Supporting Information

Electrochemical Dual Oxidative C(sp^3)–H Amination: Switchable Synthesis of Imidazo-Fused Quinazolinones

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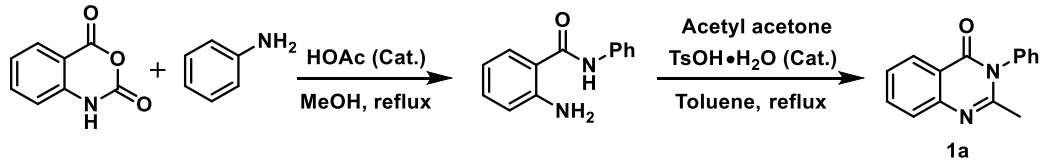
General Information

Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. NMR spectra were recorded on a Bruker AV-500 (^{1}H: 500 MHz, ^{13}C: 125 MHz, ^{19}F NMR: 470 MHz) spectrometer using TMS as internal reference. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively. GC-MS was Shimadzu QP-5050 GC-MS system. Commercially available compounds were used without further purification. GC-MS was Shimadzu QP-5050 GC-MS system. Commercially available compounds were used without further purification. All substances were known compounds and synthesized according to the literature.[1] High resolution mass spectra (HRMS) were measured using electrospray ionization (ESI) and the time-of-flight (TOF) mass analyzer. The anode electrode and cathode electrode all are Pt (1.0 × 1.0 cm^2). These electrodes are commercially available from GaossUnion, China.

Substrates Preparation

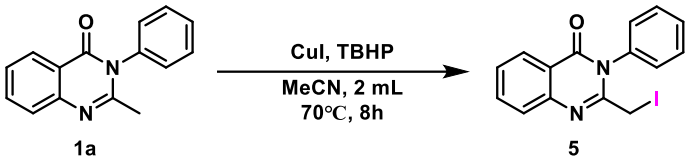
General Procedure for the preparation of methylquinazolinone derivatives.



A suspension of isatoic anhydride, 1.1 equiv of aryl- or benzyl-amine and 1% AcOH in MeOH was stirred at 75 °C for 10 h. After the reaction was completed, as indicated by TLC (eluent hexane: EtOAc = 6:4), the brown solution was filtered in a Büchner funnel that had been packed with a layer of celite and activated charcoal; the colorless solution was then evaporated under reduced pressure. Recrystallization from Et_2O afforded benzamide. [S1]

In a sealed tube equipped with a magnetic bar was charged with 2-amino benzamide derivatives (1, 3.67 mmol), acetyl acetone (4.04 mmol) and $TsOH·H_2O$ (0.73 mmol) in toluene (5 mL). The reaction mixture was stirred at 120 °C for 10 h. After completion of the reaction, the reaction mass was cooled to room temperature, diluted with EtOAc, gave a water wash and the organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash column chromatography (eluent hexane: EtOAc = 6:4) on silica gel to afford the desired product.[S2] Similarly, the other methylquinazolinones derivatives were prepared.

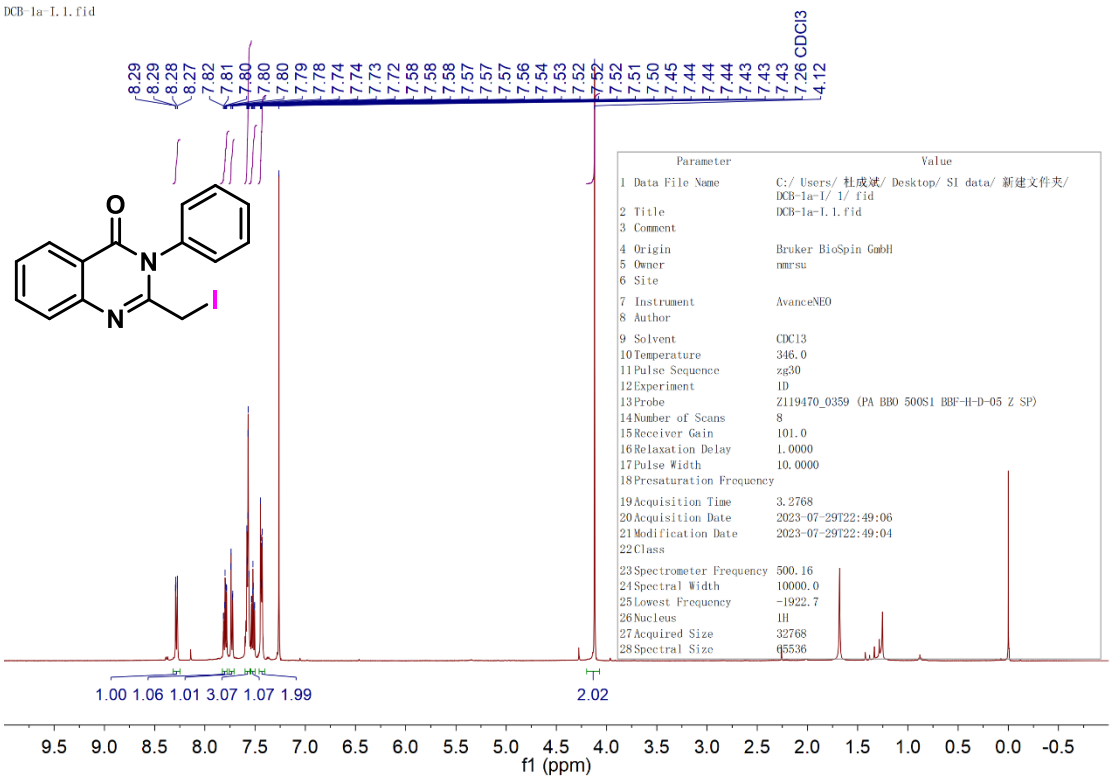
Procedure for the preparation of 5 (2-(iodomethyl)-3-phenylquinazolin-4(3*H*)-one). [S3]

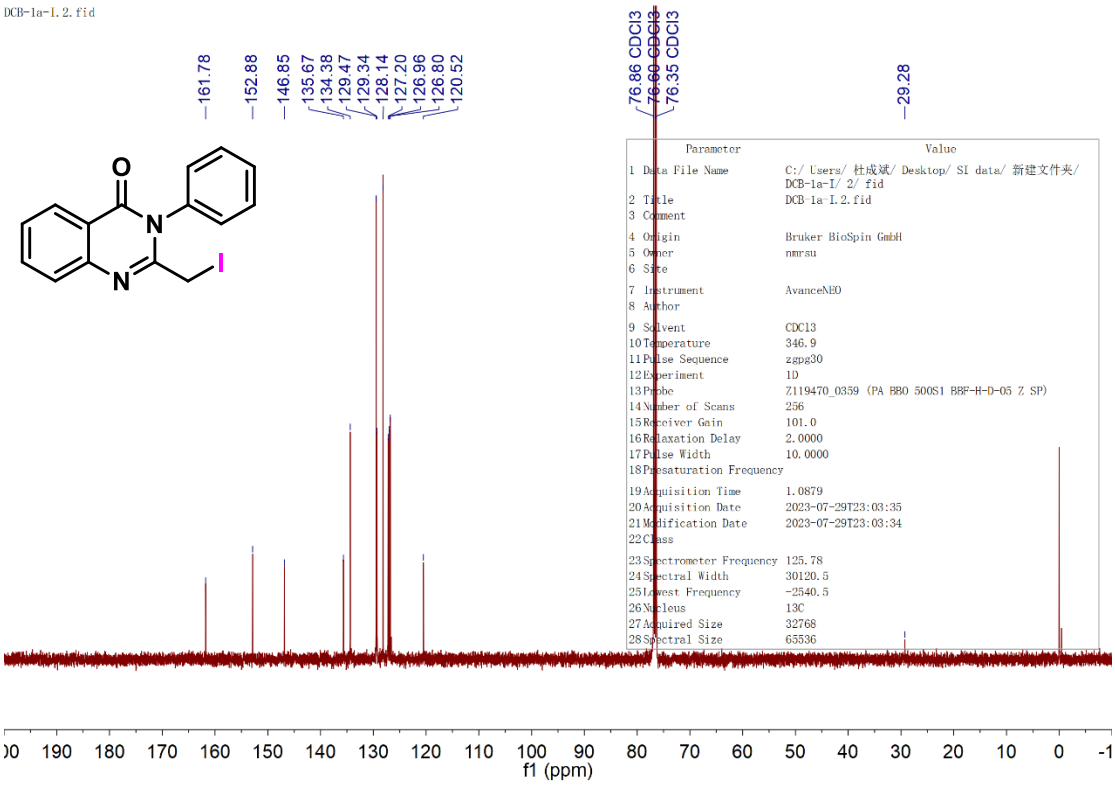


Methylquinazolinone(**1a**, 0.5mmol), CuI (0.75mmol), TBHP (8.0 eq., 70% aqueous solution) and CH_3CN (2mL) were stirred at 70 °C for 8h. Then, the reaction mixture was diluted by water and extracted with CH_2Cl_2 (3×15mL). The I_2 in organic phase was quenched by $Na_2S_2O_3$. The combined organic layers were washed with saturated NH_4Cl aqueous solution and dried over anhydrous Na_2SO_4. After filtration, the solvent was evaporated in vacuo. The desired product was obtained by

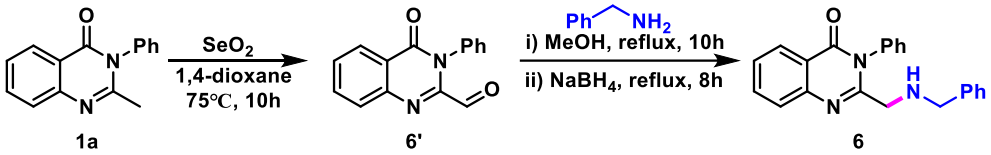
silica gel chromatography (eluent hexane: EtOAc = 6:4).

2-(iodomethyl)-3-phenylquinazolin-4(3*H*)-one (5): ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.80 (ddd, *J* = 8.5, 7.1, 1.6 Hz, 1H), 7.73 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.60 – 7.55 (m, 3H), 7.52 (ddd, *J* = 8.1, 7.1, 1.3 Hz, 1H), 7.46 – 7.41 (m, 2H), 4.12 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.8, 152.9, 146.8, 135.7, 134.4, 129.5, 129.3, 128.1, 127.2, 126.9, 126.8, 120.5, 29.3.





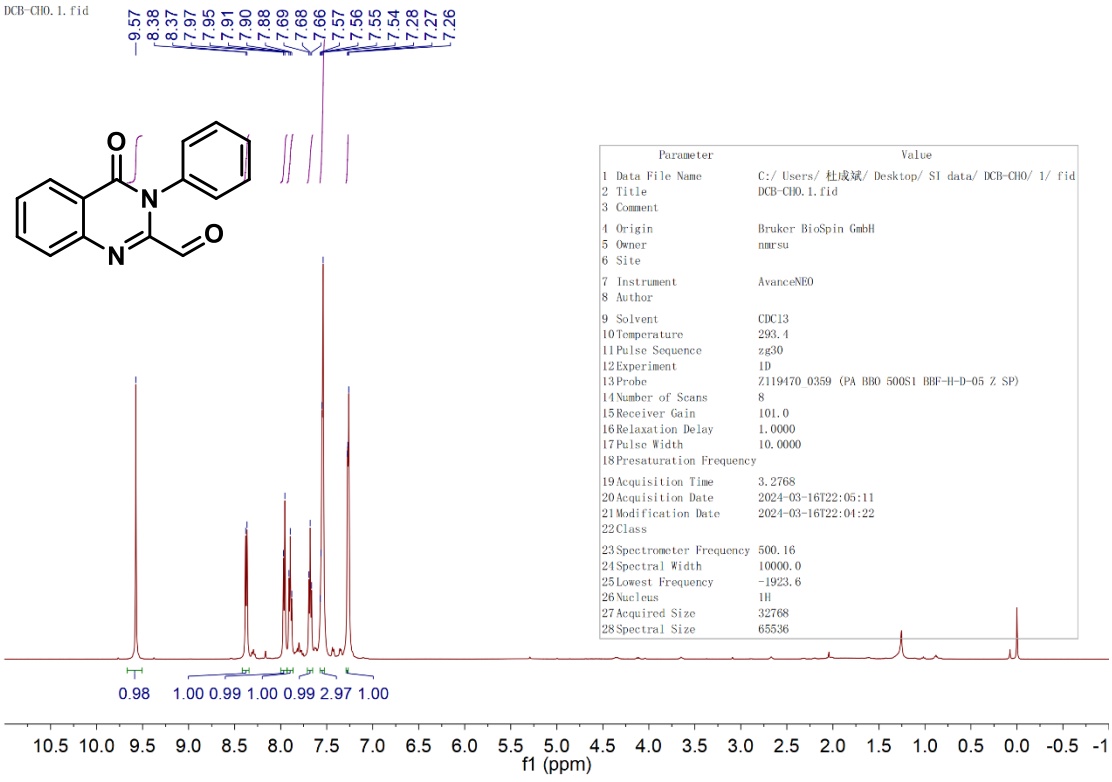
Procedure for the preparation of 6 [2-((benzylamino)methyl)-3-phenylquinazolin-4(3*H*)-one]. [S4, S5]

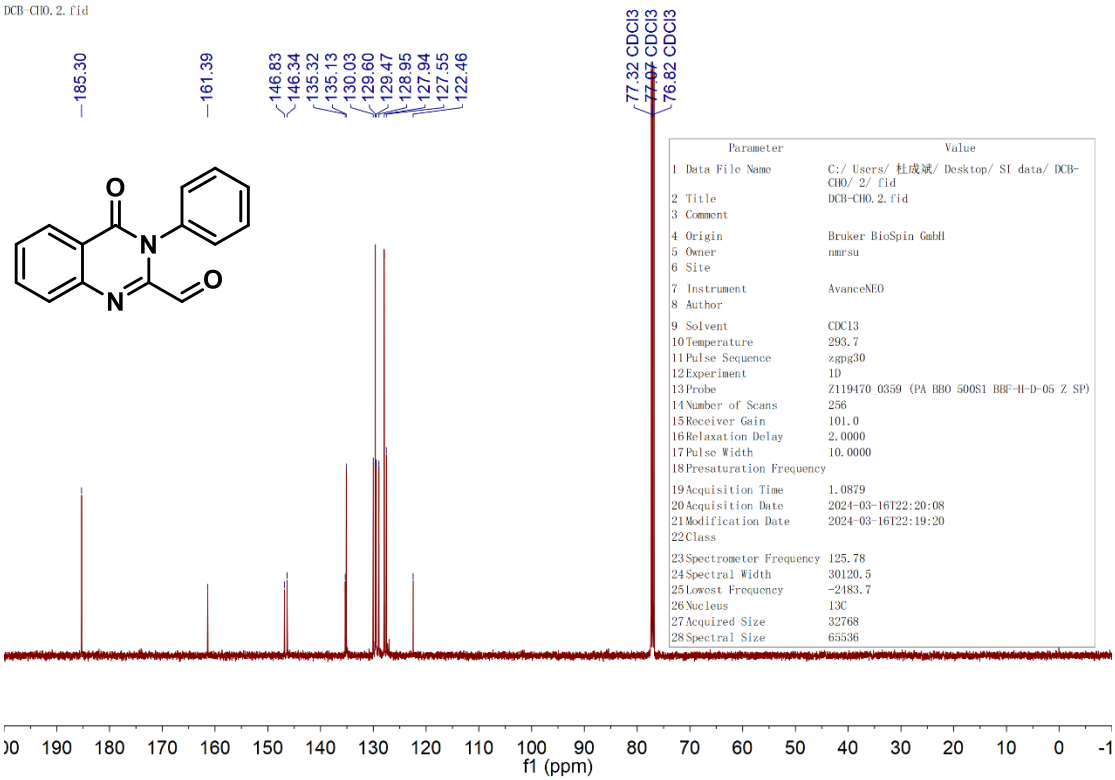


1a 6' 6

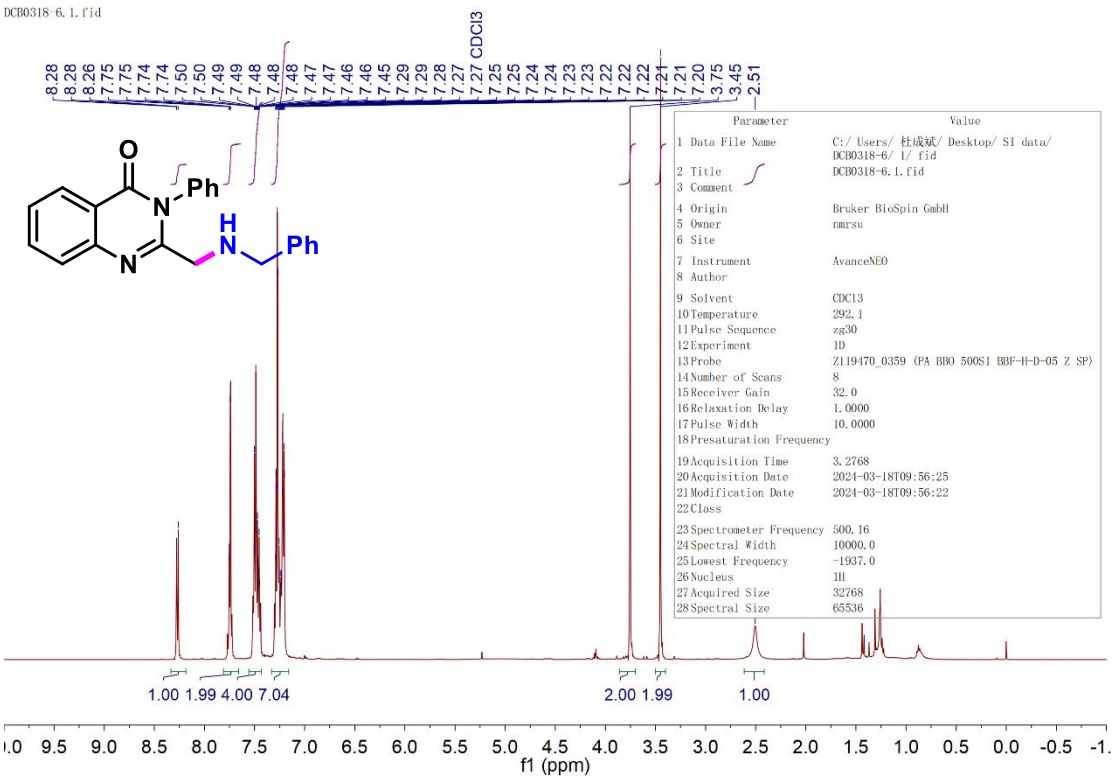
Methylquinazolinone(**1a**) was first oxidized to the aldehyde by selenium dioxide(2 equiv) in dioxane at 75 °C for 10h. After filtration, the solvent was evaporated in vacuo. The desired aldehyde (**6'**) was obtained by silica gel chromatography (eluent hexane: EtOAc = 6:4). Then, the aldehyde (**6'**) was added to 20 mL of ethanol in a 100 mL single-necked flask at room temperature, and primary amine (0.95 equiv) was added, and the mixture was heated to 80° C. and refluxed for 10 h. Cool to room temperature, weigh sodium borohydride (4 equiv) and slowly add it to the reaction system, and heat to 70° C. to react for 8 h. After returning to room temperature, it was quenched with 10% potassium carbonate solution, extracted with dichloromethane, washed with saturated brine, and dried with anhydrous Na_2SO_4. Filter and remove the solvent to obtain a grape-red liquid. The desired product was obtained by silica gel chromatography (eluent hexane: EtOAc = 6:4).

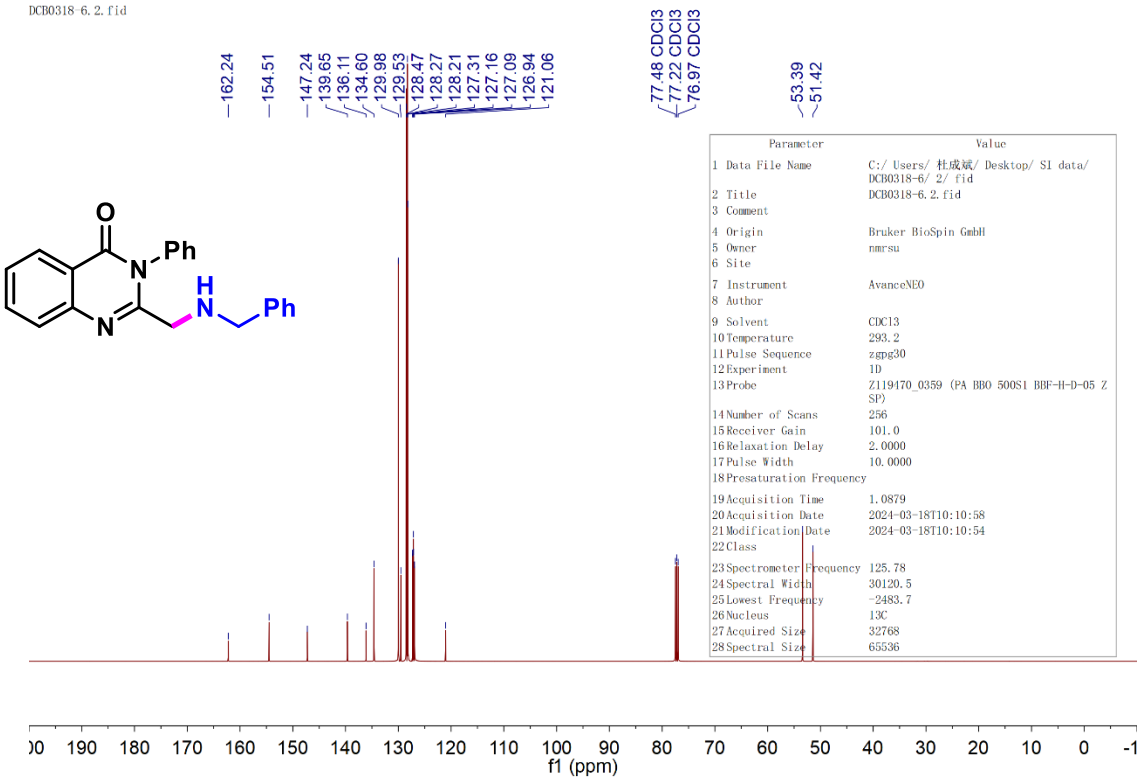
4-oxo-3-phenyl-3,4-dihydroquinazoline-2-carbaldehyde (6'): ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.57 (s, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.89 (t, *J* = 7.7 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.55 (d, *J* = 6.2 Hz, 3H), 7.27 (d, *J* = 2.6 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) 185.3, 161.4, 146.8, 146.3, 135.3, 135.1, 130.0, 129.6, 129.5, 128.9, 127.9, 127.5, 122.5.





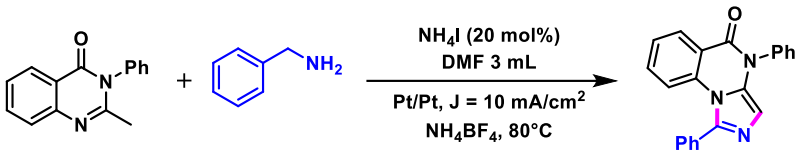
2-((benzylamino)methyl)-3-phenylquinazolin-4(3*H*)-one (6): ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 – 8.19 (m, 1H), 7.75 (dd, *J* = 6.2, 1.6 Hz, 2H), 7.56 – 7.43 (m, 4H), 7.33 – 7.16 (m, 7H), 3.75 (s, 2H), 3.45 (s, 2H), 2.51 (br, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.2, 154.5, 147.2, 139.6, 136.1, 134.6, 129.9, 129.5, 128.5, 128.3, 128.2, 127.3, 127.2, 127.1, 126.9, 121.1, 53.4, 51.4.





Optimization of Reaction Conditions

Table S1: Optimization of the *N*-hetrocycles reaction conditions. [a]



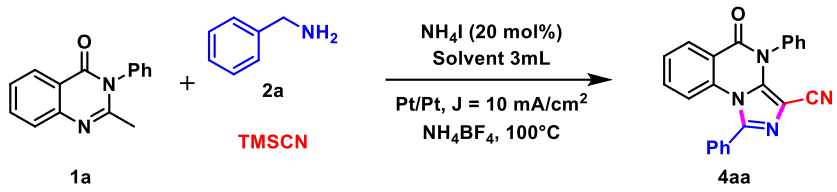
1a **2a** **3aa**

entry	variations from standard conditions	yield [b] (%)
1	none	93
2	no electricity	n. d.
3	DMA, DMSO, NMP instead DMF	32, 17, n. d. [c]
4	TEMPO, NHPI instead of NH_4I	n.d., n.d.
5	nBu_4NI, Me_4NI, KI instead of NH_4I	53, 47, 66
6	30 mol% or 10 mol% NH4I	75, 31
7	a graphite plate as cathode	46
8	a graphite plate as anode	75
9	15 mA, 6.7 h instead of 10 mA, 10 h	88
10	5 mA, 20 h instead of 10 mA, 10 h	79
11	nBu_4NBF_4, NH_4PF_6 or instead of NH_4BF_4	64, 71
12	70°C, 90°C or 100°C instead of 80°C	43, 87, 75

a Standard conditions 1: platinum plate (10 mm × 10 mm × 0.2mm) as the anode, platinum plate (10 mm × 10 mm × 0.2mm) as the cathode, undivided cell, 1a (0.3 mmol), 2a (0.9 mmol), NH_4I (20 mol%), NH_4BF_4 (0.3 mol), DMF (3.0 mL), Air, 80 °C, 10 h. *b* Isolated yields. DMA: N, N-Dimethylacetamide, DMSO: Dimethyl sulfoxide, NMP: N-Methyl pyrrolidone, TEMPO: 2,2,6,6-tetramethylpiperidine-1-oxyl, NHPI: N-hydroxyphthalimide.

c n.d. = not detected.

Table S2: Optimization of the cyanide-functionalization reaction conditions. [a]

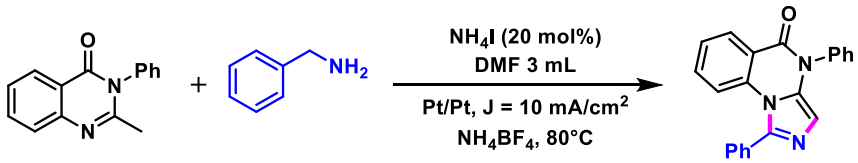


entry	Solvent	Equivalent of NH_4BF_4	Temperature(℃)	Yield (%) [b]
1	DMF	1.0	100	58
2	DMA	1.0	100	70
3	DMSO	1.0	100	43
4	DMA/DMF=2/1	1.0	100	81
5	DMA/DMF=5/1	1.0	100	89
6	DMA/DMF=10/1	1.0	100	87
7	DMA/DMF=5/1	1.0	90	72
8	DMA/DMF=5/1	1.0	110	81
9	DMA/DMF=5/1	0.5	100	82
10	**DMA/DMF=5/1**	**1.5**	**100**	**91**
11	DMA/DMF=5/1	2.0	100	85

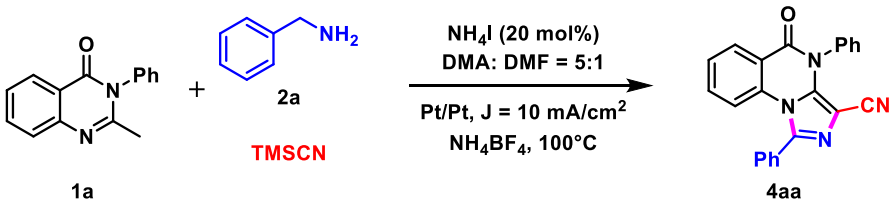
[a] Unless otherwise noted, all reactions were performed with **1a** (0.3 mmol), **2a** (0.9 mmol), NH_4I (0.06 mmol), NH_4BF_4 (0.45 mol), Trimethylsilyl cyanide (0.3 mmol), DMF (3.0 mL). The reaction was carried out at 100°C for 15 h.

[b] Isolated yield.

Experimental Procedure



Typical Procedure 1 for imidazo-fused N-heterocycles: A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one (0.3 mmol), benzylamine (0.9 mmol), ammonium tetrafluoroborate (0.3 mmol) and NH_4I (0.06 mmol) and DMF = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 80°C for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product.



Typical Procedure 2 for cyanide-functionalization imidazo-fused N-heterocycles: A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one (0.3 mmol), benzylamine (0.9 mmol), ammonium

tetrafluoroborate (0.45 mmol), Trimethylsilyl cyanide (0.9 mmol) and NH_4I (0.06 mmol) and DMA:DMF = 2.5:0.5 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 100℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product.

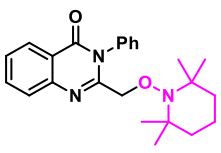
Gram-scale synthesis of 3aa: A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one (5 mmol), benzylamine (15 mmol), ammonium tetrafluoroborate (5 mmol) and NH_4I (1 mmol) and DMF = 60 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed (J = 10 mA/cm^2, I = 23 mA) under 80℃ for 2.5 days. When the reaction was finished, the solution was extracted with EtOAc (3×100 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product.

Gram-scale synthesis of 4aa: A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one (5 mmol), benzylamine (15 mmol), ammonium tetrafluoroborate (7.5 mmol), Trimethylsilyl cyanide (7.5 mmol) and NH_4I (1 mmol) and DMA = 50 mL, DMF = 10 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed (J = 10 mA/cm^2, I = 23 mA) under 100℃ for 2.5 days. When the reaction was finished, the solution was extracted with EtOAc (3×100 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product.

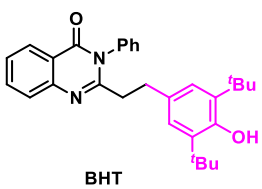
Control Experiments

Scheme 2a: for TEMPO: A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one (0.3 mmol), benzylamine (0.9 mmol), ammonium tetrafluoroborate (0.3 mmol) and NH_4I (0.06 mmol), 2,2,6,6-tetramethylpiperidinooxy(TEMPO, 0.6 mmol) and DMF = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 80℃ for corresponding time. HRMS (ESI) m/z calcd for $C_{22}H_{29}N_3O_2[M+H]^+$ 392.2333, found 392.2324.

Scheme 2a: for BHT: A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one (0.3 mmol), benzylamine (0.9 mmol), ammonium tetrafluoroborate (0.3 mmol) and NH_4I (0.06 mmol), butylated hydroxytoluene (BHT, 0.6 mmol) and DMF = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 80℃ for corresponding time. HRMS (ESI) m/z calcd for $C_{22}H_{29}N_3O_2[M+Na]^+$ 477.2512, found 477.2503.



TEMPO



BHT

Scheme 2b: A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one **(1)** (0.3 mmol), benzylamine

(0.9 mmol), ammonium tetrafluoroborate (0.3 mmol) and iodine (0.03 mmol), and DMF = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 80℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product. The cyanation reaction is carried out according to standard conditions 2.

Scheme 2c: A mixture of 2-(iodomethyl)-3-phenylquinazolin-4(3H)-one (**5**) (0.3 mmol), benzylamine (0.9 mmol), ammonium tetrafluoroborate (0.3 mmol) and NH_4I (0.06 mmol), and DMF = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 80℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product. The cyanation reaction is carried out according to standard conditions 2.

Scheme 2d: A mixture of 2-((benzylamino)methyl)-3-phenylquinazolin-4(3H)-one (**6**) (0.3 mmol), ammonium tetrafluoroborate (0.3 mmol) and NH_4I (0.06 mmol) and DMF = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 80℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product. The cyanation reaction is carried out according to standard conditions 2.

Scheme 2e: 4-oxo-3-phenyl-3,4-dihydroquinazoline-2-carbaldehyde **(6')** (0.3 mmol), benzylamine (0.9 mmol), ammonium tetrafluoroborate (0.3 mmol) and NH_4I (0.06 mmol) and DMF = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 80℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product. The cyanation reaction is carried out according to standard conditions 2.

Scheme 2f: A mixture of A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one (0.3 mmol), benzylamine (0.9 mmol) or Trimethylsilyl cyanide (0.9 mmol), ammonium tetrafluoroborate (0.3 mmol) and NH_4I (0.06 mmol) and DMF: DMA = 2.5: 0.5 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 100℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 3:1) to afford the desired product.

The Proof of Mechanism Experiment.

Constant potential experiment: A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one (0.3 mmol), benzylamine (0.9 mmol), ammonium tetrafluoroborate (0.3 mmol) and NH_4I (0.06 mmol) and DMF = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant potential of 0.9V [the first oxidation potential of iodide ion 0.7V vs. Ag/AgCl (0.199V)] under 80℃ for 75h. And we can get the desired product **3aa** with a yield of 49.7%, which indicated the iodin free radical is the catalyst of the system.

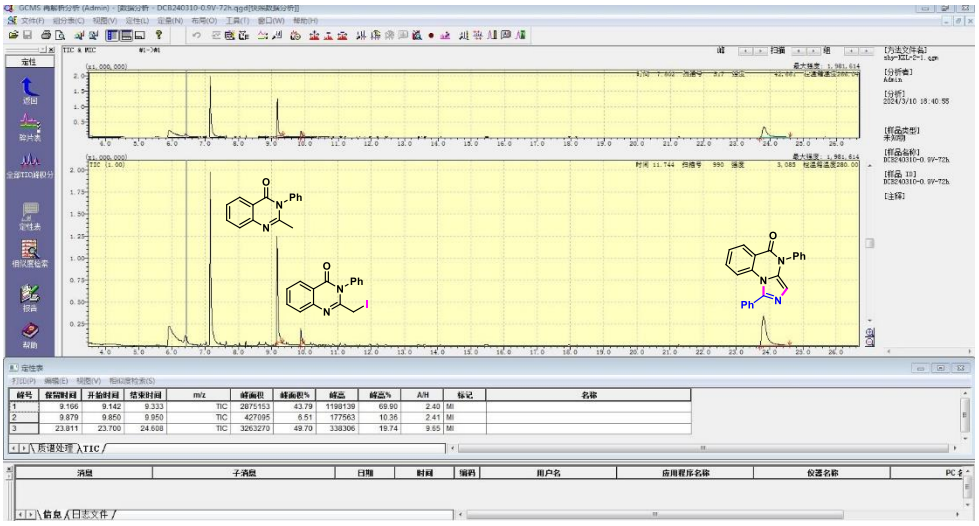


Figure S1. The GC-MS result of constant potential experiment

Nitrogen atmosphere experiment: A mixture of 2-methyl-3-phenylquinazolin-4-(3*H*)-one (0.3 mmol), benzylamine (0.9 mmol), ammonium tetrafluoroborate (0.3 mmol) and NH_4I (0.06 mmol), and DMF = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 80℃. And we can get the desired product **3aa** with a yield of 62.2%, which indicated O_2 is not necessary for the reaction and we think the mechanism of the iodide intermediates is suitable.

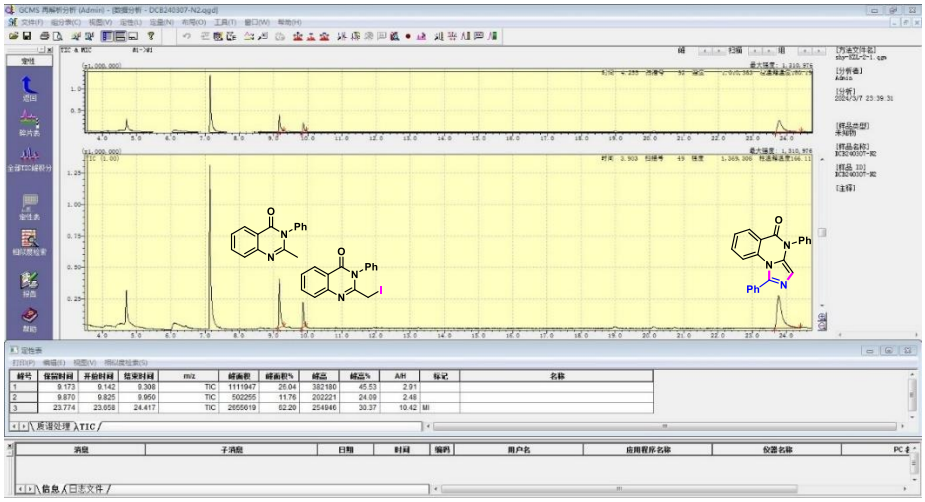


Figure S2. The GC-MS result of nitrogen atmosphere experiment

Cyclic Voltammetry Studies

Cyclic voltammetry data were measured with a Shanghai Chenhua potentiostat (CHI760E).
Working electrode: The working electrode is a 3 mm diameter Pt disk working electrode. Polished with 0.3 μm aluminum oxide and then sonicated in distilled water before drying.
Reference electrode: The reference electrode consisted of a silver wire covered with silver chloride immersed in a saturated solution of potassium chloride.
Counter electrode: The counter electrode is a platinum wire that was polished with sand paper.

