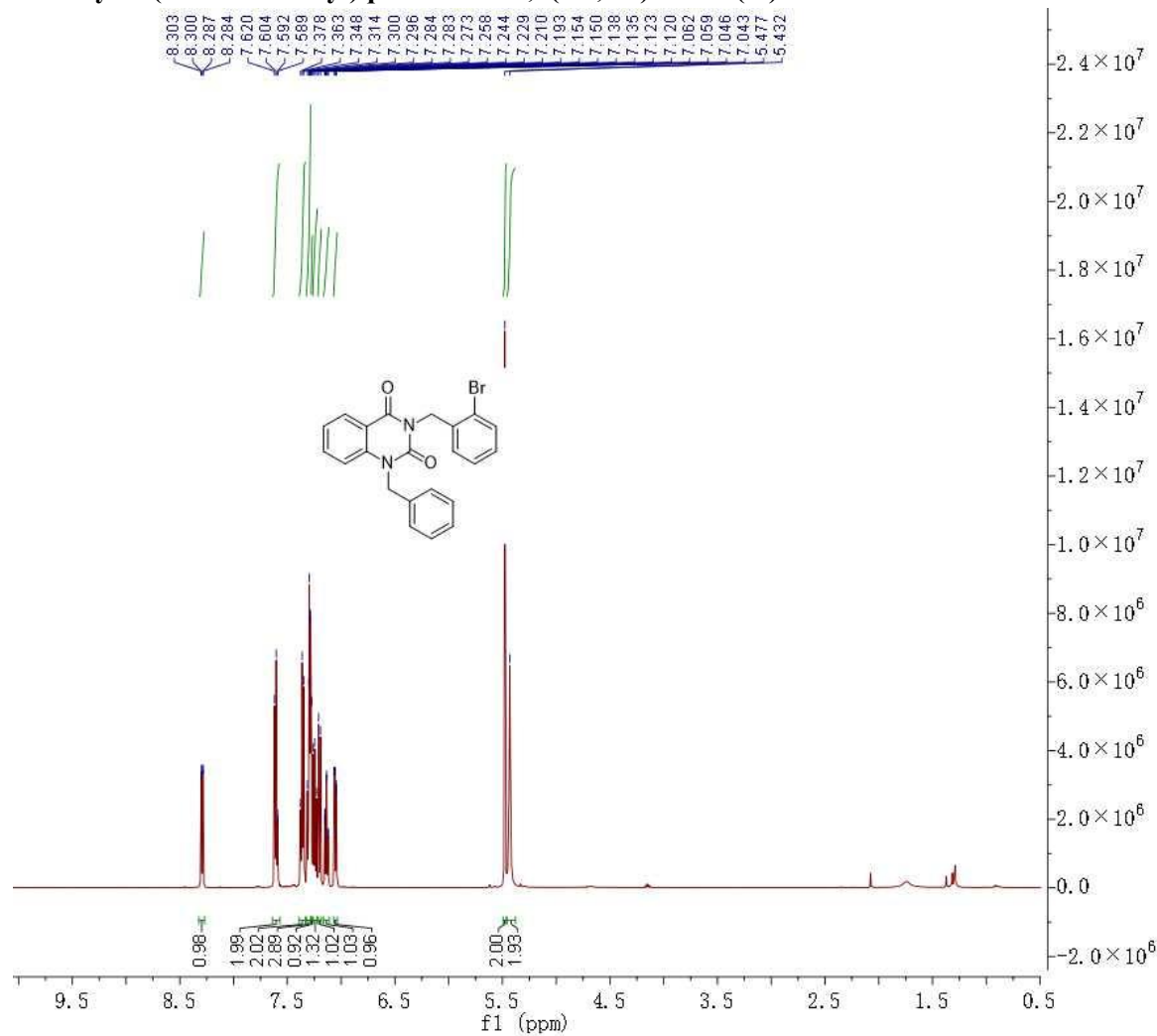


Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	293.8
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer	500.15
Frequency	
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536

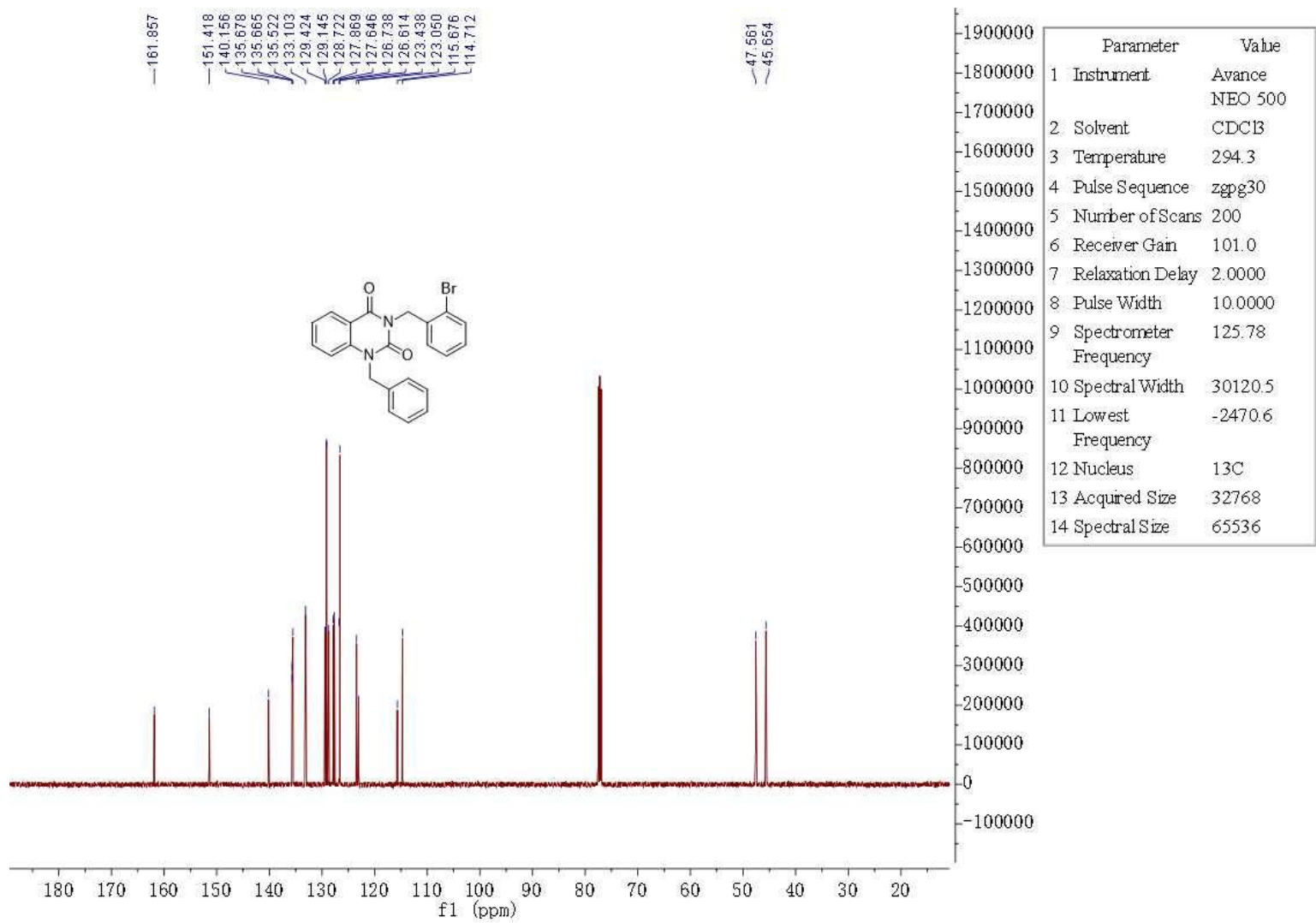


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.5
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2484.0
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

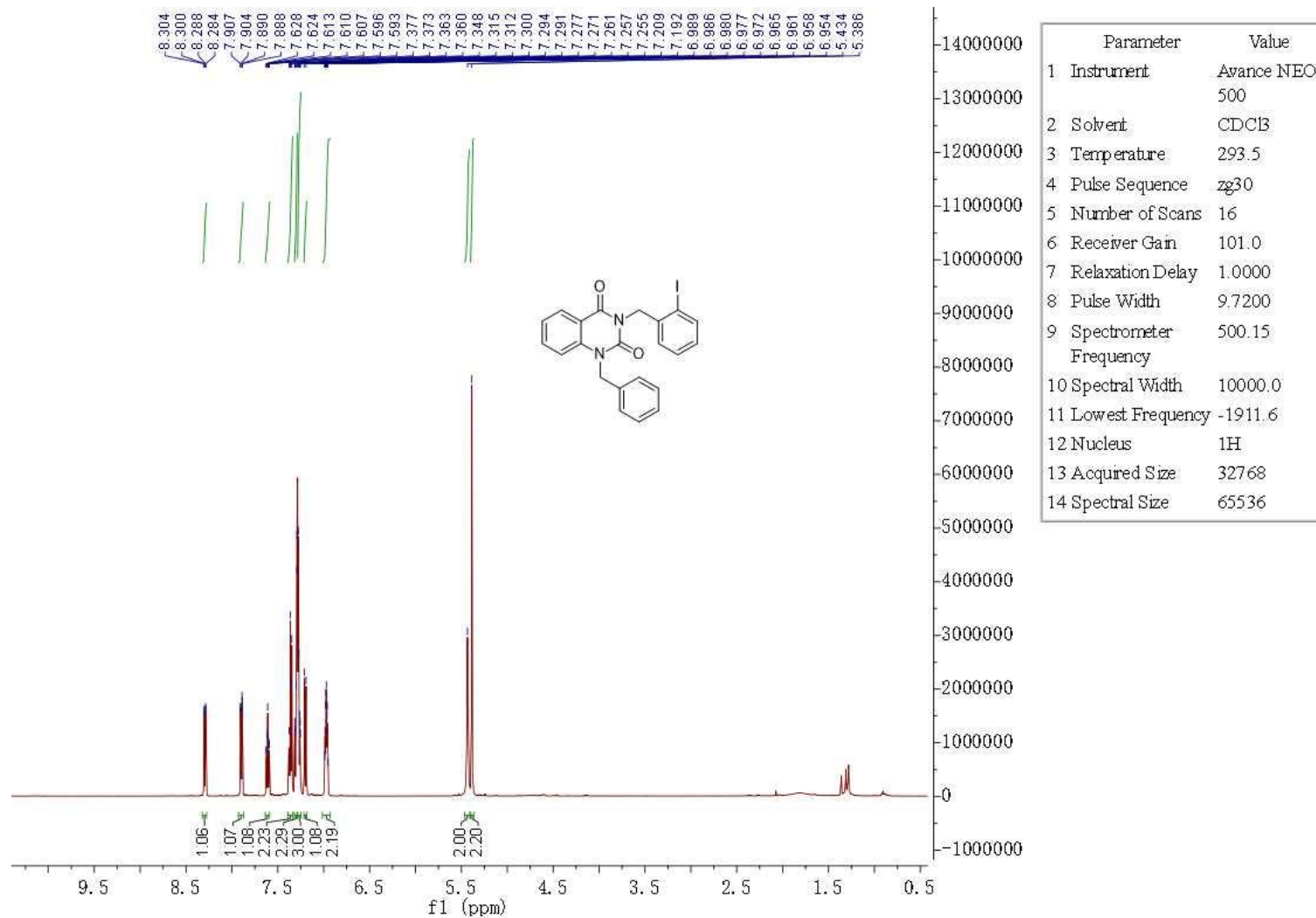
1-benzyl-3-(2-bromobenzyl)quinazoline-2,4(1H,3H)-dione (5f)

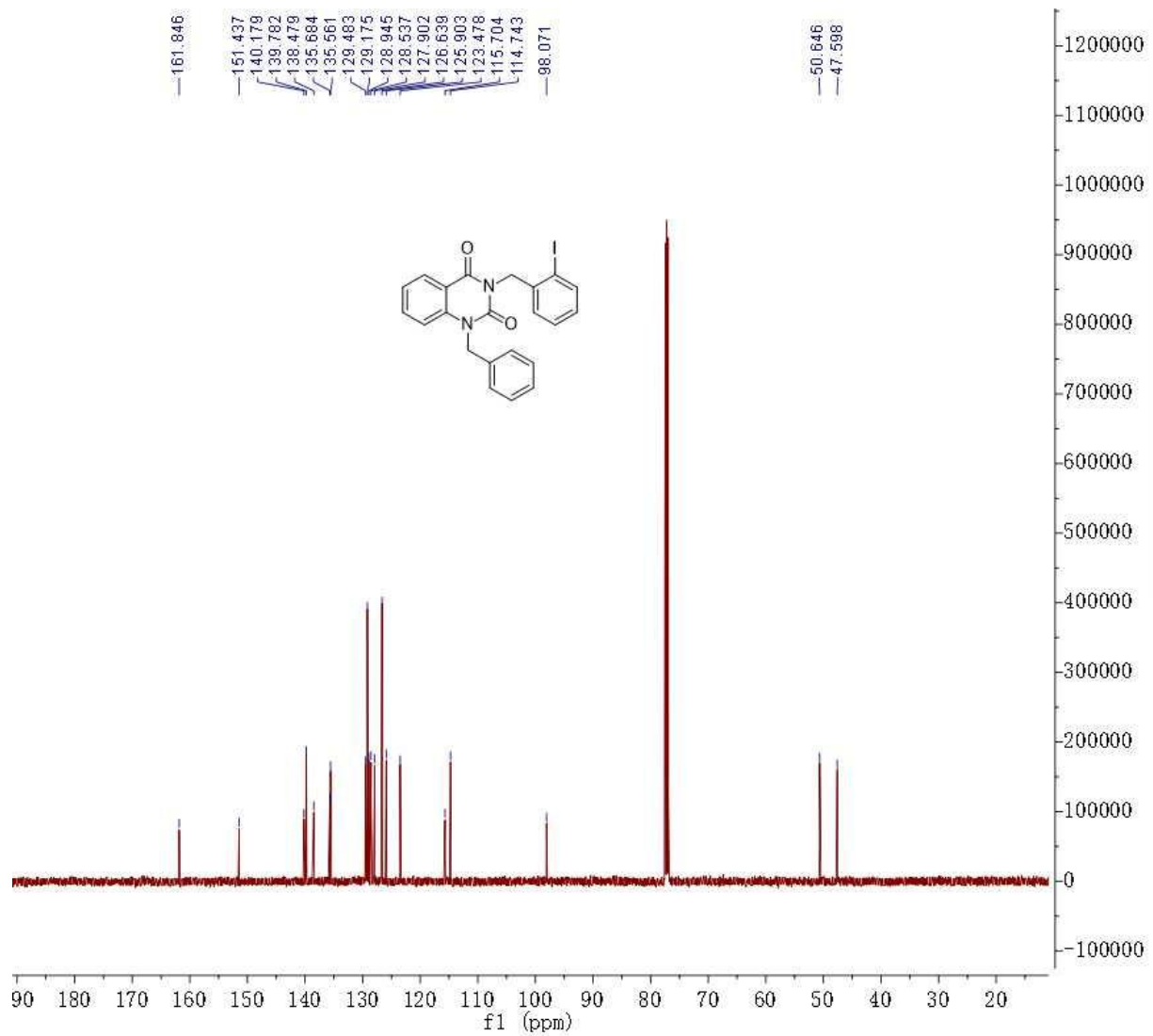


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	293.6
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer	500.15
Frequency	
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



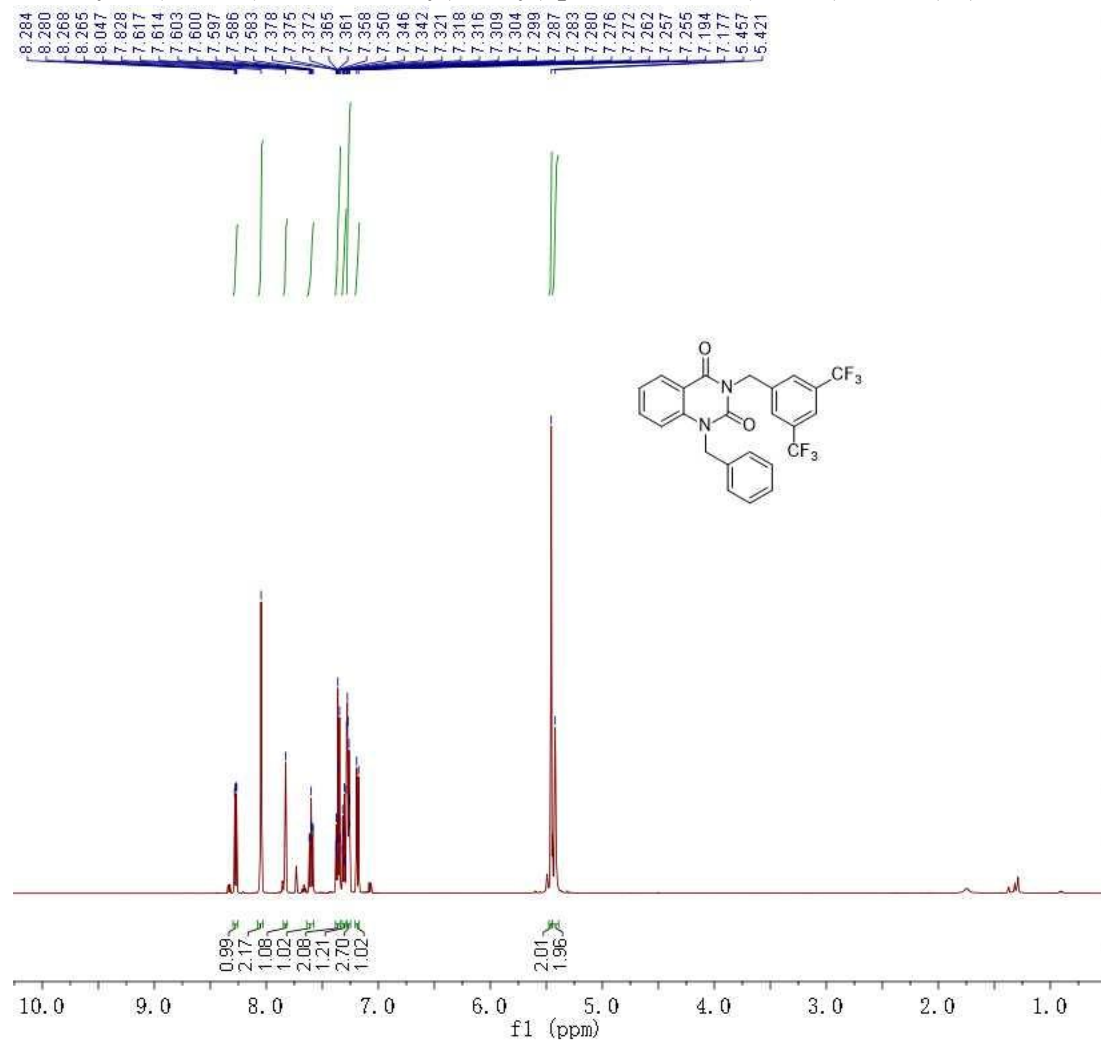
1-benzyl-3-(2-iodobenzyl)quinazoline-2,4(1H,3H)-dione (5g)