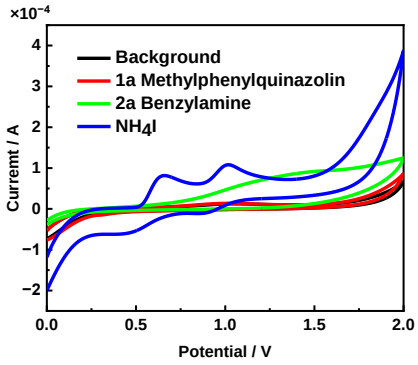


Figure S3. Cyclic voltammograms of **1a** in 0.1 M NH_4BF_4/DMF using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes, at a scan rate of 100 mV/s: background (curve a), 1a (5 mmol/L) (curve b), 2a (15 mmol/L) (curve c), and NH_4I (2 mmol/L) (curve d).

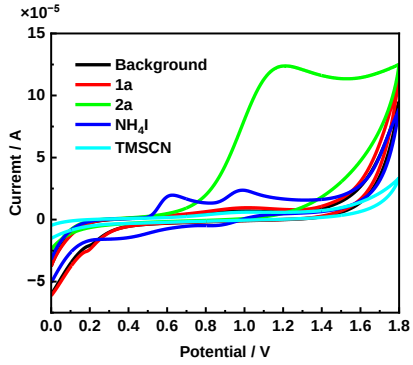


Figure S4. Cyclic voltammograms of **1a** and TMSCN in 0.1 M NH_4BF_4/(DMA+DMF) using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes, at a scan rate of 100 mV/s: background (curve a), **1a** (5 mmol/L) (curve b), **2a** (15 mmol/L) (curve c), NH_4I (2 mmol/L) (curve d), and TMSCN (15 mmol/L) (curve e).

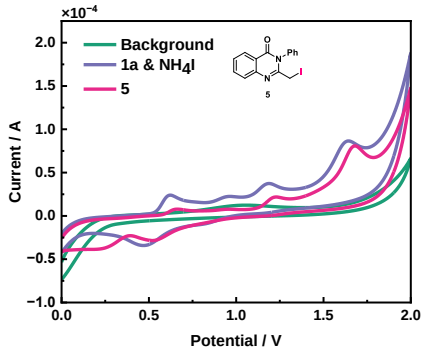


Figure S5. Cyclic voltammograms of **1a** in 0.1 M NH_4BF_4/DMF using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes, at a scan rate of 100 mV/s: background (curve a), **1a**(5 mmol/L) and NH_4I (2

mmol/L) (curve b) and **5** (5 mmol/L) (curve c).

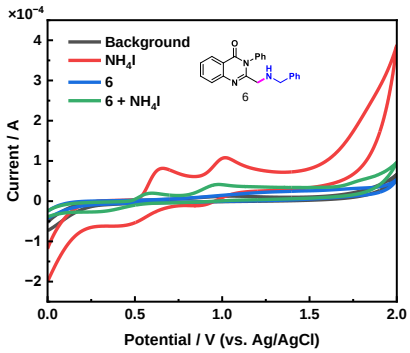
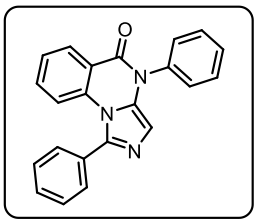


Figure S6. Cyclic voltammograms of **1a** in 0.1 M NH_4BF_4/DMF using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes, at a scan rate of 100 mV/s: background (curve a), NH_4I (2 mmol/L) (curve b) and **6** (5 mmol/L) (curve c) and the mixture of 6 and NH_4I (curve d).

Figure S3 and **Figure S4** showed that no obvious oxidation wave of 2-methyl-3-phenylquinazolin-4-(3H)-one **1a** was observed (curve b in Fig. **S3**, curve b in Fig. **S4**). This result was perhaps due to the inertness of the C(sp^3)–H bond, and CV results indicated that the iodide anion should be oxidized first compared to benzylamine, and the following transformation can be initiated from this oxidized iodide ion, which should be the intermediate of this reaction.When **1a** was mixed with NH_4I, the results showed multiple new oxidation peak signals appeared, which indicated that iodine species could activate **1a** under electrochemical conditions. It coincided with the curve of iodinate **5**, which implied that compound **5** was a possible intermediate in the reaction. (Fig. **S5**) And no obvious oxidation wave of 6, which indicted iodide anion was important for the next stage to get the desired products. (Fig. **S6**)

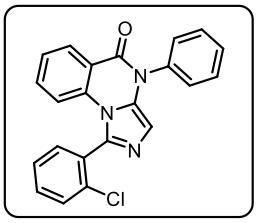
Detail Descriptions for Products

1,4-diphenylimidazo[1,5-a]quinazolin-5(4H)-one (3aa)[S6]



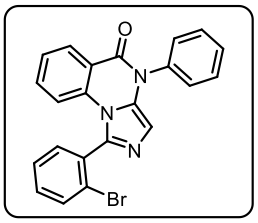
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 93% yield, 94.1 mg. m.p. 216 - 217℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.7 Hz, 1H), 7.72-7.45 (m, 10H), 7.39 (dt, *J* = 22.5, 6.9 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 1H), 6.29 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.8, 140.0, 136.3, 135.8, 134.0, 133.8, 132.6, 130.2, 130.0, 129.8, 129.6, 129.4, 129.0, 128.0, 125.9, 118.1, 116.6, 109.8. HRMS (ESI) m/z calcd for $C_{22}H_{15}N_3O$ $[M+H]^+$ 338.1288, found 338.1294.

1-(2-chlorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ab)



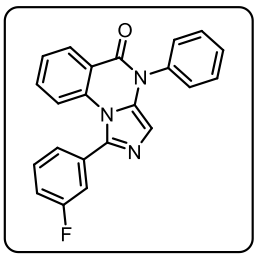
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 85% yield, 94.8 mg. m.p. 225 - 226℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.42 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.68 – 7.38 (m, 11H), 7.01 (d, *J* = 8.3 Hz, 1H), 6.35 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.7, 136.6, 136.2, 135.7, 135.3, 134.3, 133.7, 132.5, 132.2, 131.6, 130.2, 130.1, 129.5, 128.0, 127.7, 126.1, 117.9, 115.2, 109.9. HRMS (ESI) m/z calcd for $C_{22}H_{14}ClN_3O$ $[M+H]^+$ 372.0898, found 372.0904.

1-(2-bromophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ac)



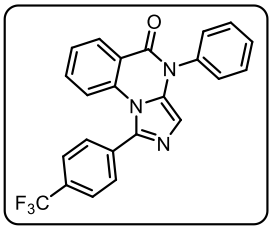
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 84% yield, 104.9mg. m.p. 238 - 239℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 (d, *J* = 7.7 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.65 – 7.38 (m, 10H), 6.97 (d, *J* = 8.3 Hz, 1H), 6.35 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.7, 137.8, 136.2, 135.6, 134.4, 134.3, 133.5, 133.2, 132.6, 131.8, 130.2, 130.1, 129.5, 128.2, 128.0, 126.1, 125.3, 117.8, 115.3, 109.7. HRMS (ESI) m/z calcd for $C_{22}H_{14}BrN_3O$ $[M+H]^+$ 415.0320, found 410.0327.

1-(3-fluorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ad)



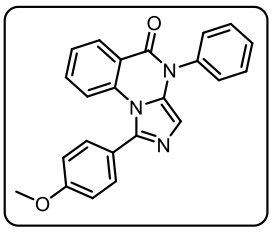
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 92% yield, 98.1 mg. m.p. 220 - 221℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.42 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 2H), 7.57 – 7.47 (m, 5H), 7.43 (d, *J* = 7.3 Hz, 2H), 7.37 (dt, *J* = 9.2, 2.0 Hz, 1H), 7.32 (d, *J* = 8.3 Hz, 1H), 7.24 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.30 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$):δ 162.8 (d, *J* = 248.5 Hz), 157.7, 138.6, 138.6, 136.1, 135.5, 134.4 (d, *J* = 8.2 Hz), 134.3, 133.9, 130.7 (d, *J* = 8.4 Hz), 130.4, 130.0 (d, *J* = 116.8 Hz), 127.9, 126.2, 125.4 (d, *J* = 3.1 Hz), 118.2, 116.9 (d, *J* = 8.5 Hz), 116.8 (d, *J* = 10.1 Hz), 116.5, 110.0. ^{19}F NMR (470 MHz, $CDCl_3$) δ -111.2. HRMS (ESI) m/z calcd for $C_{22}H_{14}FN_3O$ $[M+H]^+$ 356.1194, found 356.1201.

4-phenyl-1-(4-(trifluoromethyl)phenyl)imidazo[1,5-a]quinazolin-5(4H)-one (3ae)



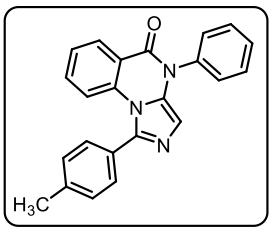
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 85% yield, 103.3 mg. m.p. 170 - 171°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.42 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.79 (s, 4H), 7.63 – 7.48 (m, 6H), 7.45 – 7.40 (m, 1H), 7.34 – 7.28 (m, 1H), 6.33 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$):δ 157.7, 138.5, 136.0, 135.4, 134.6, 133.9, 131.5 (q, *J* = 33.0 Hz), 130.5, 130.2, 129.9, 129.5, 129.4, 128.7, 127.9, 127.5, 126.4, 126.0 (q, *J* = 3.7 Hz), 122.8 (q, *J* = 272.4 Hz) 118.3, 116.5, 110.5. ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.7. HRMS (ESI) m/z calcd for $C_{23}H_{14}F_3N_3O$ $[M+H]^+$ 406.1162, found 406.1168.

1-(4-methoxyphenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3af)



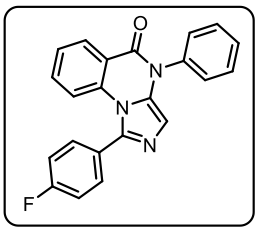
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 98% yield, 108.0 mg. m.p. 243 - 244°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.39 (d, *J* = 7.9 Hz, 1H), 7.67 – 7.29 (m, 10H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.27 (s, 1H), 3.91 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.7, 157.7, 140.0, 136.3, 135.9, 133.8, 131.1, 130.2, 130.1, 129.4, 127.9, 125.9, 124.7, 118.2, 116.5, 114.5, 109.4, 55.4. HRMS (ESI) m/z calcd for $C_{23}H_{17}N_3O_2$ $[M+H]^+$ 368.1394, found 368.1401.

4-phenyl-1-(p-tolyl)imidazo[1,5-a]quinazolin-5(4H)-one (3ag)



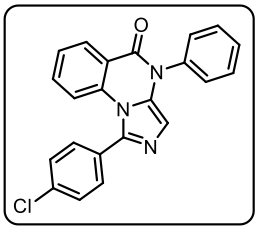
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 96% yield, 101.2 mg. m.p. 238 - 239°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.39 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 2H), 7.55-7.48 (m, 5H), 7.44-7.31 (m, 5H), 6.26 (s, 1H), 2.47 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.8, 140.2, 139.9, 136.2, 135.9, 133.9, 133.8, 130.2, 130.1, 129.8, 129.6, 129.5, 129.4, 128.0, 125.9, 118.1, 116.6, 109.6, 21.6. HRMS (ESI) m/z calcd for $C_{23}H_{17}N_3O$ $[M+H]^+$ 352.1444, found 352.1450.

1-(4-fluorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ah)



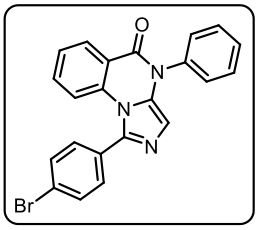
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 93% yield, 99.1 mg. m.p. 221 - 222°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.66 – 7.40 (m, 9H), 7.29 – 7.19 (m, 3H), 6.28 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 1163.5 (d, *J* = 250.4 Hz), 157.7, 138.9, 135.9 (d, *J* = 57.0 Hz), 134.1, 133.9, 131.7 (d, *J* = 8.4 Hz), 130.4, 130.1, 129.5, 128.7, 127.9, 126.1, 118.2, 116.4 (d, *J* = 2.3 Hz), 116.2, 109.8. ^{19}F NMR (470 MHz, $CDCl_3$) δ -110.3. HRMS (ESI) m/z calcd for $C_{22}H_{14}FN_3O$ $[M+H]^+$ 356.1194, found 356.1201.

1-(4-chlorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ai)



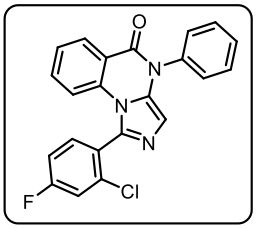
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 92% yield, 102.6 mg. m.p. 225 - 226℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.62 – 7.56 (m, 4H), 7.56 – 7.46 (m, 6H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 6.29 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.7, 138.8, 136.1, 135.9, 135.6, 134.3, 133.9, 130.9, 130.4, 130.1, 129.6, 129.5, 129.4, 127.9, 126.2, 118.2, 116.5, 110.0. HRMS (ESI) m/z calcd for $C_{22}H_{14}ClN_3O$ $[M+H]^+$ 372.0898, found 372.0904.

1-(4-bromophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3aj)



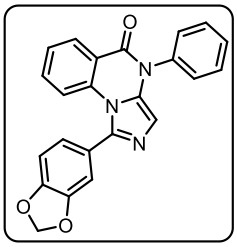
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 90% yield, 112.4 mg. m.p. 246 - 247℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 (d, *J* = 7.8 Hz, 1H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.60 (t, *J* = 7.6 Hz, 2H), 7.52 (dq, *J* = 16.0, 7.5 Hz, 6H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 6.29 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.7, 138.8, 136.1, 135.6, 134.3, 133.9, 132.3, 131.4, 131.2, 130.5, 130.1, 129.5, 127.9, 126.2, 124.2, 118.2, 116.5, 110.0. HRMS (ESI) m/z calcd for $C_{22}H_{14}BrN_3O$ $[M+H]^+$ 416.0393, found 416.0399.

1-(2-chloro-4-fluorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ak)



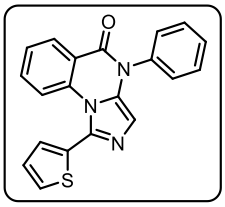
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 87% yield, 104.1 mg. m.p. 232 - 234℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.42 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.61 (q, *J* = 8.1 Hz, 3H), 7.55 – 7.48 (m, 4H), 7.46 – 7.42 (m, 1H), 7.36 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.27 (td, *J* = 9.6, 2.2 Hz, 2H), 6.35 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.4 (d, *J* = 253.5 Hz), 157.6, 137.3 (d, *J* = 9.8 Hz), 136.1, 135.6, 134.5, 134.2, 132.8 (d, *J* = 2.9 Hz), 132.8, 130.3, 130.1, 129.5, 127.9, 126.3, 125.6, 125.6, 119.8 (d, *J* = 15.3 Hz), 118.1, 117.1 (d, *J* = 24.4 Hz), 115.2, 110.6. ^{19}F NMR (470 MHz, $CDCl_3$) δ -109.4. HRMS (ESI) m/z calcd for $C_{22}H_{13}ClFN_3O$ $[M+H]^+$ 390.0804, found 390.0810.

1-(benzo[d][1,3]dioxol-5-yl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3al)



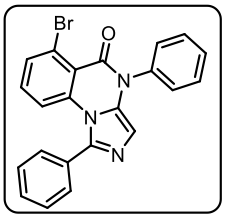
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 87% yield, 99.5 mg. m.p. 238 - 239℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.39 (d, *J* = 7.9 Hz, 1H), 7.67 – 7.32 (m, 8H), 7.20 – 6.87 (m, 3H), 6.25 (s, 1H), 6.08 (s, 2H).^{13}C NMR (125 MHz, $CDCl_3$): δ 157.7, 148.9, 148.1, 139.6, 136.2, 135.8, 133.8, 130.3, 130.1, 129.4, 128.0, 125.9, 123.9, 118.2, 116.6, 110.0, 109.5, 108.9, 101.6. HRMS (ESI) m/z calcd for $C_{23}H_{15}N_3O_3$ $[M+H]^+$ 382.1186, found 382.1194.

4-phenyl-1-(thiophen-2-yl)imidazo[1,5-a]quinazolin-5(4H)-one (3am)



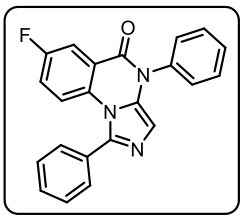
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 83% yield, 85.5 mg. m.p. 221 - 223℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.40 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.62 – 7.56 (m, 3H), 7.55 – 7.47 (m, 4H), 7.44 – 7.33 (m, 3H), 7.20 (dd, *J* = 5.2, 3.5 Hz, 1H), 6.31 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.7, 136.1, 135.7, 134.4, 134.1, 132.8, 132.6, 130.2, 130.1, 130.1, 129.5, 128.8, 127.9, 127.6, 126.2, 118.1, 116.2, 110.3. HRMS (ESI) m/z calcd for $C_{20}H_{13}N_3OS$ $[M+H]^+$ 344.0852, found 344.0858.

6-bromo-1,4-diphenylimidazo[1,5-a]quinazolin-5(4H)-one (3ba)



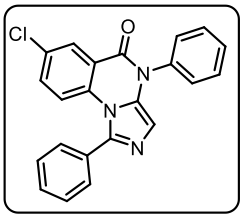
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 94% yield, 117.4 mg. m.p. 242 - 244℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 6.6 Hz, 4H), 7.55 – 7.47 (m, 6H), 7.42 – 7.32 (m, 2H), 7.18 (t, *J* = 8.2 Hz, 1H), 6.23 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.2, 140.2, 138.0, 136.2, 133.6, 133.6, 133.2, 132.4, 130.1, 129.8, 129.4, 129.4, 129.1, 128.1, 125.4, 116.8, 116.0, 109.3. HRMS (ESI) m/z calcd for $C_{22}H_{14}BrN_3O$ $[M+H]^+$ 416.0393, found 416.0399.

7-fluoro-1,4-diphenylimidazo[1,5-a]quinazolin-5(4H)-one (3ca)



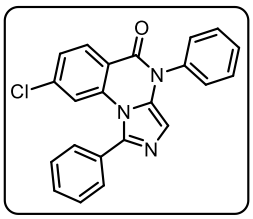
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 89% yield, 94.9 mg. m.p. 222 - 223℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.06 (d, *J* = 8.3 Hz, 1H), 7.66 – 7.43 (m, 10H), 7.28 (d, *J* = 14.3 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 6.30 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9 (d, *J* = 248.3 Hz), 156.8, 139.8, 135.9, 133.7, 132.3, 130.1, 129.9, 129.6, 129.6, 129.2, 127.8, 121.3 (d, *J* = 23.6 Hz), 120.2, 120.2, 118.7 (d, *J* = 7.4 Hz), 116.1 (d, *J* = 24.5 Hz), 109.9. HRMS (ESI) m/z calcd for $C_{22}H_{14}FN_3O$ $[M+H]^+$ 356.1194, found 356.1189.

7-chloro-1,4-diphenylimidazo[1,5-a]quinazolin-5(4H)-one (3da)



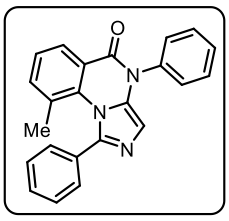
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 86% yield, 95.9 mg. m.p. 226 - 227℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.32 (s, 1H), 7.64 – 7.47 (m, 10H), 7.39 – 7.35 (m, 1H), 7.21 (d, *J* = 8.9 Hz, 1H), 6.28 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.7, 140.0, 135.9, 134.2, 133.8, 133.7, 132.1, 131.8, 130.2, 130.1, 129.7, 129.6, 129.6, 129.2, 127.8, 119.6, 118.2, 110.0. HRMS (ESI) m/z calcd for $C_{22}H_{14}ClN_3O$ $[M+H]^+$ 372.0898, found 372.0895.

8-chloro-1,4-diphenylimidazo[1,5-a]quinazolin-5(4H)-one (3ea)



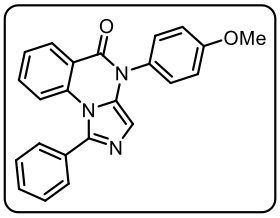
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 84% yield, 93.1 mg. m.p. 210 - 212°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.31 (d, *J* = 8.4 Hz, 1H), 7.63 – 7.53 (m, 8H), 7.51 – 7.48 (m, 2H), 7.34 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.23 (d, *J* = 1.9 Hz, 1H), 6.28 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.1, 140.2, 136.4, 135.9, 134.0, 131.9, 131.6, 130.2, 130.2, 130.0, 129.6, 129.3, 127.9, 126.4, 116.9, 116.6, 115.5, 110.0. HRMS (ESI) m/z calcd for $C_{22}H_{14}ClN_3O$ $[M+H]^+$ 372.0898, found 372.0902.

9-methyl-1,4-diphenylimidazo[1,5-a]quinazolin-5(4H)-one (3fa)



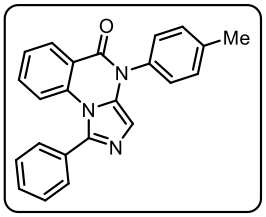
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 75% yield, 79.1 mg. m.p. 203 - 205°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.19 (d, *J* = 2.2 Hz, 1H), 7.66 – 7.57 (m, 4H), 7.52 (dt, *J* = 10.7, 7.3 Hz, 6H), 7.25 – 7.15 (m, 2H), 6.28 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.9, 139.8, 136.4, 136.0, 134.6, 133.9, 133.6, 132.6, 130.0, 130.0, 129.6, 129.6, 129.3, 128.9, 128.0, 117.9, 116.5, 109.7, 20.8.. HRMS (ESI) m/z calcd for $C_{23}H_{17}N_3O$ $[M+H]^+$ 352.1444, found 352.1450.

4-(4-methoxyphenyl)-1-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ga)



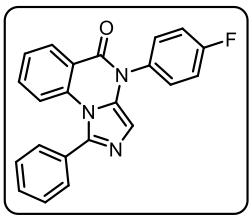
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 96% yield, 105.8 mg. m.p. 233 - 234°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.39 (dd, *J* = 7.6, 1.9 Hz, 1H), 7.65 – 7.60 (m, 2H), 7.53 (h, *J* = 6.4, 5.5 Hz, 3H), 7.44 – 7.37 (m, 4H), 7.28 (d, *J* = 10.2 Hz, 1H), 7.09 (d, *J* = 8.6 Hz, 2H), 6.30 (s, 1H), 3.89 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.0 158.0, 140.0, 135.7, 134.3, 133.7, 132.5, 130.2, 129.8, 129.6, 129.0, 129.0, 128.7, 125.9, 118.2, 116.6, 115.3, 109.7, 55.6. HRMS (ESI) m/z calcd for $C_{23}H_{17}N_3O_3$ $[M+H]^+$ 368.1394, found 368.1400.

1-phenyl-4-(p-tolyl)imidazo[1,5-a]quinazolin-5(4H)-one (3ha)



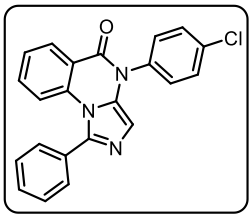
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 90% yield, 94.9 mg. m.p. 243 - 244°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.39 (dd, *J* = 7.7, 1.9 Hz, 1H), 7.68 – 7.59 (m, 2H), 7.52 (tt, *J* = 6.3, 3.1 Hz, 3H), 7.44 – 7.33 (m, 6H), 7.28 (d, *J* = 8.4 Hz, 1H), 6.30 (s, 1H), 2.46 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.8, 139.9, 139.4, 135.8, 134.2, 133.7, 133.6, 132.6, 130.7, 130.3, 129.8, 129.6, 129.0, 127.6, 125.9, 118.2, 116.6, 109.8, 21.4. HRMS (ESI) m/z calcd for $C_{23}H_{17}N_3O$ $[M+H]^+$ 352.1444, found 352.1448.

4-(4-fluorophenyl)-1-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ia)



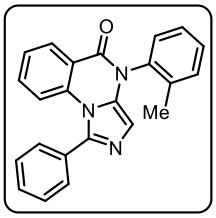
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 92% yield, 98.1 mg. m.p. 216 - 217°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.39 (dd, *J* = 7.7, 1.9 Hz, 1H), 7.67 – 7.60 (m, 2H), 7.59 – 7.47 (m, 5H), 7.47 – 7.38 (m, 2H), 7.33 – 7.27 (m, 3H), 6.29 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.5 (d, *J* = 250.4 Hz), 162.6, 157.7, 138.9, 135.9 (d, *J* = 57.0 Hz), 134.1, 133.9, 131.71 (d, *J* = 8.4 Hz), 130.4, 130.1, 129.5, 128.7, 127.9, 126.1, 118.2, 116.4 (d, *J* = 2.3 Hz), 116.2, 109.7. ^{19}F NMR (470 MHz, $CDCl_3$) δ -111.2. HRMS (ESI) m/z calcd for $C_{22}H_{14}FN_3O$ $[M+H]^+$ 356.1194, found 356.1201.

4-(4-chlorophenyl)-1-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ja)



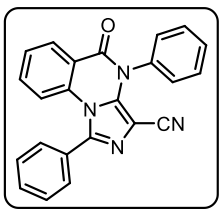
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 89% yield, 99.3 mg. m.p. 226 - 227°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.37 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.64 – 7.59 (m, 2H), 7.59 – 7.52 (m, 5H), 7.47 – 7.39 (m, 4H), 7.28 (d, *J* = 8.1 Hz, 1H), 6.30 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 140.3, 135.8, 135.3, 134.6, 134.0, 133.6, 132.4, 130.4, 130.3, 129.9, 129.6, 129.4, 129.1, 126.1, 117.9, 116.7, 109.7. HRMS (ESI) m/z calcd for $C_{22}H_{14}ClN_3O$ $[M+H]^+$ 372.0898, found 372.0904.

1-phenyl-4-(o-tolyl)imidazo[1,5-a]quinazolin-5(4H)-one (3ka)



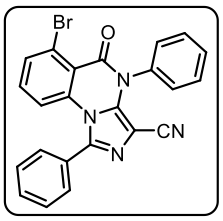
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a white solid. 81% yield, 85.4 mg. m.p. 206 - 208°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 (d, *J* = 7.6 Hz, 1H), 7.65 (dd, *J* = 6.6, 2.8 Hz, 2H), 7.56 – 7.50 (m, 3H), 7.46 – 7.36 (m, 6H), 7.32 (d, *J* = 8.3 Hz, 1H), 6.16 (s, 1H), 2.25 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.3, 140.1, 136.2, 135.9, 135.1, 133.8, 133.4, 132.6, 131.7, 130.3, 129.8, 129.8, 129.7, 129.0, 128.2, 127.7, 125.9, 118.0, 116.6, 109.6, 17.5. HRMS (ESI) m/z calcd for $C_{23}H_{17}N_3O$ $[M+H]^+$ 352.1444, found 352.1449.

5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4aa)



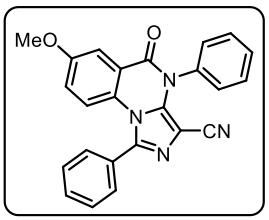
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 91% yield, 98.9 mg. m.p. 275 - 277°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.46 – 8.37 (m, 1H), 7.68 – 7.55 (m, 8H), 7.53 – 7.46 (m, 4H), 7.27 (d, *J* = 6.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.8, 141.0, 138.9, 135.0, 134.5, 134.4, 131.0, 130.9, 130.8, 130.5, 130.4, 129.6, 129.4, 128.9, 127.3, 117.9, 117.0, 112.4, 95.6. HRMS (ESI) m/z calcd for $C_{23}H_{14}N_4O$ $[M+H]^+$ 363.1240, found 362.1246.

6-bromo-5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ba)



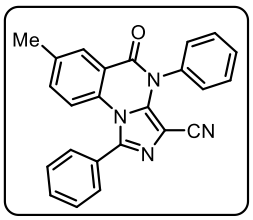
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 80% yield, 105.9 mg. m.p. 282 - 284°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.81 – 7.77 (m, 1H), 7.65 (h, *J* = 2.7 Hz, 3H), 7.62 – 7.53 (m, 5H), 7.50 – 7.47 (m, 2H), 7.35 – 7.32 (m, 1H), 7.28 – 7.24 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.1, 141.1, 138.5, 137.2, 134.8, 134.3, 133.7, 131.0, 130.8, 130.3, 129.4, 129.4, 128.9, 127.7, 125.8, 117.1, 115.9, 112.2, 95.2. HRMS (ESI) m/z calcd for $C_{23}H_{13}BrN_4O$ $[M+H]^+$ 441.0346, found 441.0352.

7-methoxy-5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ca)



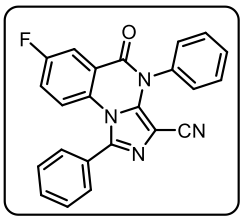
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 91% yield, 107.1 mg. m.p. 284 - 286°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.80 (d, *J* = 3.1 Hz, 1H), 7.68 – 7.45 (m, 10H), 7.18 (d, *J* = 9.3 Hz, 1H), 7.04 (dd, *J* = 9.3, 3.1 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.2, 157.8, 140.5, 138.4, 134.5, 131.0, 130.8, 130.8, 130.3, 129.6, 129.3, 128.9, 128.8, 122.6, 119.1, 118.6, 112.6, 111.6, 95.4, 77.4, 77.1, 76.9, 56.0. HRMS (ESI) m/z calcd for $C_{24}H_{16}N_4O_2$ $[M+H]^+$ 393.1346, found 393.1352.

7-methyl-5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4da)



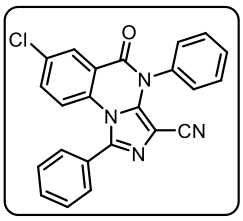
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 84% yield, 94.8 mg. m.p. 284 - 285°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.18 (s, 1H), 7.66 – 7.59 (m, 5H), 7.56 (d, *J* = 7.2 Hz, 2H), 7.48 (dd, *J* = 6.3, 3.1 Hz, 2H), 7.30 (q, *J* = 11.3, 9.5 Hz, 2H), 7.14 (d, *J* = 8.7 Hz, 1H), 2.43 (s, 3H).; ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.9, 140.8, 138.8, 137.7, 135.5, 134.5, 132.8, 130.9, 130.7, 130.3, 130.1, 129.6, 129.3, 128.9, 127.8, 117.6, 116.9, 112.60, 95.5, 20.9. HRMS (ESI) m/z calcd for $C_{24}H_{16}N_4O$ $[M+H]^+$ 377.1397, found 377.1403.

7-fluoro-5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ea)



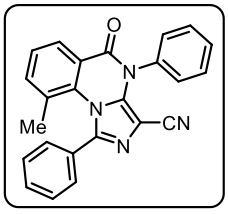
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 94% yield, 107.3 mg. m.p. 287 - 289°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.07 (dd, *J* = 8.0, 3.0 Hz, 1H), 7.70 – 7.56 (m, 8H), 7.49 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.27 – 7.16 (m, 2H).^{13}C NMR (125 MHz, $CDCl_3$):δ 160.5 (d, *J* = 251.0 Hz), 156.9, 156.9, 140.7, 138.4, 134.2, 131.4 (d, *J* = 2.7 Hz), 131.1, 131.0, 130.6, 130.4, 129.6, 129.5, 128.8, 122.2 (d, *J* = 23.8 Hz), 120.0 (d, *J* = 7.9 Hz), 119.3 (d, *J* = 7.6 Hz), 116.3 (d, *J* = 24.6 Hz), 112.2, 95.9. ^{19}F NMR (470 MHz, $CDCl_3$) δ -111.3. HRMS (ESI) m/z calcd for $C_{23}H_{13}FN_4O$ $[M+H]^+$ 381.1146, found 381.1152.

7-chloro-5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4fa)



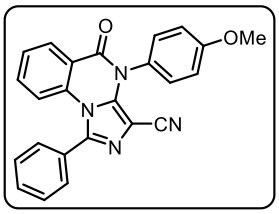
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 92% yield, 109.5 mg. m.p. 282 - 284℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.36 (d, *J* = 2.6 Hz, 1H), 7.68 – 7.54 (m, 8H), 7.50 – 7.42 (m, 3H), 7.20 (d, *J* = 9.1 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.8, 140.9, 138.5, 134.6, 134.2, 133.4, 133.4, 131.2, 131.0, 130.5, 130.4, 129.9, 129.6, 129.5, 128.8, 119.3, 118.5, 112.2, 96.0. HRMS (ESI) m/z calcd for $C_{23}H_{13}ClN_4O$ $[M+H]^+$ 397.0851, found 397.0856.

9-methyl-5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ga)



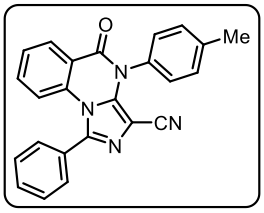
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 73% yield, 82.4 mg. m.p. 251 - 252℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.24 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.64 – 7.60 (m, 3H), 7.51 – 7.41 (m, 8H), 7.33 (dd, *J* = 9.0, 3.4 Hz, 1H), 1.73 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.4, 143.3, 139.7, 138.1, 134.2, 131.7, 130.8, 130.1, 129.9, 129.2, 129.0, 128.9, 128.3, 127.8, 127.7, 126.7, 121.1, 112.6, 96.1, 21.1. HRMS (ESI) m/z calcd for $C_{24}H_{16}N_4O$ $[M+H]^+$ 377.1397, found 377.1403.

4-(4-methoxyphenyl)-5-oxo-1-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ha)



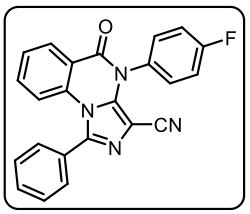
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 94% yield, 110.3 mg. m.p. 295 - 297℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.42 (dd, *J* = 6.4, 3.3 Hz, 1H), 7.74 – 7.44 (m, 8H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 3.90 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.3, 158.1, 140.9, 139.4, 135.0, 134.4, 130.9, 130.7, 130.5, 129.9, 129.6, 129.3, 127.2, 126.9, 117.9, 116.9, 115.5, 112.6, 95.7, 55.6. HRMS (ESI) m/z calcd for $C_{24}H_{16}N_4O_2$ $[M+H]^+$ 393.1346, found 393.1352.

5-oxo-1-phenyl-4-(p-tolyl)-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ia)



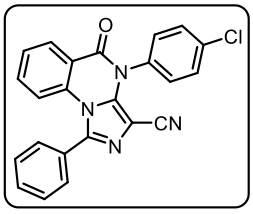
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 93% yield, 105.0 mg. m.p. 302 - 303℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.47 – 8.38 (m, 1H), 7.67 – 7.54 (m, 5H), 7.52 – 7.43 (m, 4H), 7.39 – 7.35 (m, 2H), 7.30 – 7.27 (m, 1H), 2.50 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): ^{1} δ 157.9, 141.3, 140.9, 139.0, 134.9, 134.4, 131.7, 130.9, 130.9, 130.8, 130.5, 129.6, 129.3, 128.5, 127.2, 117.9, 116.9, 112.6, 95.6, 21.5. HRMS (ESI) m/z calcd for $C_{24}H_{16}N_4O$ $[M+H]^+$ 377.1397, found 377.1403.