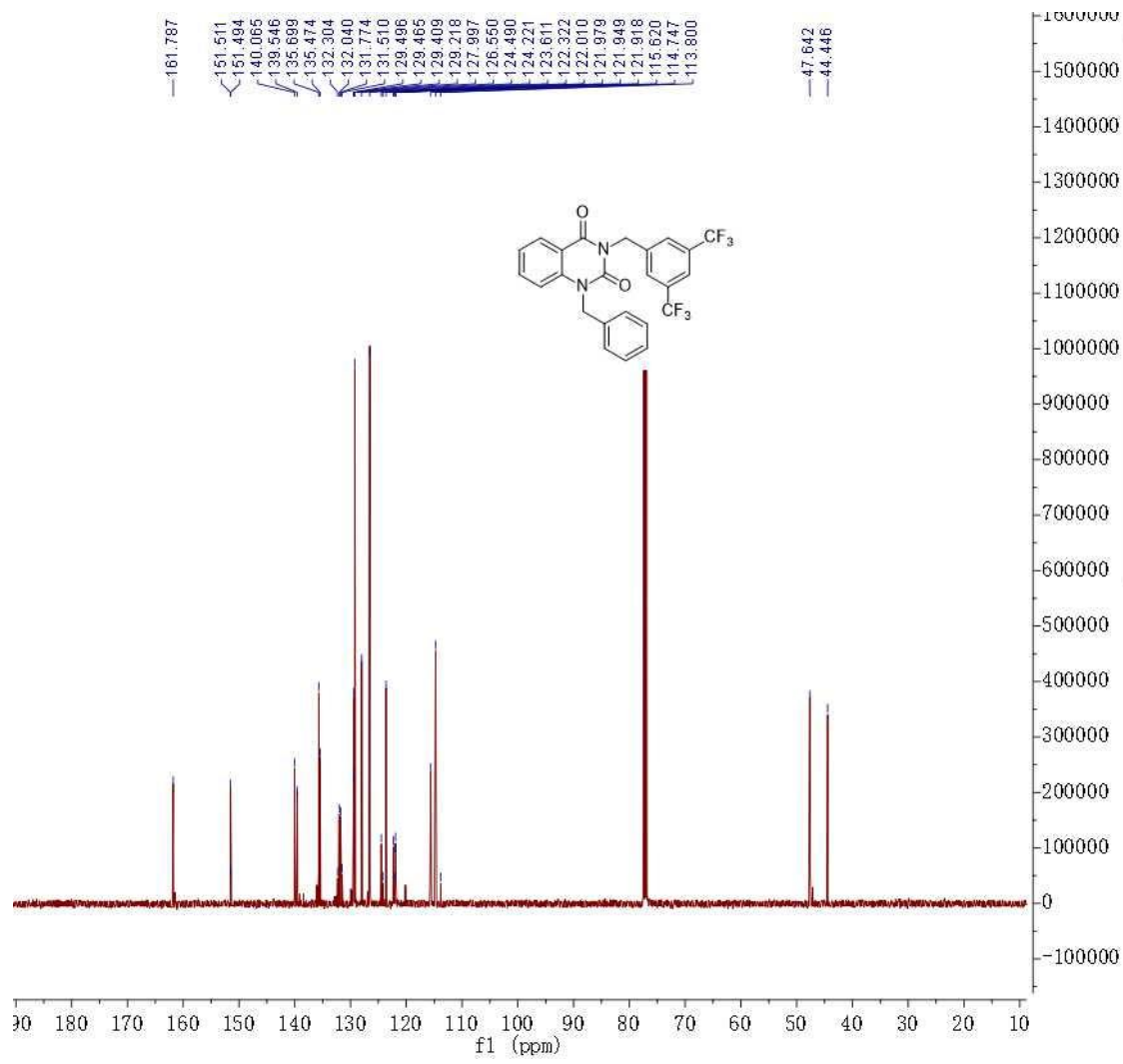


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl ₃
3 Temperature	294.3
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2466.9
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536

1-benzyl-3-(3,5-bis(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (5h)

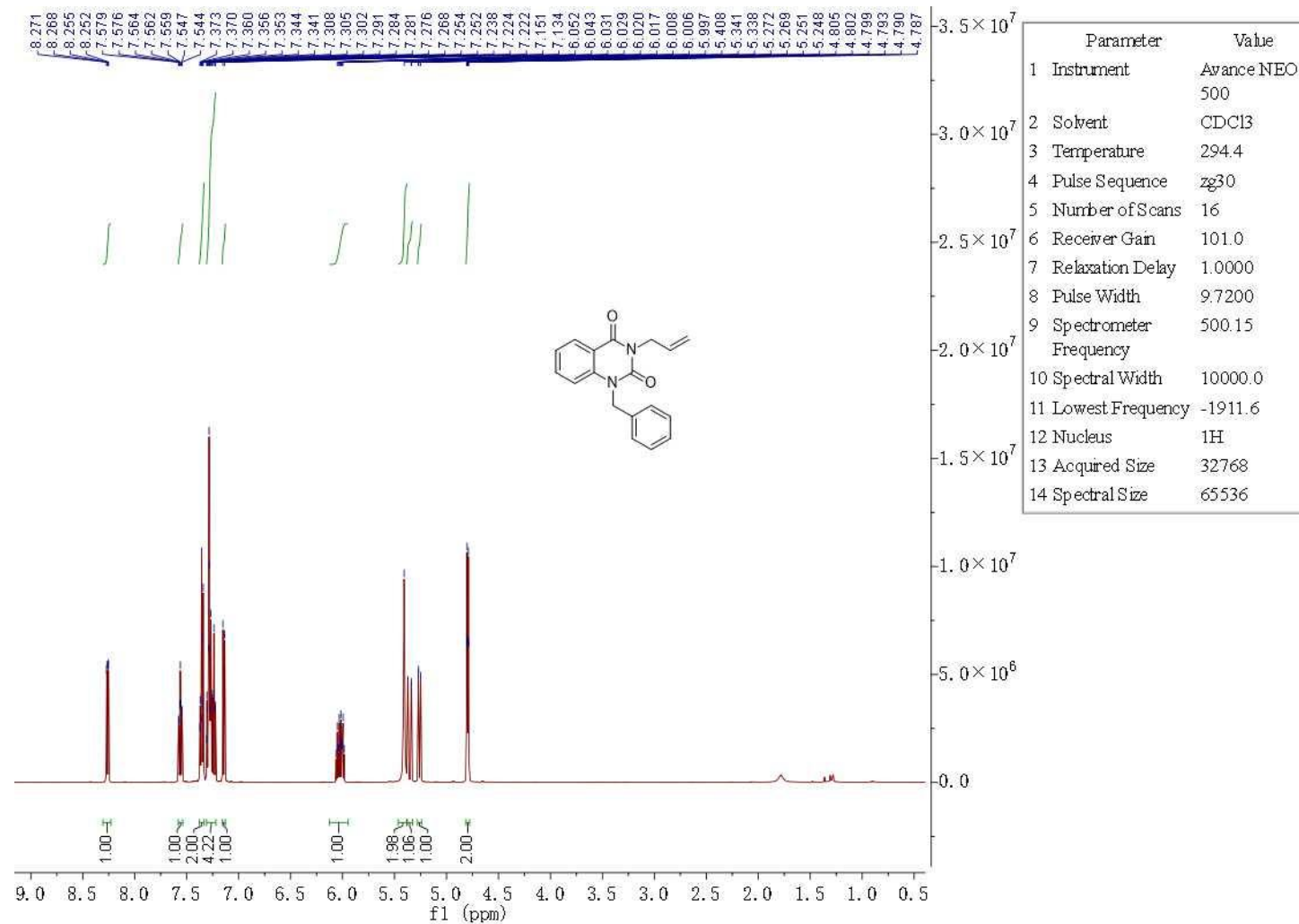


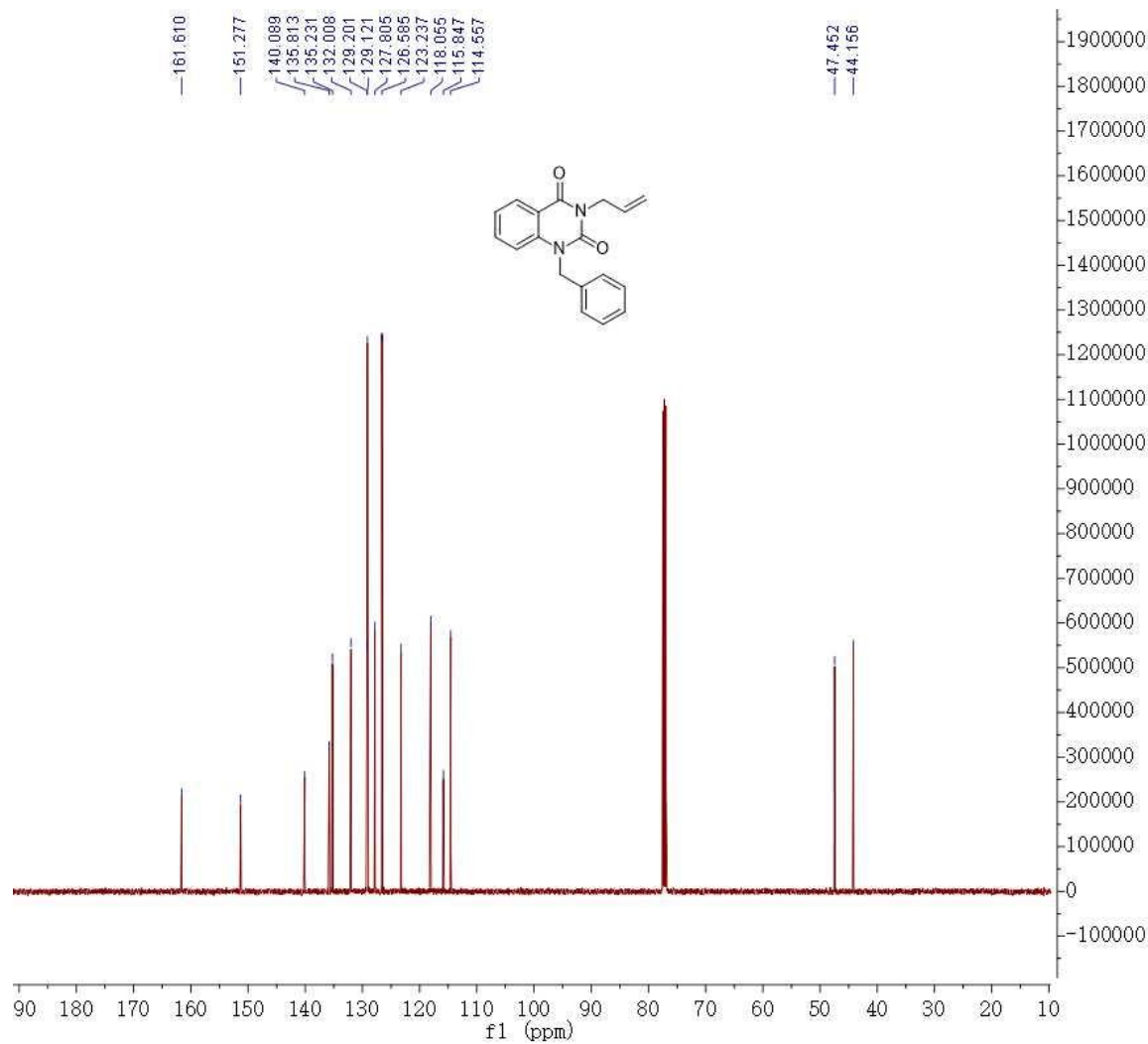
Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	293.6
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer Frequency	500.15
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.1
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2466.0
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

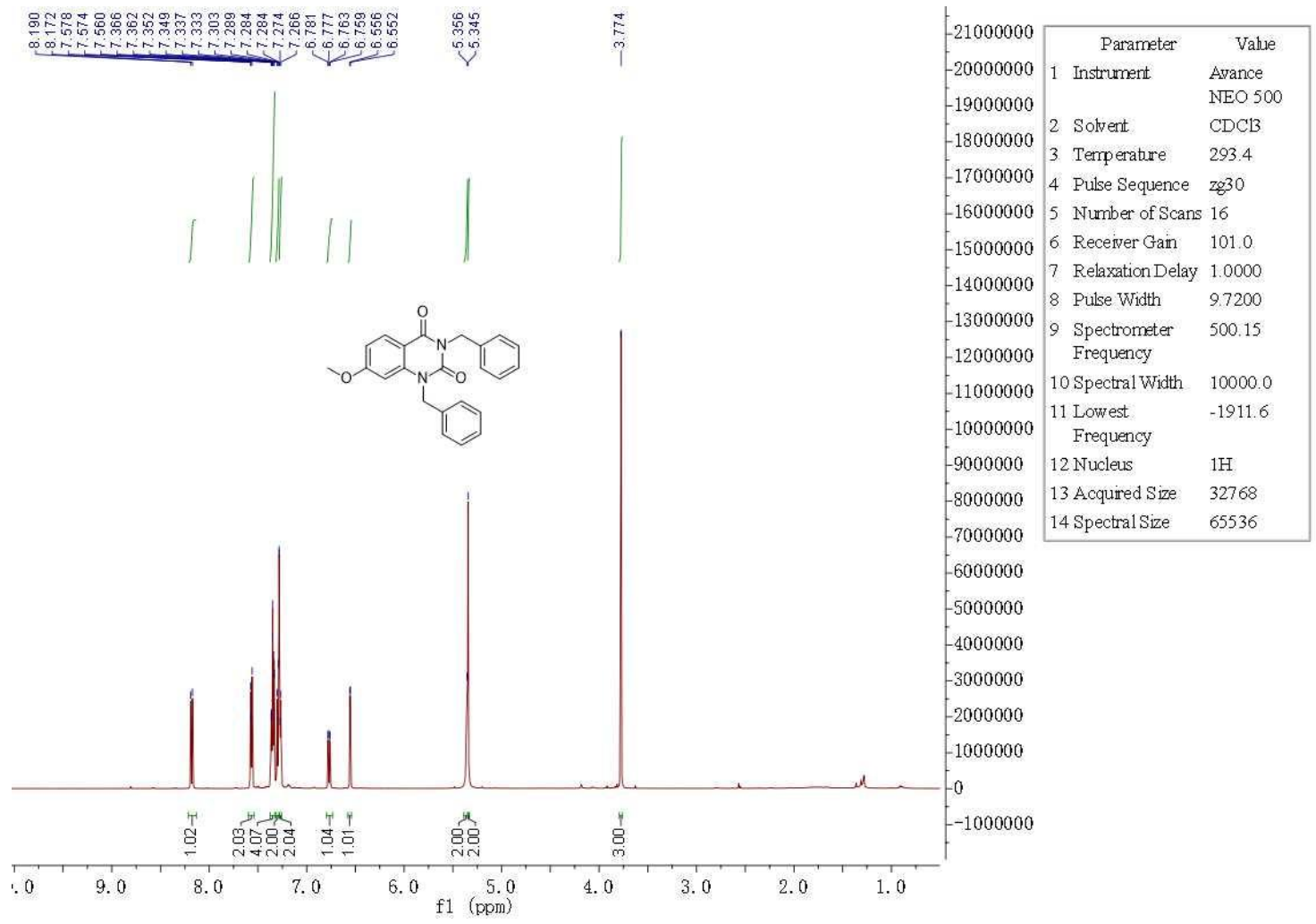
3-allyl-1-benzylquinazoline-2,4(1H,3H)-dione (5i)

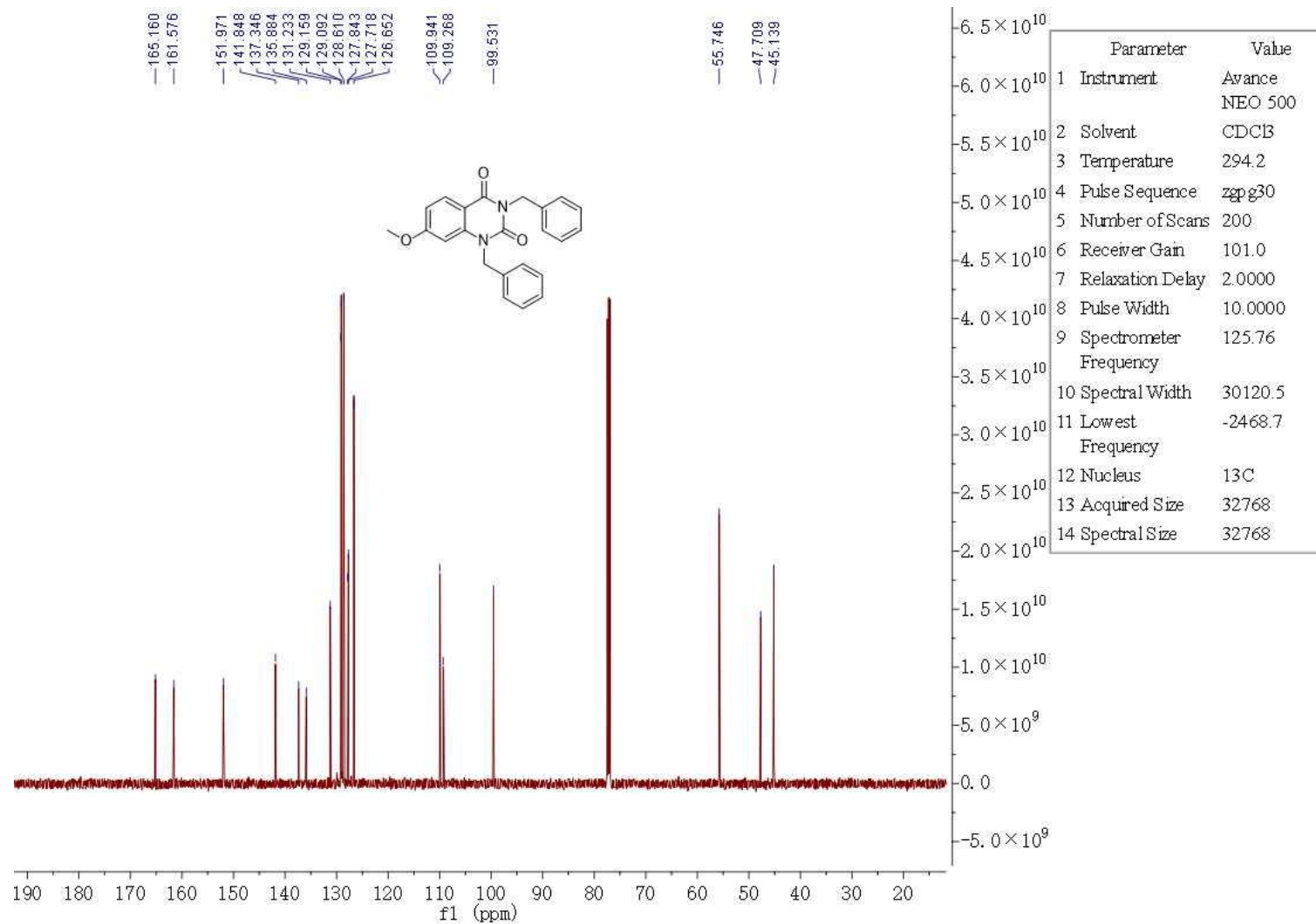




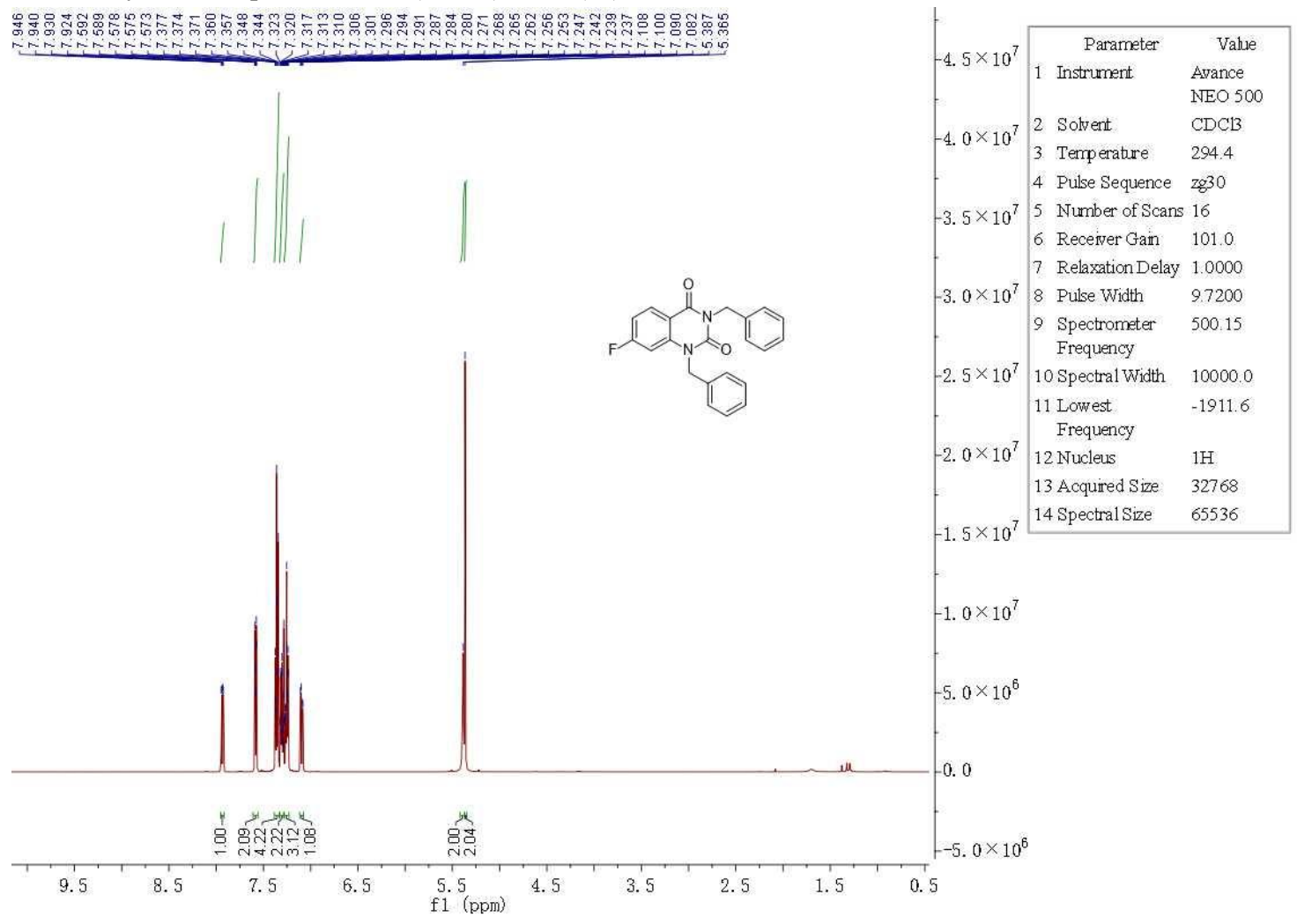
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	295.0
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2469.5
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

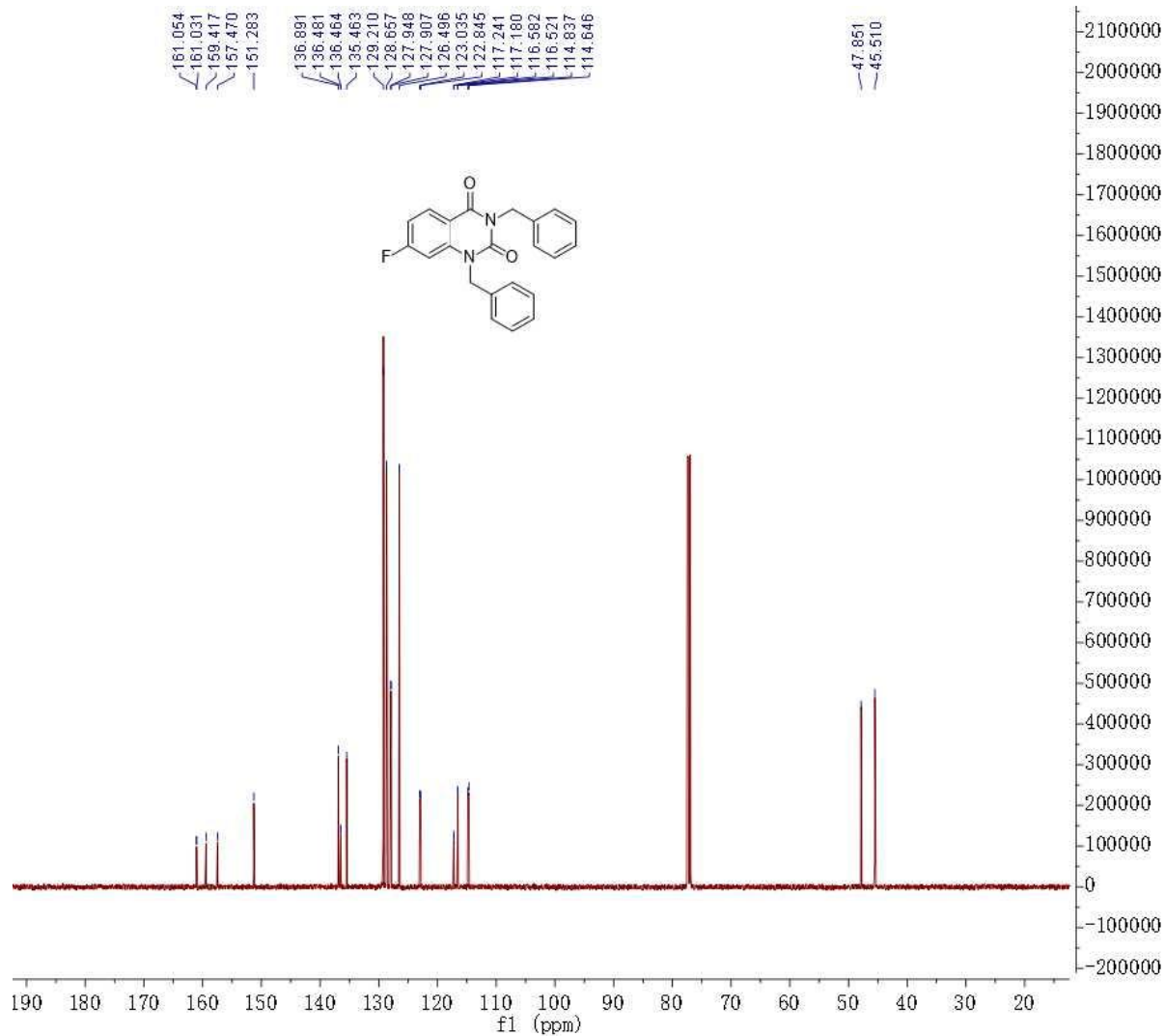
1,3-dibenzyl-7-methoxyquinazoline-2,4(1H,3H)-dione (5j)





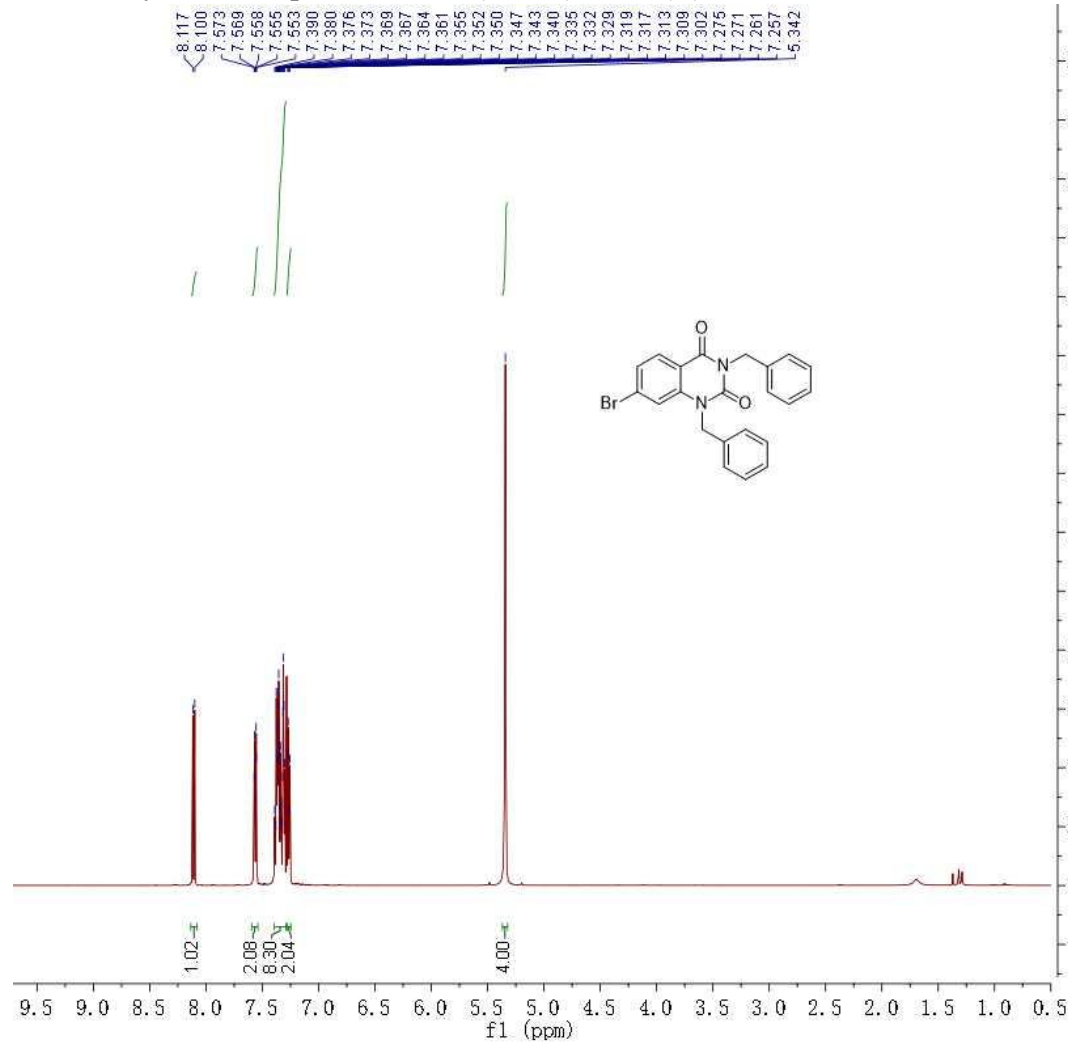
1,3-dibenzyl-7-fluoroquinazoline-2,4(1H,3H)-dione (5k)



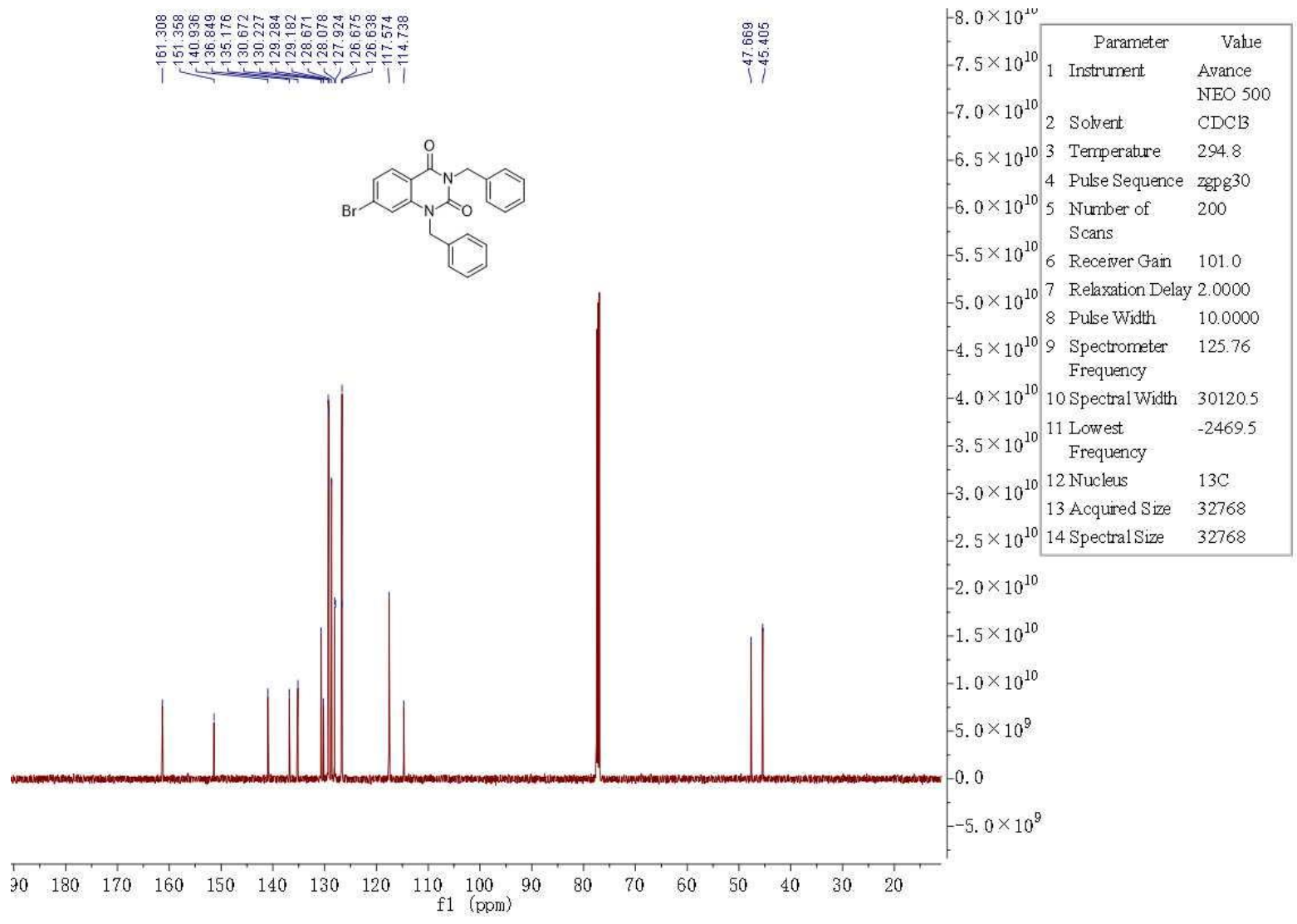


Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	295.1
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2469.9
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

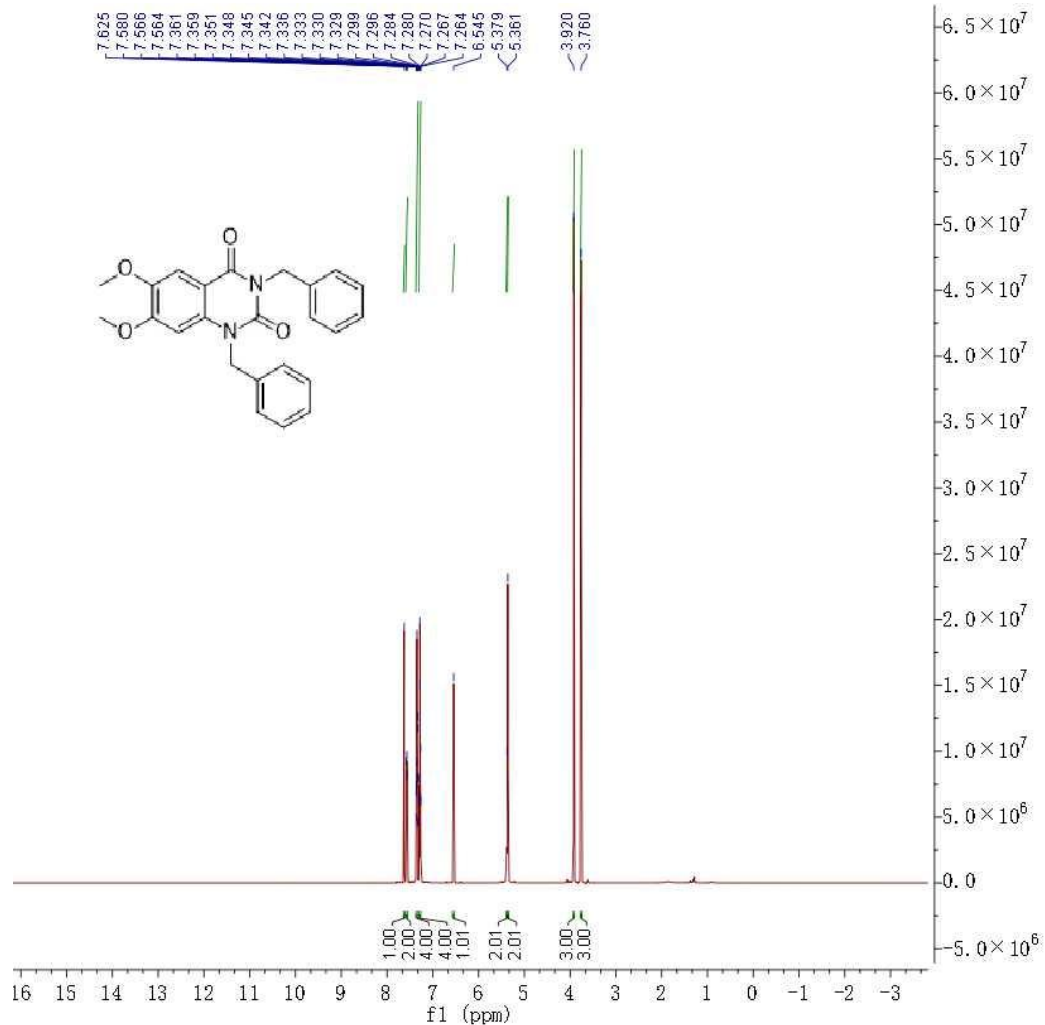
1,3-dibenzyl-7-bromoquinazoline-2,4(1H,3H)-dione (5l)