4-(4-fluorophenyl)-5-oxo-1-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ja)



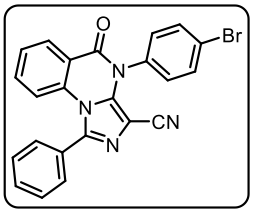
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 89% yield, 101.7 mg. m.p. 283 - 284℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.43 – 8.38 (m, 1H), 7.66 – 7.56 (m, 5H), 7.53 – 7.46 (m, 4H), 7.36 – 7.31 (m, 2H), 7.28 (td, *J* = 3.3, 2.7, 1.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.8 (d, *J* = 251.6 Hz), 157.9, 141.2, 138.9, 135.0, 134.7, 131.0, 130.9 (d, *J* = 7.1 Hz), 130.8, 130.4, 130.2 (d, *J* = 3.2 Hz), 129.5 (d, *J* = 25.7 Hz), 127.4, 117.7, 117.6, 117.4, 117.0, 112.5, 95.6. HRMS (ESI) m/z calcd for $C_{23}H_{13}FN_3O$ $[M+H]^+$ 381.1146, found 381.1152.

4-(4-chlorophenyl)-5-oxo-1-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ka)



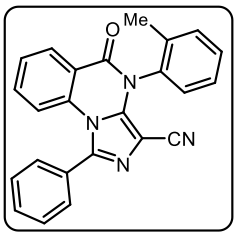
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 87% yield, 103.6 mg. m.p. 269 - 271℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.46 – 8.38 (m, 1H), 7.65 – 7.56 (m, 7H), 7.54 – 7.49 (m, 2H), 7.46 – 7.42 (m, 2H), 7.31 – 7.27 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.7, 141.1, 138.5, 137.1, 135.0, 134.7, 1327, 130.9, 130.8, 130.6, 130.5, 130.3, 129.6, 129.4, 127.4, 117.7, 117.0, 112.5, 95.6. HRMS (ESI) m/z calcd for $C_{23}H_{13}ClN_4O$ $[M+H]^+$ 397.0851, found 397.0857.

4-(4-bromophenyl)-5-oxo-1-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4la)



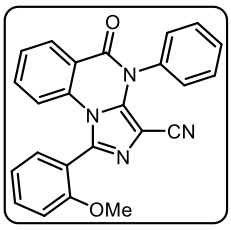
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 88% yield, 116.5 mg. m.p. 275 - 276℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.40 – 8.30 (m, 1H), 7.62 – 7.47 (m, 7H), 7.44 (p, *J* = 6.0 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.21 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$):δ 156.7, 140.1, 137.5, 136.1, 133.9, 133.6, 131.6, 129.8, 129.7, 129.6, 129.4, 129.3, 128.5, 128.3, 126.4, 116.6, 115.9, 111.5, 94.6. HRMS (ESI) m/z calcd for $C_{23}H_{13}BrN_4O$ $[M+H]^+$ 441.0346, found 441.0352.

5-oxo-1-phenyl-4-(o-tolyl)-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ma)



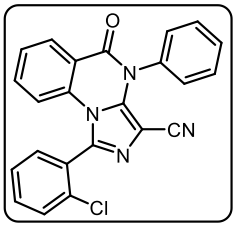
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 82% yield, 92.6 mg. m.p. 261 - 262℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.47 – 8.36 (m, 1H), 7.65 – 7.43 (m, 10H), 7.36 (dd, *J* = 17.2, 7.7 Hz, 2H), 2.27 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.3, 141.1, 138.4, 137.0, 135.1, 134.6, 133.4, 131.7, 131.3, 130.8, 130.5, 129.6, 129.3, 128.9, 128.9, 128.3, 127.9, 127.8, 127.3, 117.7, 116.9, 112.2, 95.4, 17.4. HRMS (ESI) m/z calcd for $C_{24}H_{16}N_4O$ $[M+H]^+$ 377.1397, found 377.1403.

1-(2-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ab)



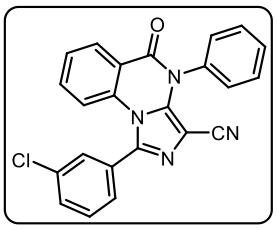
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 81% yield, 95.4 mg. m.p. 261 - 262℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.40 (dd, *J* = 7.1, 2.3 Hz, 1H), 7.69 – 7.43 (m, 9H), 7.26 – 7.23 (m, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 7.04 (d, *J* = 8.3 Hz, 1H), 3.66 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.9, 138.6, 138.4, 135.5, 134.5, 134.5, 132.7, 131.8, 130.9, 130.3, 129.9, 127.1, 121.5, 120.8, 120.4, 117.5, 115.9, 112.6, 111.2, 110.5, 95.6, 55.5. HRMS (ESI) m/z calcd for $C_{24}H_{16}N_4O_2$ $[M+H]^+$ 393.1346, found 393.1352.

1-(2-chlorophenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ac)



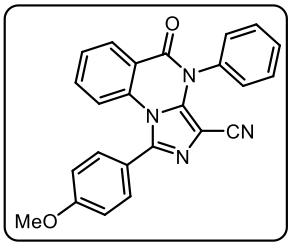
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 95% yield, 113.1 mg. m.p. 274 - 275℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 – 8.39 (m, 1H), 7.69 – 7.47 (m, 11H), 7.07 – 7.00 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.7, 138.6, 137.7, 135.1, 135.0, 134.9, 134.4, 132.4, 132.3, 131.0, 130.7, 130.4, 130.3, 130.2, 129.1, 127.9, 127.4, 117.6, 115.5, 112.3, 95.8. HRMS (ESI) m/z calcd for $C_{23}H_{13}ClN_4O$ $[M+H]^+$ 397.0851, found 397.0857.

1-(3-chlorophenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ad)



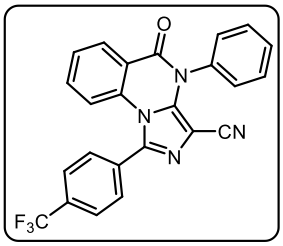
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 92% yield, 109.5 mg. m.p. 261 - 262℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.45 – 8.37 (m, 1H), 7.68 – 7.59 (m, 6H), 7.56 (dd, *J* = 8.5, 6.3 Hz, 2H), 7.49 (dd, *J* = 5.9, 3.3 Hz, 3H), 7.31 – 7.26 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.8, 141.0, 138.9, 135.0, 134.5, 134.4, 131.0, 130.9, 130.8, 130.4, 130.3, 129.6, 129.3, 128.9, 127.8, 127.6, 127.3, 117.9, 117.0, 112.5, 95.6.HRMS (ESI) m/z calcd for $C_{23}H_{13}ClN_4O$ $[M+H]^+$ 397.0851, found 397.0857.

1-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ae)



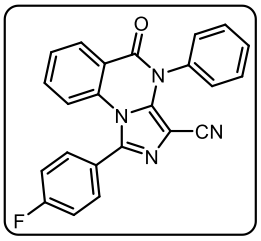
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 89% yield, 104.8 mg. m.p. 262 - 264℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.65 (h, *J* = 2.1 Hz, 3H), 7.57 – 7.42 (m, 6H), 7.34 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.14 – 7.04 (m, 2H), 3.92 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.4, 157.8, 141.0, 138.8, 135.2, 134.5, 134.5, 131.1, 130.9, 130.4, 130.3, 128.9, 127.2, 122.9, 117.9, 116.9, 114.7, 112.5, 95.4, 55.5. HRMS (ESI) m/z calcd for $C_{24}H_{16}N_4O_2$ $[M+H]^+$ 393.1346, found 393.1352.

5-oxo-4-phenyl-1-(4-(trifluoromethyl)phenyl)-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4af)



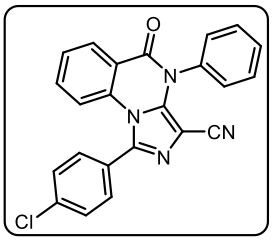
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 87% yield, 112.3 mg. m.p. 258 - 259℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.44 (dd, *J* = 7.5, 2.1 Hz, 1H), 7.87 – 7.78 (m, 4H), 7.66 (dt, *J* = 4.5, 2.7 Hz, 3H), 7.58 – 7.47 (m, 4H), 7.28 (d, *J* = 1.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$):δ 157.7, 138.4, 136.0, 135.4, 134.6, 133.9, 131.5 (q, *J* = 33.0 Hz), 130.5, 130.2, 129.9, 129.5, 128.7, 127.9, 127.1, 126.0 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 272.4 Hz), 118.3, 116.5, 110.4. ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.8. HRMS (ESI) m/z calcd for $C_{24}H_{13}F_3N_4O$ $[M+H]^+$ 431.1114, found 431.1116.

1-(4-fluorophenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ag)



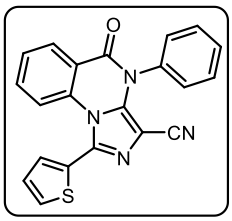
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 85% yield, 97.0 mg. m.p. 256 - 258℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.42 (dd, *J* = 7.3, 2.2 Hz, 1H), 7.63 (ddd, *J* = 13.9, 5.8, 2.4 Hz, 5H), 7.56 – 7.47 (m, 4H), 7.29 – 7.25 (m, 3H).; ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.0 (d, *J* = 252.3 Hz), 157.7, 139.9, 138.9, 134.9, 134.6, 134.4, 131.8 (d, *J* = 8.6 Hz), 131.0, 130.6, 130.3, 128.9, 127.4, 127.0 (d, *J* = 3.6 Hz), 117.9, 116.7 (d, *J* = 1.6 Hz), 116.6, 112.3, 95.7. ^{19}F NMR (470 MHz, $CDCl_3$) δ -108.2. HRMS (ESI) m/z calcd for $C_{23}H_{13}FN_4O$ $[M+H]^+$ 381.1146, found 381.1152.

1-(4-chlorophenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ah)



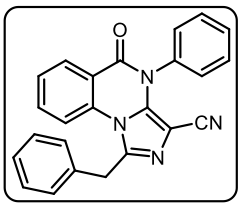
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 87% yield, 103.6 mg. m.p. 303 - 304℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.43 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.66 (p, *J* = 3.6, 3.1 Hz, 3H), 7.59 – 7.47 (m, 8H), 7.30 (dd, *J* = 8.2, 1.3 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.7, 139.8, 139.0, 137.1, 134.8, 134.6, 134.3, 131.1, 130.9, 130.6, 130.4, 129.7, 129.3, 128.9, 127.5, 117.9, 116.8, 112.3, 95.9. HRMS (ESI) m/z calcd for $C_{23}H_{13}ClN_4O$ $[M+H]^+$ 397.0851, found 397.0857.

5-oxo-4-phenyl-1-(thiophen-2-yl)-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ai)



The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 85% yield, 94.0 mg. m.p. 265 - 267℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.44 (d, *J* = 7.9 Hz, 1H), 7.68 (t, *J* = 3.9 Hz, 3H), 7.65 – 7.40 (m, 6H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.27 (d, *J* = 4.2 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.8, 139.1, 134.9, 134.8, 134.3, 134.0, 131.1, 131.1, 130.5, 130.4, 130.4, 129.9, 128.9, 127.9, 127.5, 117.8, 116.6, 112.2, 96.0. HRMS (ESI) m/z calcd for $C_{21}H_{12}N_4OS$ $[M+H]^+$ 368.0732, found 368.0738.

1-benzyl-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4aj)



The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 3:1) to give the product as a light yellow solid. 75% yield, 84.7 mg. m.p. 273 - 275℃. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.43 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.83 (d, *J* = 8.6 Hz, 1H), 7.72 – 7.43 (m, 7H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.30 – 7.23 (m, 2H), 7.21 (s, 1H), 4.63 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.6, 140.2, 138.9, 135.0, 134.7, 134.7, 134.5, 130.9, 130.5, 130.3, 129.3, 128.9, 128.0, 127.5, 127.1, 117.7, 116.5, 112.5, 94.7, 37.4. HRMS (ESI) m/z calcd for $C_{24}H_{16}N_4O$ $[M+H]^+$ 377.1397, found 377.1403.

Supporting Reference

[S1] Priyanka Singh, Navpreet Kaur, and Prabal Banerjee. *J. Org. Chem.* **2020**, *85*, 3393–3406.

[S2] Chiranjeevi Bingi, Kaushik Yadav Kola, Ashok Kala, Jagadeesh Babu Nanubolu, Krishnaiah Atmakur. *Tetrahedron Letters*, **2017**, *58*, 1071–1074.

[S3] Wen Zhu Bi, Chen Qu, Xiao Lan Chen, Sheng Kai Wei, Ling Bo Qu, Shu Yun Liu, Kai Sun, Yu Fen Zhao. Tetrahedron, **2018**, *74*, 1908e1917

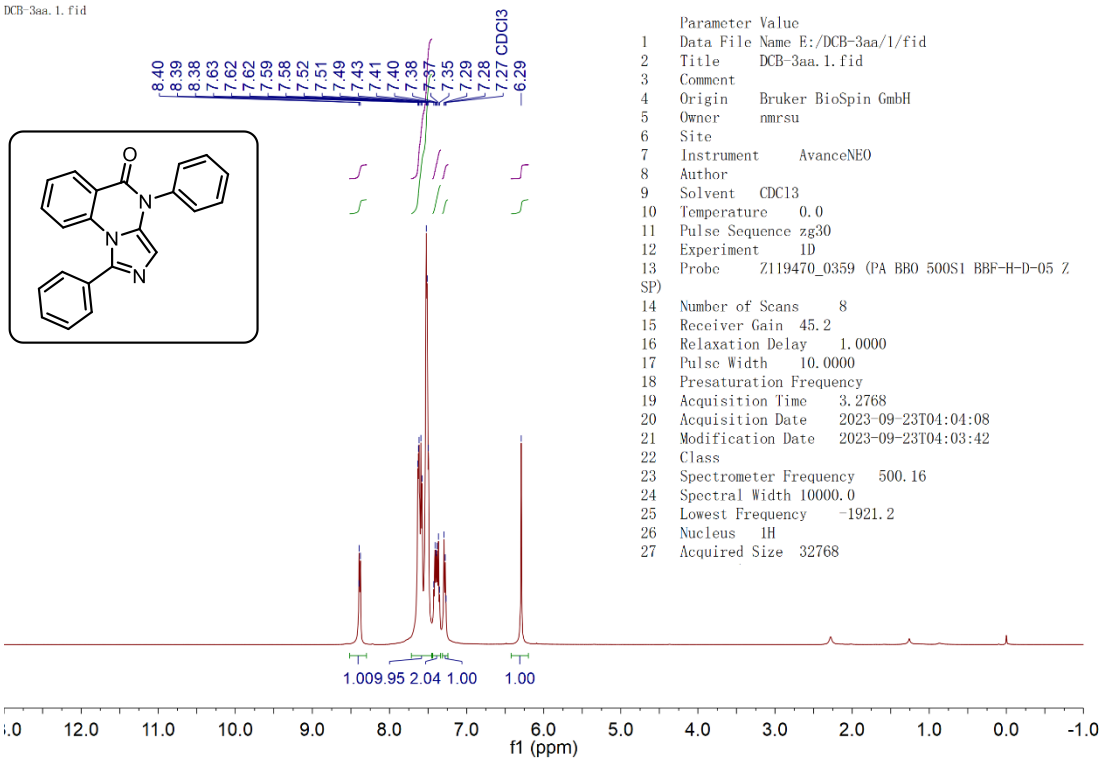
[S4] Yang Yang, Haobing Wang and Haiyan Ma. *Chem. Asian J.* **2017**, *12*, 239 –247.

[S5] Céline Valant, Emeline Maillet, Jean-Jacques Bourguignon, Bernard Bucher, Valérie Utard, Jean-Luc Galzi, and Marcel Hibert. *Journal of Medicinal Chemistry.* **2009,** *52*,, 5999-6011.

[S6] K. Donthiboina, H. K. Namballa, S. P. Shaik, J. B. Nanubolu, N. Shankaraiah and A. Kamal. *Org. Biomol. Chem.*, 2018, **16**, 1720-1727.

Copies of Product NMR Spectra

1,4-diphenylimidazo[1,5-a]quinazolin-5(4H)-one (3aa)



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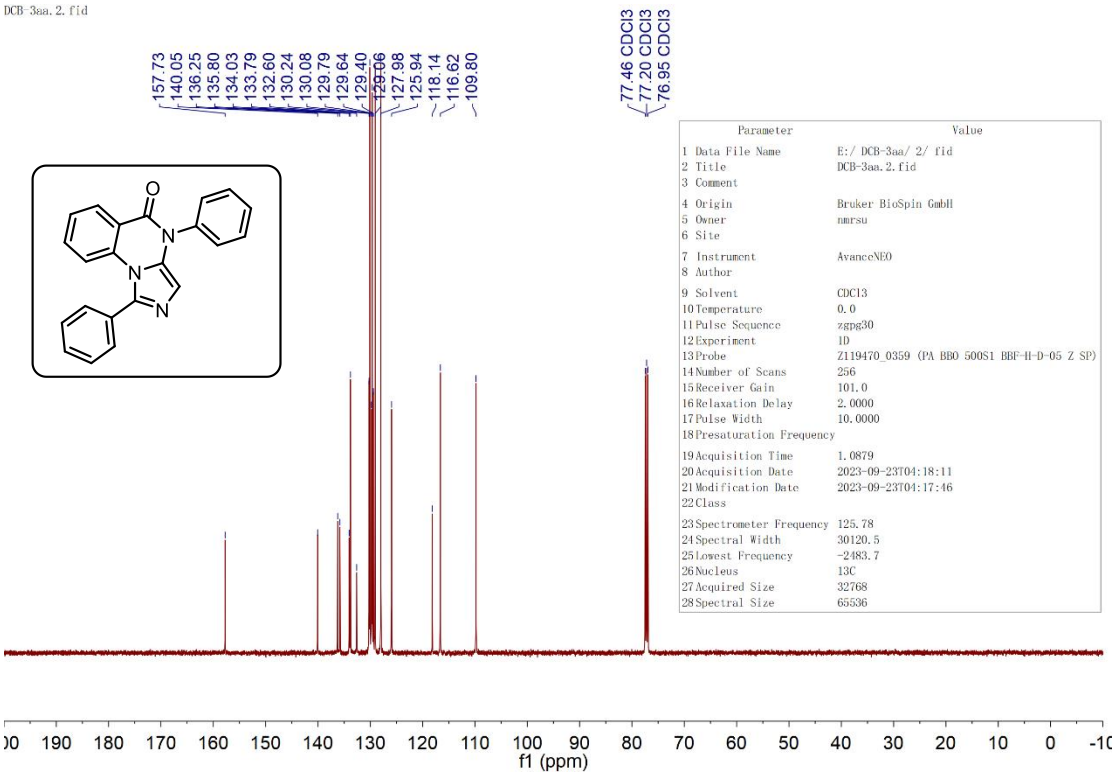
26	Nucleus	1H
27	Acquired Size	32768



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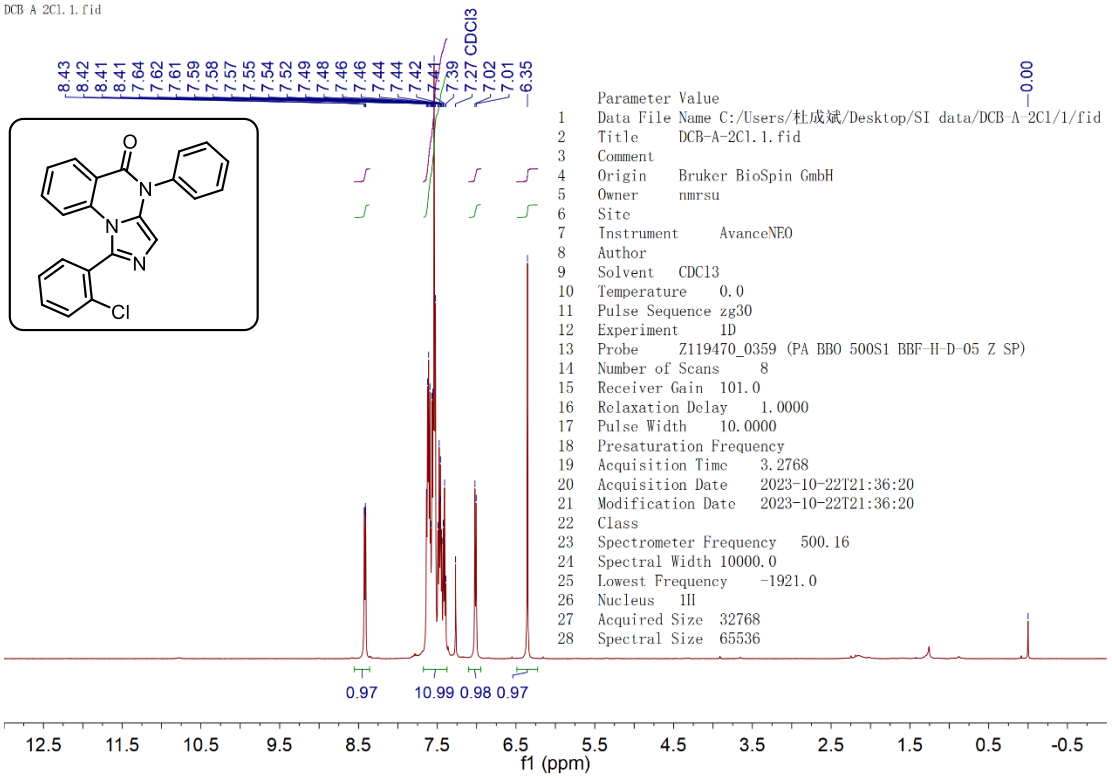
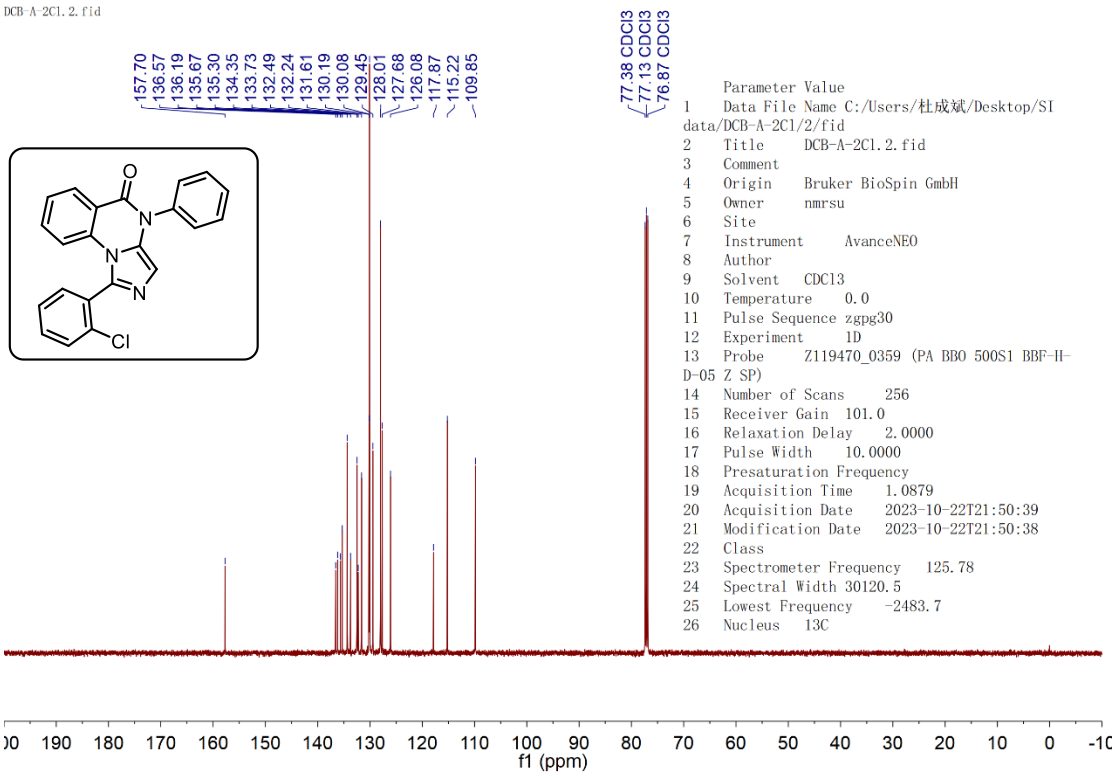
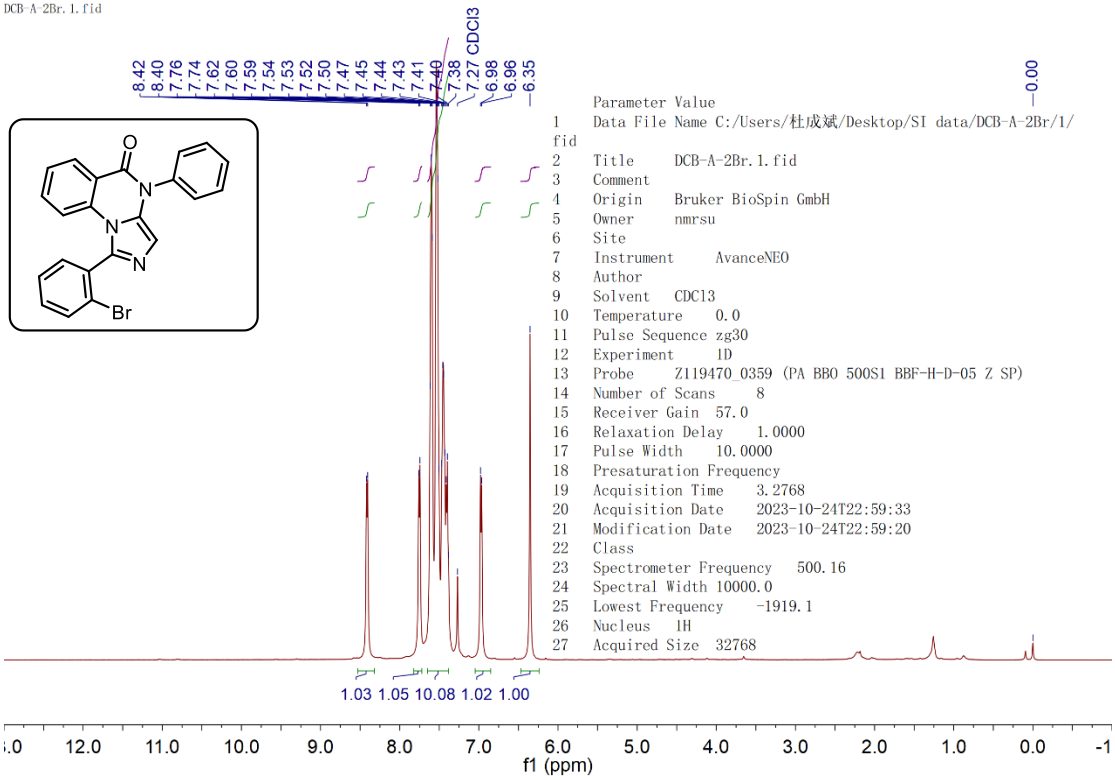
1	Data File Name	E:/ DCB-3aa/ 2/ fid
2	Title	DCB-3aa.2.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	256
15	Receiver Gain	101.0
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.0879
20	Acquisition Date	2023-09-23T04:18:11
21	Modification Date	2023-09-23T04:17:46
22	Class	
23	Spectrometer Frequency	125.78
24	Spectral Width	30120.5
25	Lowest Frequency	-2483.7
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

1-(2-chlorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ab)



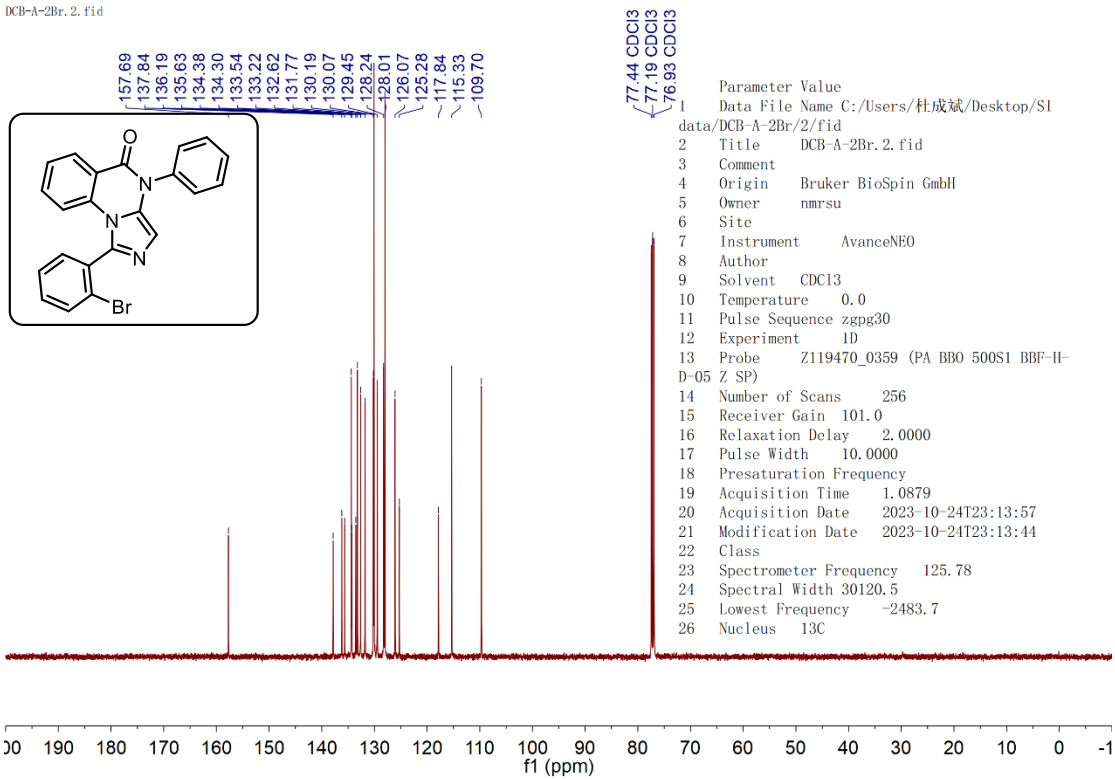


1-(2-bromophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ac)



Parameter Value

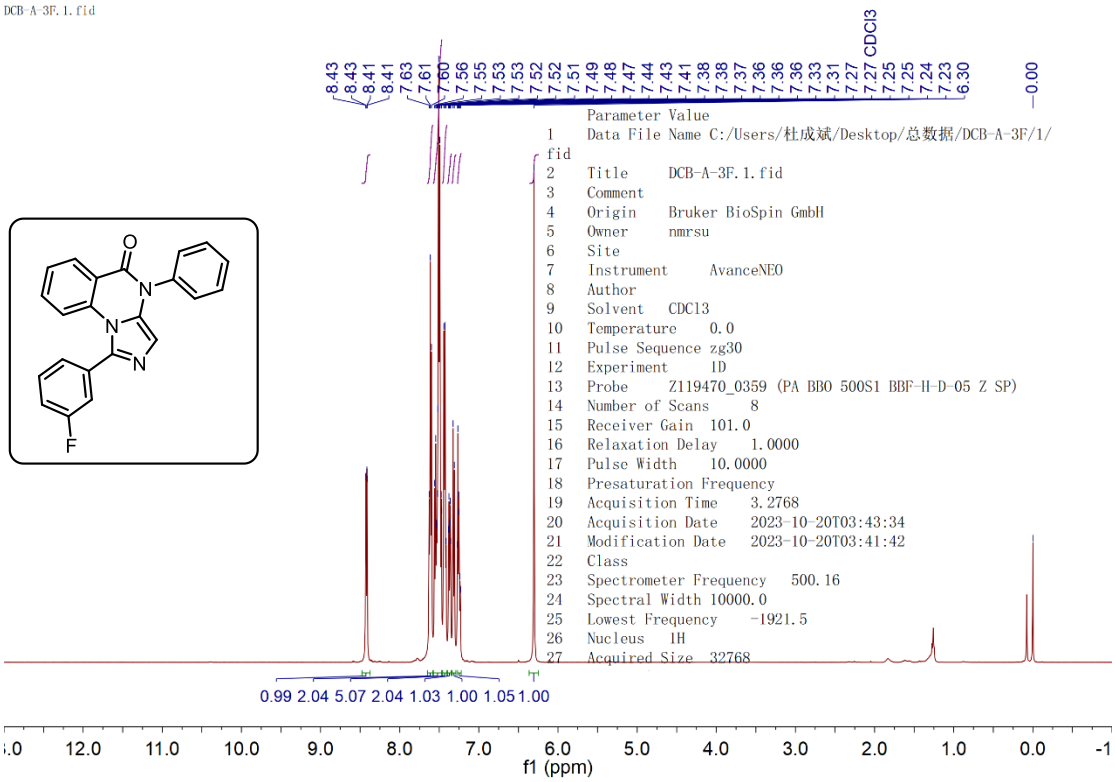
1	Data File Name	C:/Users/杜成斌/Desktop/SI data/DCB-A-2Br/1/fid
2	Title	DCB-A-2Br.1.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	8
15	Receiver Gain	57.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.2768
20	Acquisition Date	2023-10-24T22:59:33
21	Modification Date	2023-10-24T22:59:20
22	Class	
23	Spectrometer Frequency	500.16
24	Spectral Width	10000.0
25	Lowest Frequency	-1919.1
26	Nucleus	1H
27	Acquired Size	32768

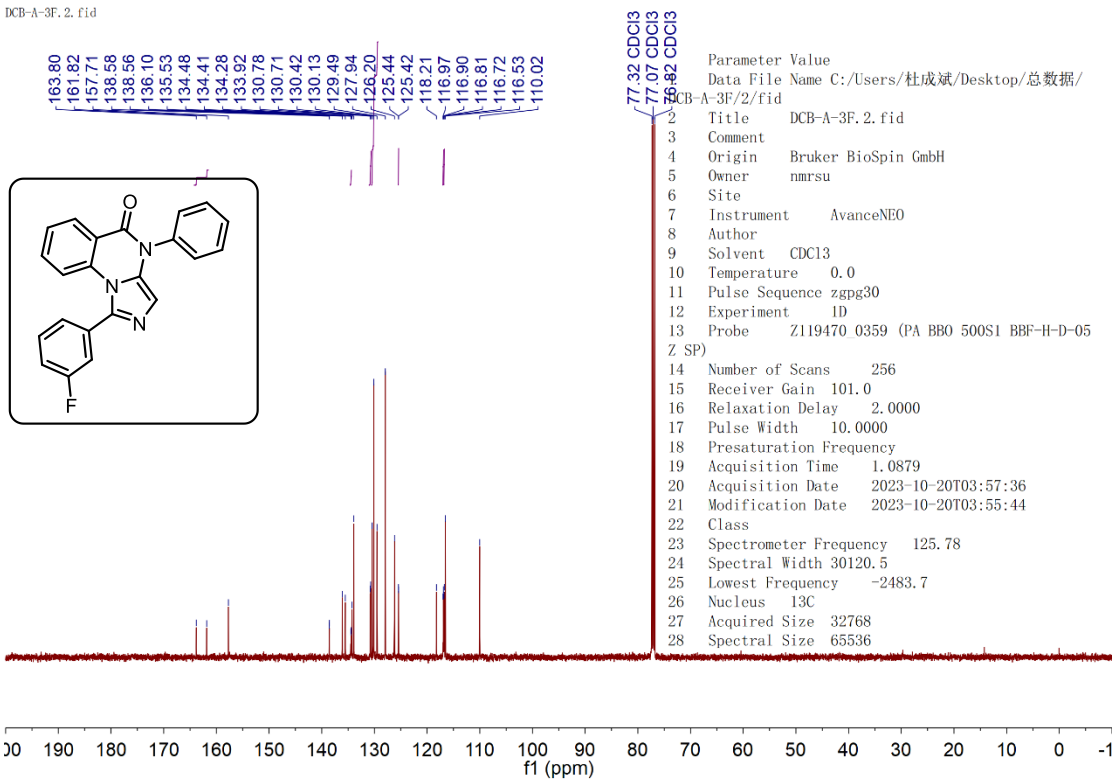


Parameter Value

1	Data File Name	C:/Users/杜成斌/Desktop/SI data/DCB-A-2Br/2/fid
2	Title	DCB-A-2Br.2.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	256
15	Receiver Gain	101.0
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.0879
20	Acquisition Date	2023-10-24T23:13:57
21	Modification Date	2023-10-24T23:13:44
22	Class	
23	Spectrometer Frequency	125.78
24	Spectral Width	30120.5
25	Lowest Frequency	-2483.7
26	Nucleus	13C