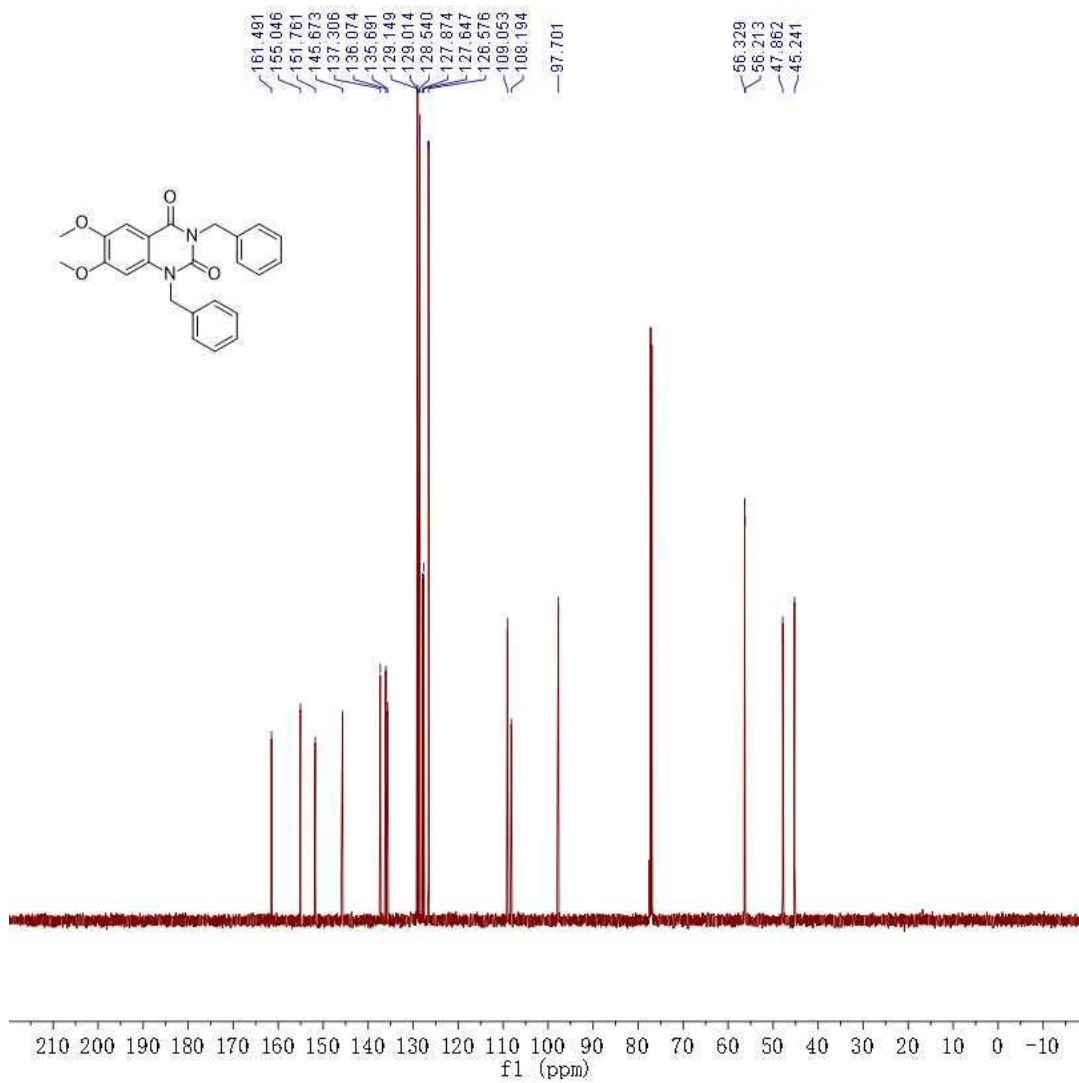
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.1
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer Frequency	500.15
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



1,3-dibenzyl-6,7-dimethoxyquinazoline-2,4(1H,3H)-dione (5m)

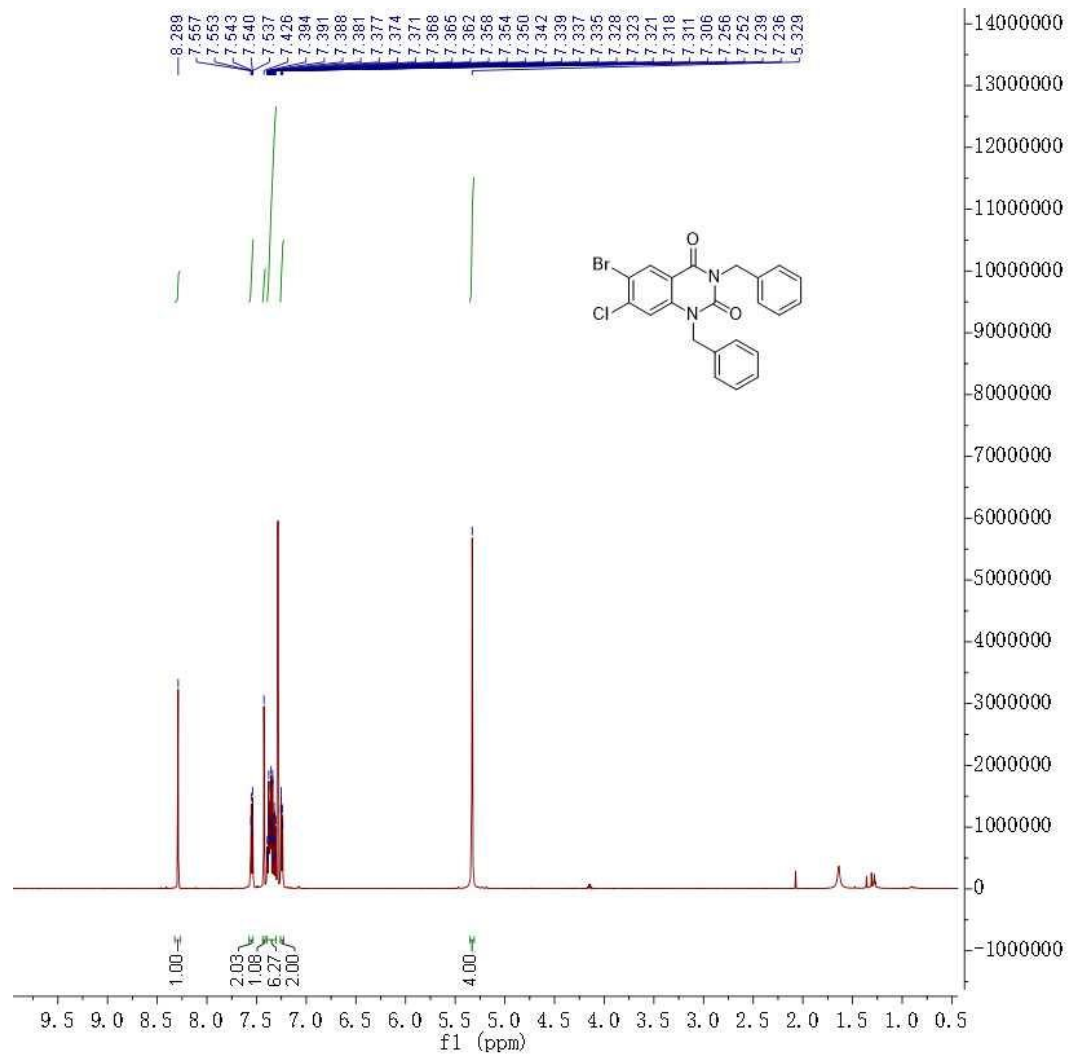


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.5
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	69.3
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer Frequency	500.15
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536

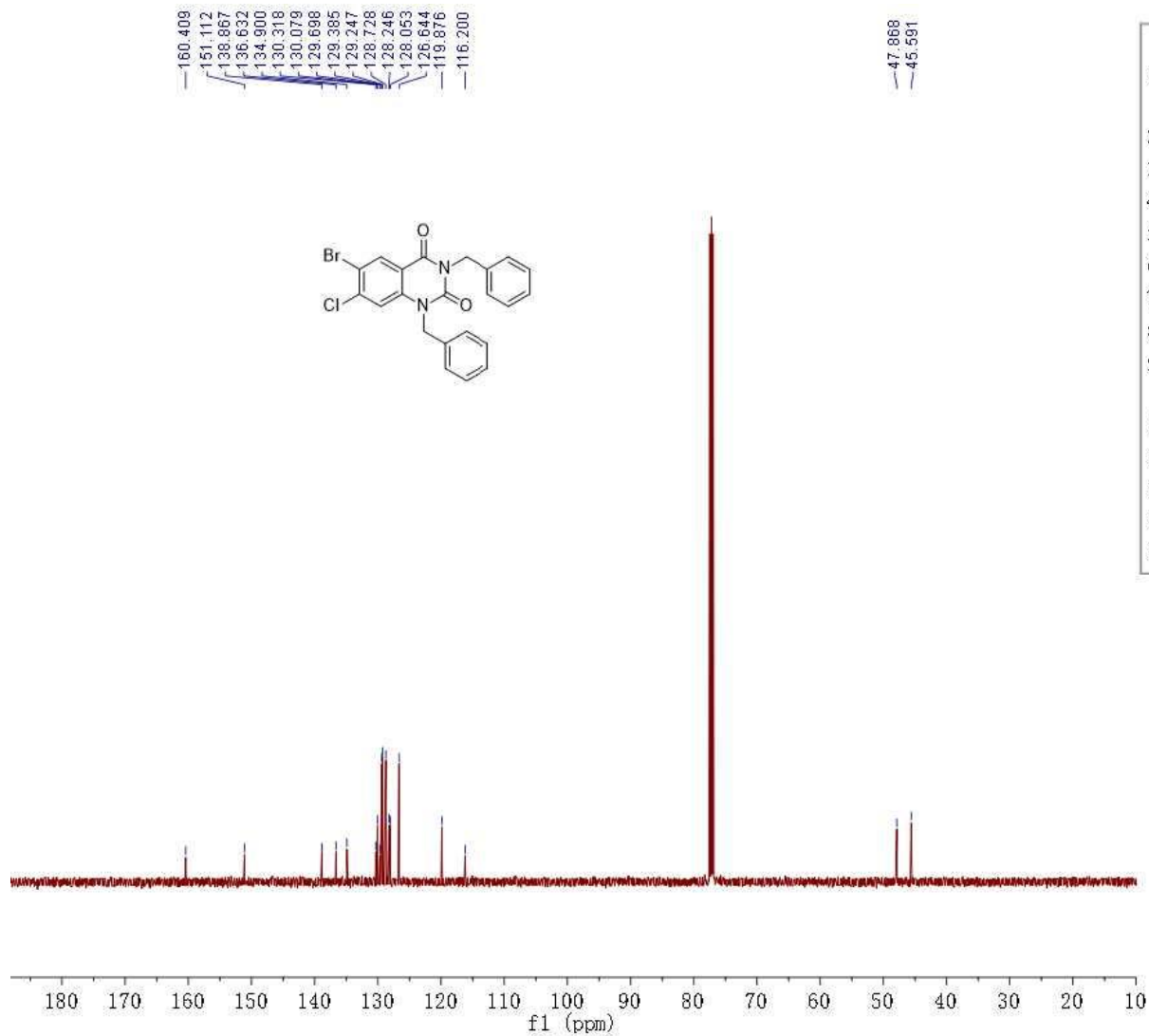


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCB
3 Temperature	294.9
4 Pulse Sequence	zgpg30
5 Number of Scans	60
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest Frequency	-2476.0
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536

1,3-dibenzyl-6-bromo-7-chloroquinazoline-2,4(1H,3H)-dione (5n)

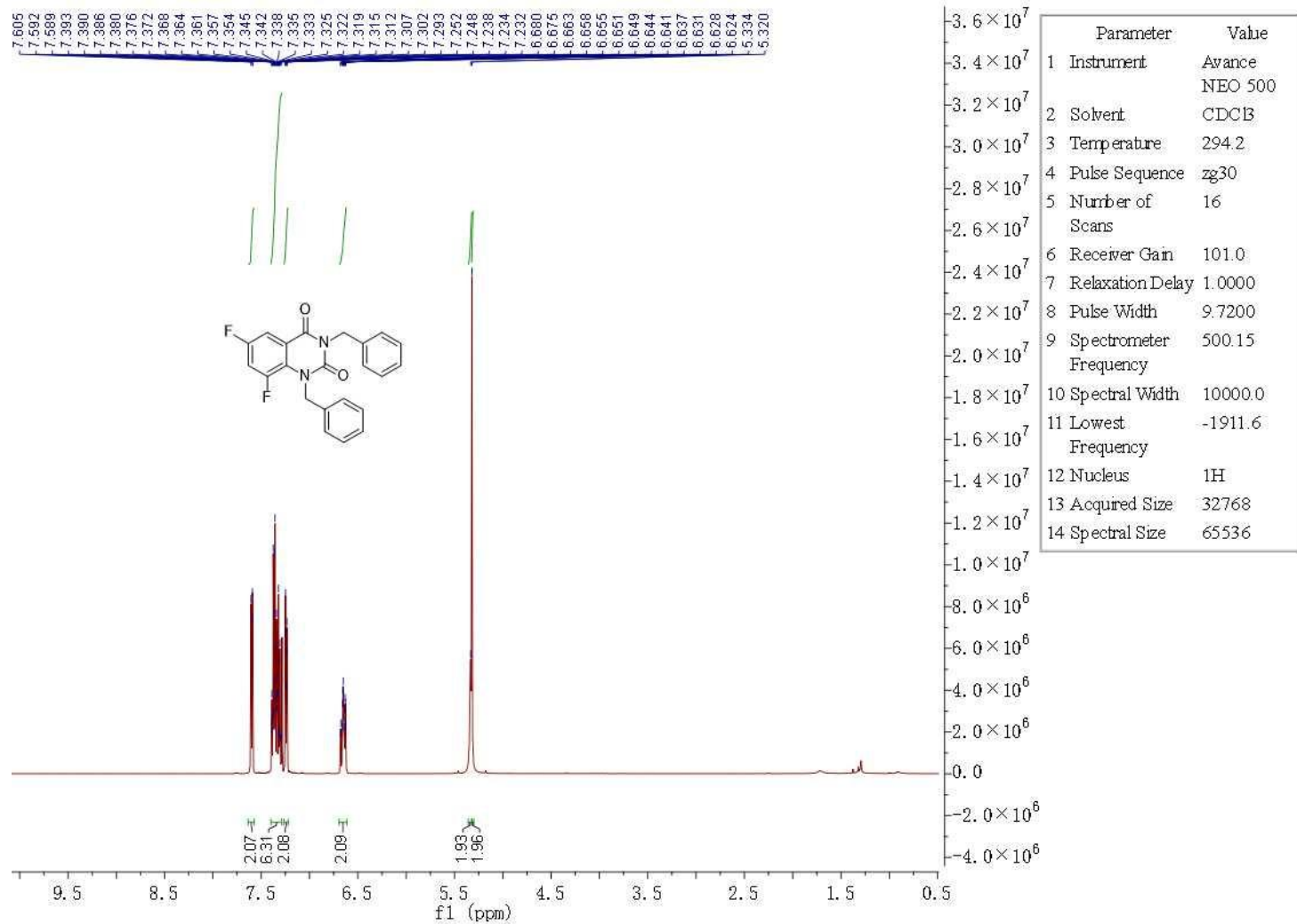


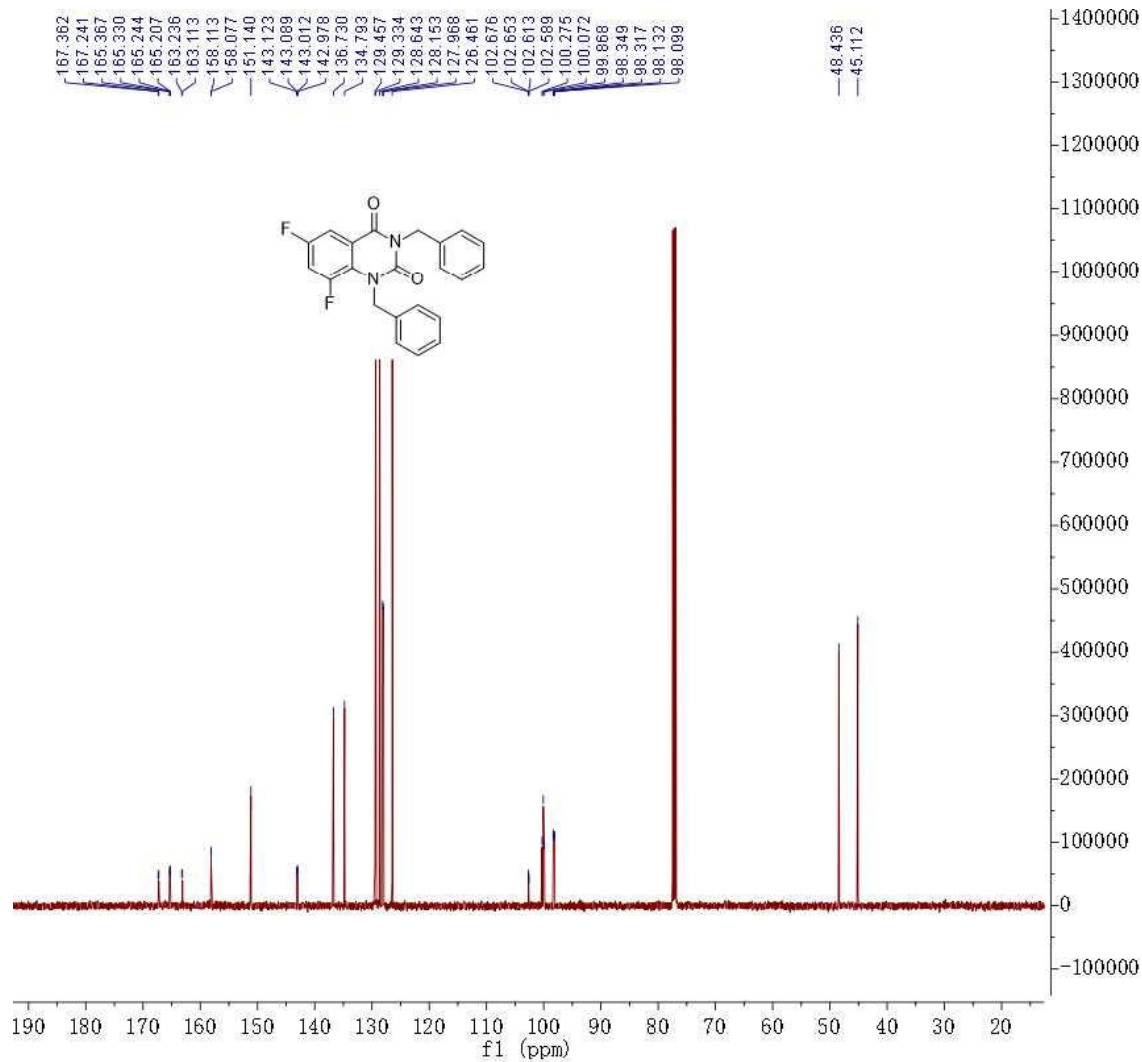
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.8
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer	500.15
Frequency	
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



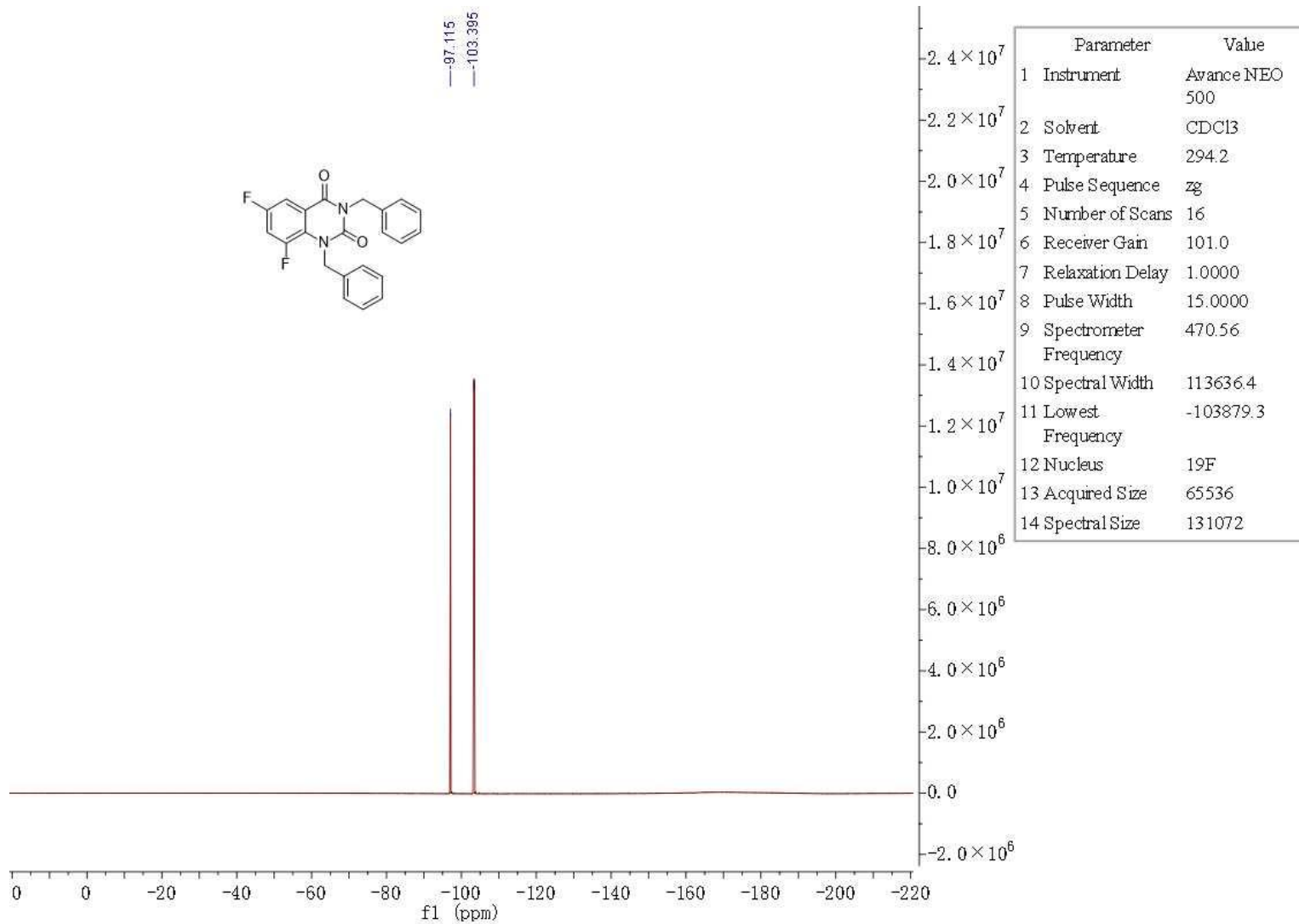
Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	295.2
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest Frequency	-2464.2
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

1,3-dibenzyl-6,8-difluoroquinazoline-2,4(1H,3H)-dione (5o)

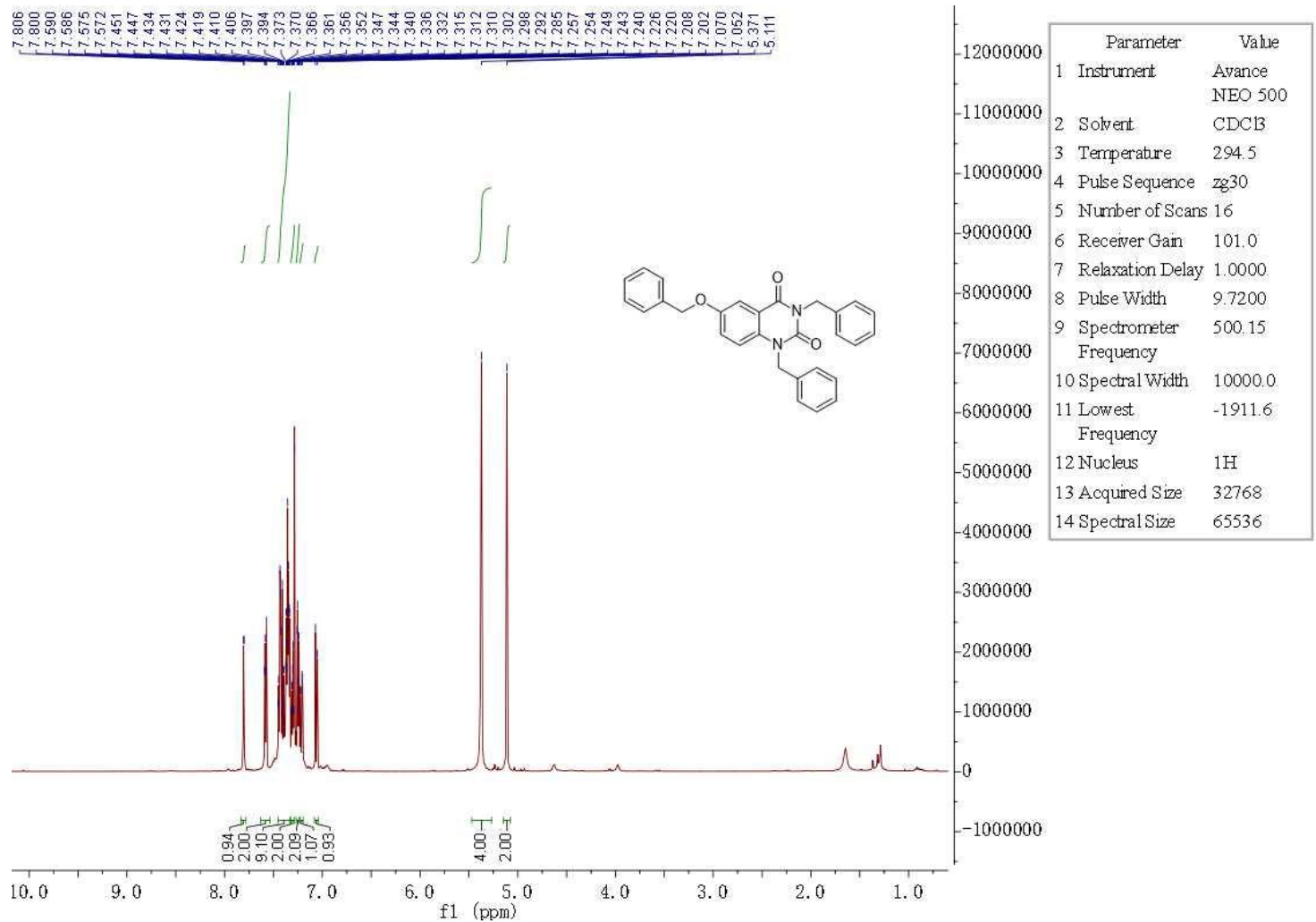


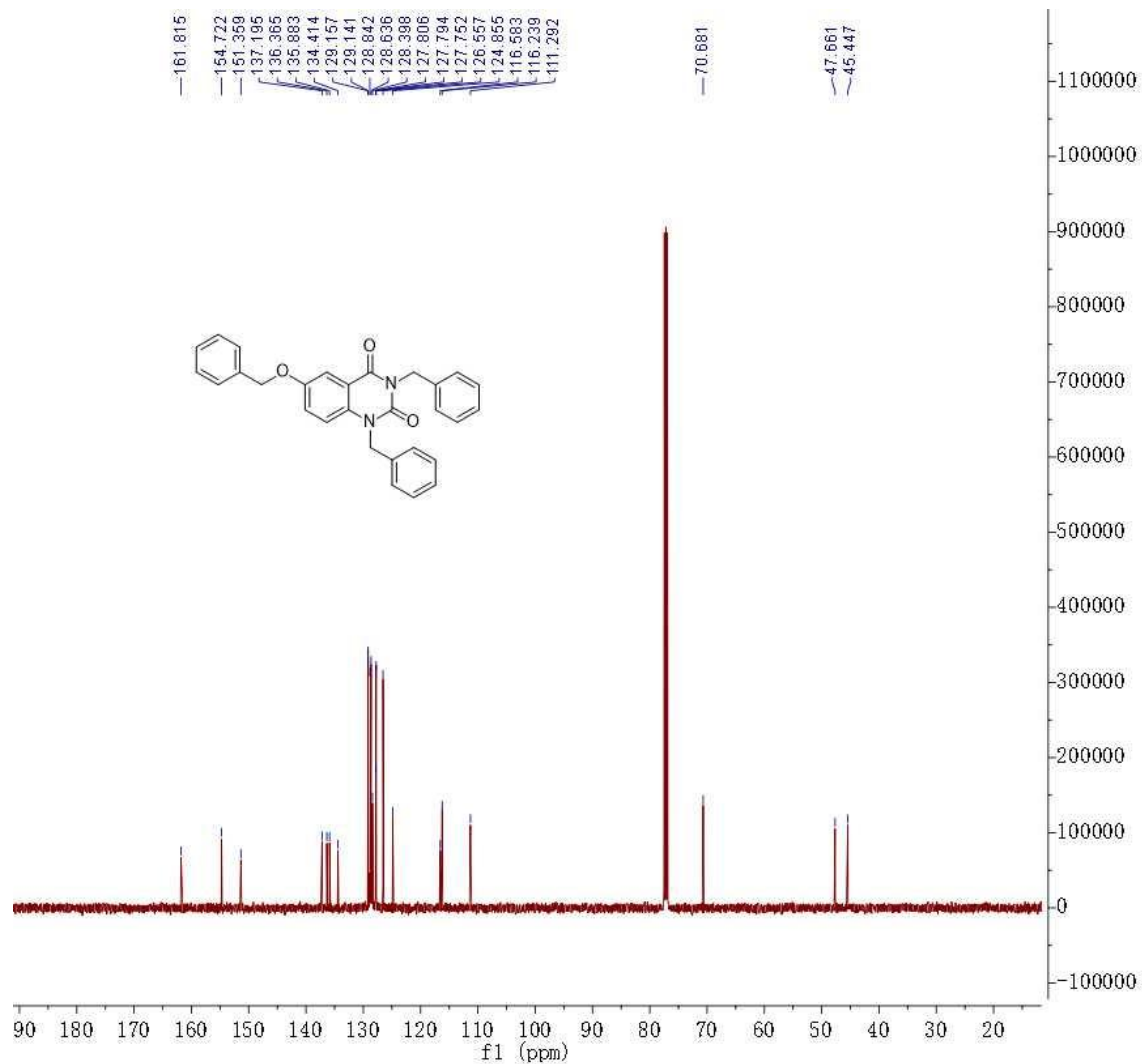


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCB
3 Temperature	294.7
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2469.9
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536



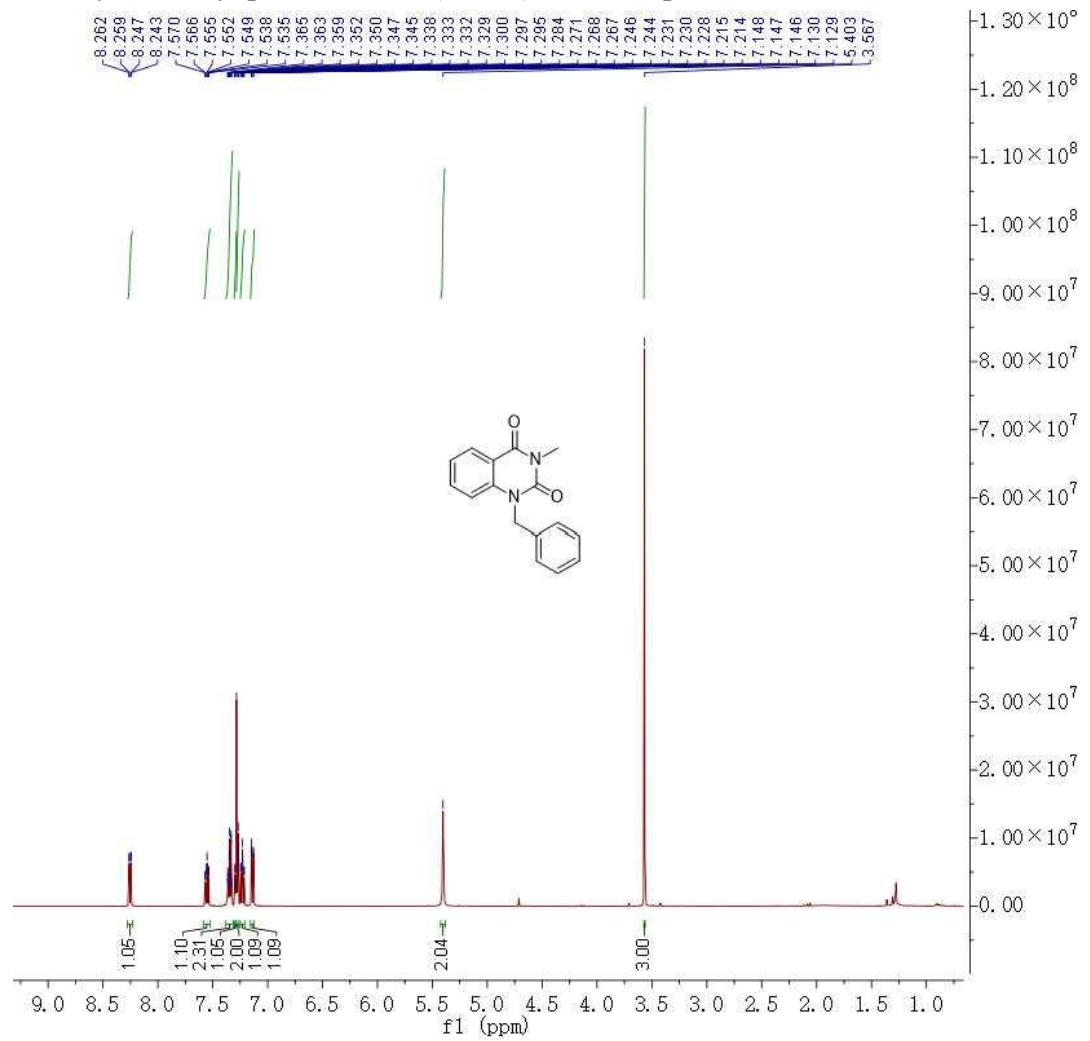
1,3-dibenzyl-6-(benzyloxy)quinazoline-2,4(1H,3H)-dione (5p)



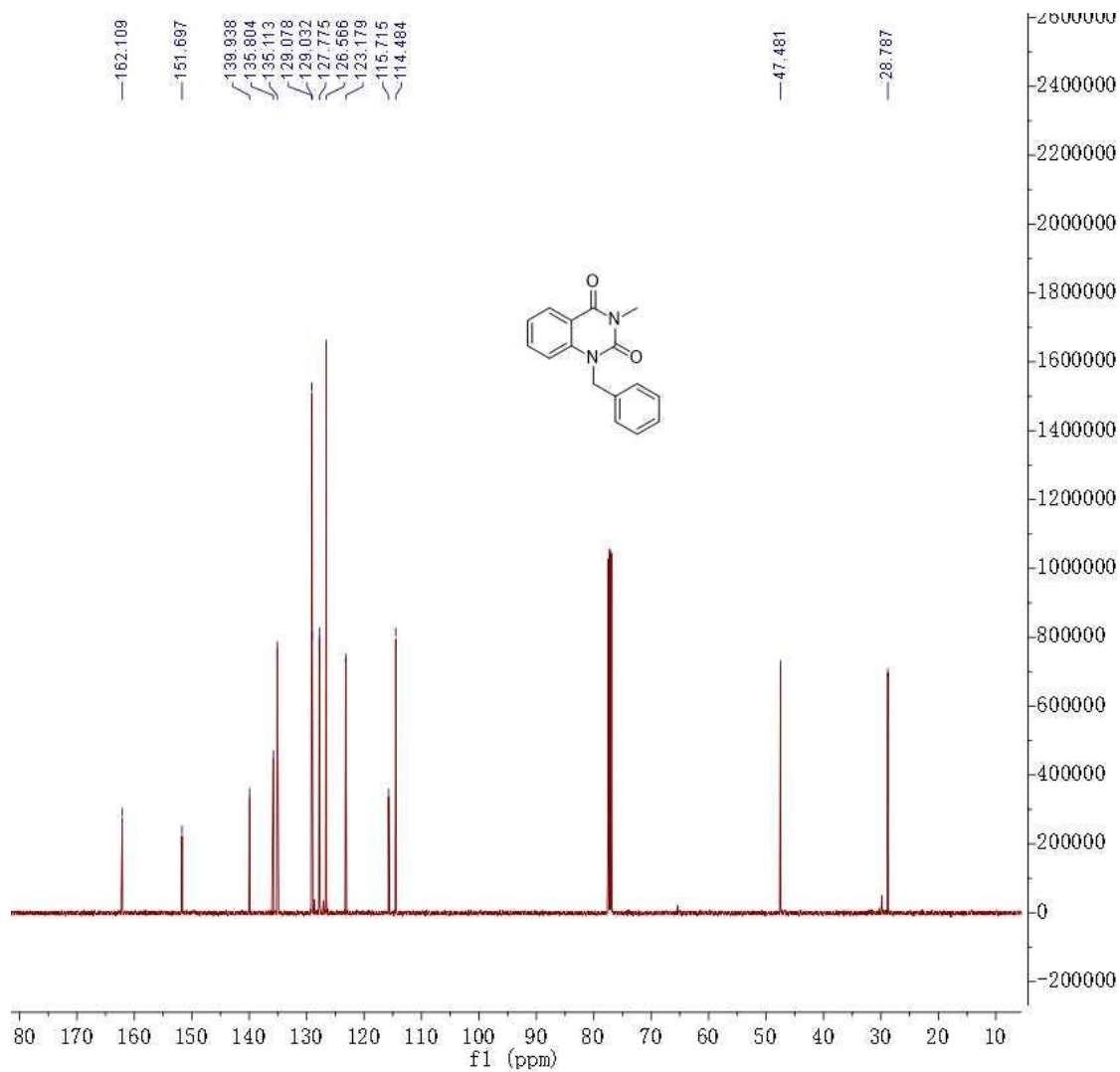


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	295.2
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2466.6
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