1-(3-fluorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ad)





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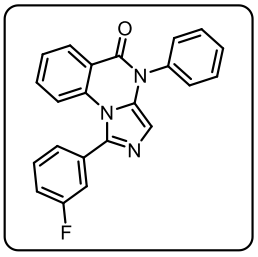
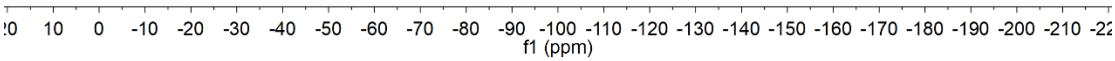
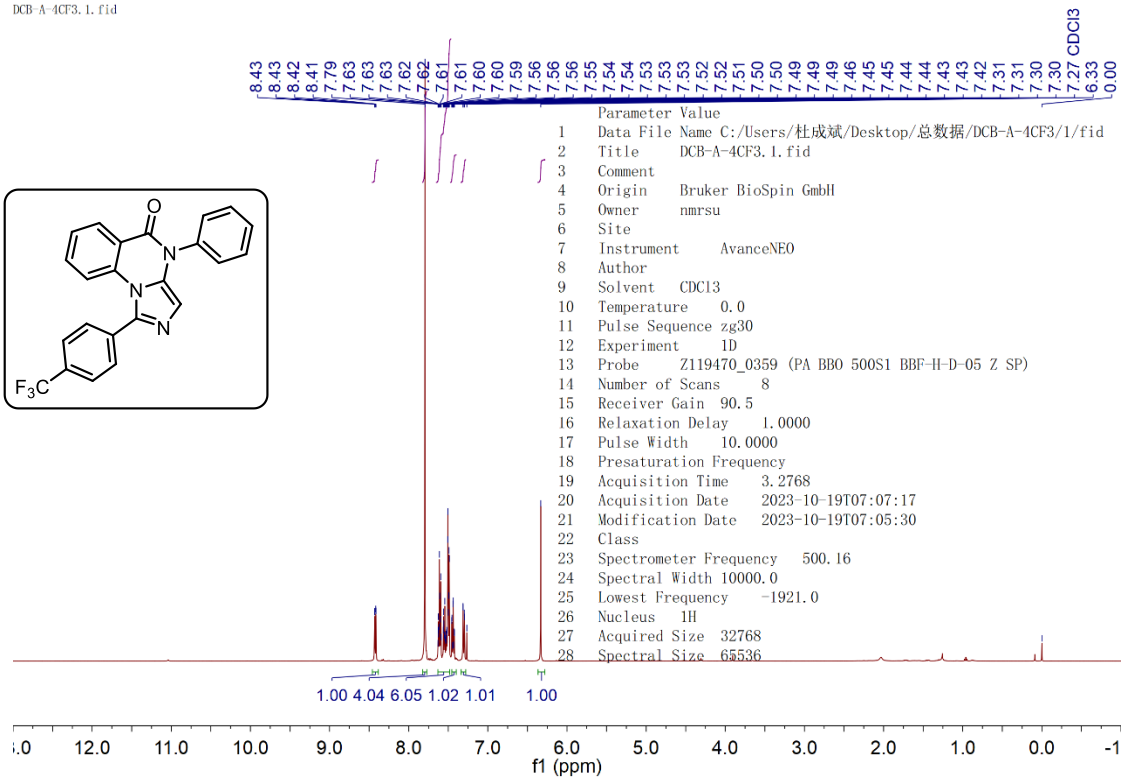


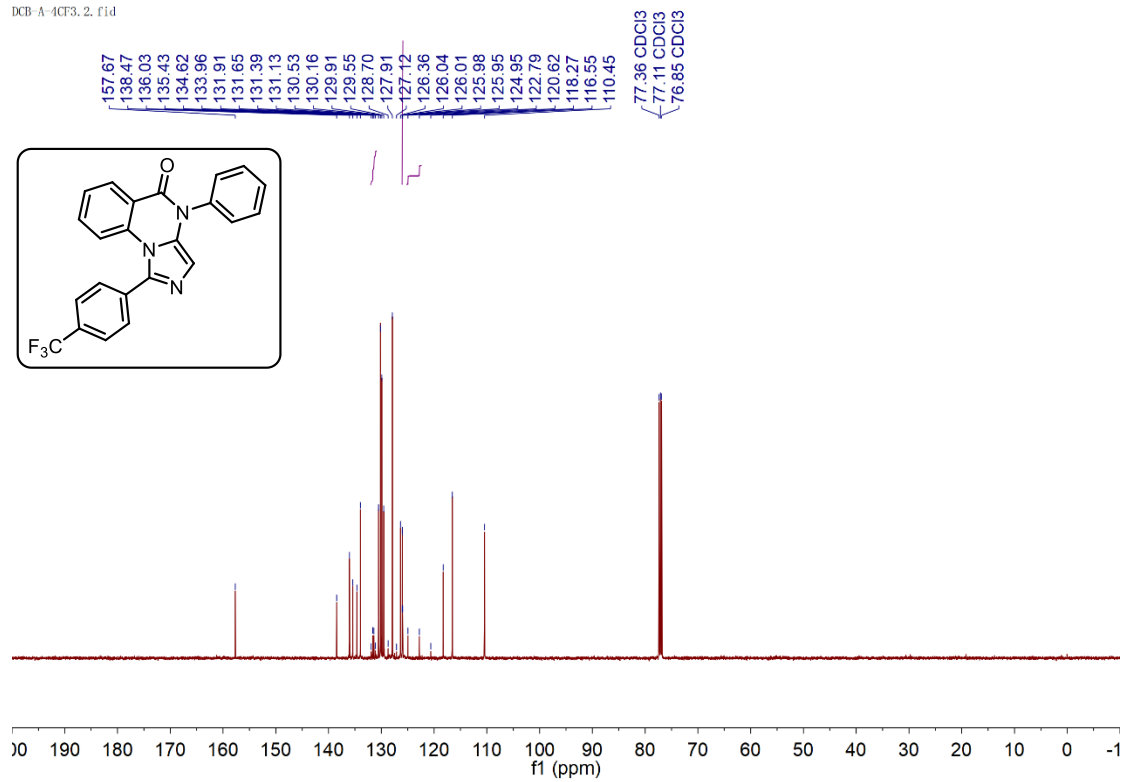
-111.23

	Parameter	Value
1	Data File Name	C:/Users/杜成斌/Desktop/总数据/DCB-A-3F/3/fid
2	Title	DCB-A-3F.3.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	0.0
11	Pulse Sequence	zgig
12	Experiment	1D
13	Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	16
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	15.0000
18	Presaturation Frequency	
19	Acquisition Time	0.5767
20	Acquisition Date	2023-10-20T03:59:14
21	Modification Date	2023-10-20T03:57:22
22	Class	
23	Spectrometer Frequency	470.57
24	Spectral Width	113636.4
25	Lowest Frequency	-103880.2
26	Nucleus	19F
27	Acquired Size	65536
28	Spectral Size	131072



4-phenyl-1-(4-(trifluoromethyl)phenyl)imidazo[1,5-a]quinazolin-5(4H)-one (3ae)





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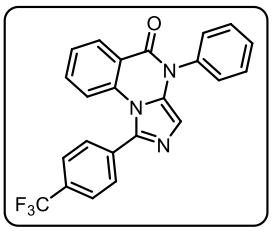
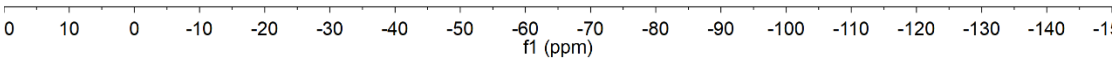
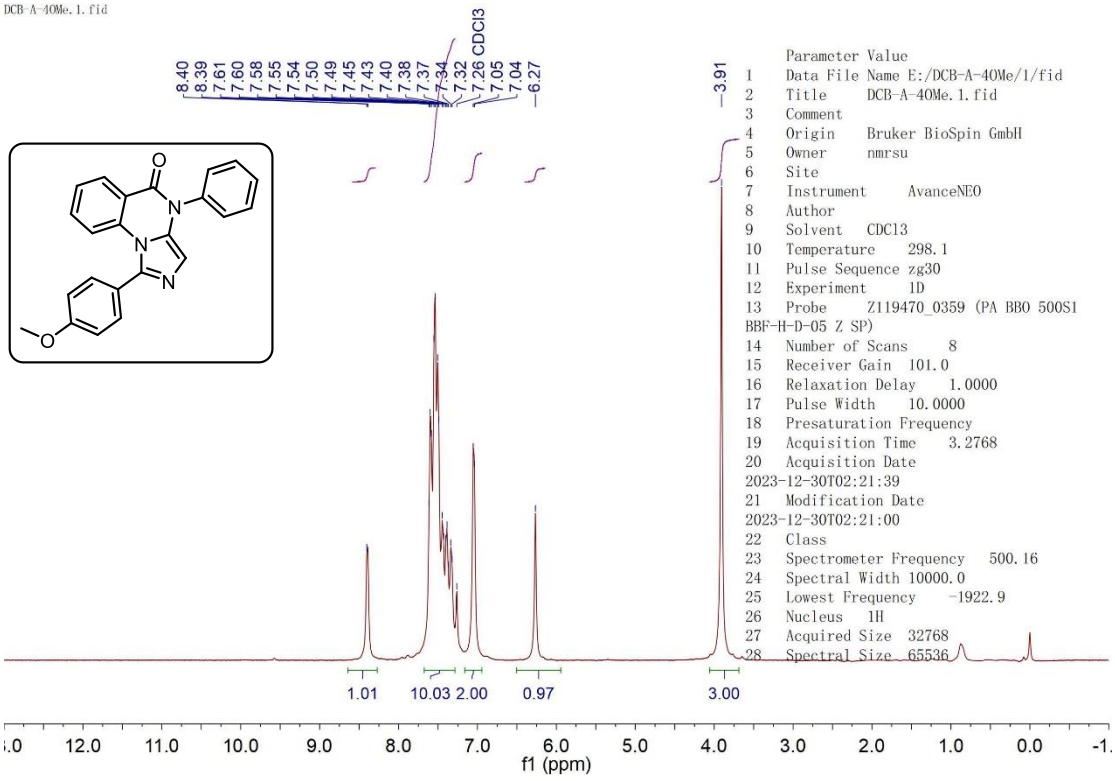


-62.67

	Parameter	Value
1	Data File Name	C:/Users/杜成斌/Desktop/总数据/DCB-A-4CF3/3/fid
2	Title	DCB-A-4CF3.3.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	0.0
11	Pulse Sequence	zgig
12	Experiment	1D
13	Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	16
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	15.0000
18	Presaturation Frequency	
19	Acquisition Time	0.5767
20	Acquisition Date	2023-10-19T07:23:05
21	Modification Date	2023-10-19T07:21:18
22	Class	
23	Spectrometer Frequency	470.57
24	Spectral Width	113636.4
25	Lowest Frequency	-103880.2
26	Nucleus	19F
27	Acquired Size	65536



1-(4-methoxyphenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3af)



Parameter Value

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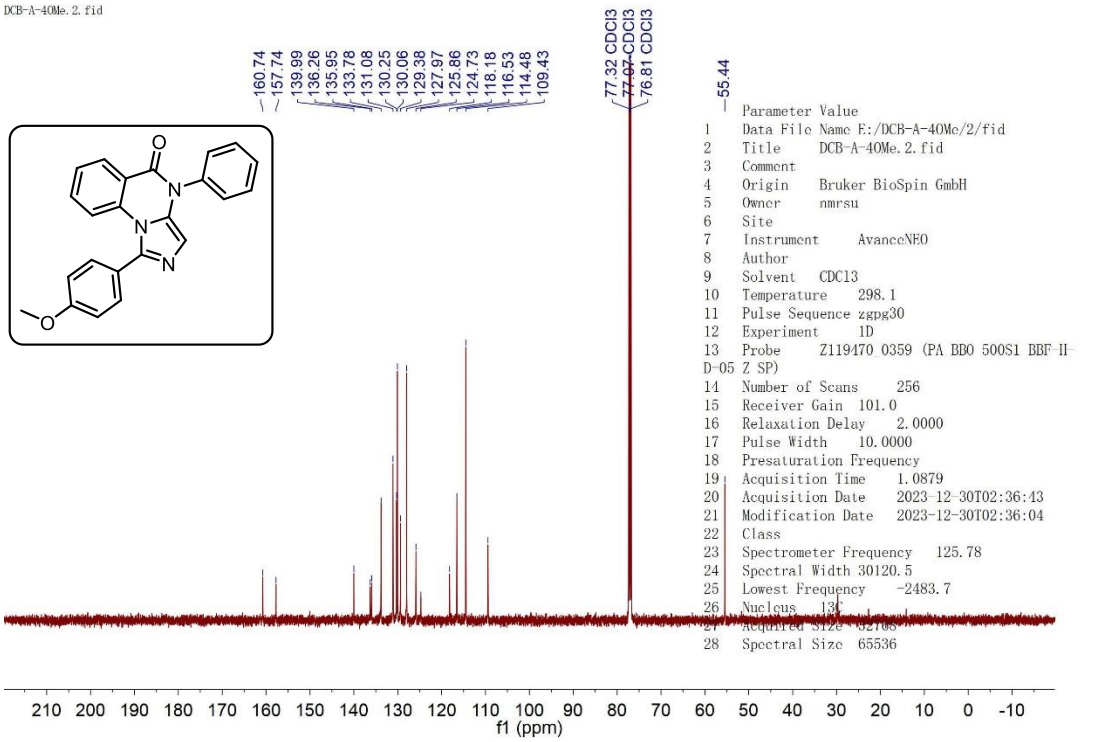
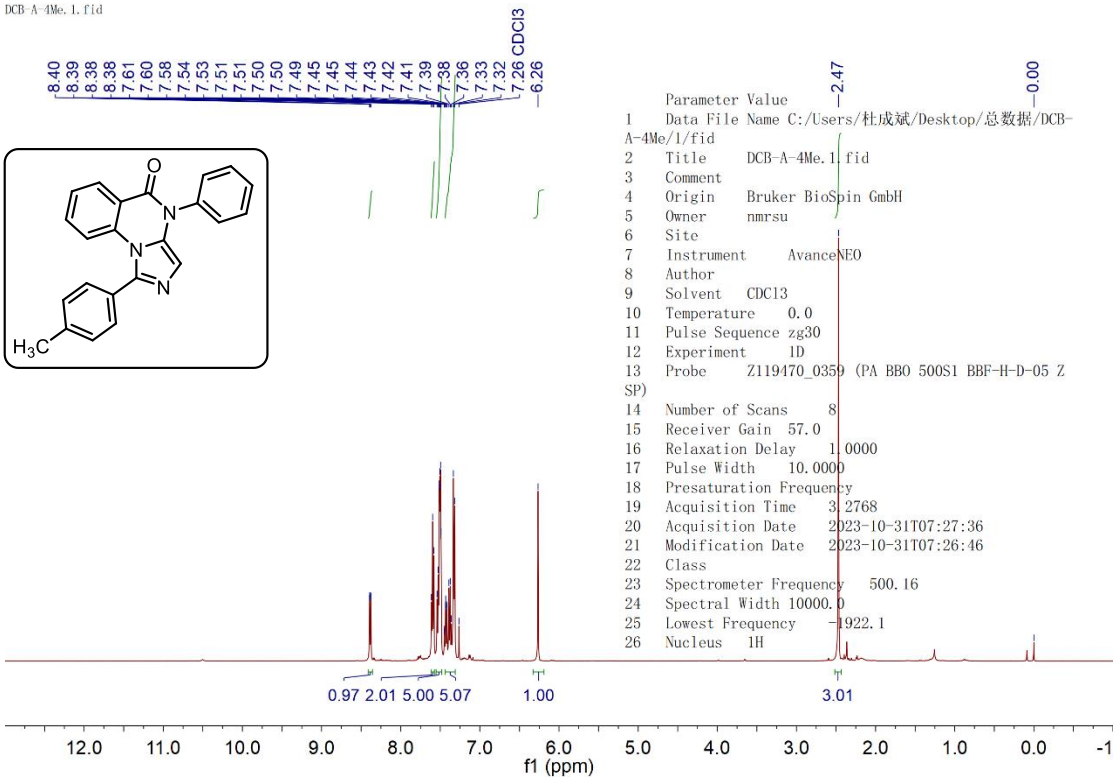
2	Title	DCB-A-4OMe.1.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	8
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.2768
20	Acquisition Date	2023-12-30T02:21:39
21	Modification Date	2023-12-30T02:21:00
22	Class	
23	Spectrometer Frequency	500.16
24	Spectral Width	10000.0
25	Lowest Frequency	-1922.9
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

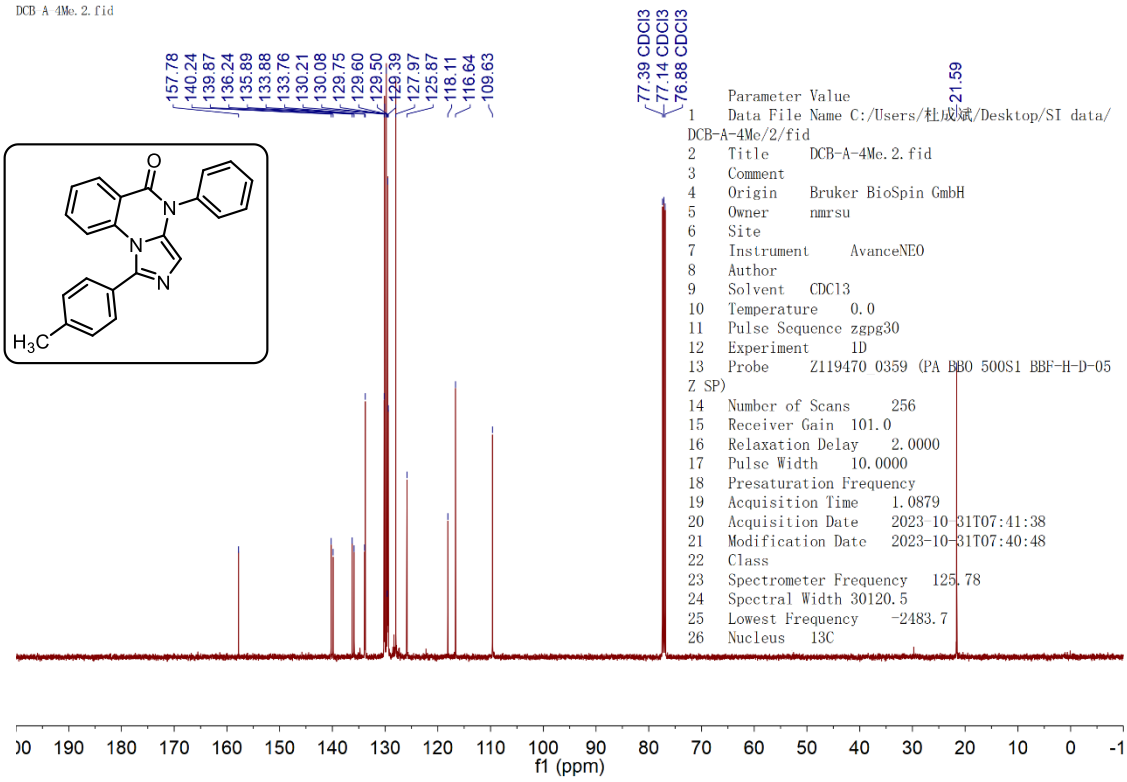


Parameter Value

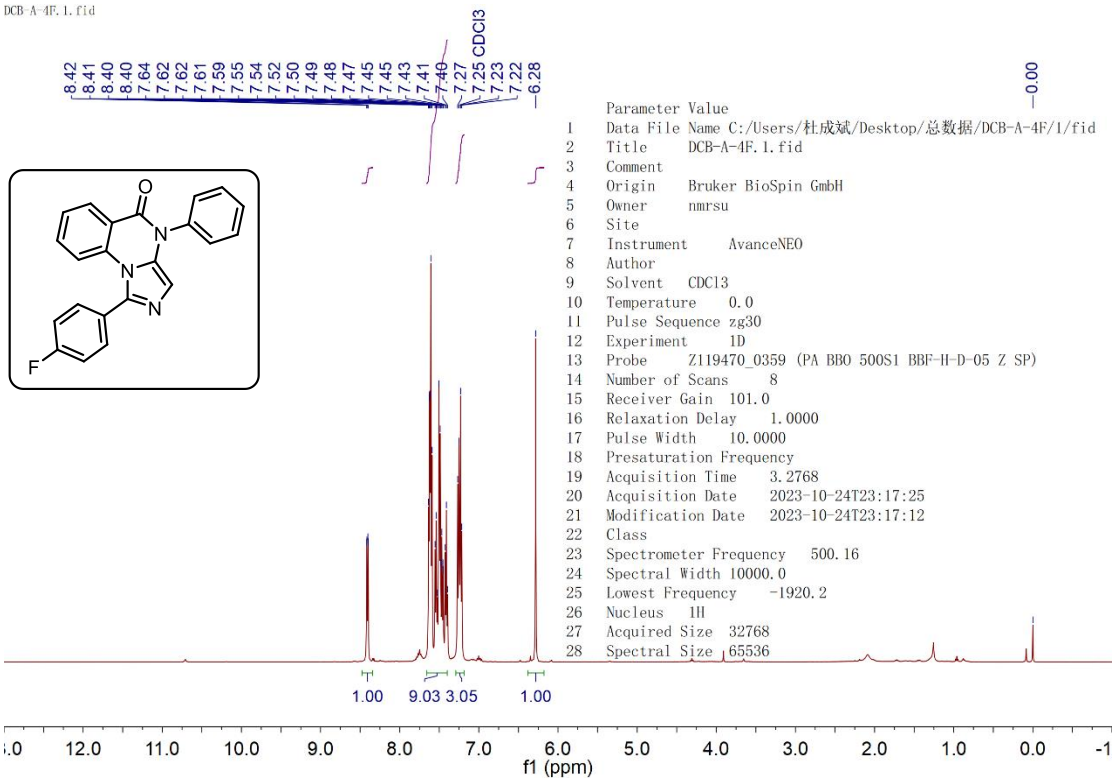
1	Data File Name	E:/DCB-A-4OMe/2/fid
2	Title	DCB-A-4OMe.2.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	256
15	Receiver Gain	101.0
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.0879
20	Acquisition Date	2023-12-30T02:36:43
21	Modification Date	2023-12-30T02:36:04
22	Class	
23	Spectrometer Frequency	125.78
24	Spectral Width	30120.5
25	Lowest Frequency	-2483.7
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

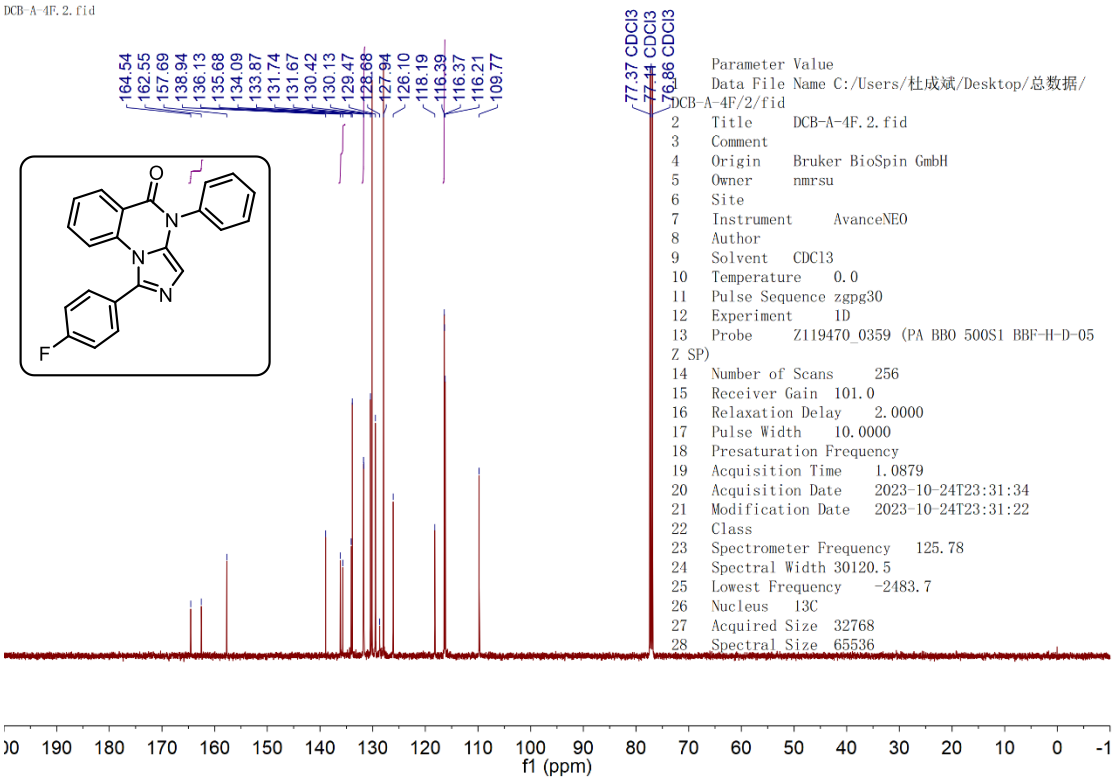
4-phenyl-1-(p-tolyl)imidazo[1,5-a]quinazolin-5(4H)-one (3ag)



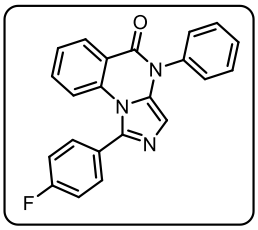


1-(4-fluorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ah)





DCB A 4F.3.fid



-110.25

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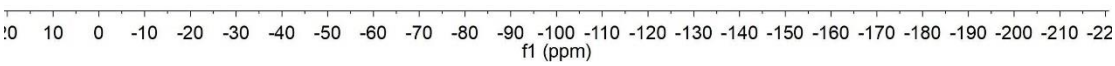
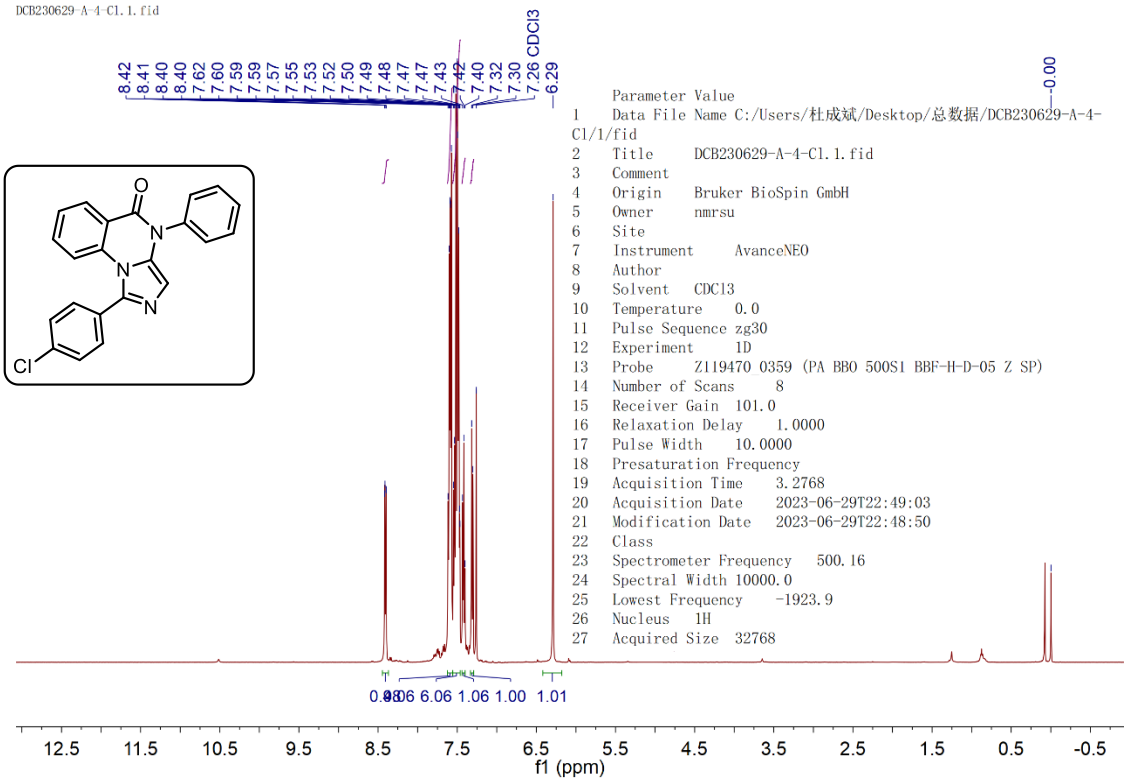
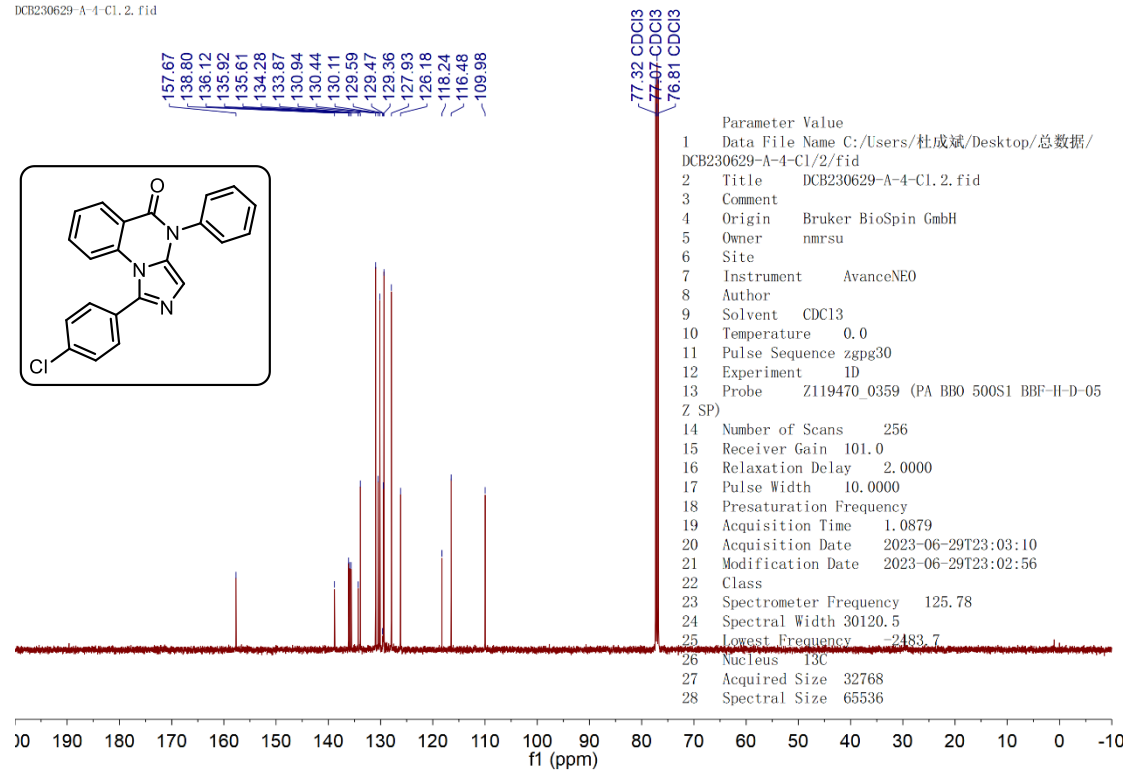
2	Title	DCB-A-4F.3.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	0.0
11	Pulse Sequence	zgig
12	Experiment	1D
13	Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	16
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	15.0000
18	Presaturation Frequency	
19	Acquisition Time	0.5767
20	Acquisition Date	2023-10-24T23:33:21
21	Modification Date	2023-10-24T23:33:08
22	Class	
23	Spectrometer Frequency	470.57
24	Spectral Width	113636.4
25	Lowest Frequency	-103880.2
26	Nucleus	19F
27	Acquired Size	65536
28	Spectral Size	131072

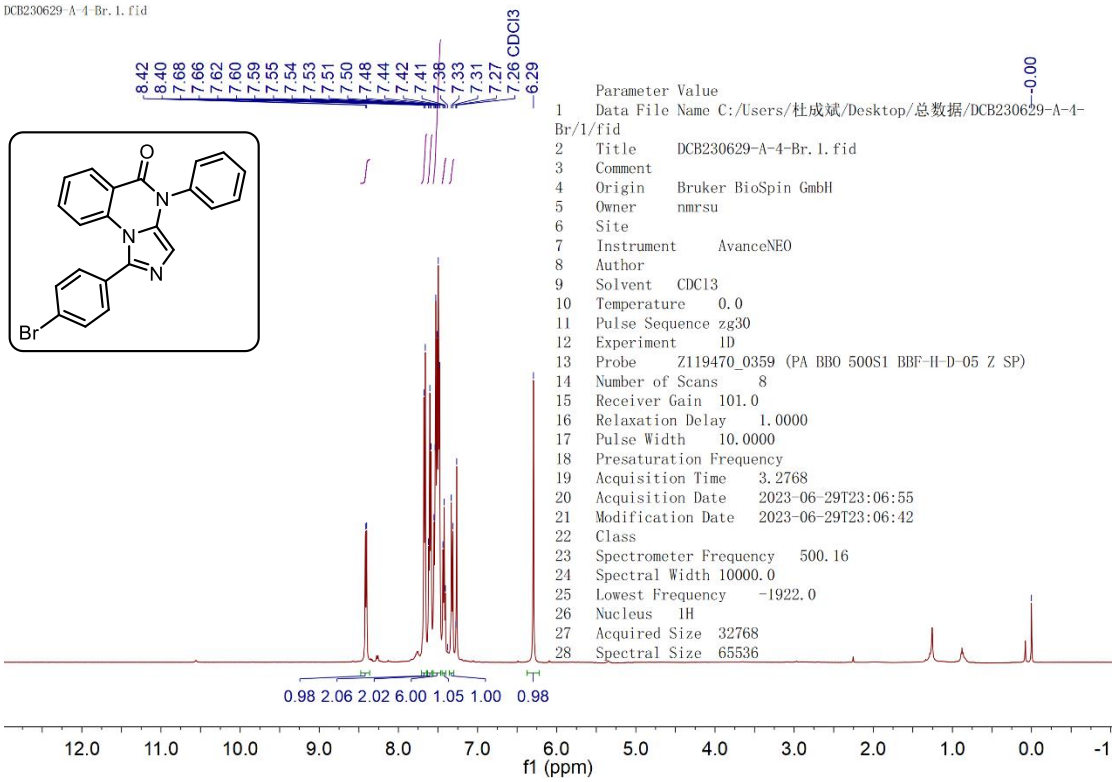


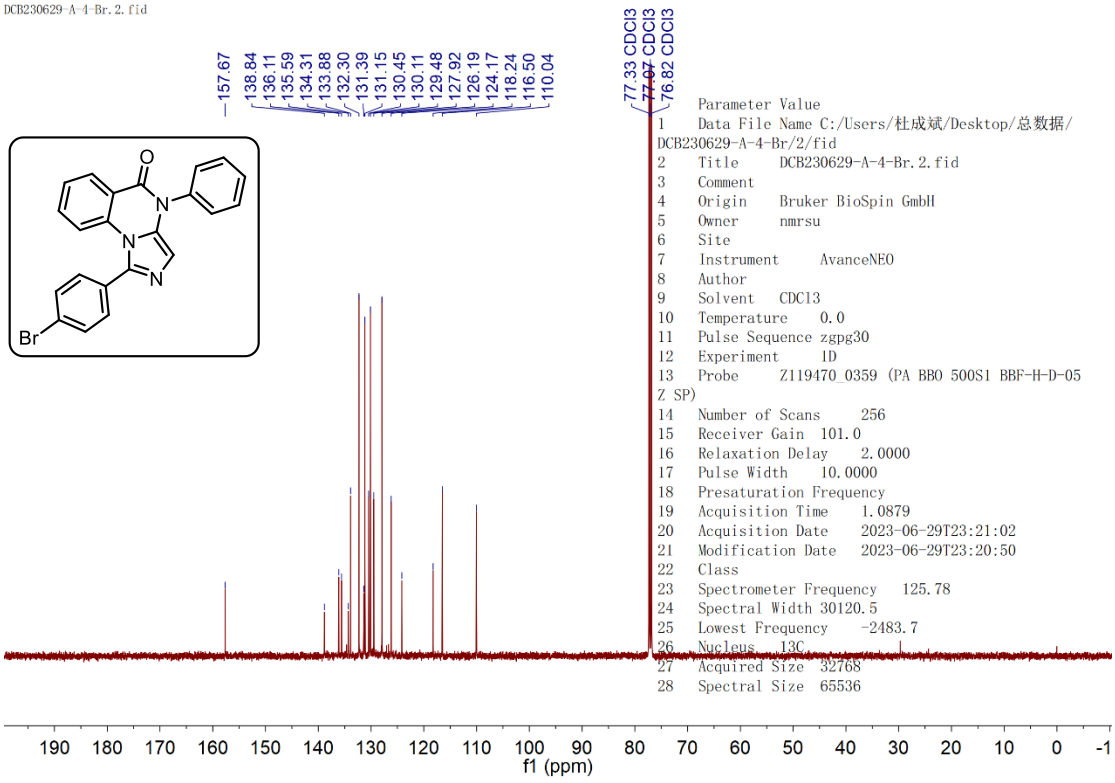
1-(4-chlorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ai)