1-benzyl-3-methylquinazoline-2,4(1H,3H)-dione (5q)

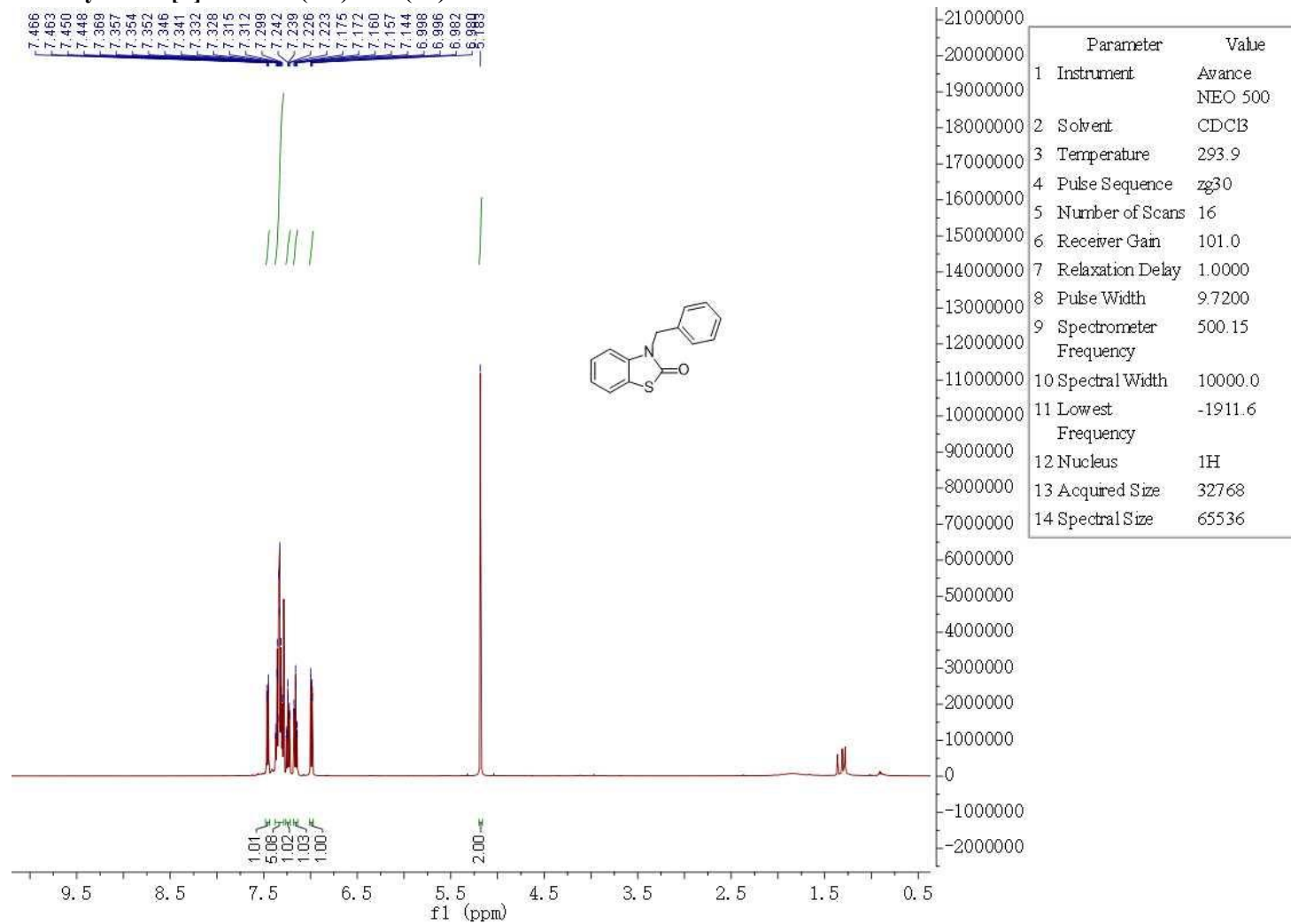


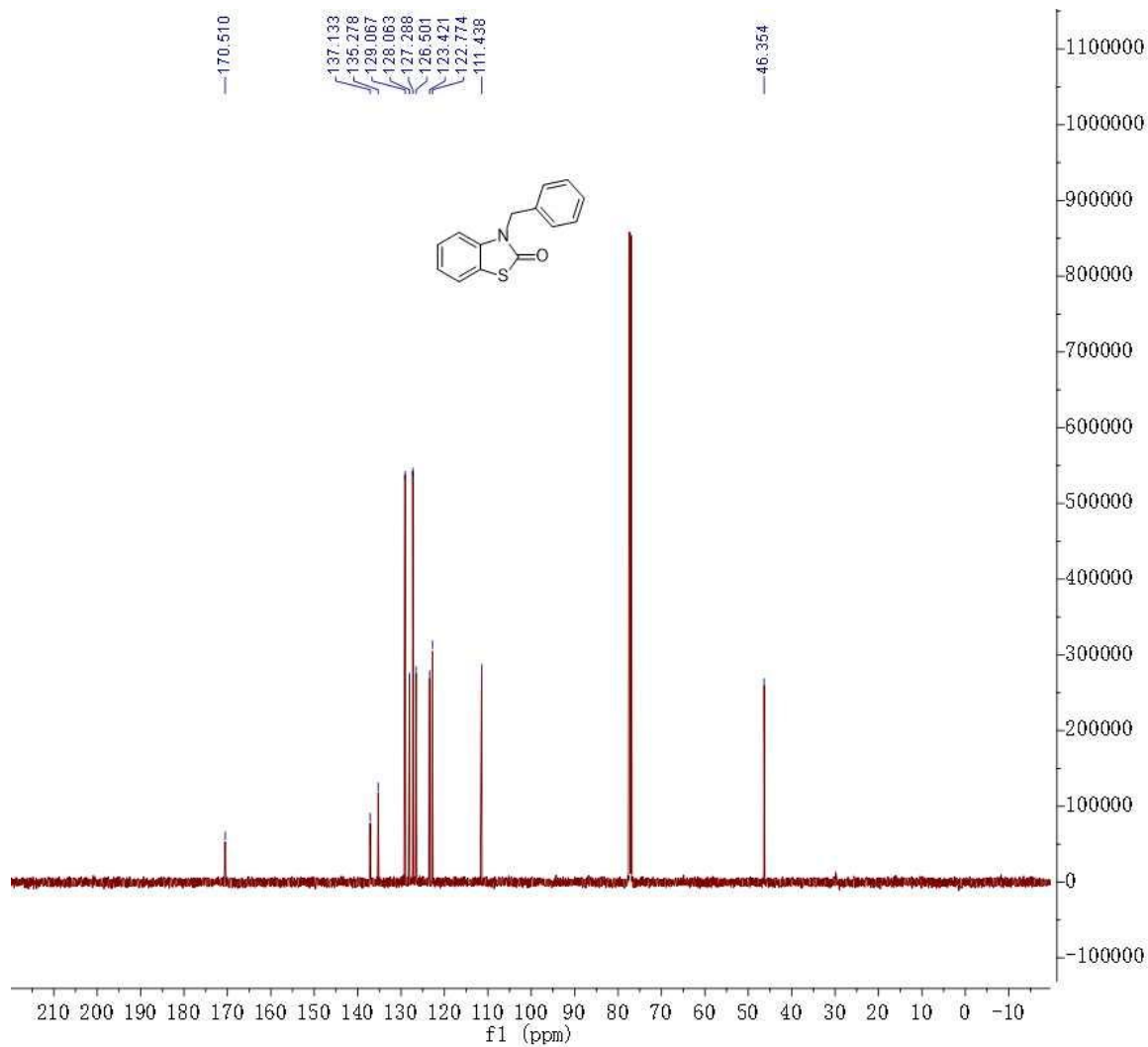
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	296.2
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	86.7
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer	500.15
Frequency	
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	296.1
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest Frequency	-2471.9
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

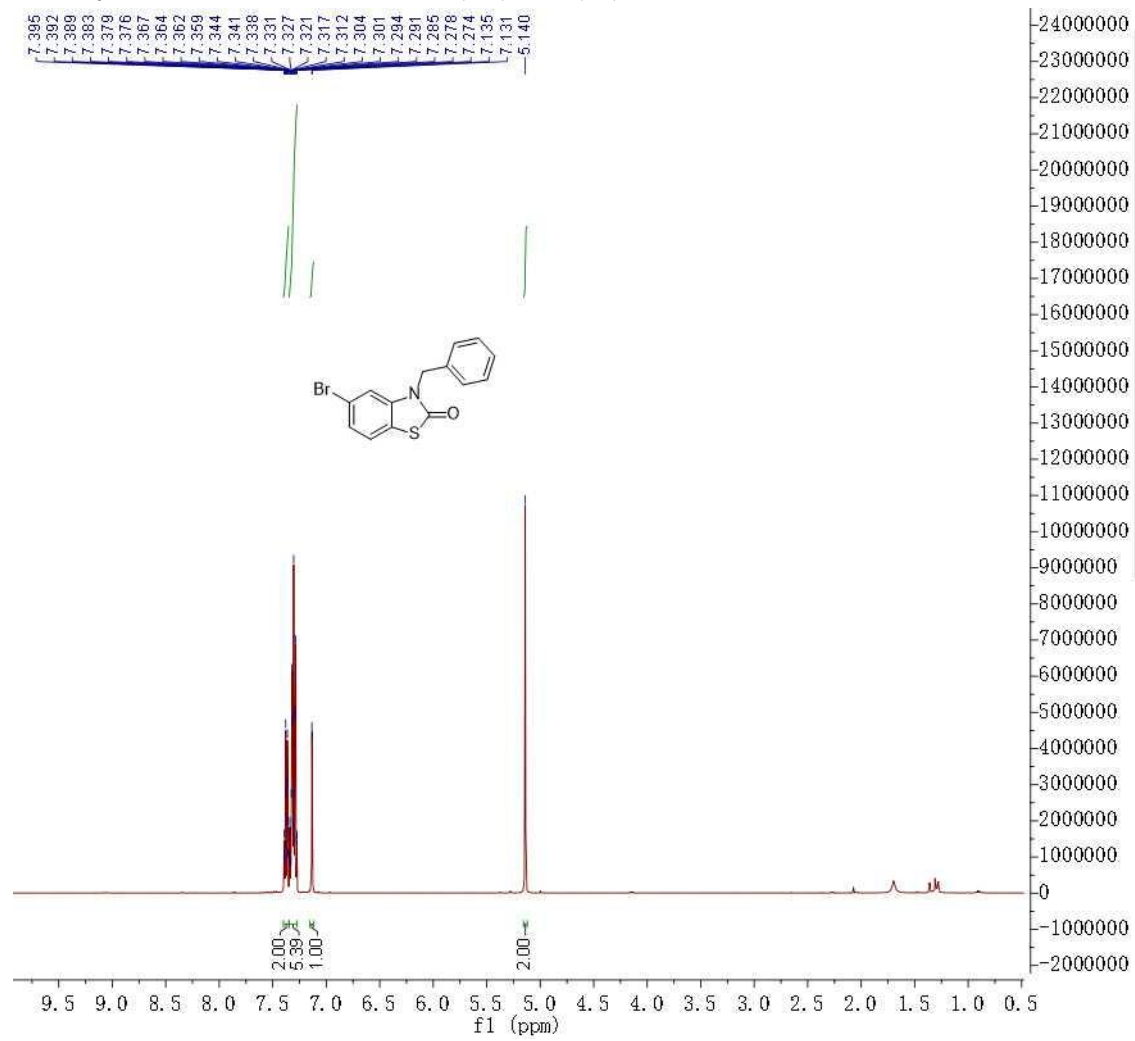
3-benzylbenzo[d]thiazol-2(3H)-one (7a)



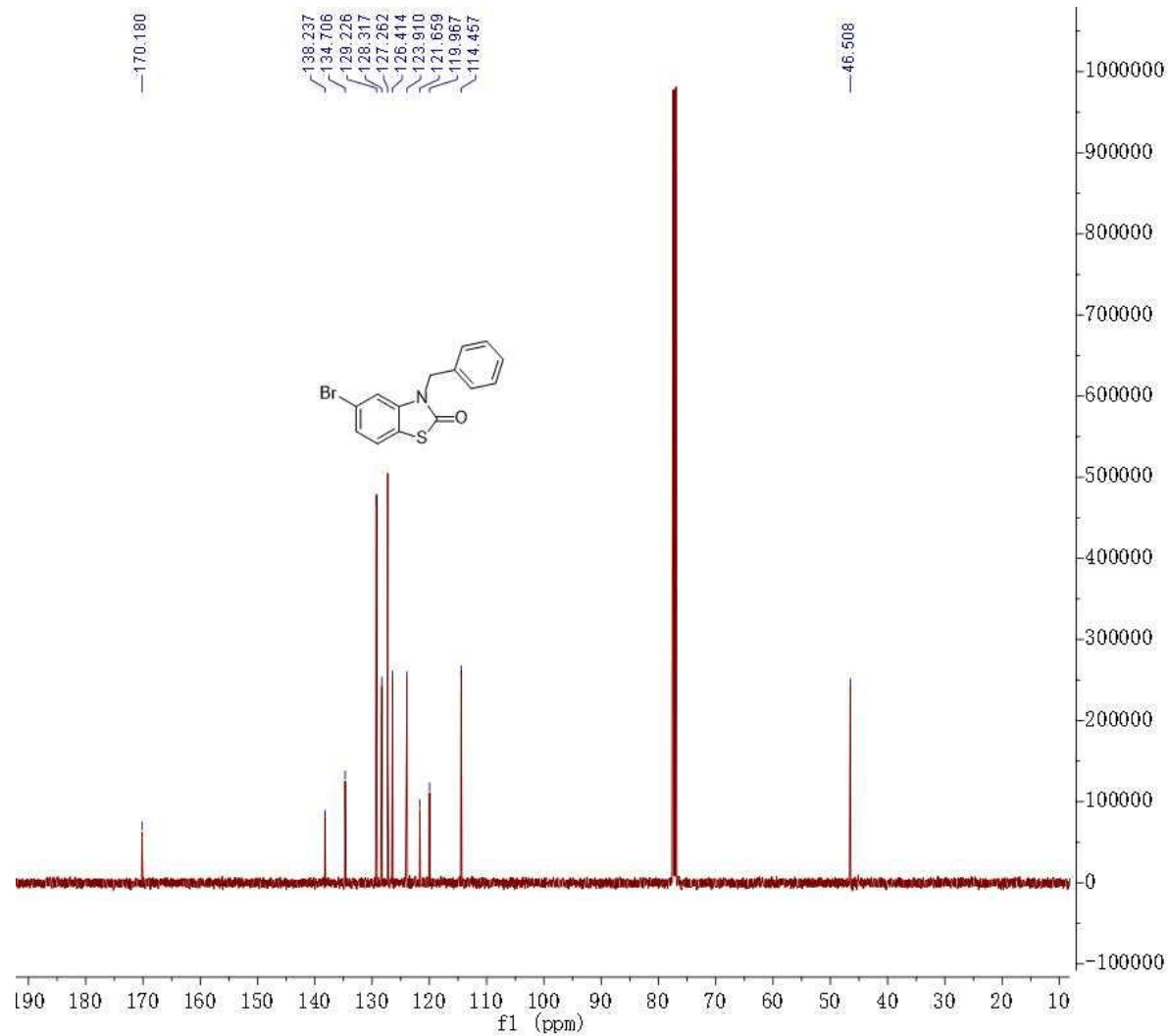


Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	294.8
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2466.6
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

3-benzyl-6-bromobenzo[d]thiazol-2(3H)-one (7b)

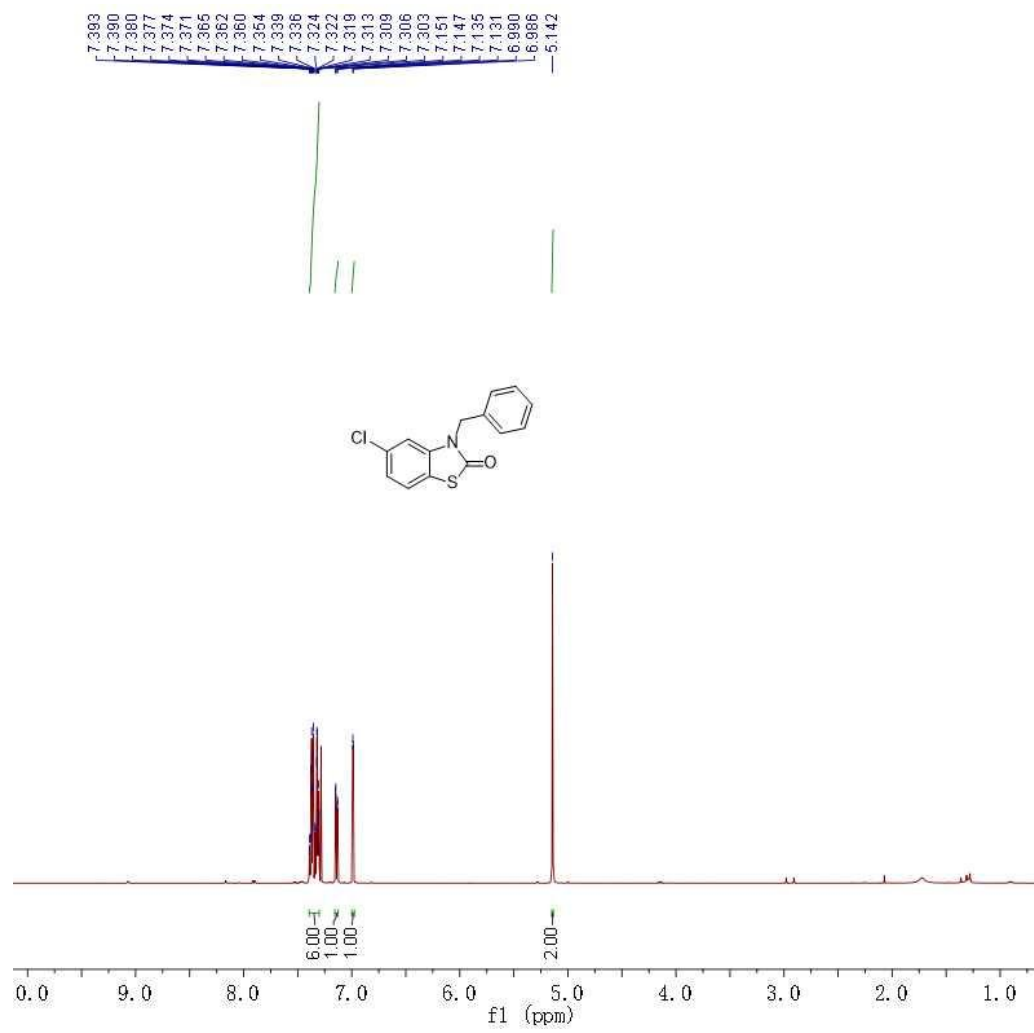


Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.5
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer Frequency	500.15
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536

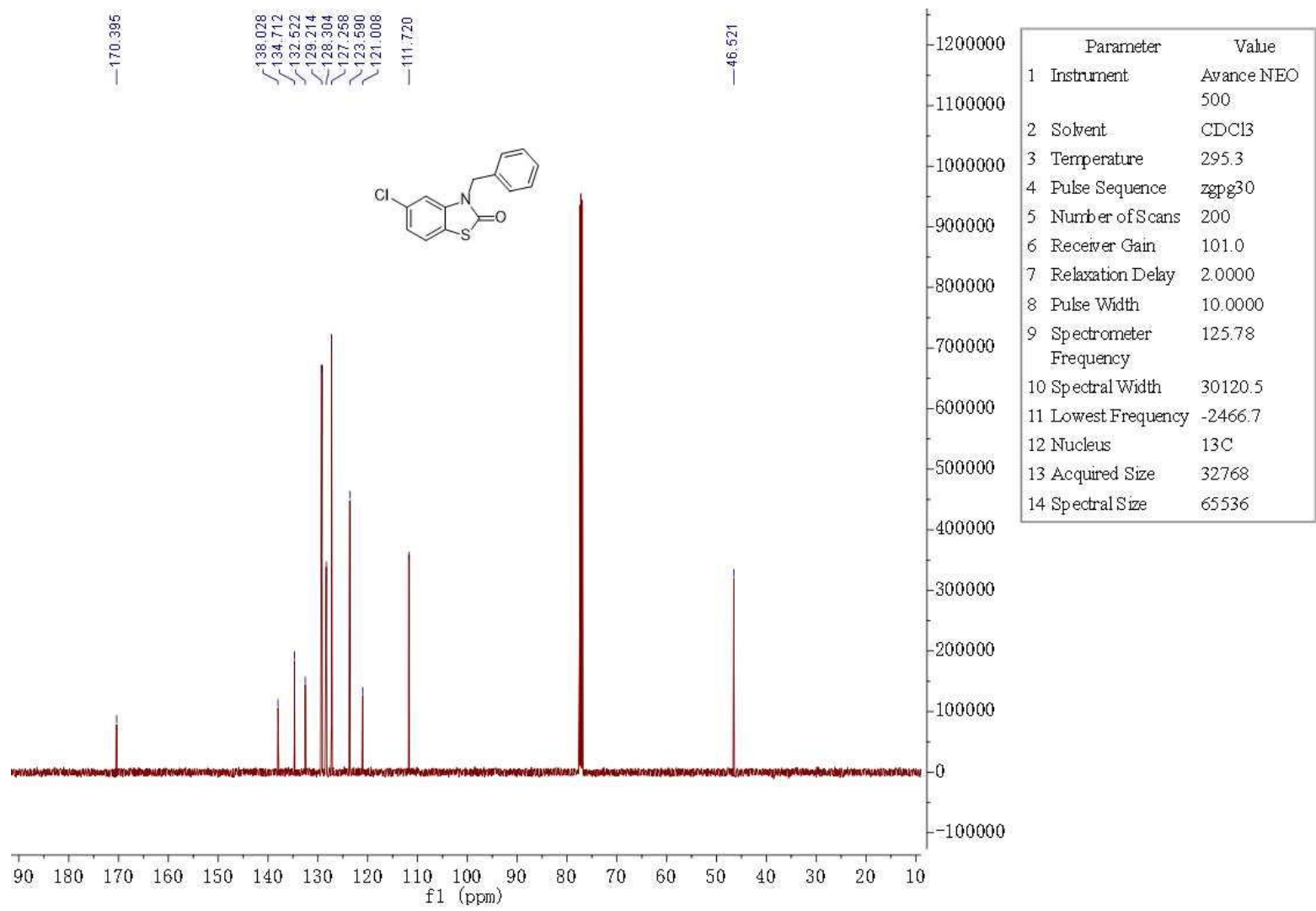


Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl ₃
3 Temperature	295.1
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2465.7
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536

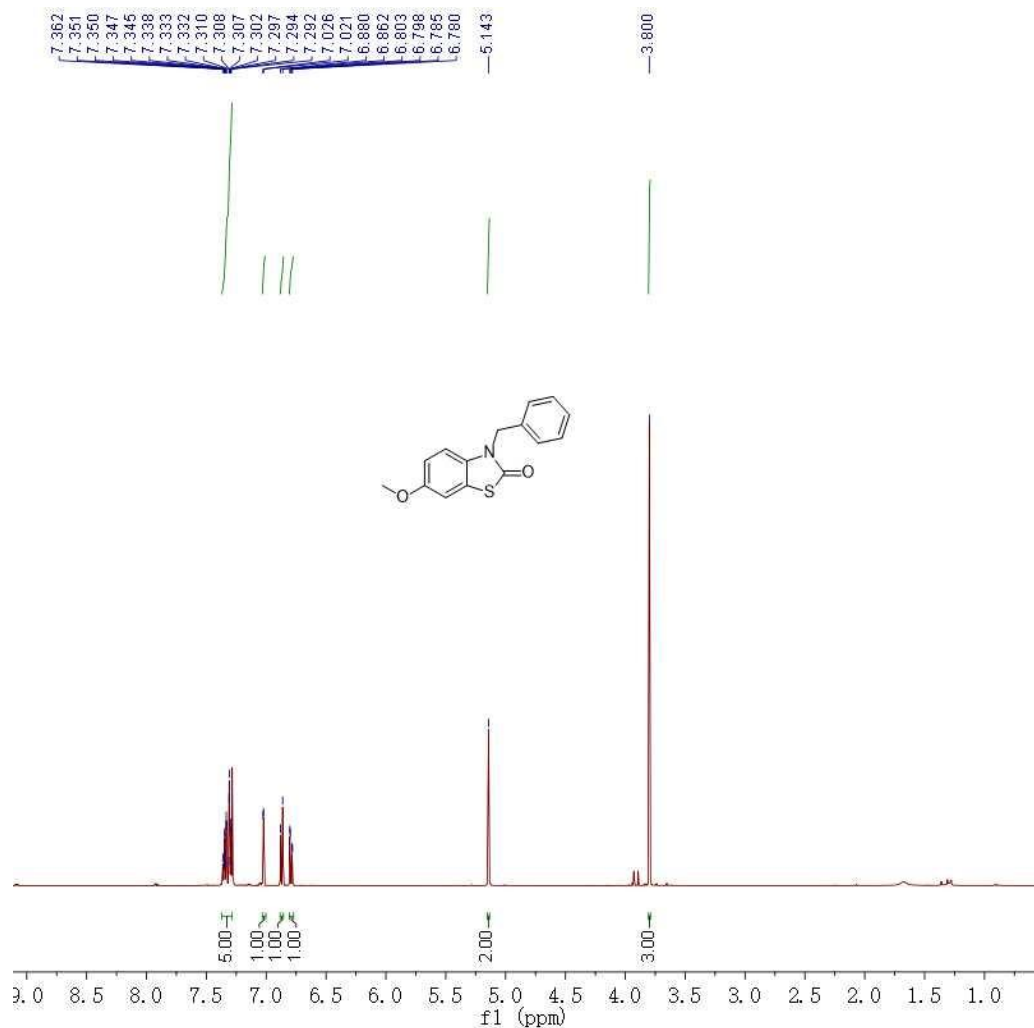
3-benzyl-6-chlorobenzo[d]thiazol-2(3H)-one (7c)



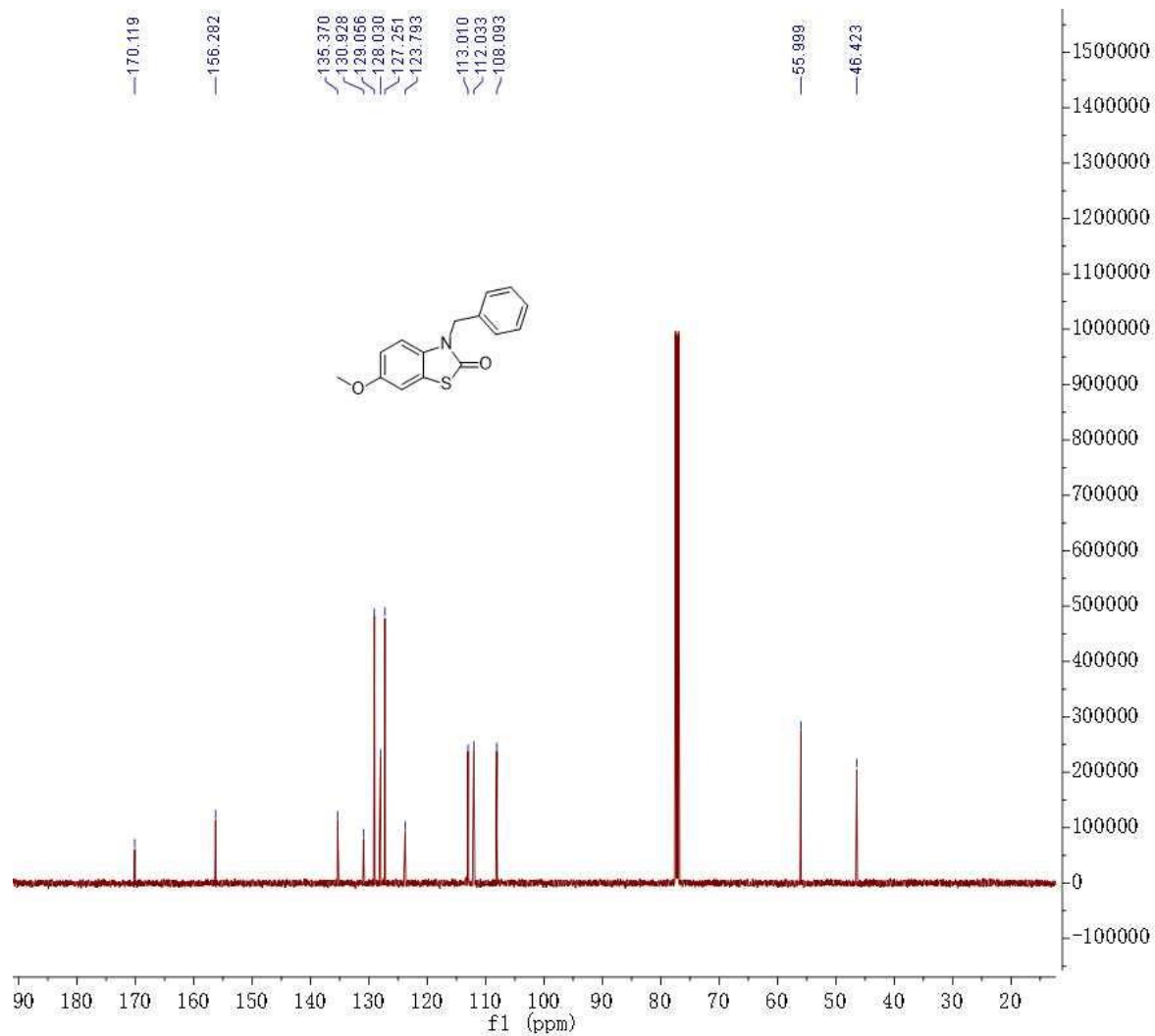
Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CDCl3
3 Temperature	294.4
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer Frequency	500.15
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



3-benzyl-6-methoxybenzo[d]thiazol-2(3H)-one (7d)

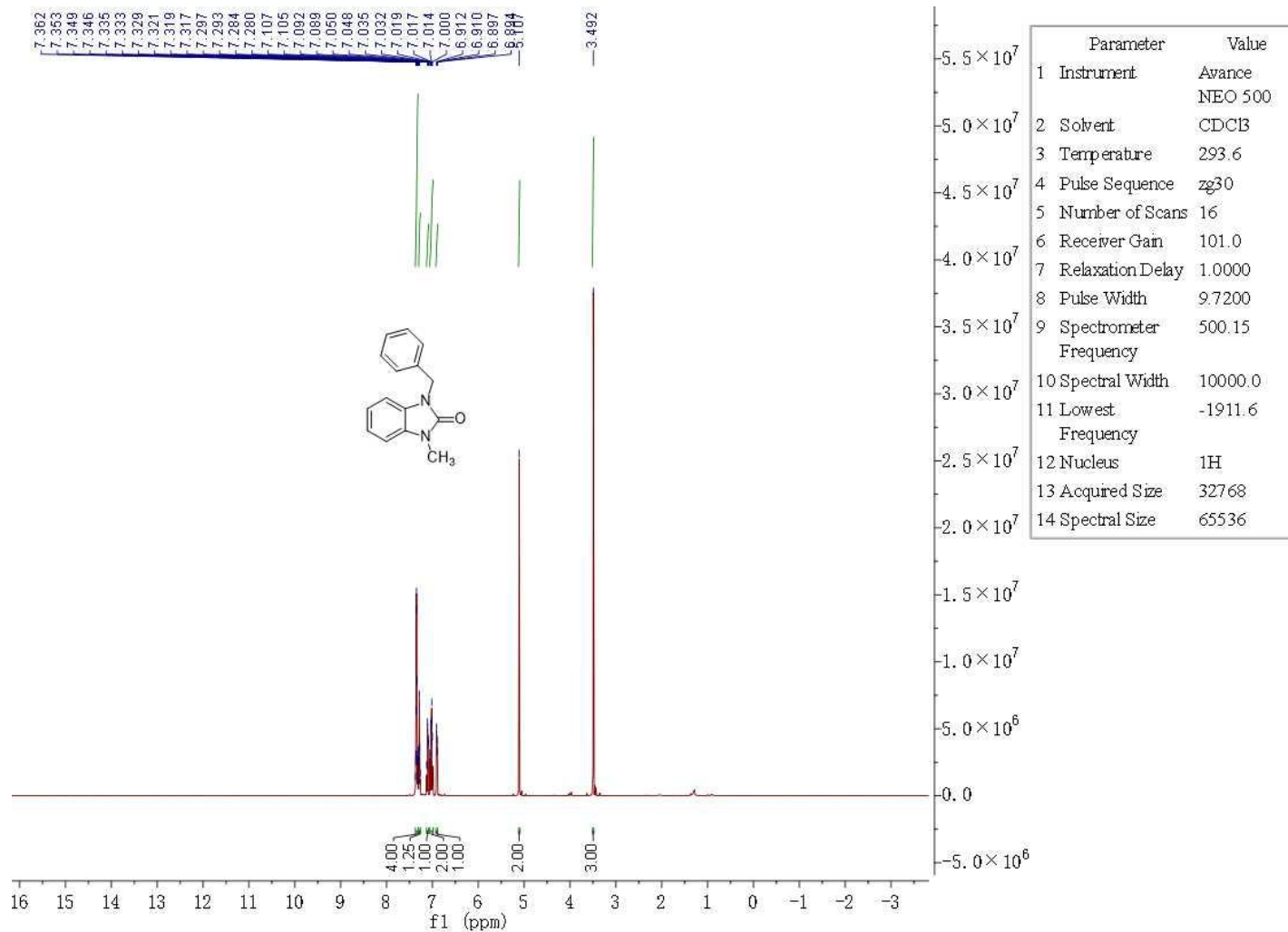


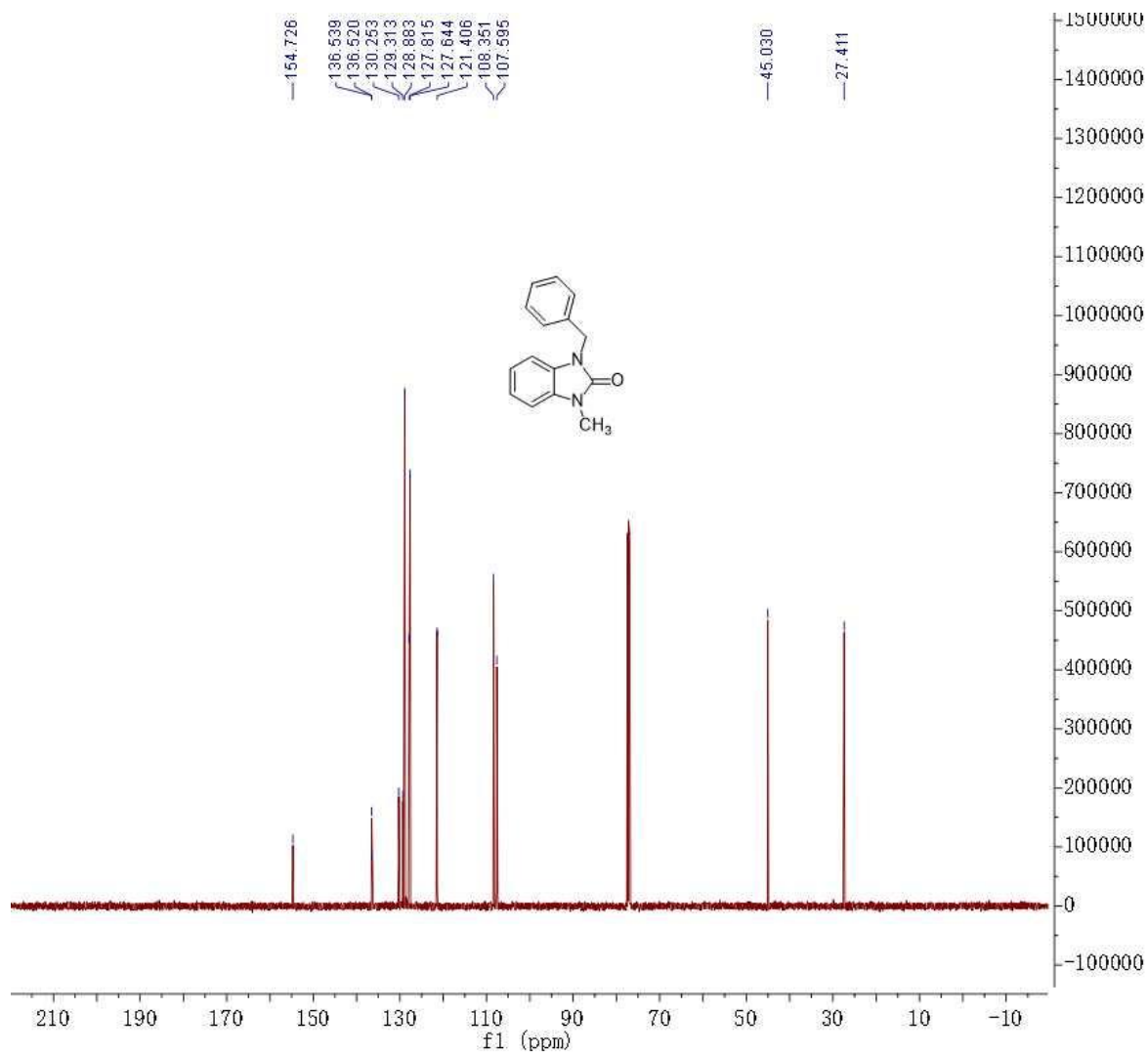
Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	294.6
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer Frequency	500.15
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