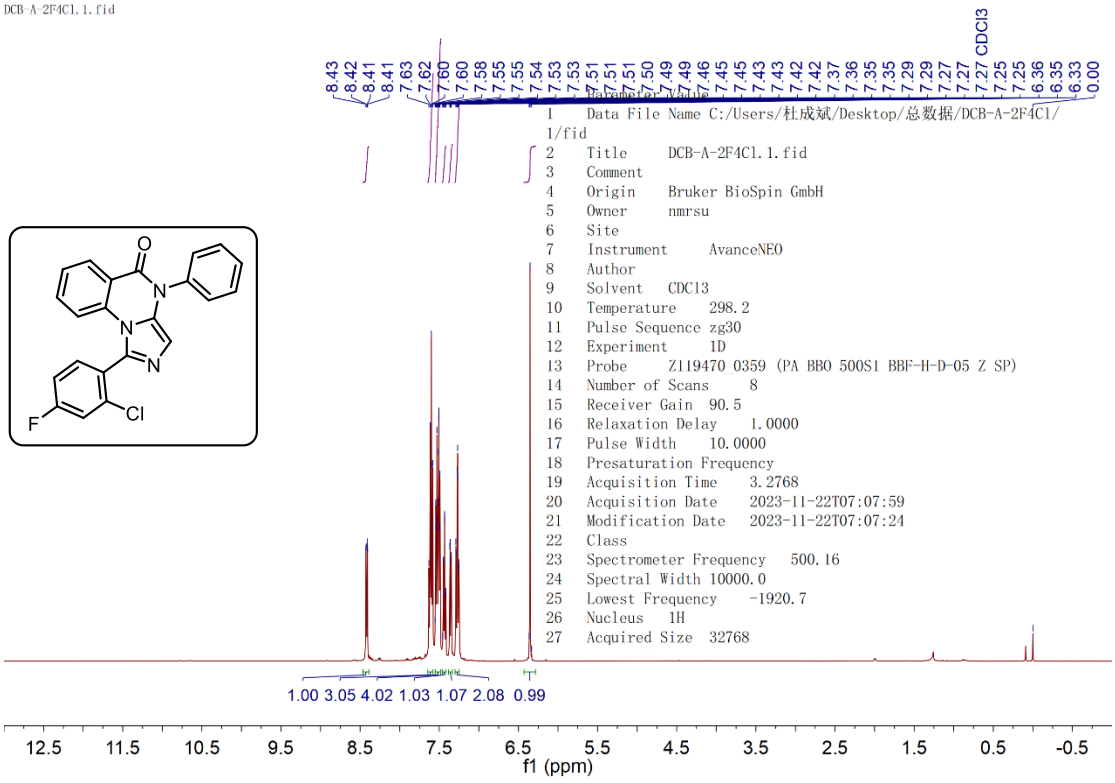


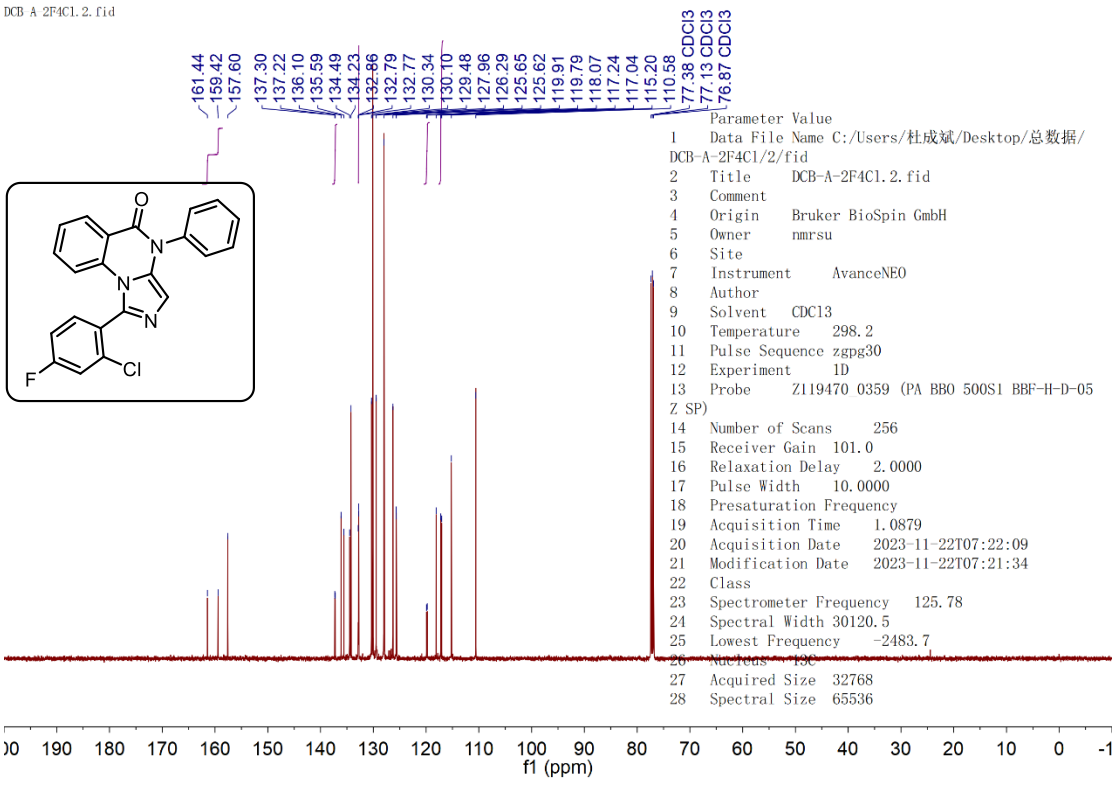
1-(4-bromophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3aj)



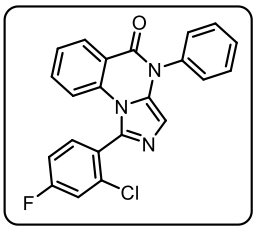


1-(2-chloro-4-fluorophenyl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3ak)





DCB-A-2F4Cl.3.fid



-109.39

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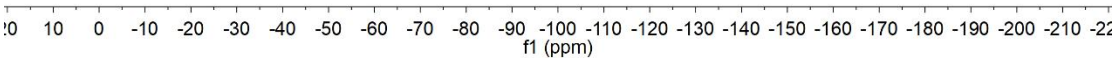
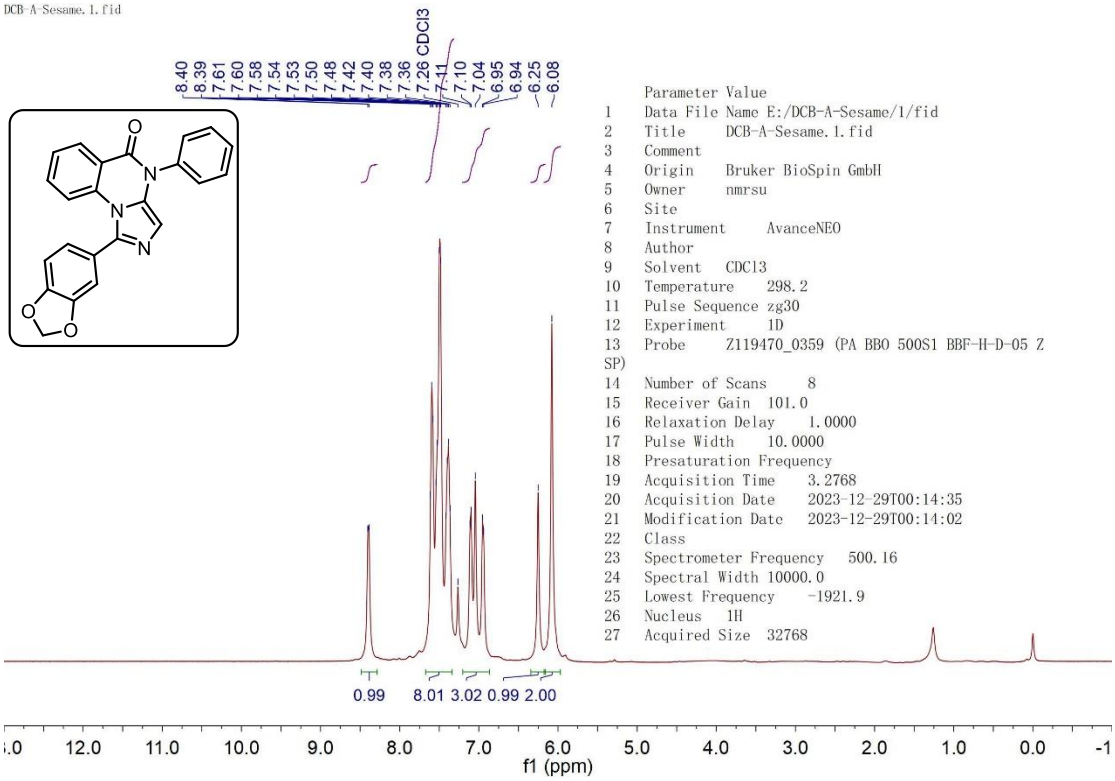
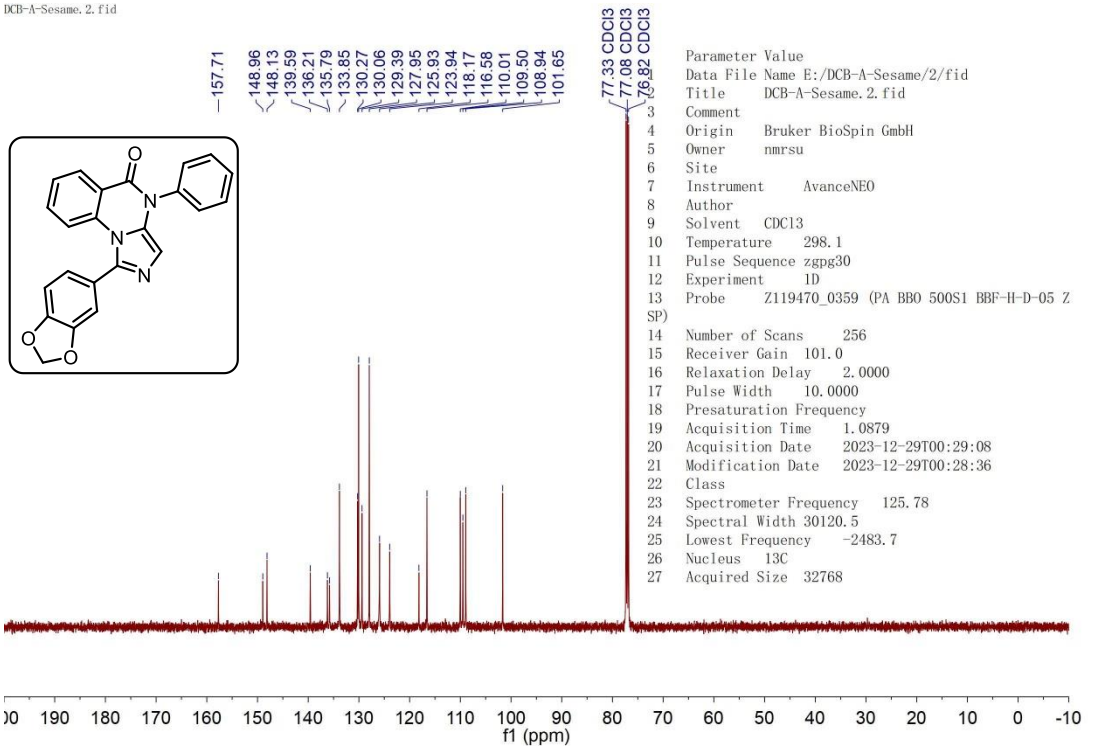
1	Data File Name	C:/Users/杜成斌/Desktop/总数据/DCB-A-2F4Cl/3/fid
2	Title	DCB-A-2F4Cl.3.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	298.2
11	Pulse Sequence	zgig
12	Experiment	1D
13	Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	16
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	15.0000
18	Presaturation Frequency	
19	Acquisition Time	0.5767
20	Acquisition Date	2023-11-22T07:23:53
21	Modification Date	2023-11-22T07:23:18
22	Class	
23	Spectrometer Frequency	470.57
24	Spectral Width	113636.4
25	Lowest Frequency	-103880.2
26	Nucleus	19F
27	Acquired Size	65536
28	Spectral Size	131072

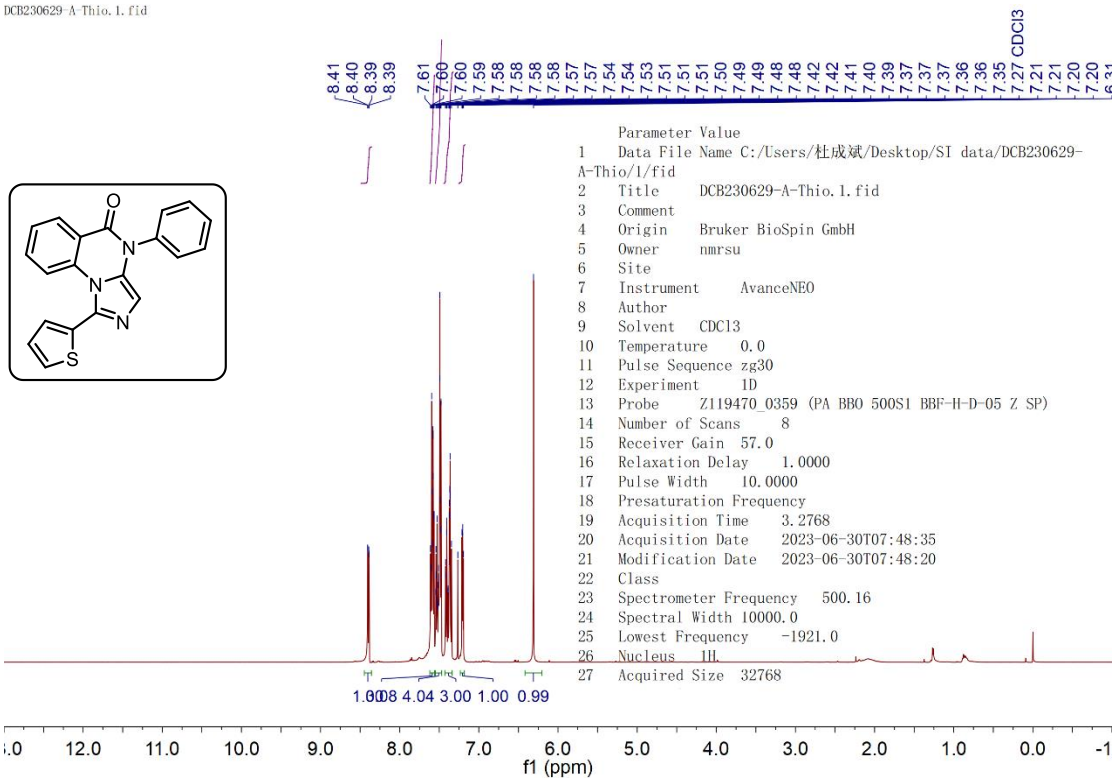


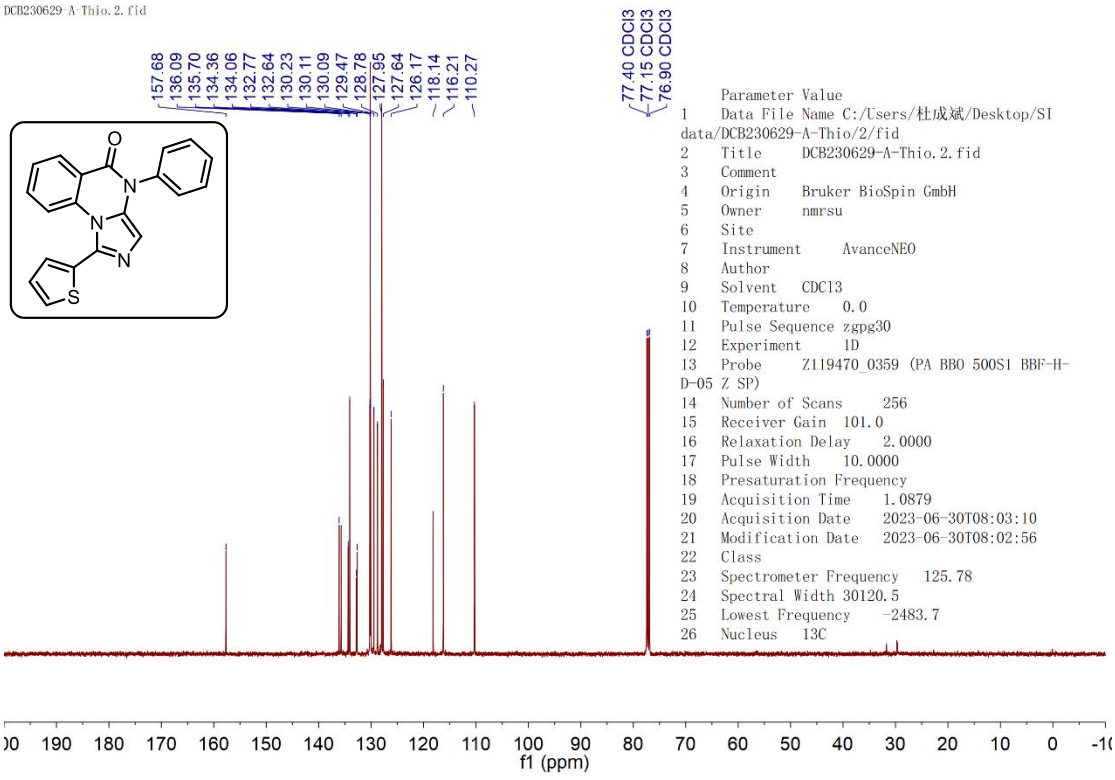
1-(benzo[d][1,3]dioxol-5-yl)-4-phenylimidazo[1,5-a]quinazolin-5(4H)-one (3al)



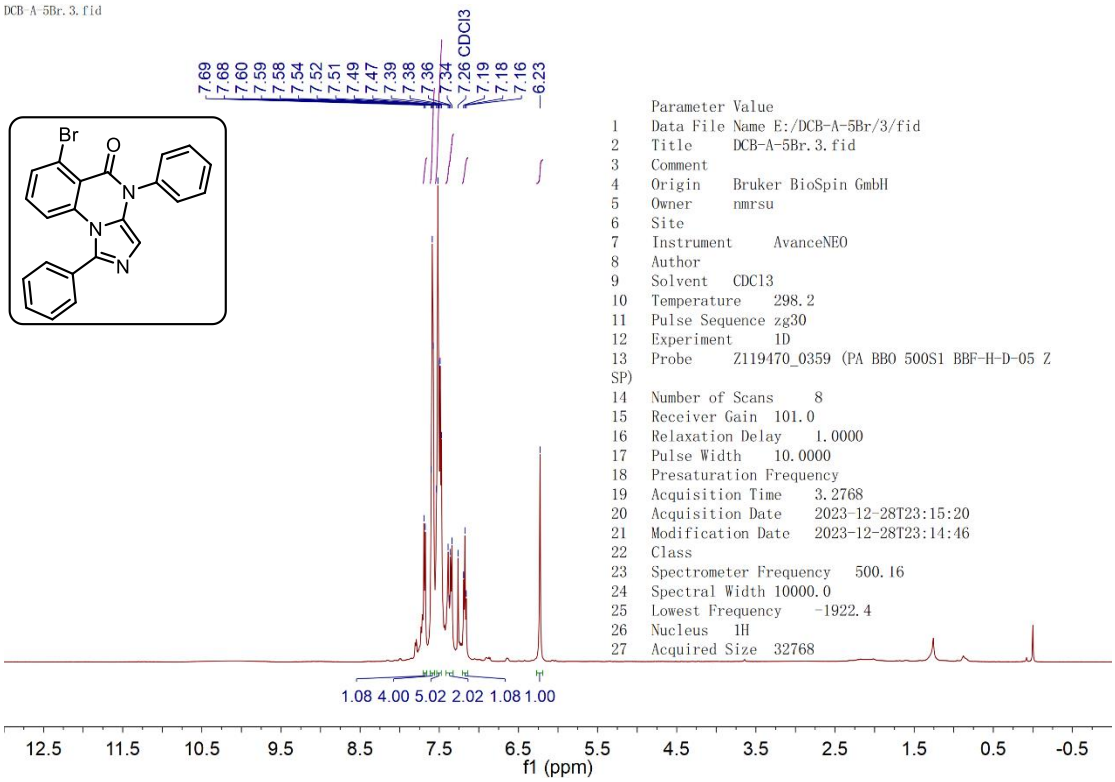


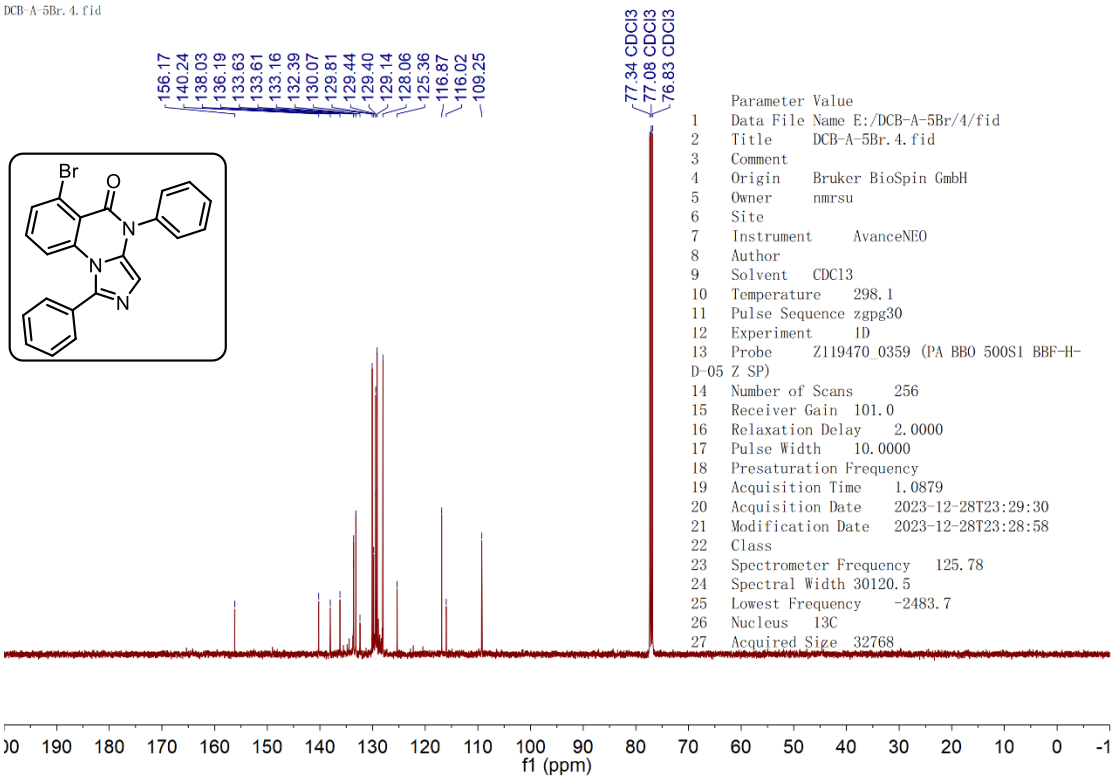
4-phenyl-1-(thiophen-2-yl)imidazo[1,5-a]quinazolin-5(4H)-one (3am)





6-bromo-1,4-diphenylimidazo[1,5-a]quinazolin-5(4H)-one (3ba)





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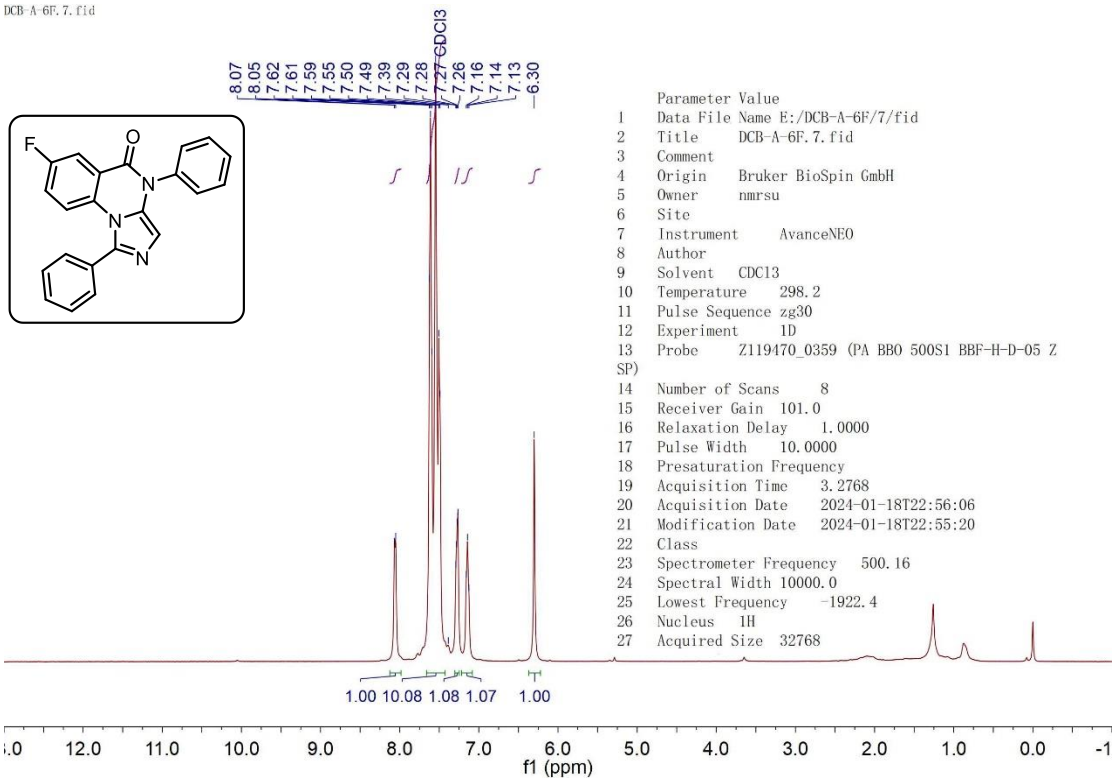

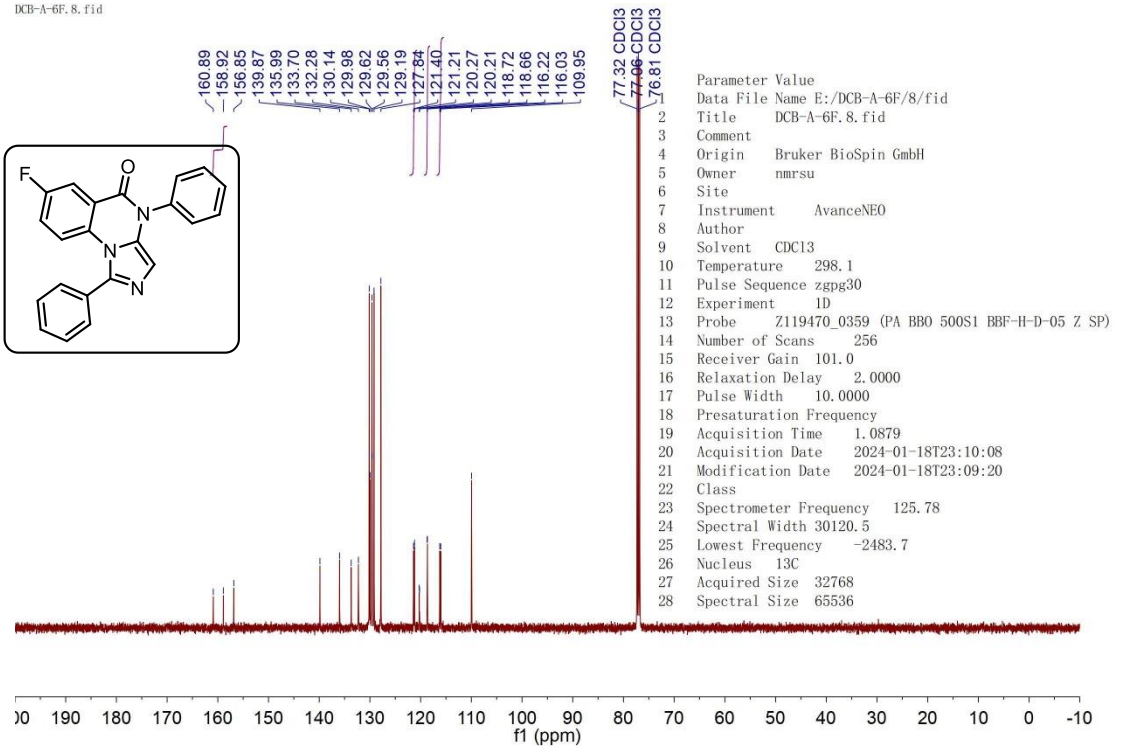

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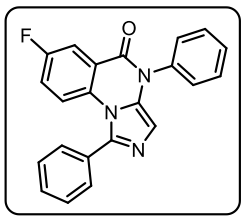

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8	Author	
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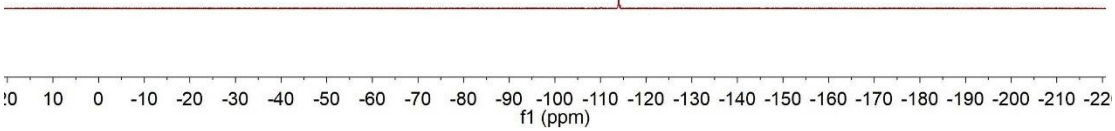

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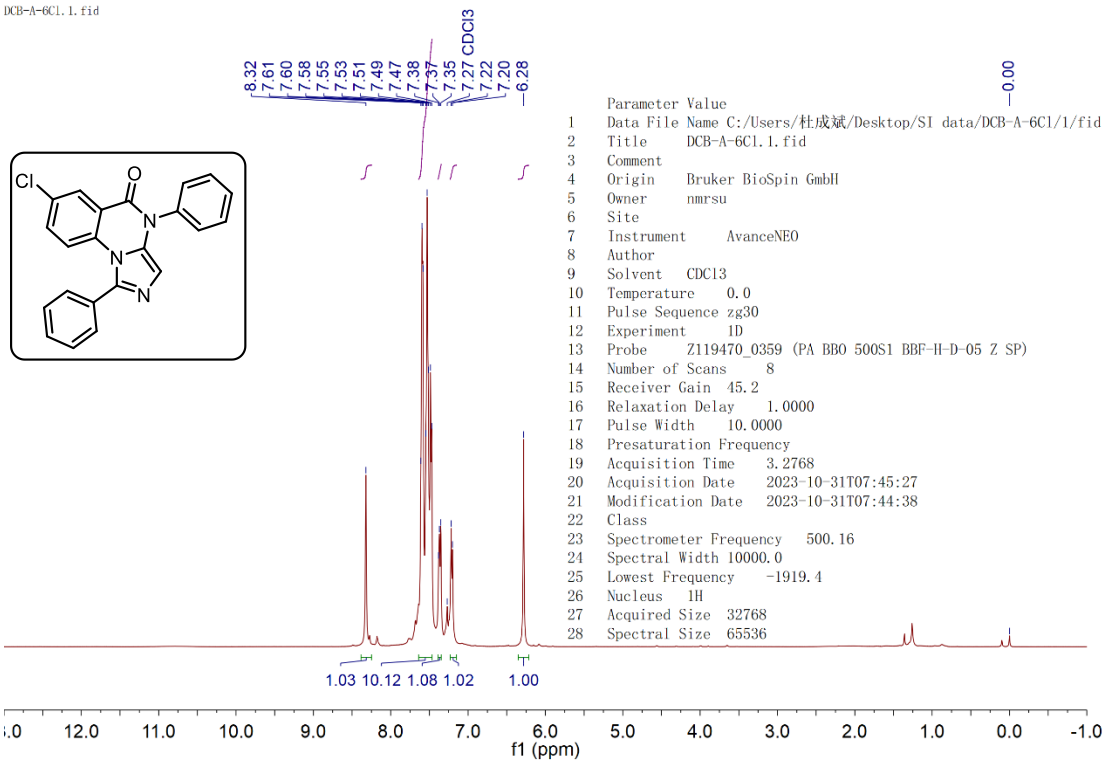

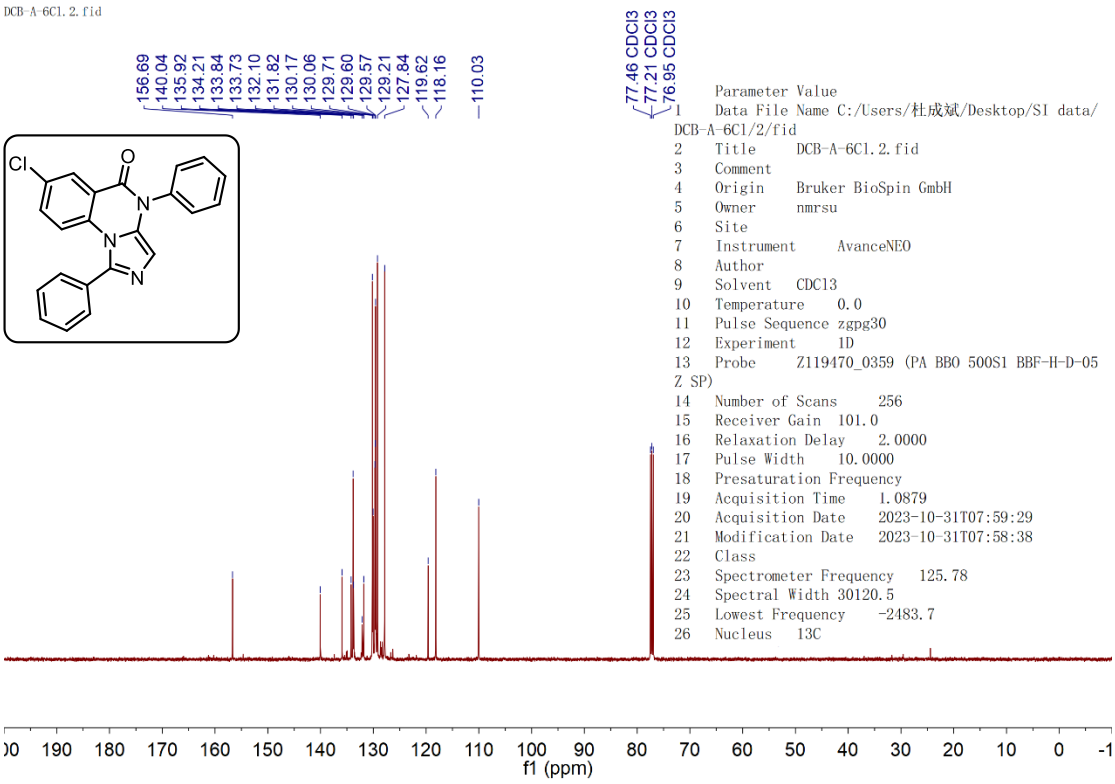

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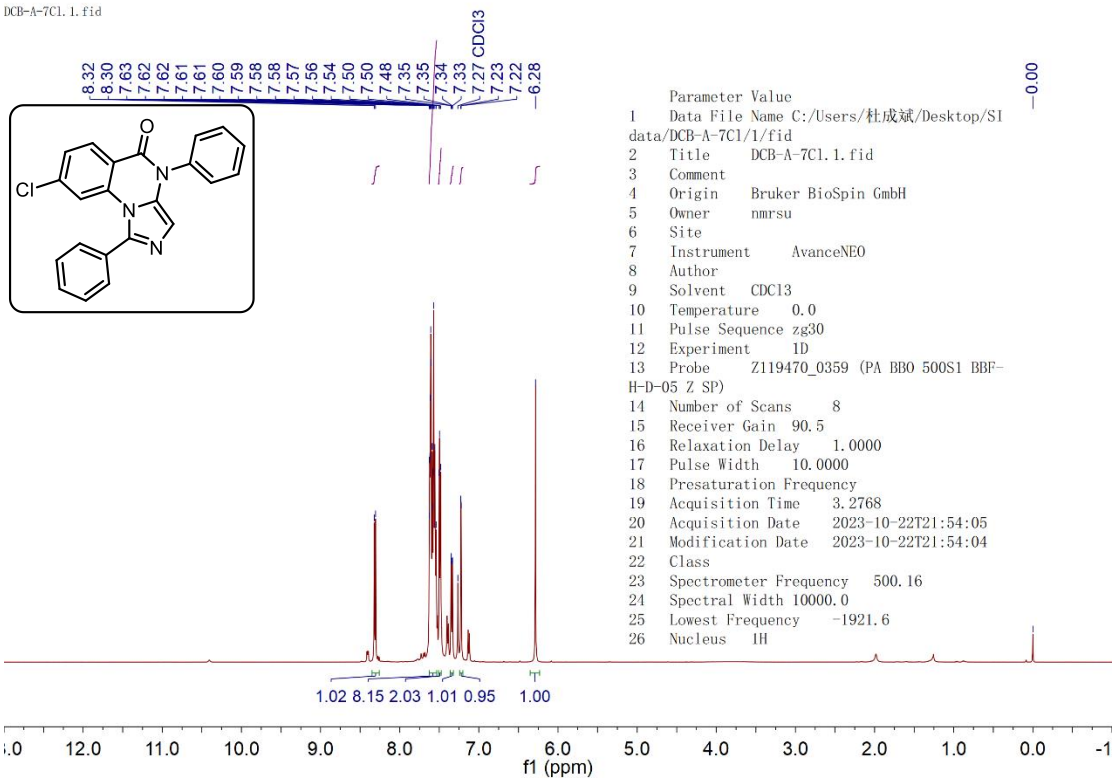

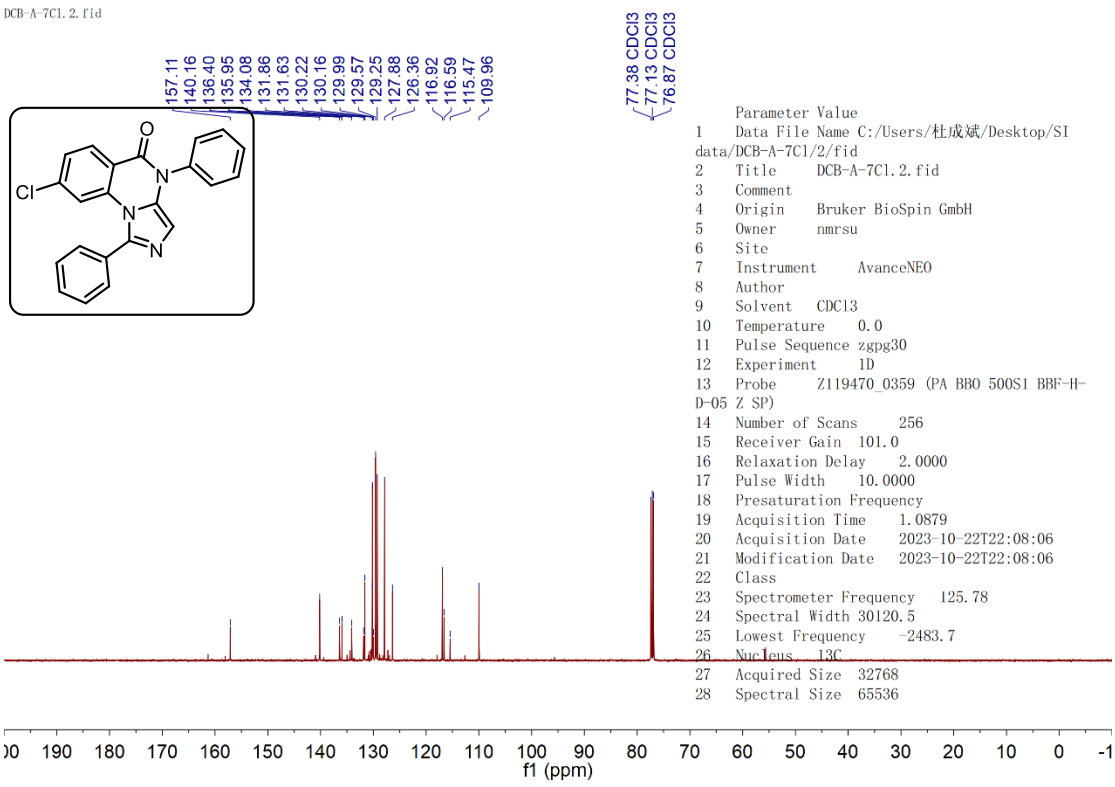

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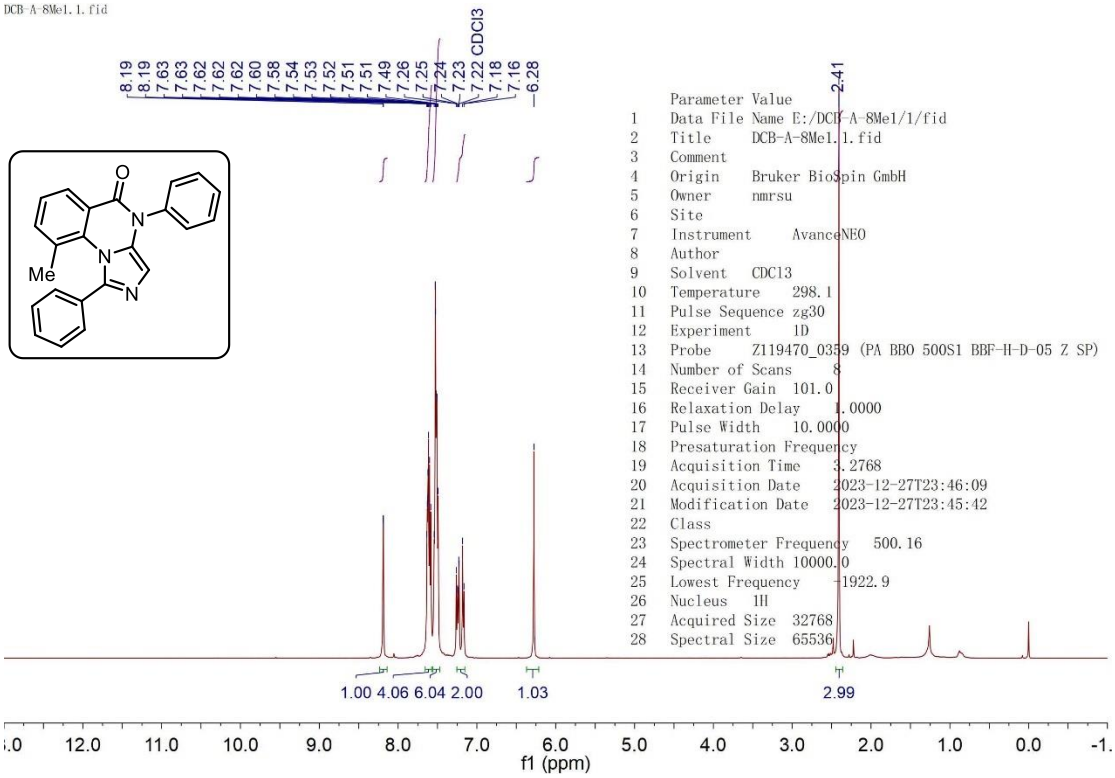

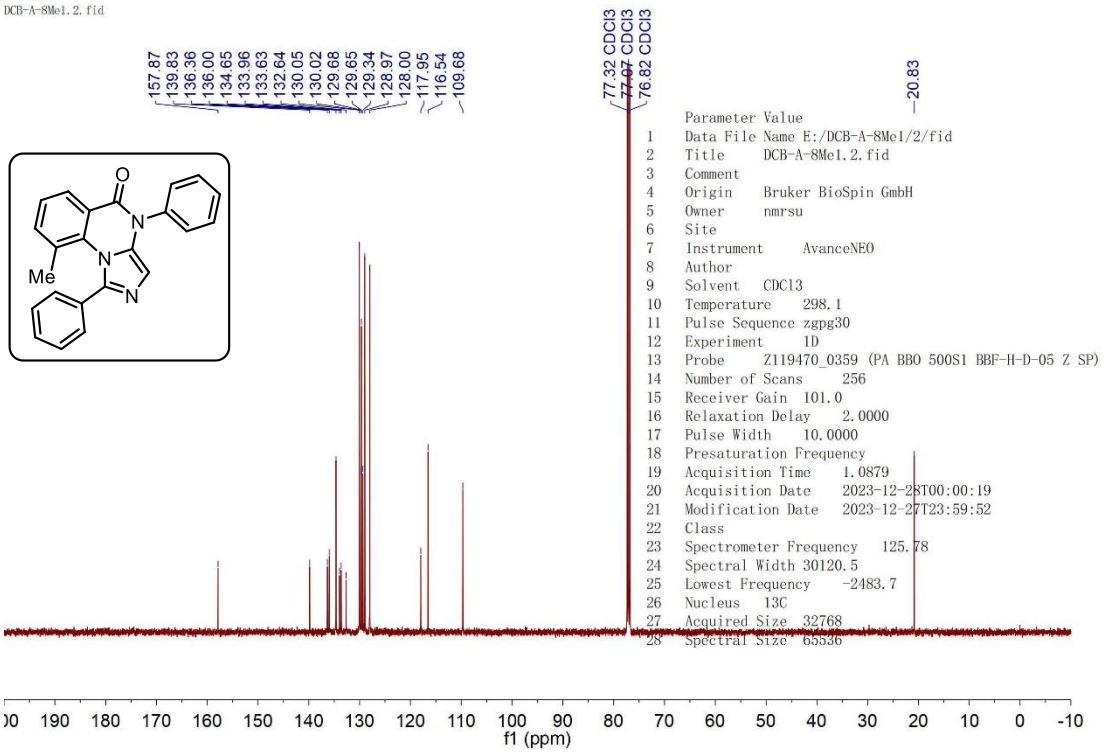

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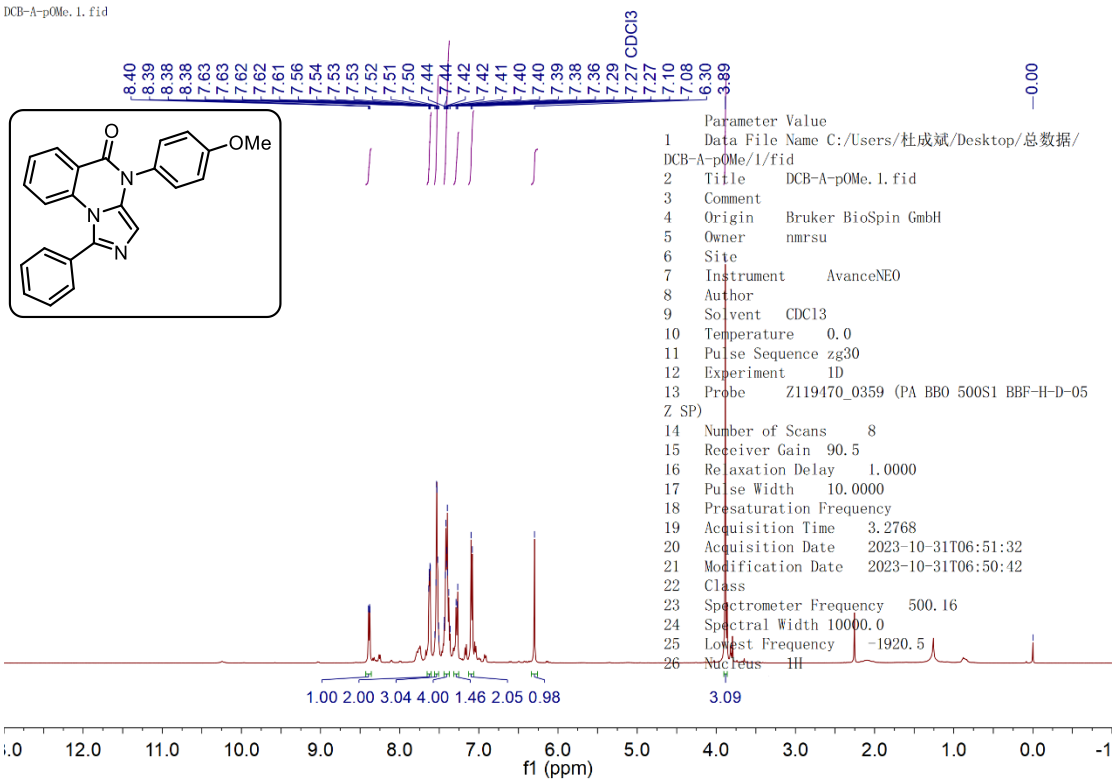

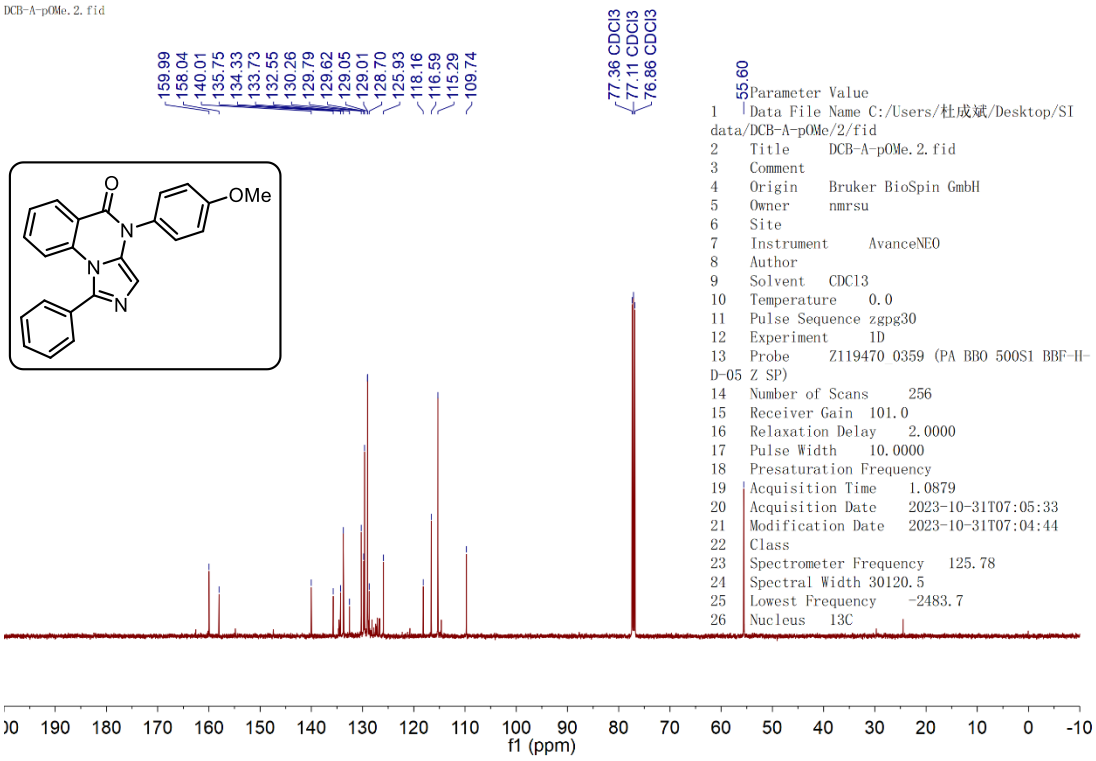

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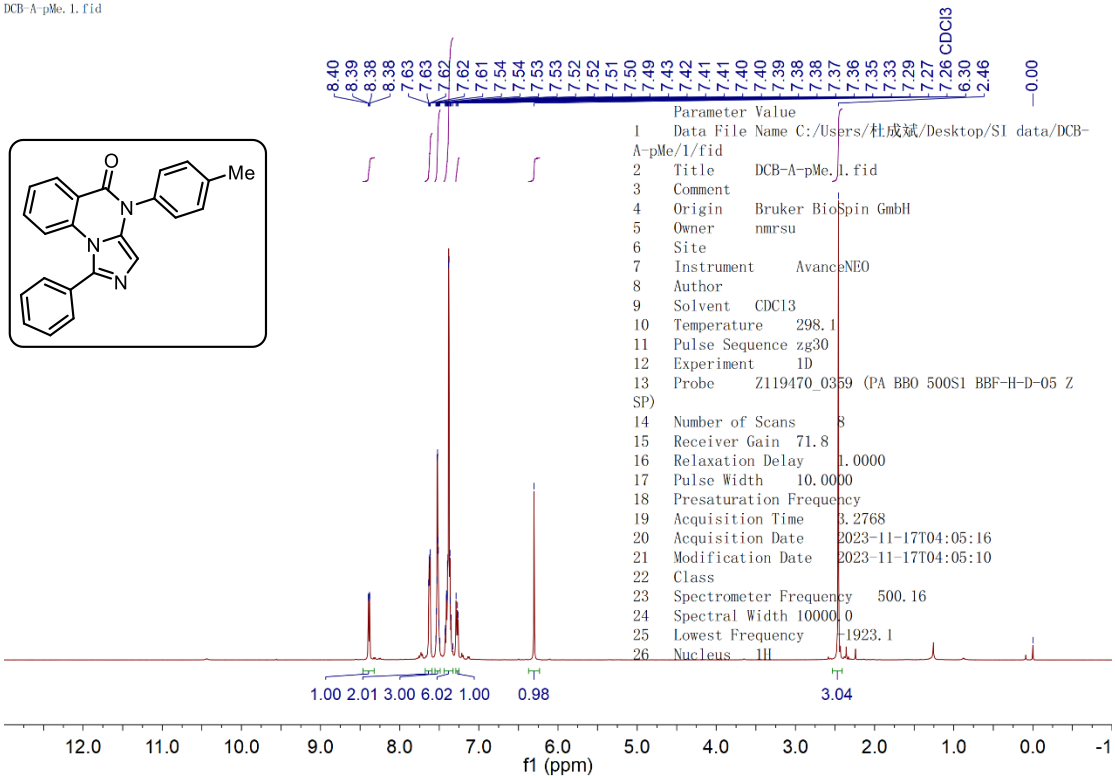

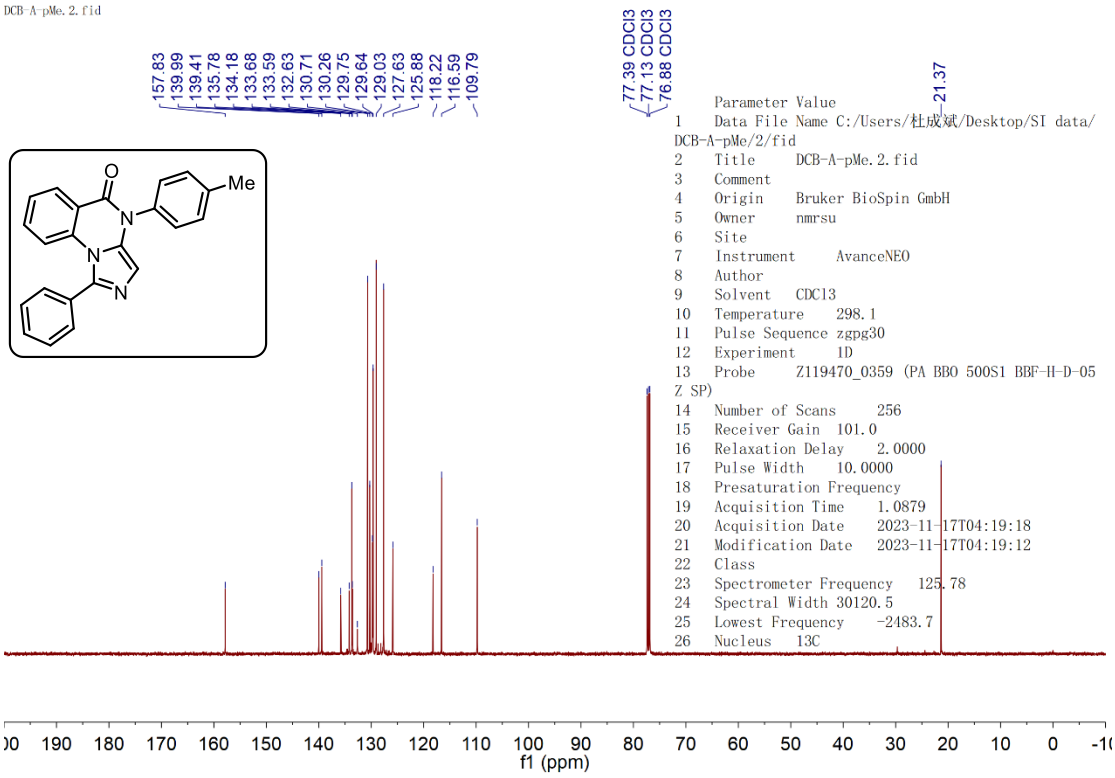

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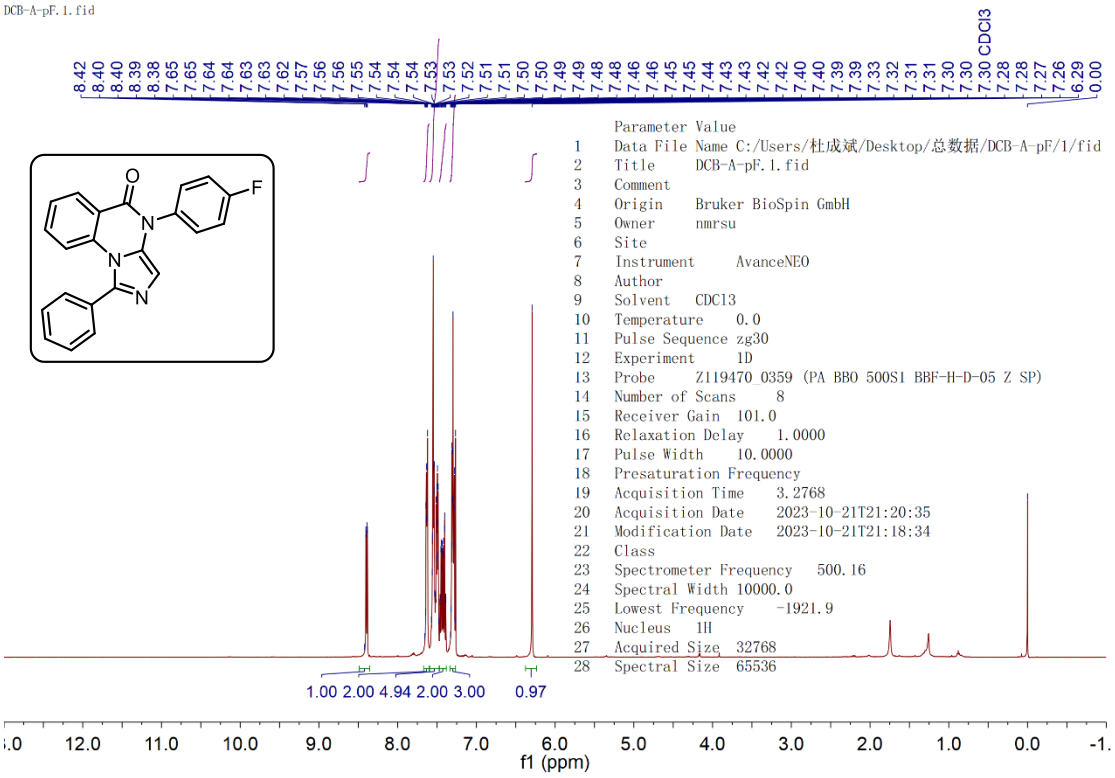

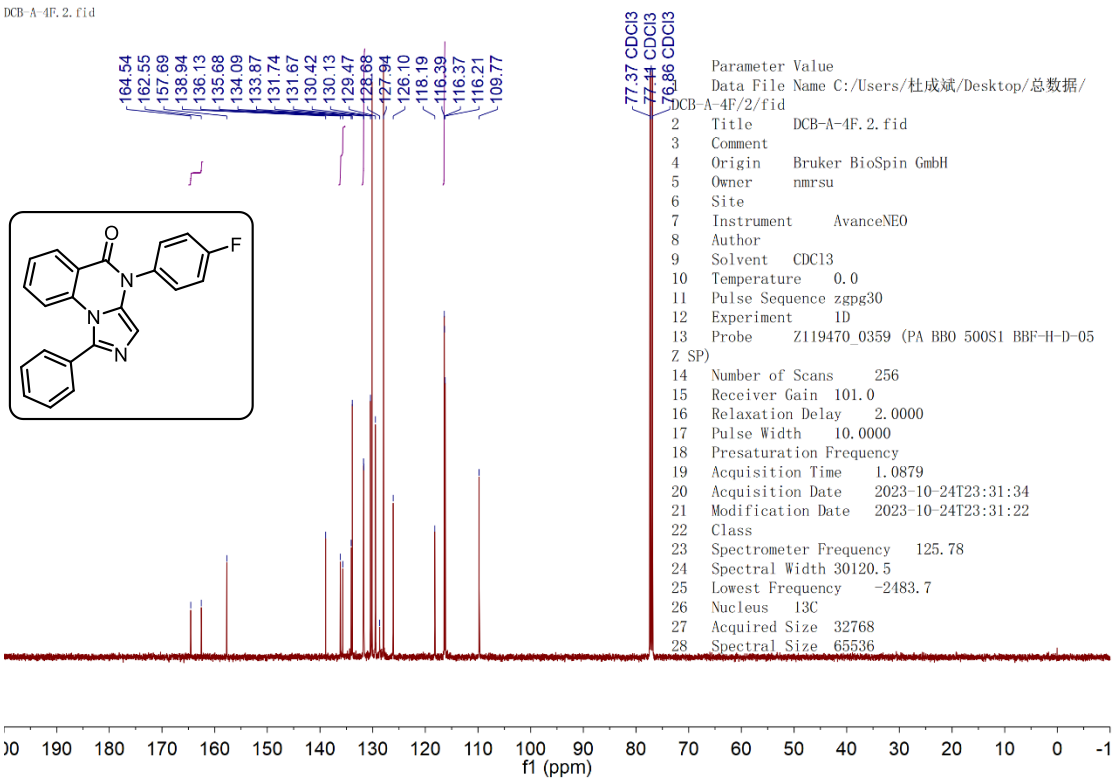

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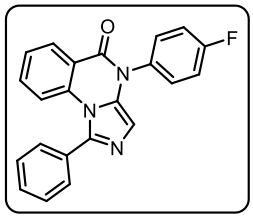

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11	Pulse Sequence	zgig
12	Experiment	1D
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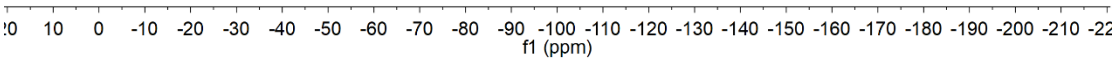

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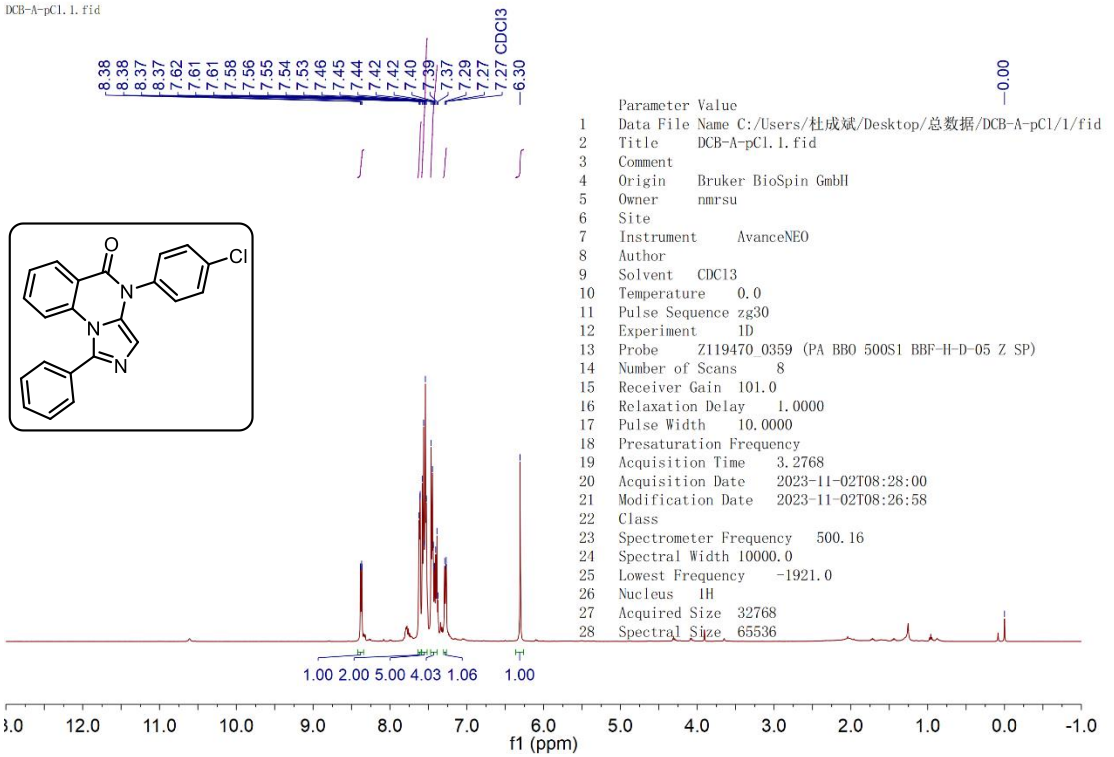
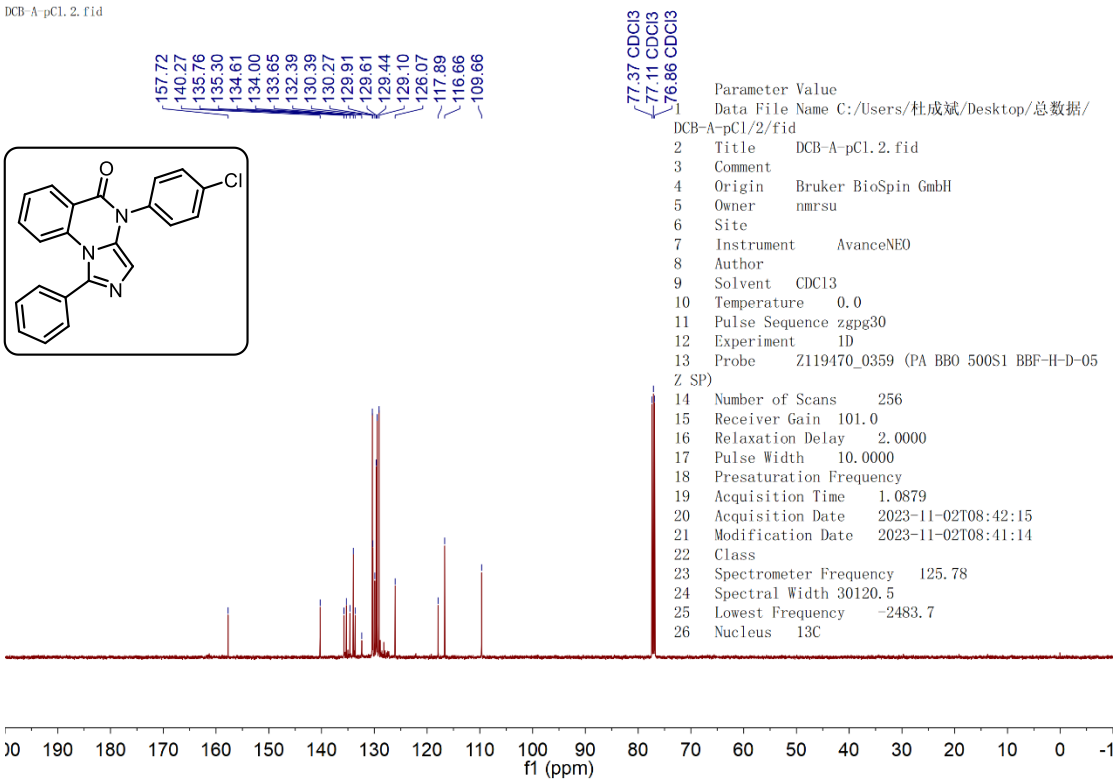
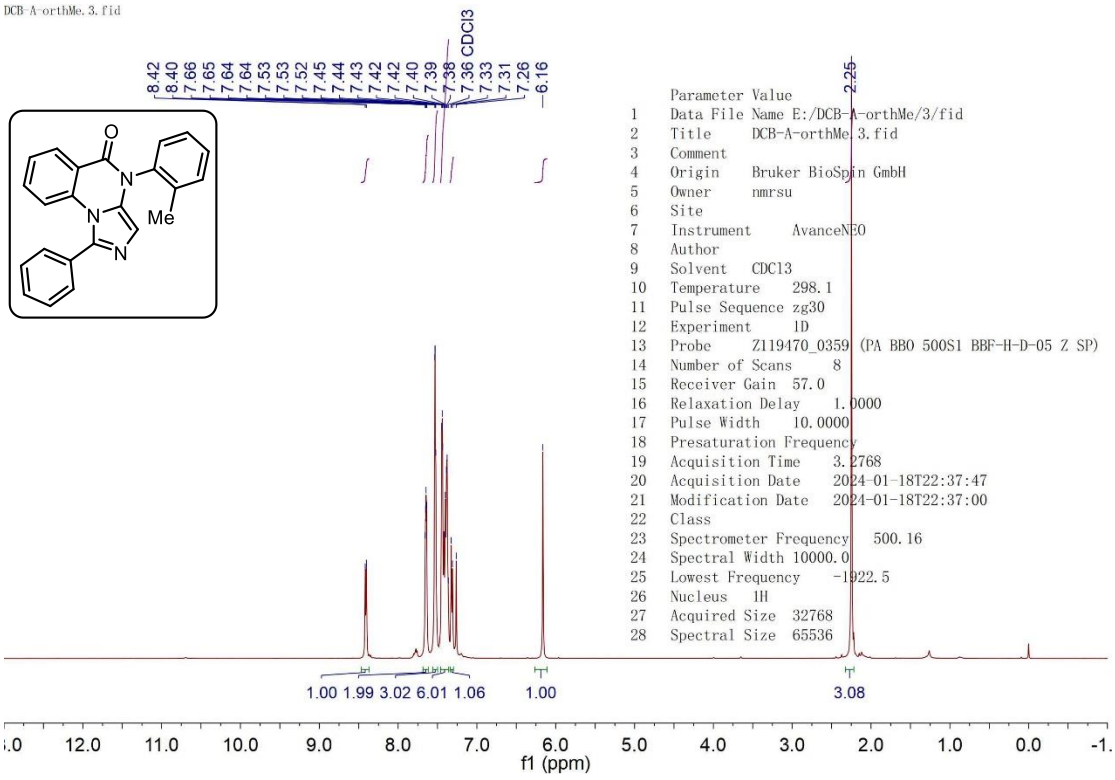
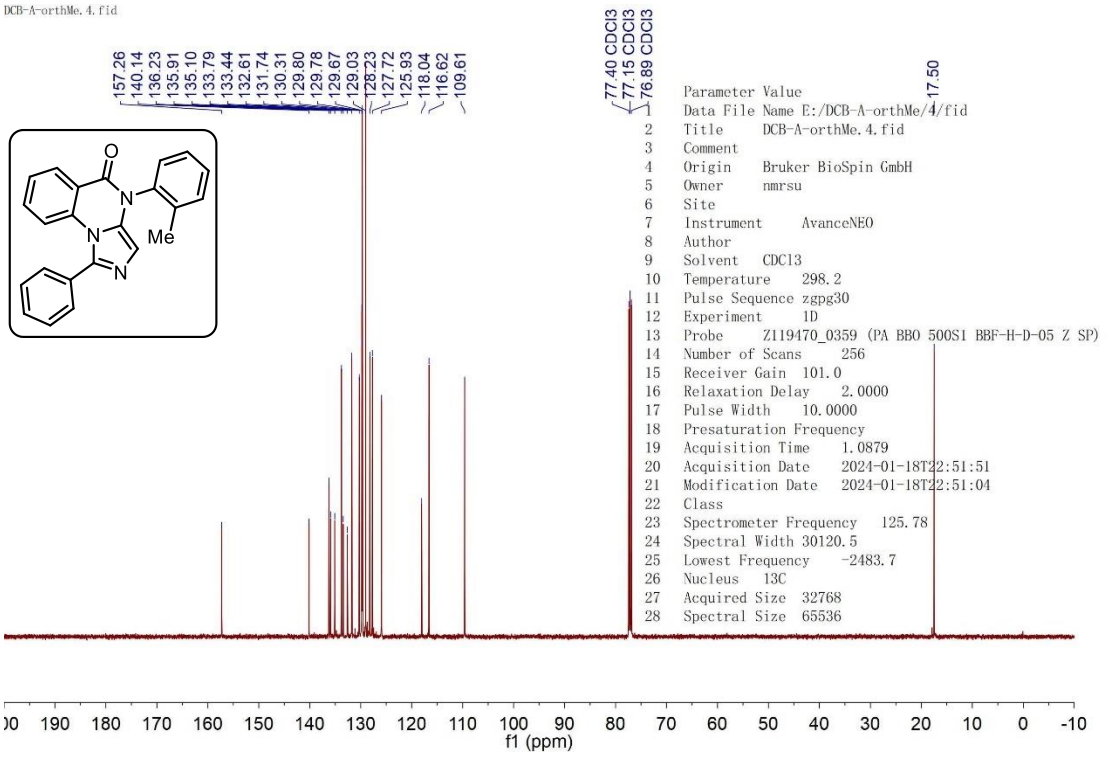