Parameter	Value
1 Instrument	Avance
	NEO 500
2 Solvent	CDCl3
3 Temperature	295.0
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest	-2465.7
Frequency	
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

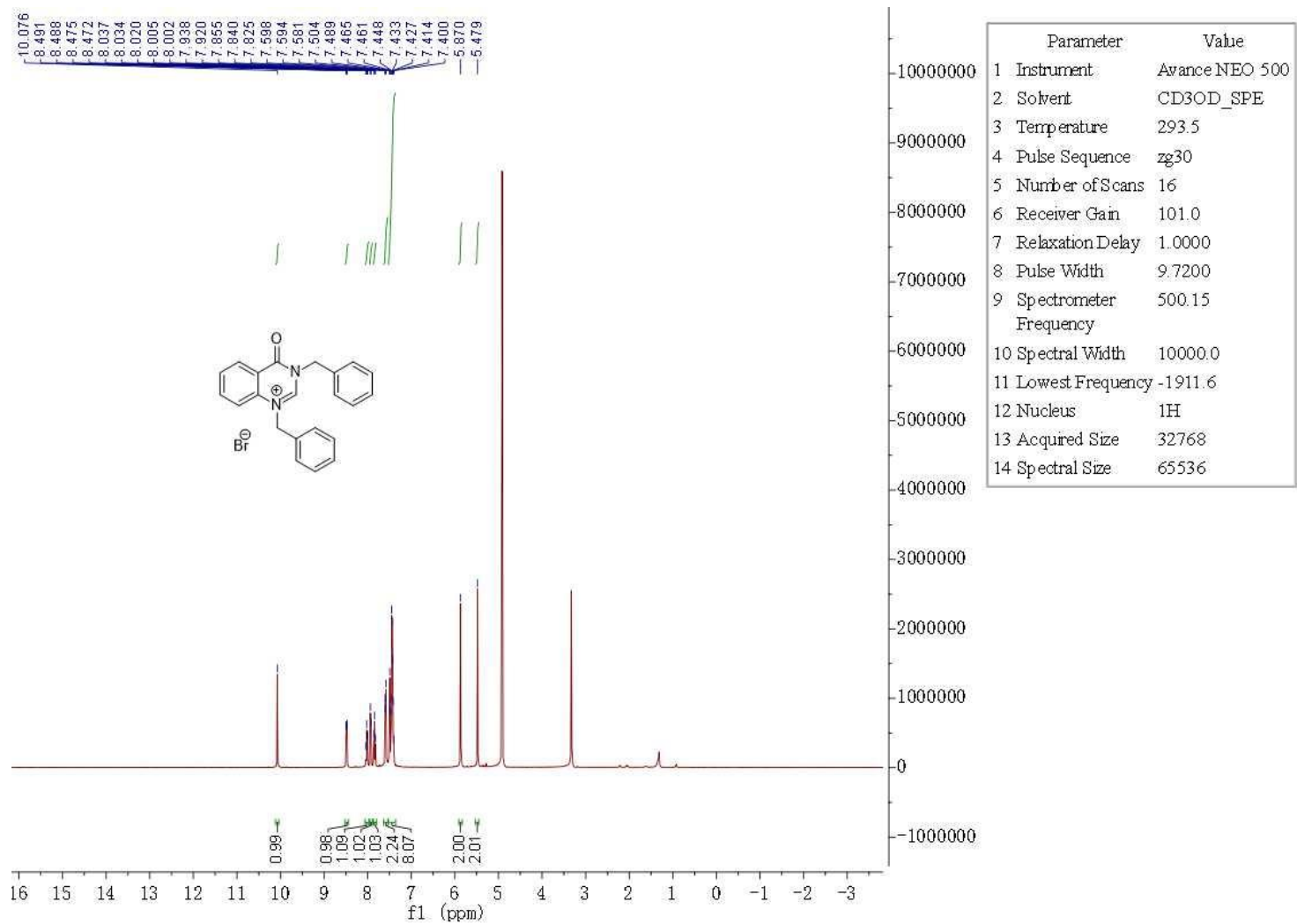
1-benzyl-3-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (7e)

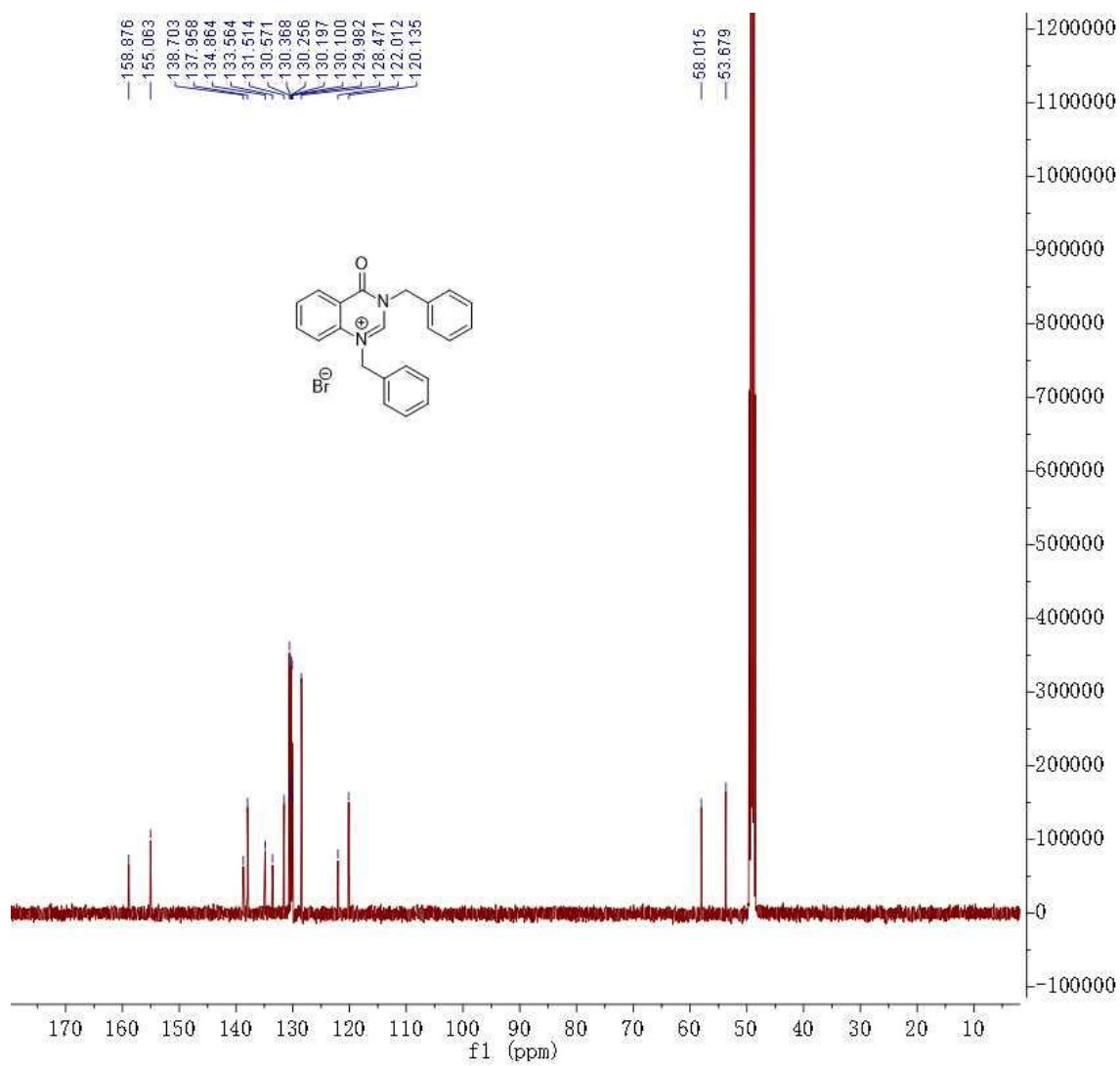




Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl ₃
3 Temperature	294.2
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest Frequency	-2468.2
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536

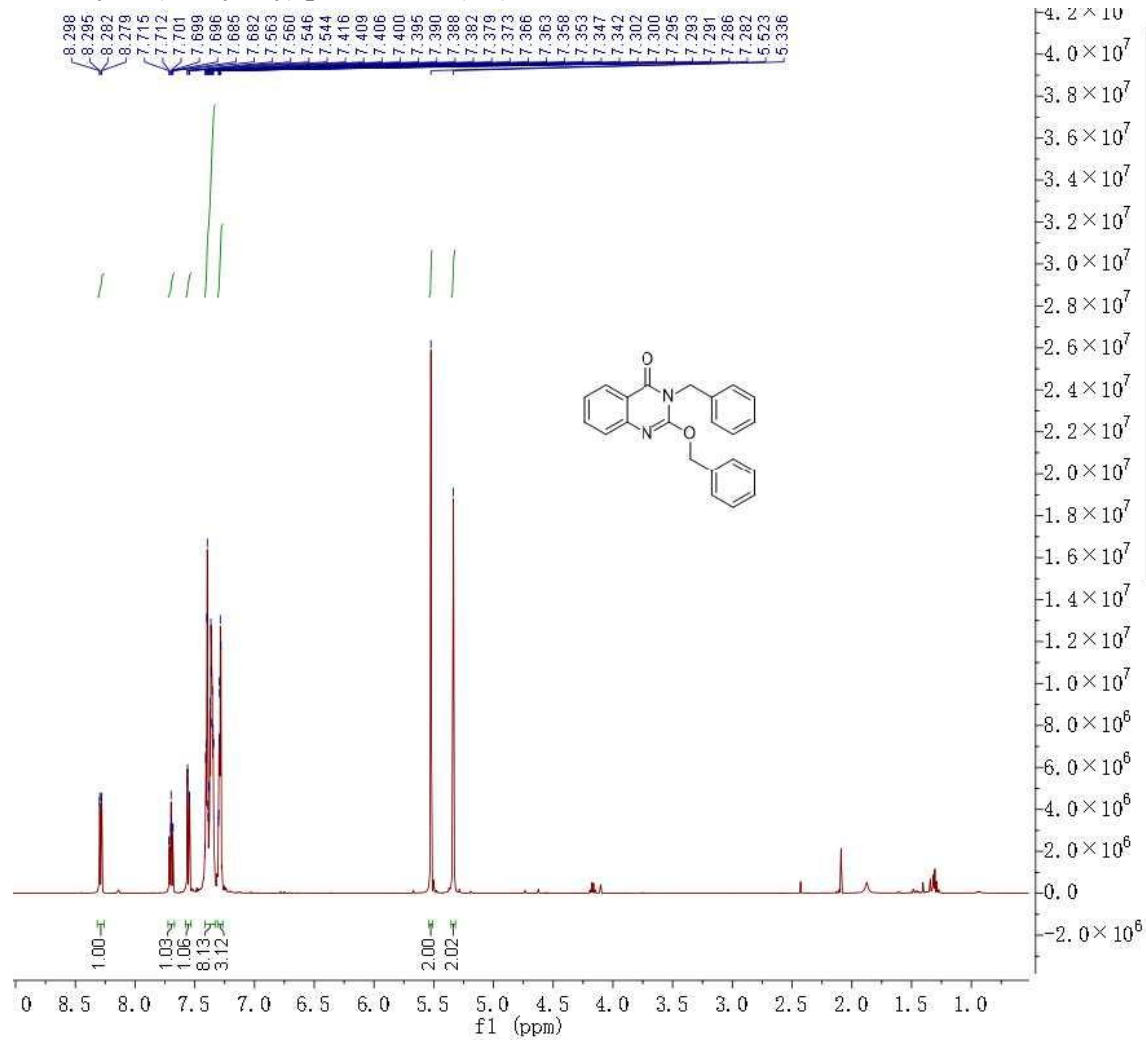
1,3-dibenzyl-4-oxo-3,4-dihydroquinazolin-1-ium bromide (8)



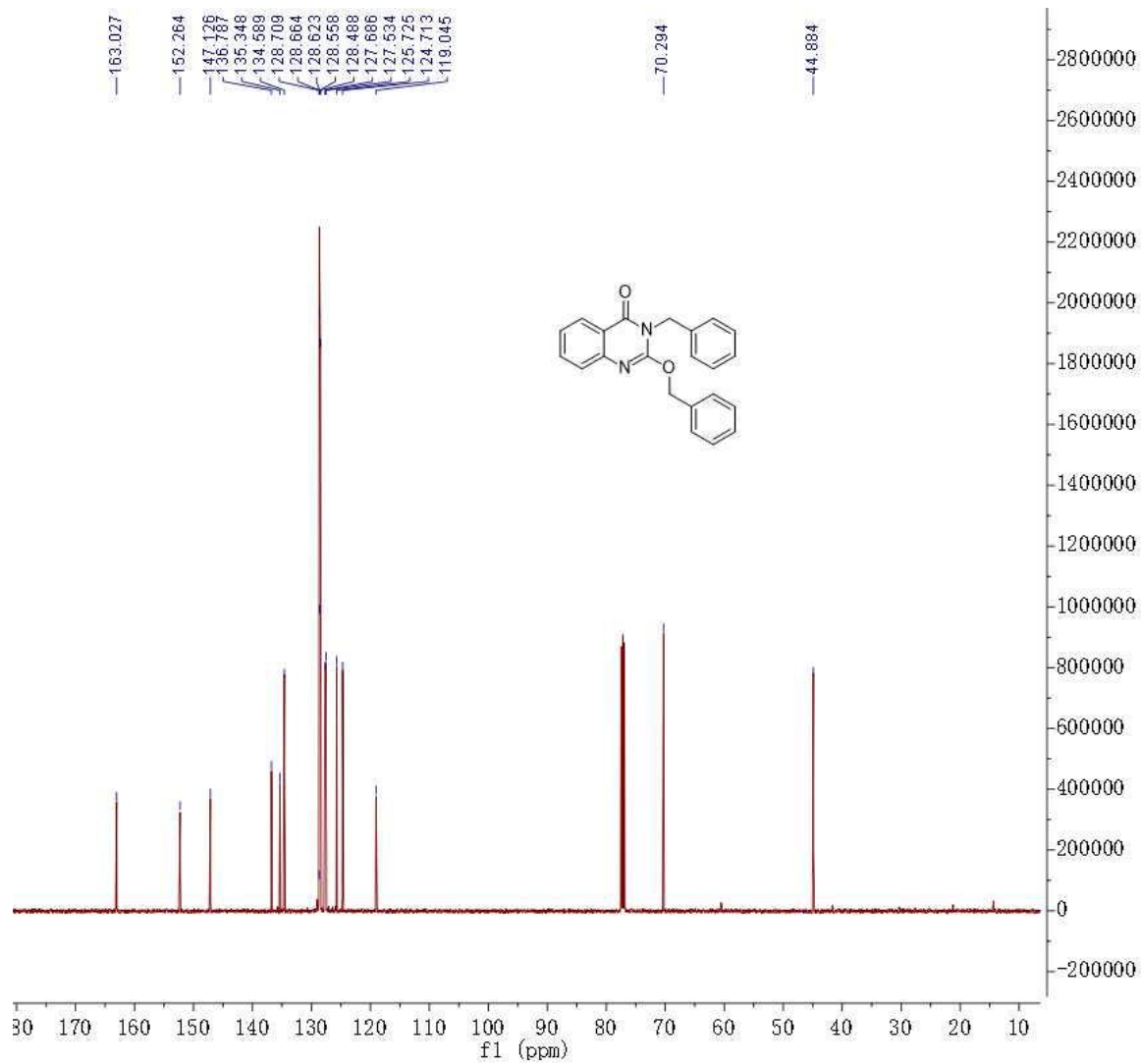


Parameter	Value
1 Instrument	Avance NEO 500
2 Solvent	CD3OD_SPE
3 Temperature	295.5
4 Pulse Sequence	zgpg30
5 Number of Scans	500
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.78
10 Spectral Width	30120.5
11 Lowest Frequency	-2308.8
12 Nucleus	^{13}C
13 Acquired Size	32768
14 Spectral Size	65536

3-benzyl-2-(benzyloxy)quinazolin-4(3H)-one (9)



Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	296.2
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	67.1
7 Relaxation Delay	1.0000
8 Pulse Width	9.7200
9 Spectrometer Frequency	500.15
10 Spectral Width	10000.0
11 Lowest Frequency	-1911.6
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



Parameter	Value
1 Instrument	Avance NEO
2 Solvent	CDCl3
3 Temperature	296.2
4 Pulse Sequence	zgpg30
5 Number of Scans	200
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer	125.78
Frequency	
10 Spectral Width	30120.5
11 Lowest Frequency	-2475.5
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536