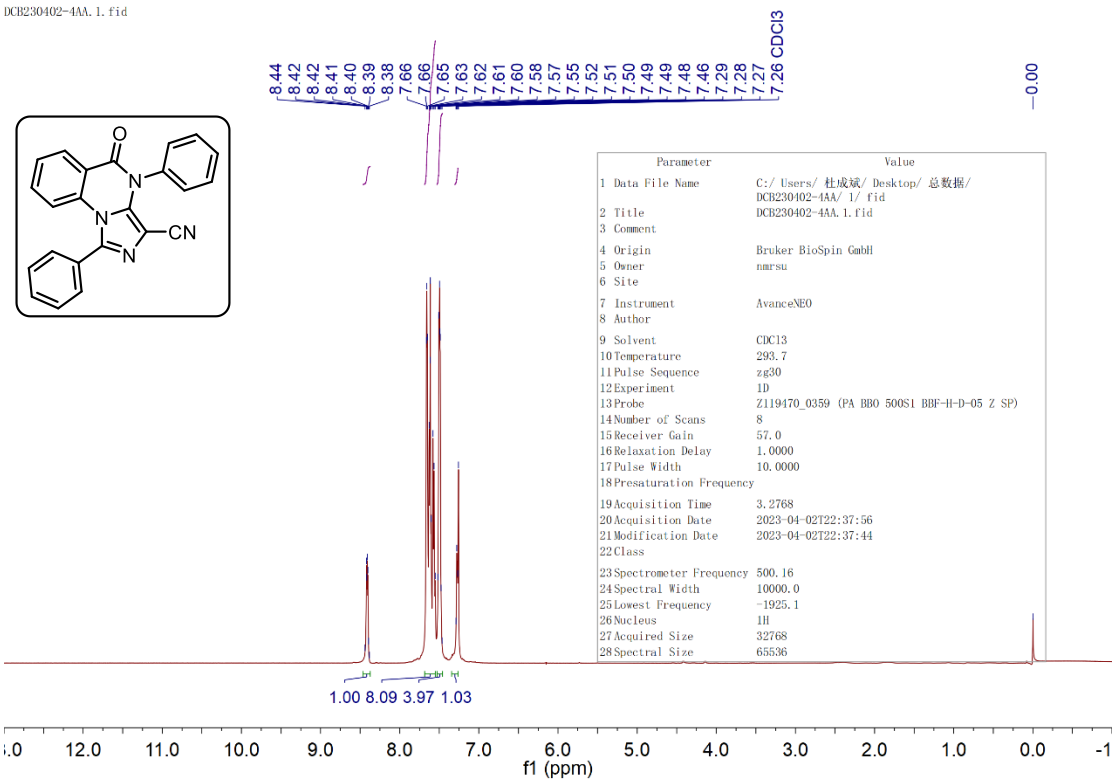


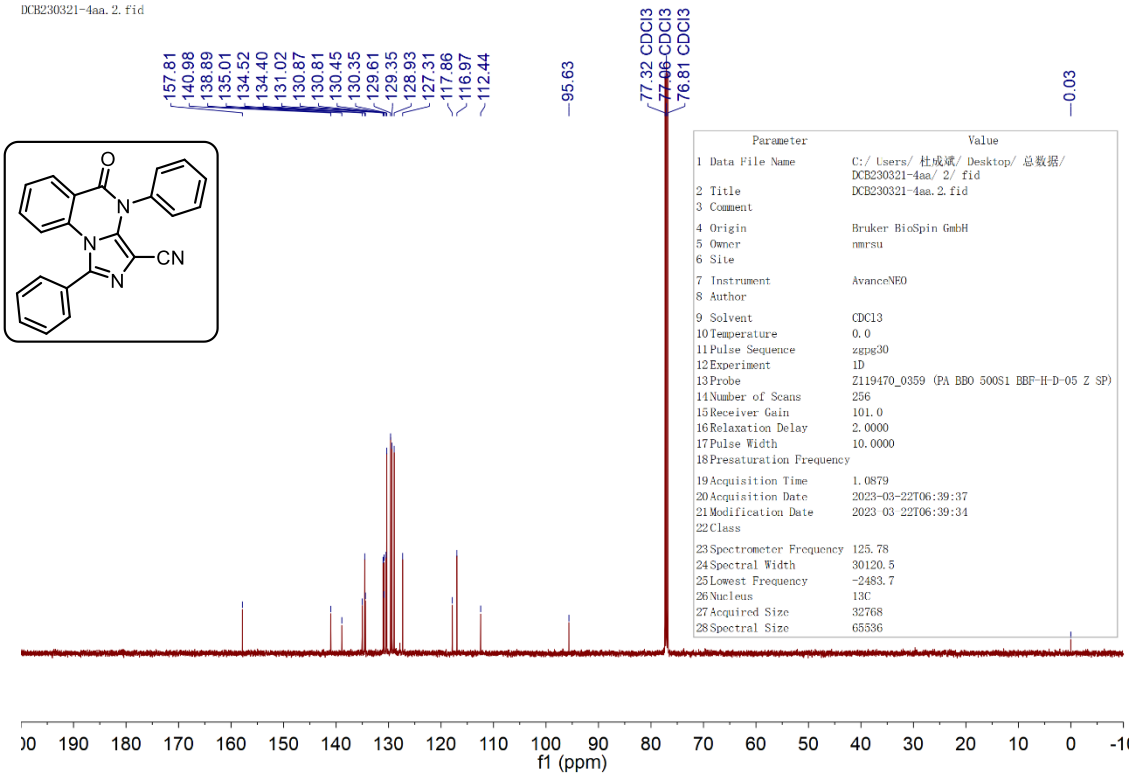
1-phenyl-4-(o-tolyl)imidazo[1,5-a]quinazolin-5(4H)-one (3ka)



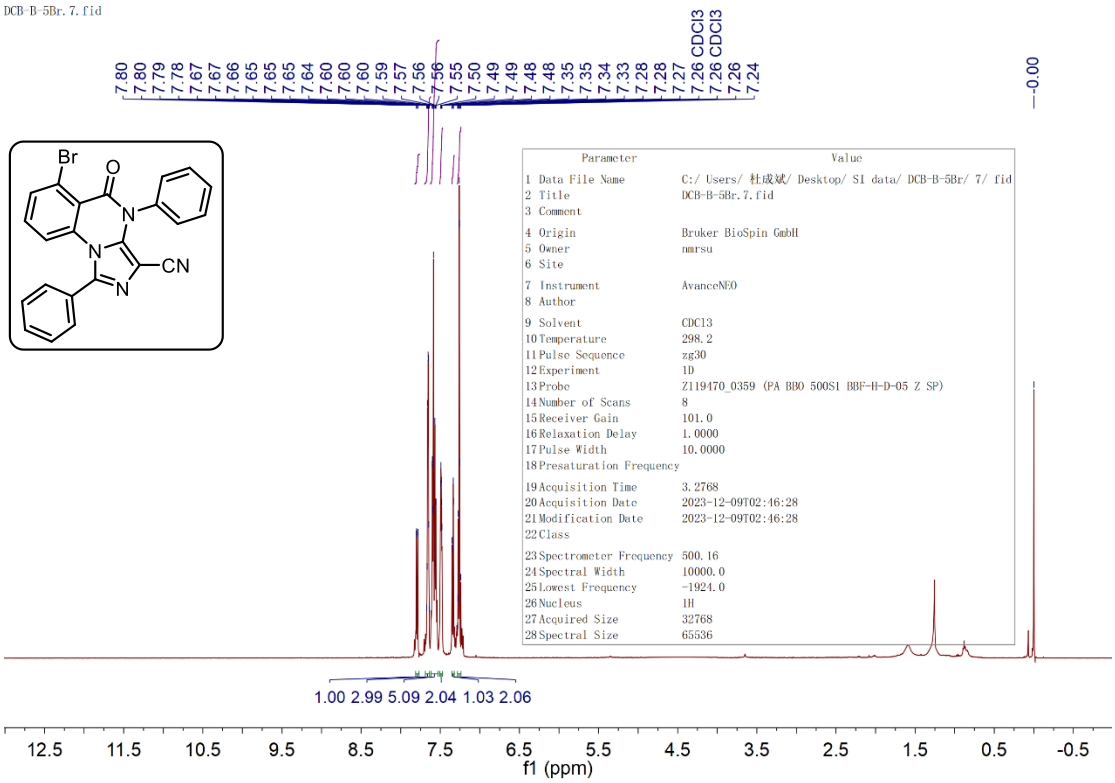


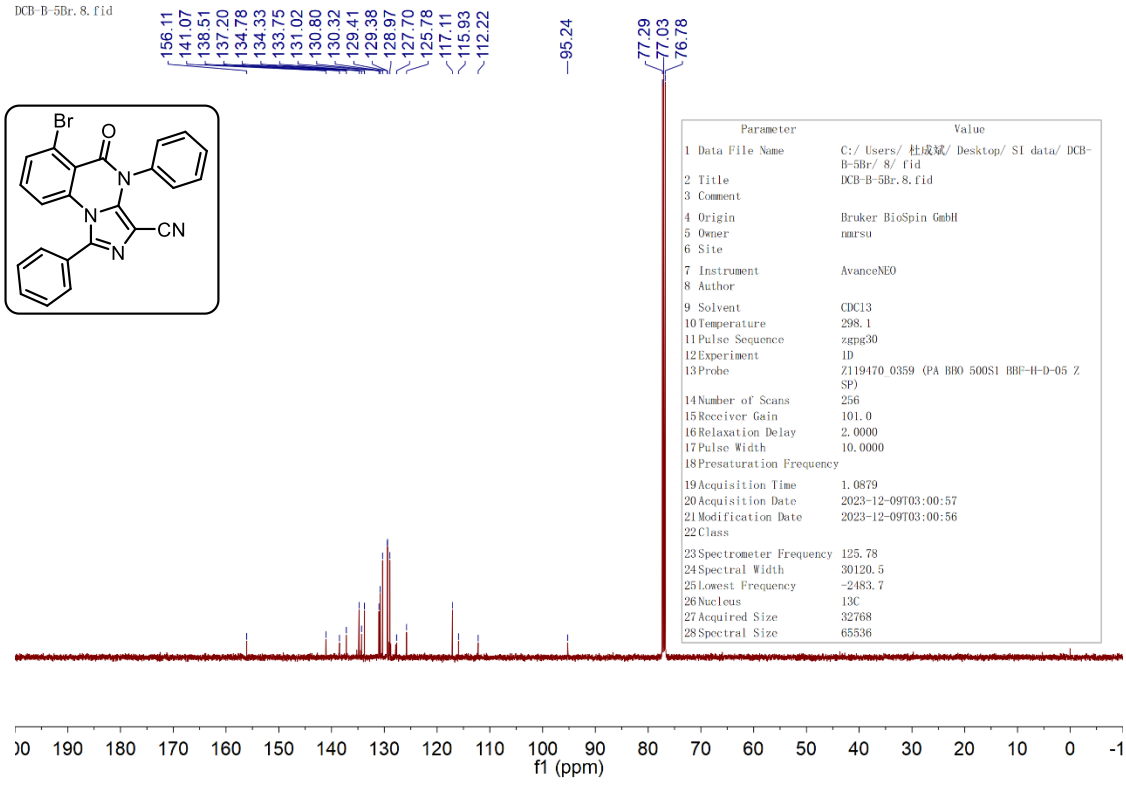
5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4aa)





6-bromo-5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ba)





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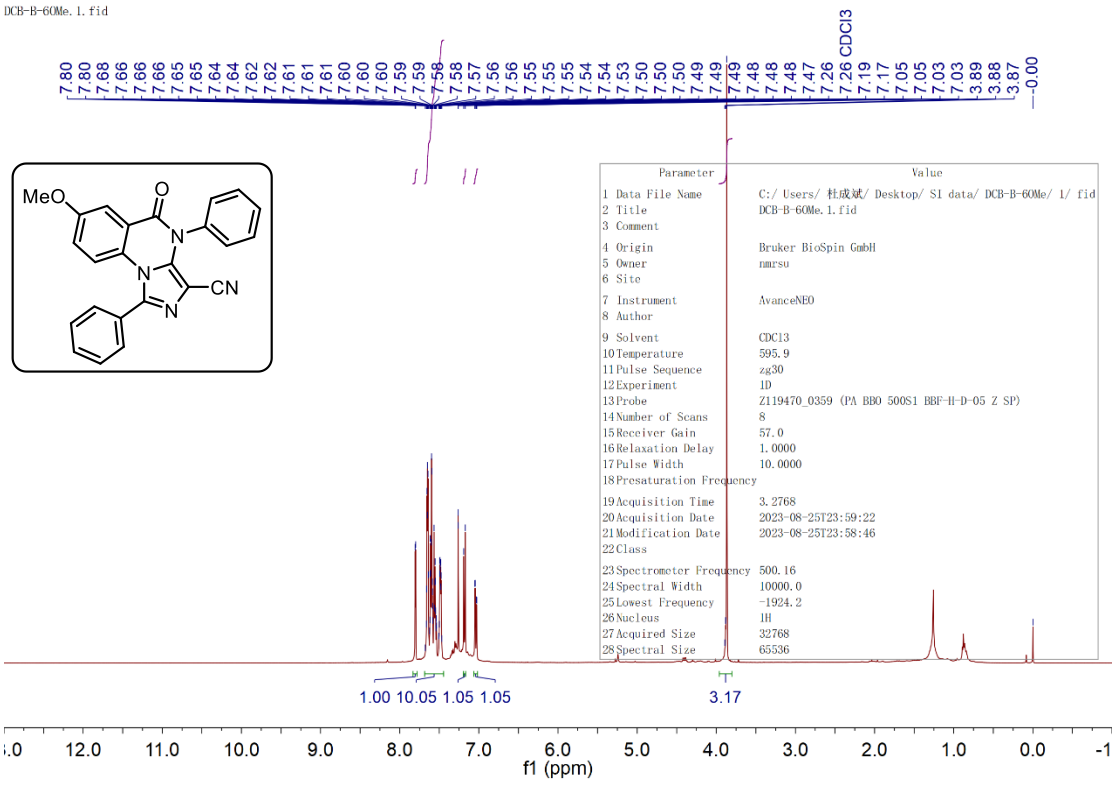

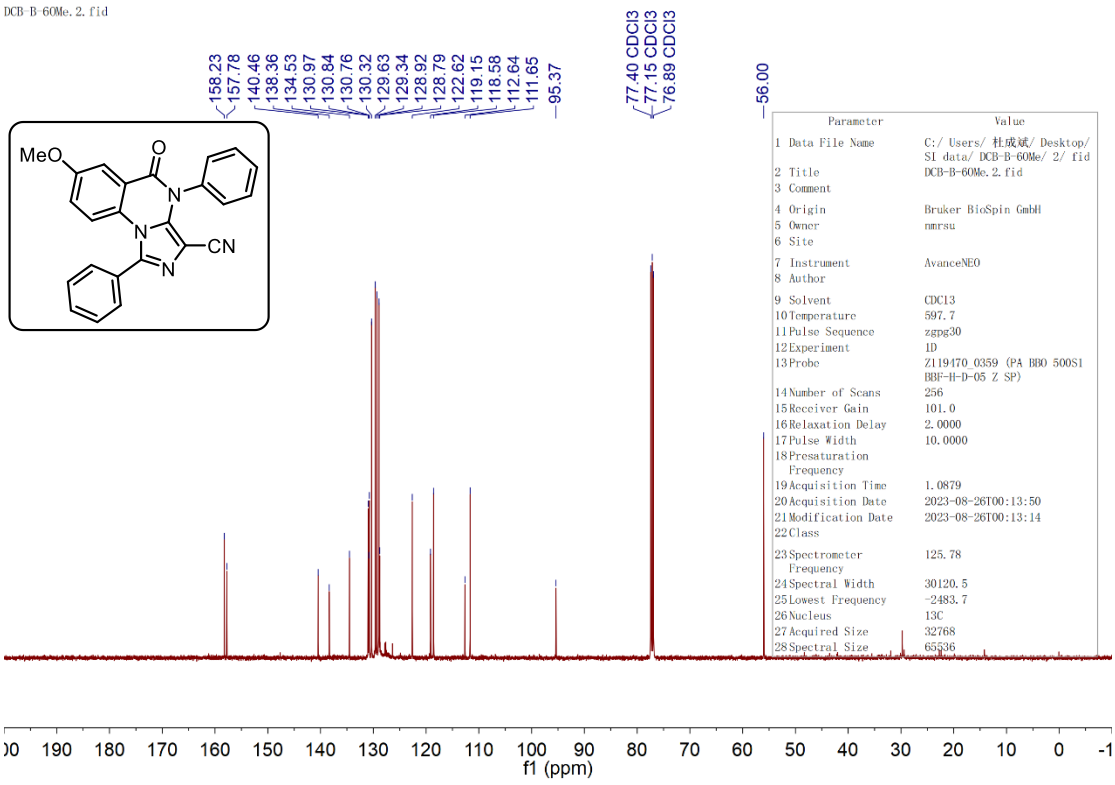

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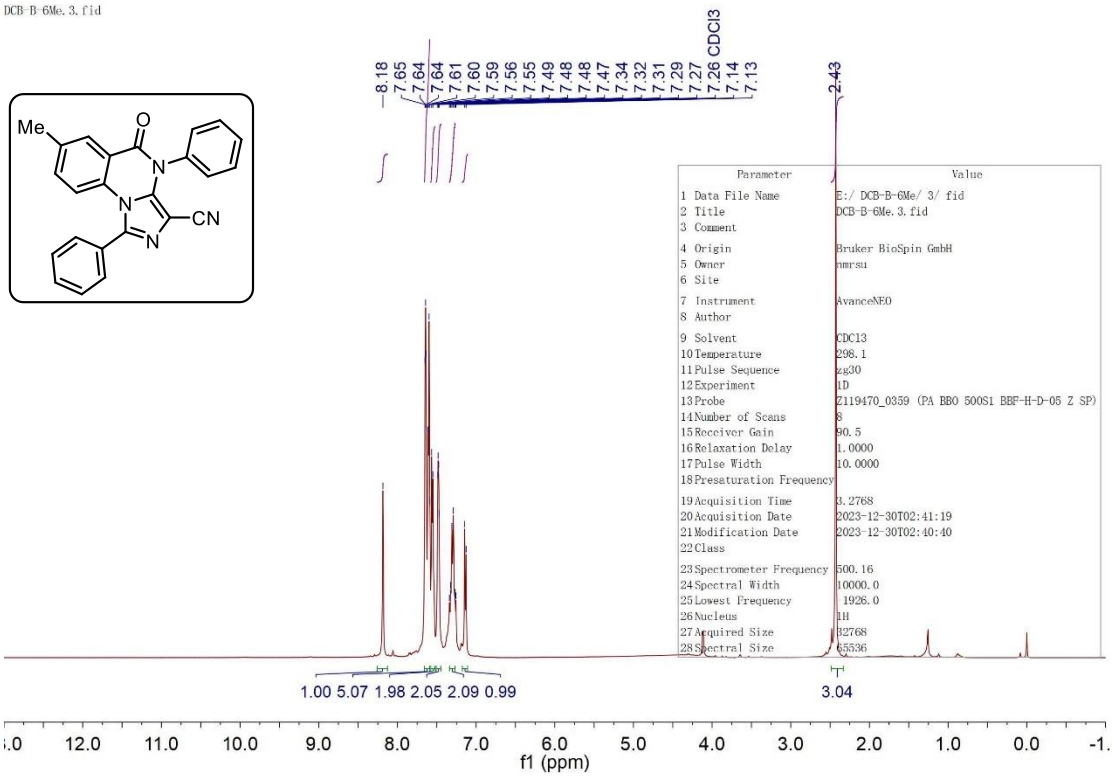

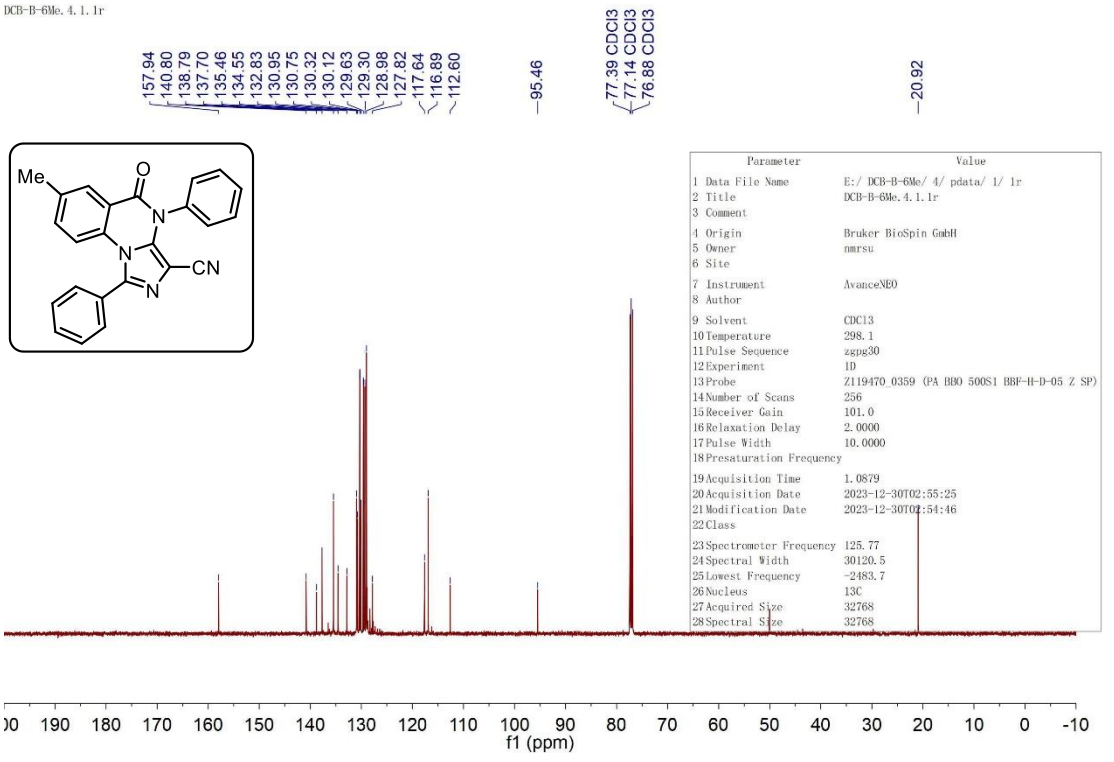

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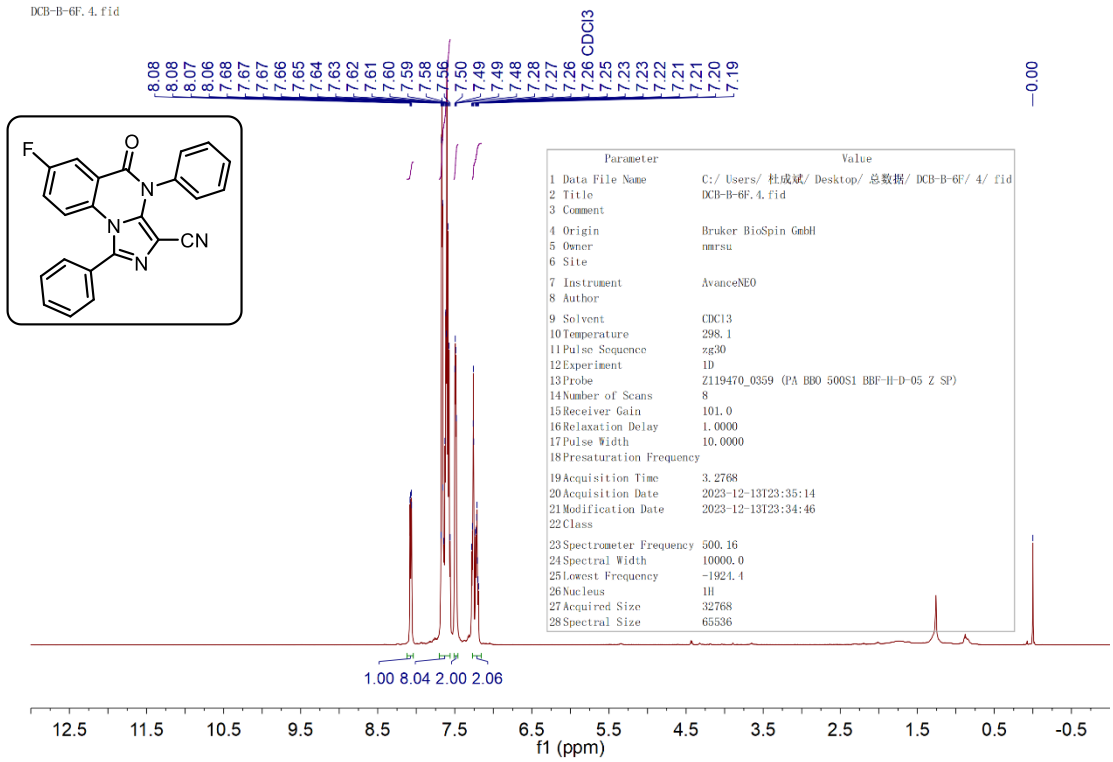

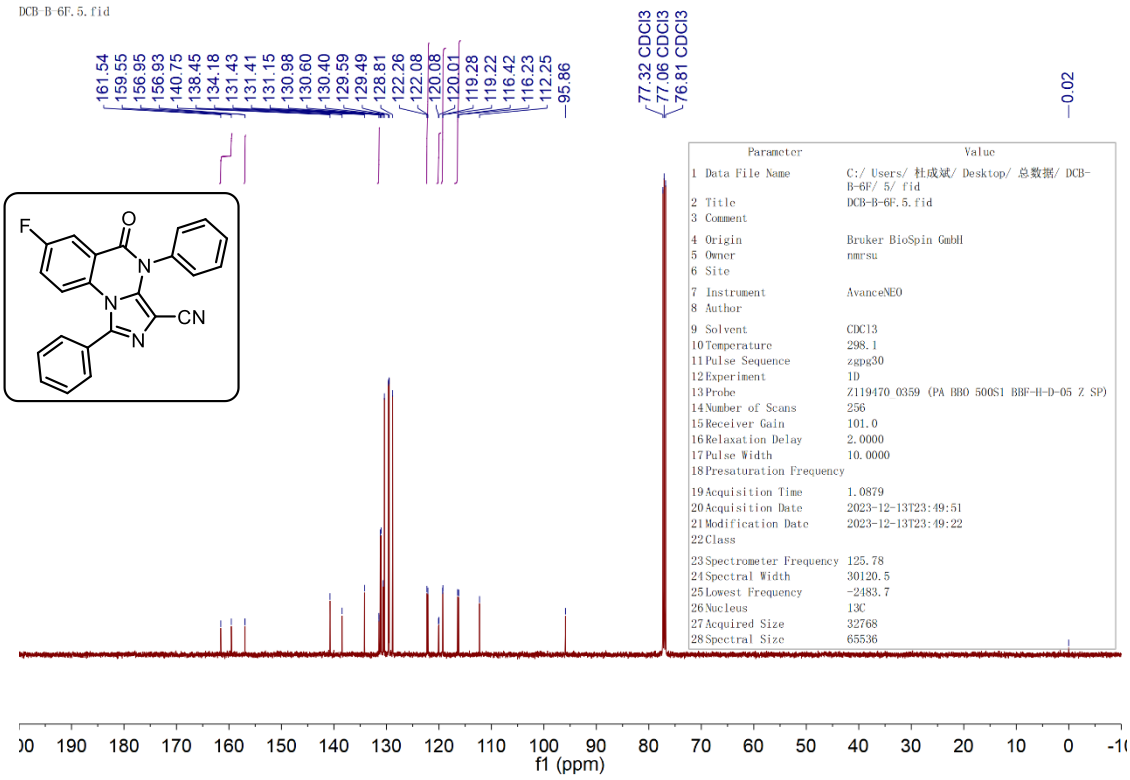

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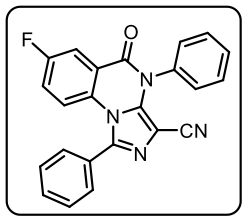

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11 Pulse Sequence	zgig
12 Experiment	1D
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14 Number of Scans	16
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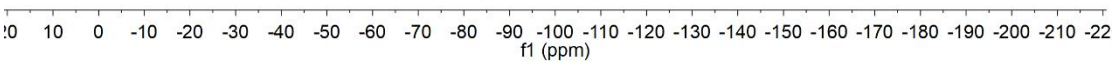

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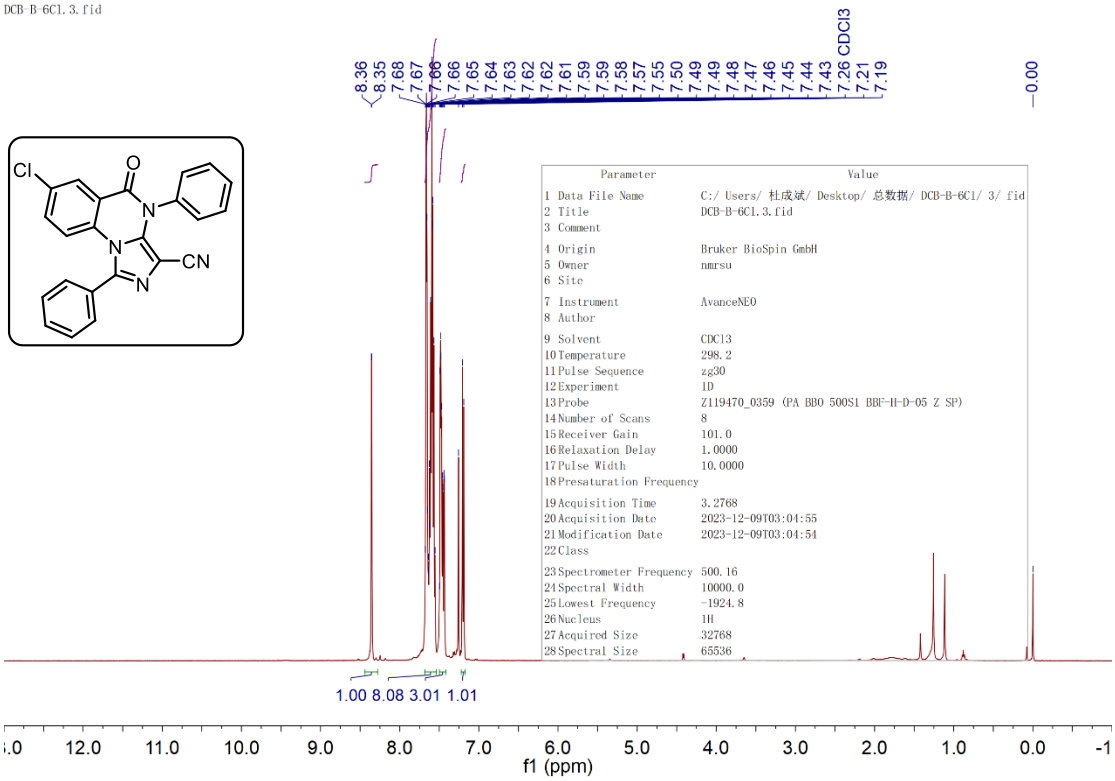
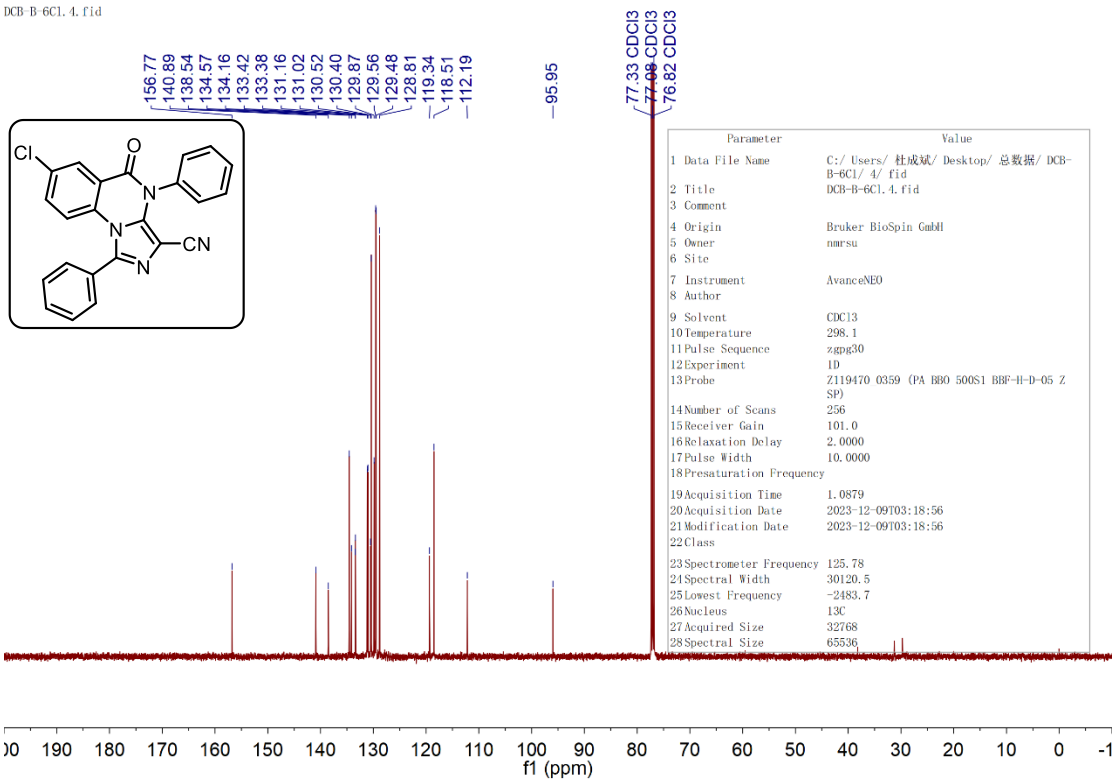
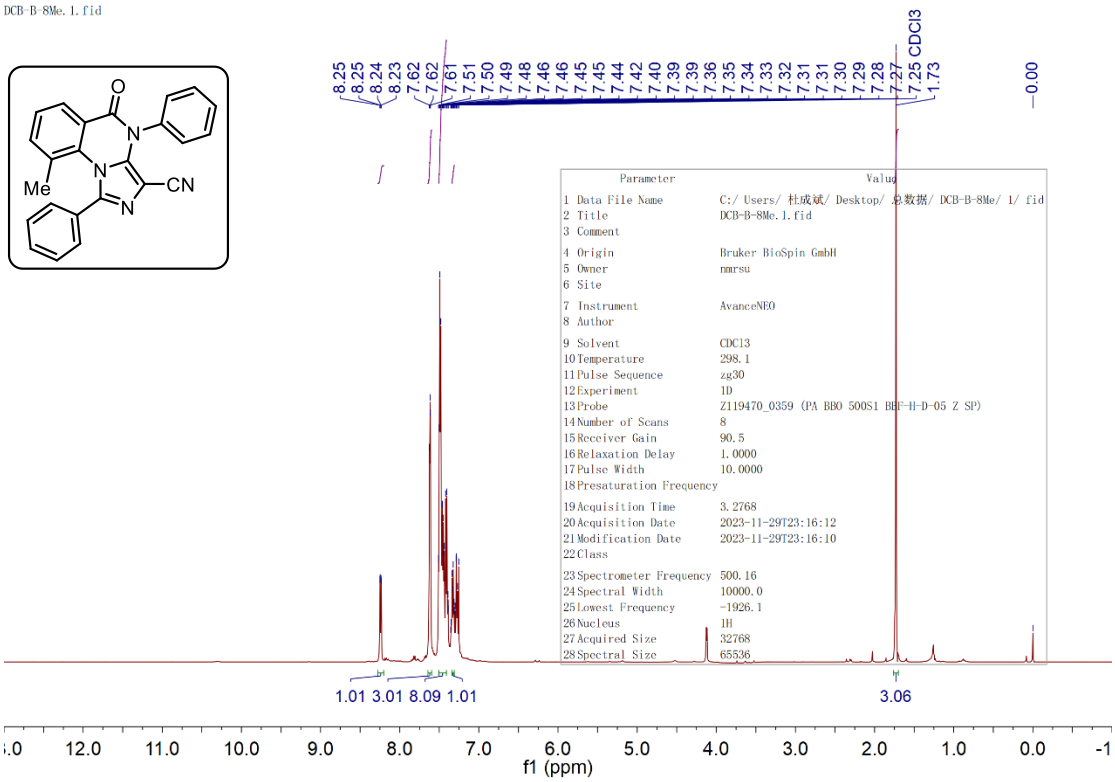
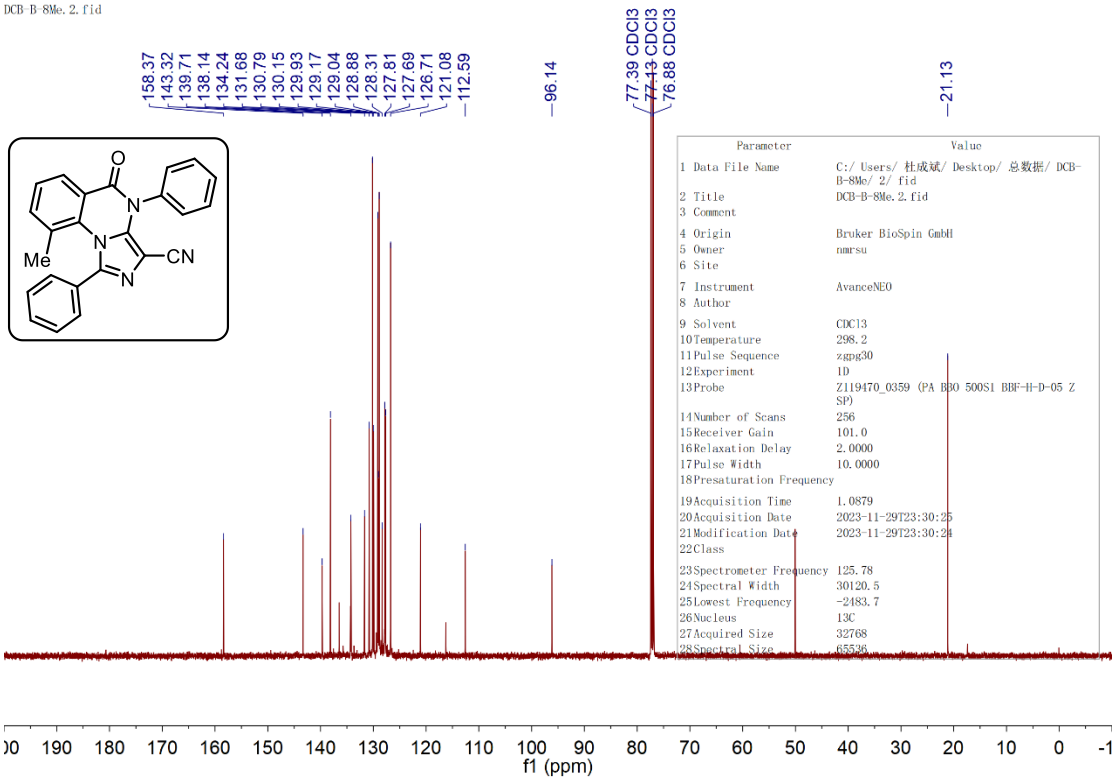




9-methyl-5-oxo-1,4-diphenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ga)





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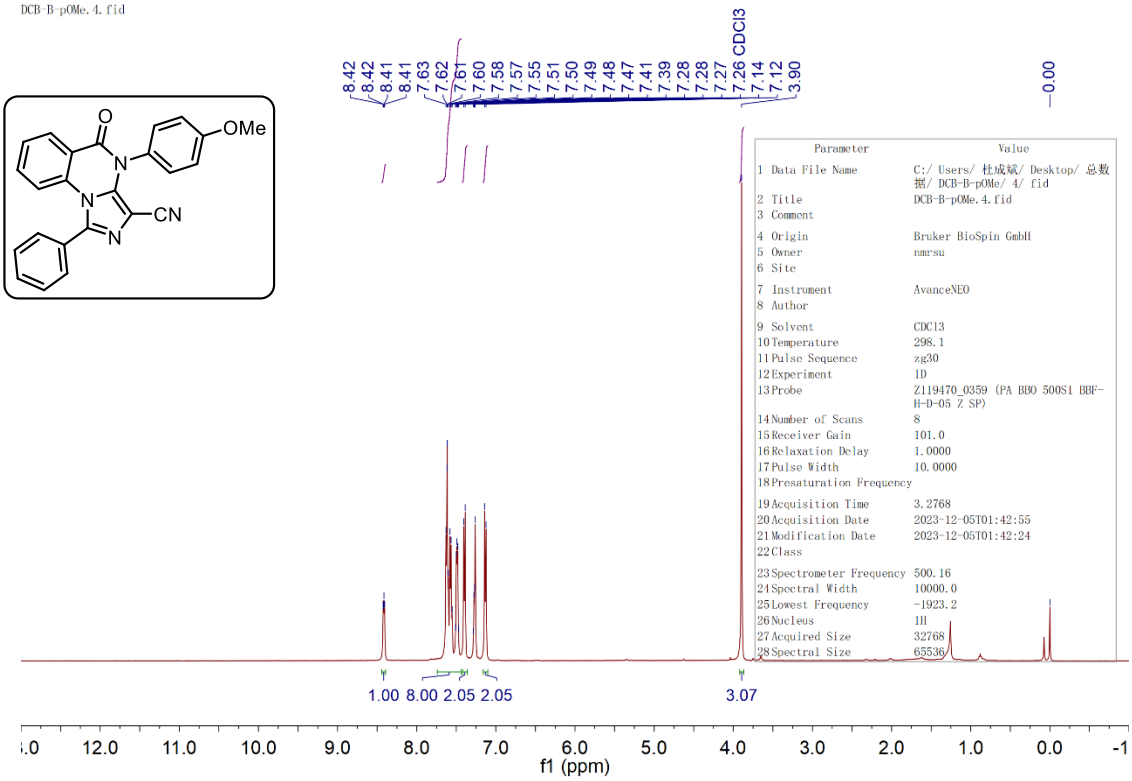

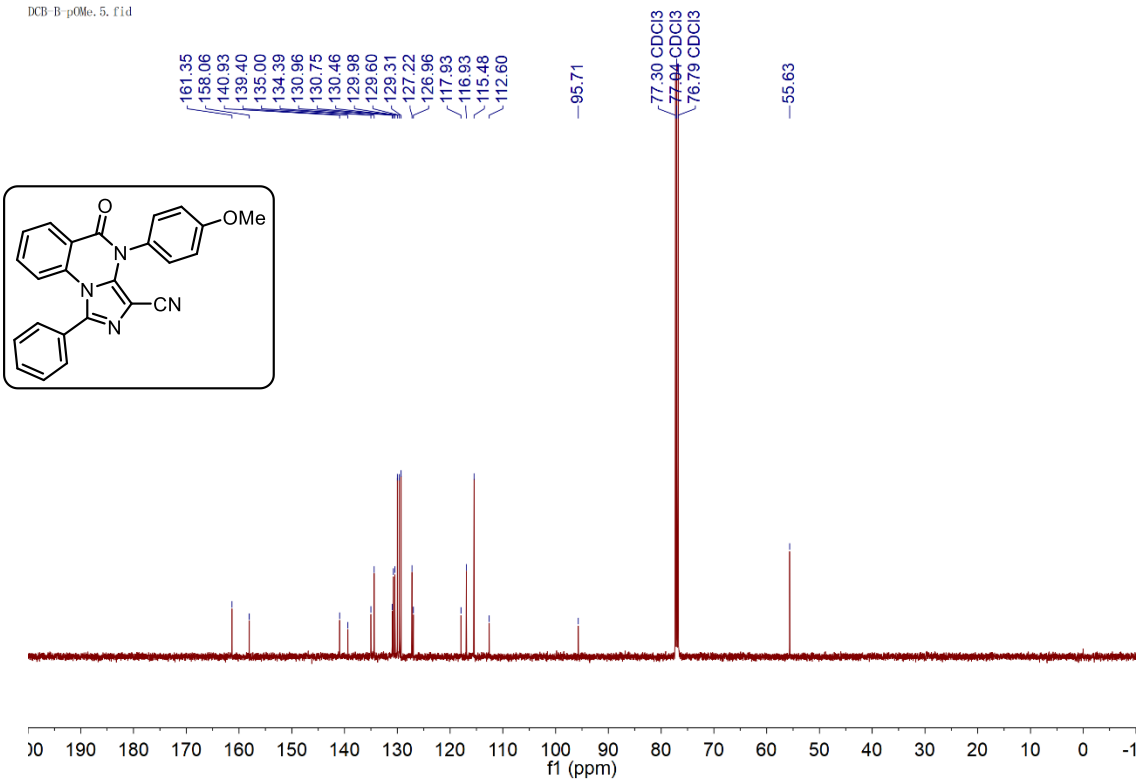

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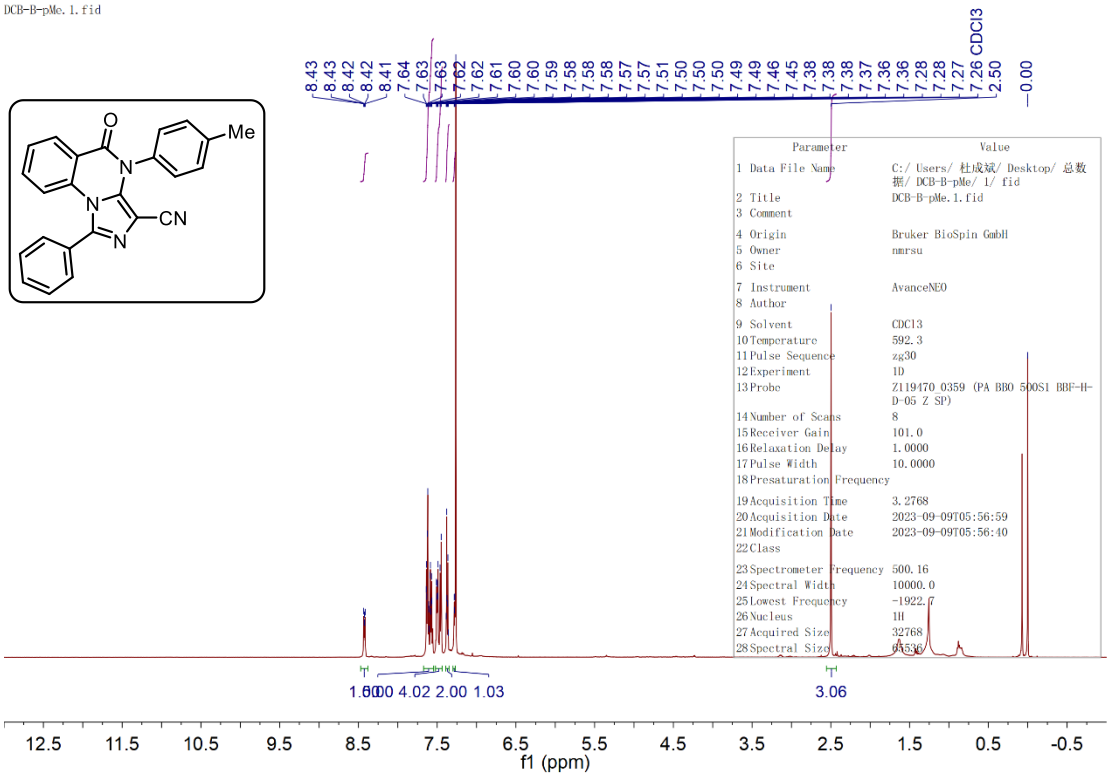

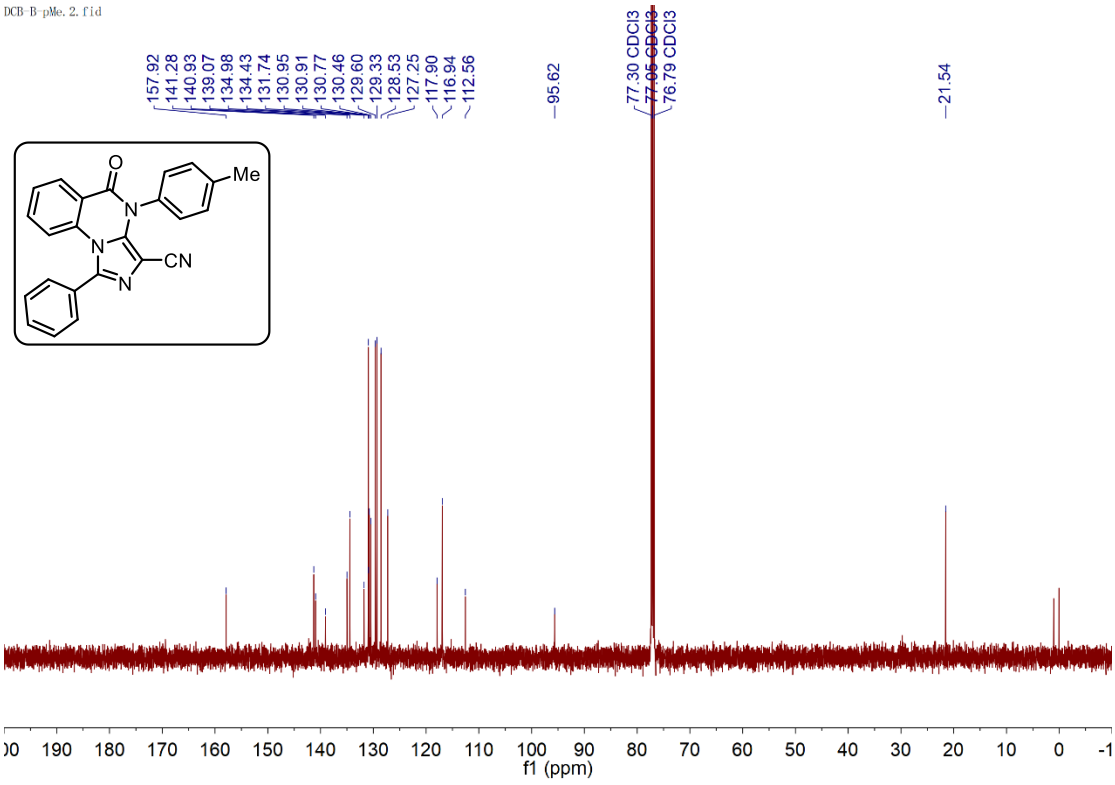

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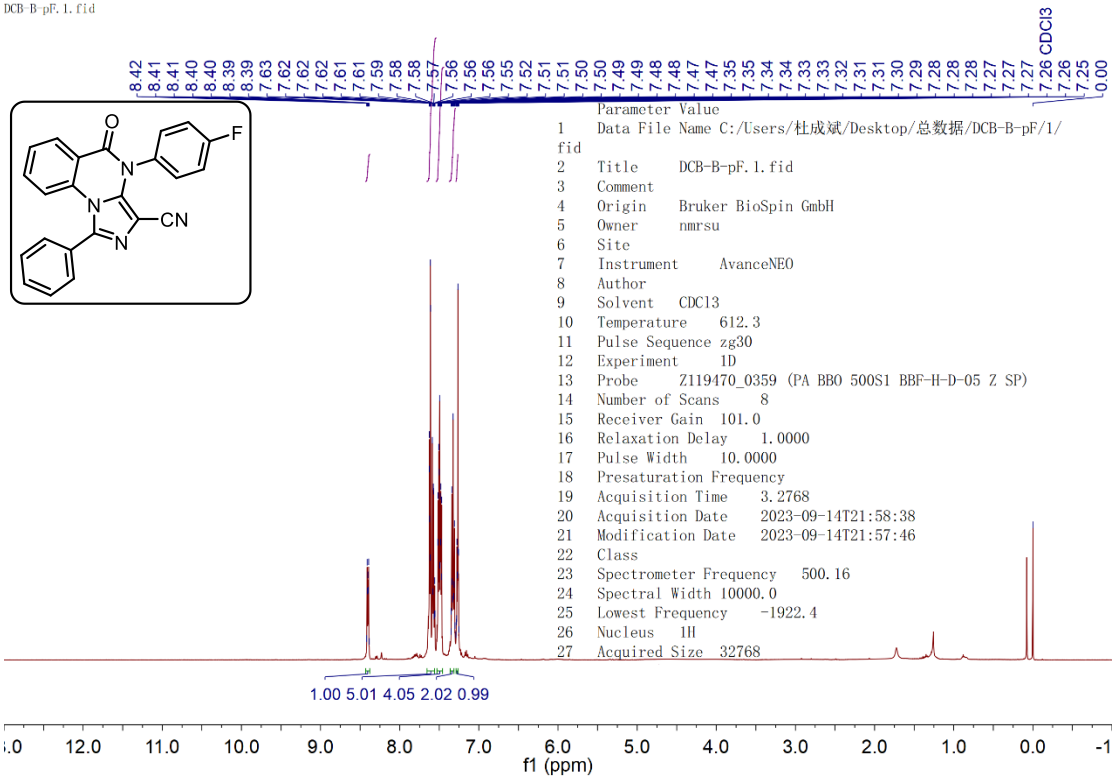
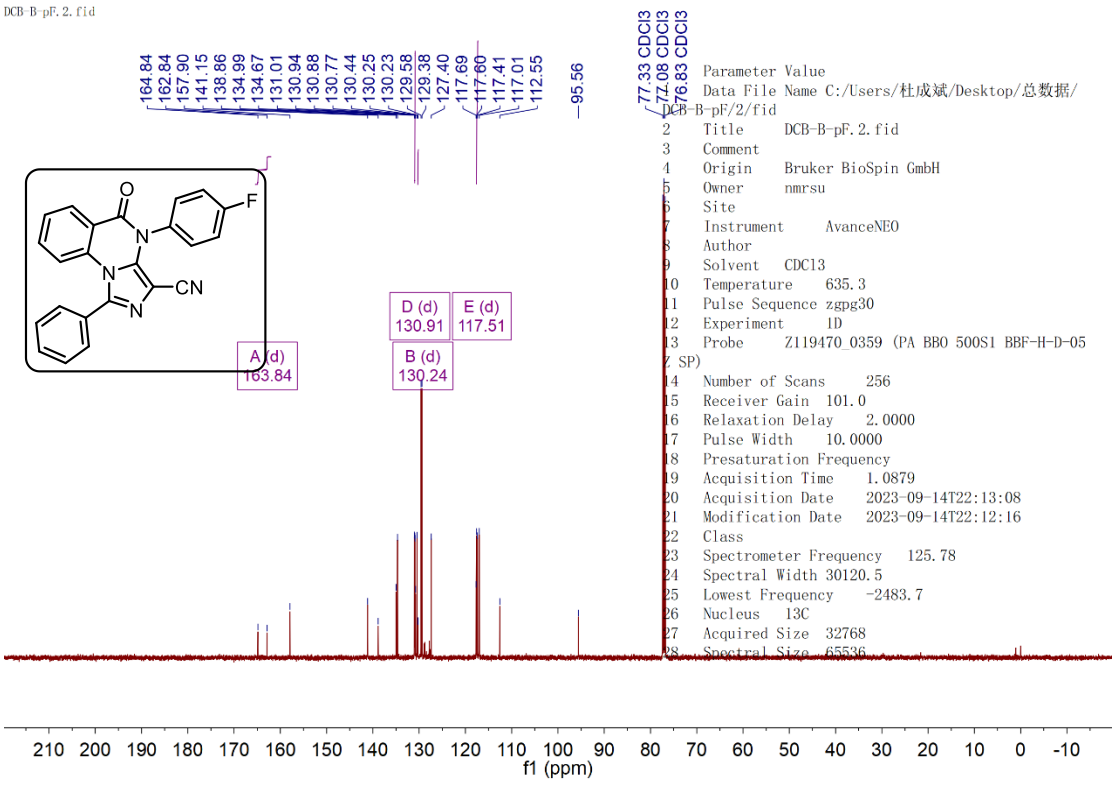
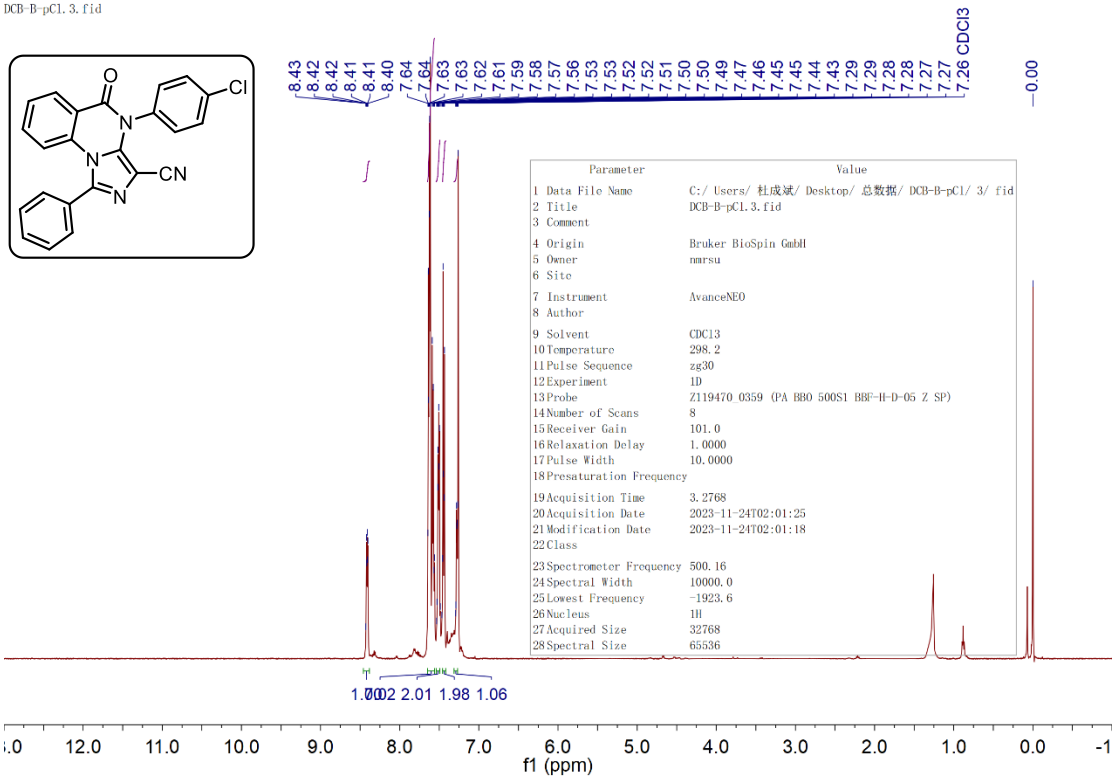
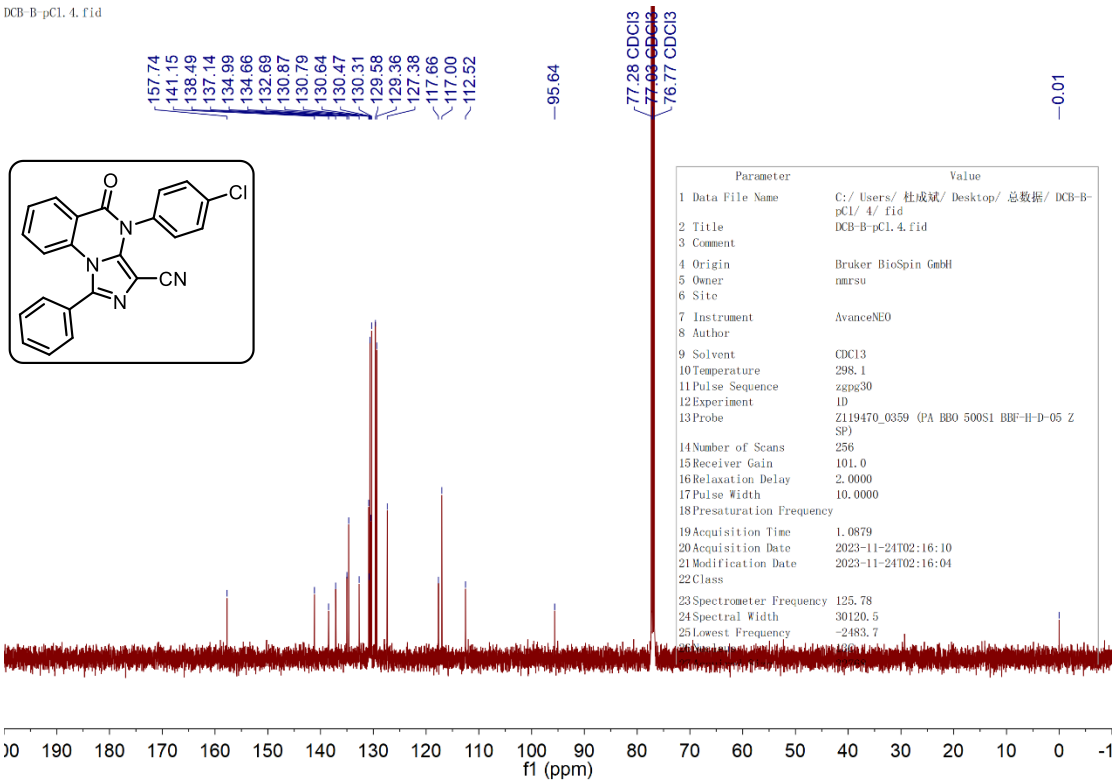


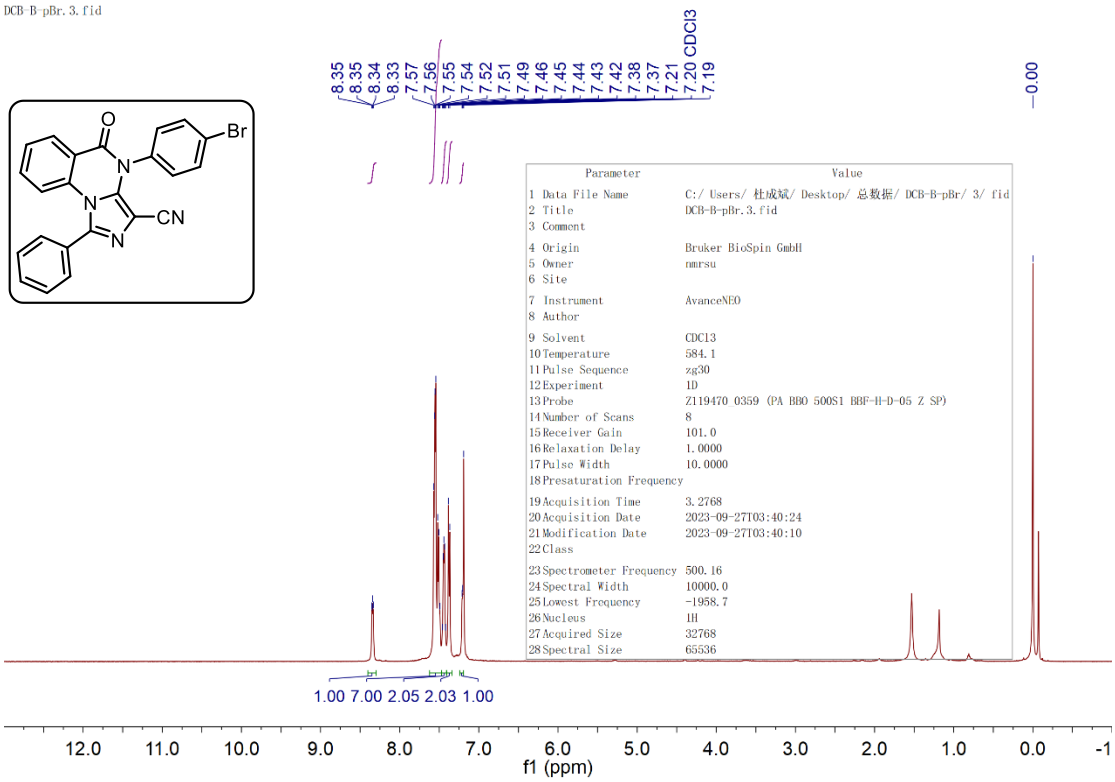


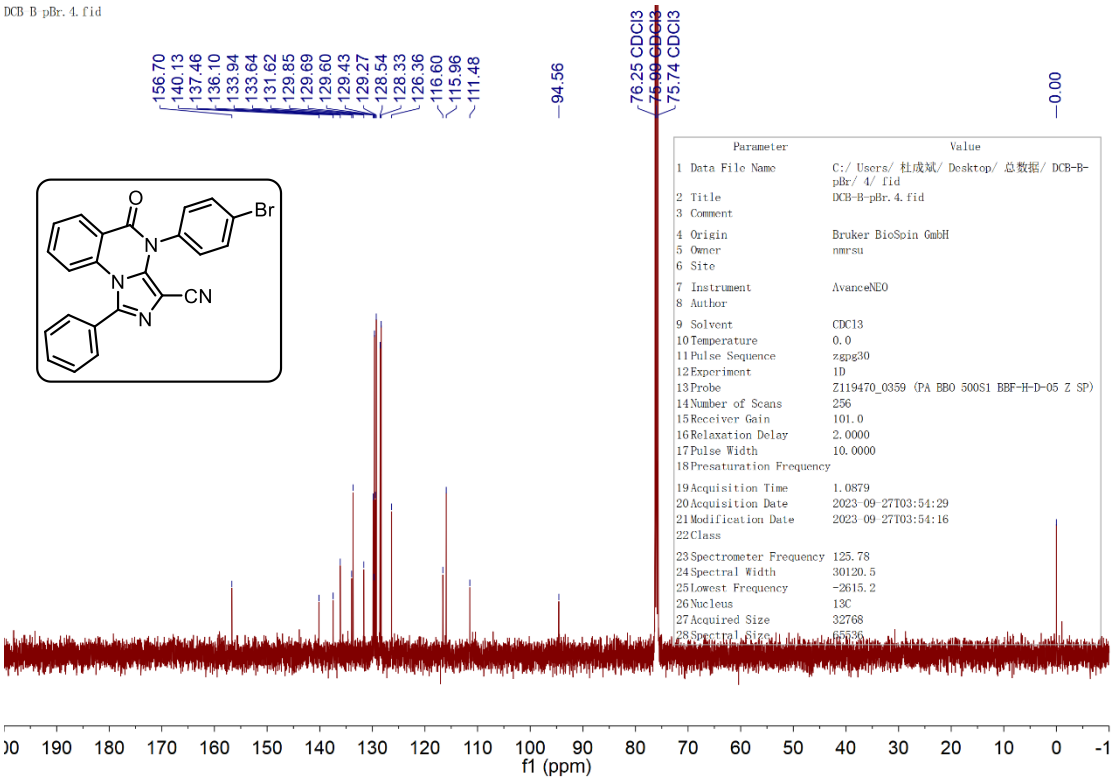
4-(4-chlorophenyl)-5-oxo-1-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ka)



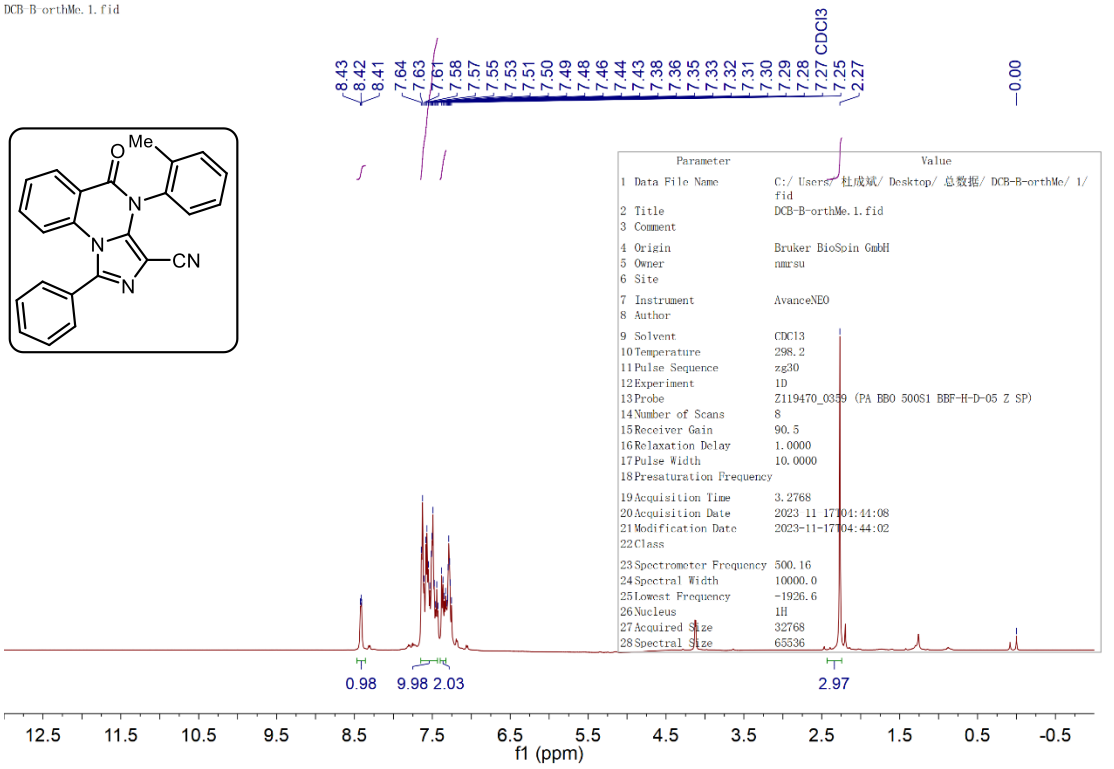


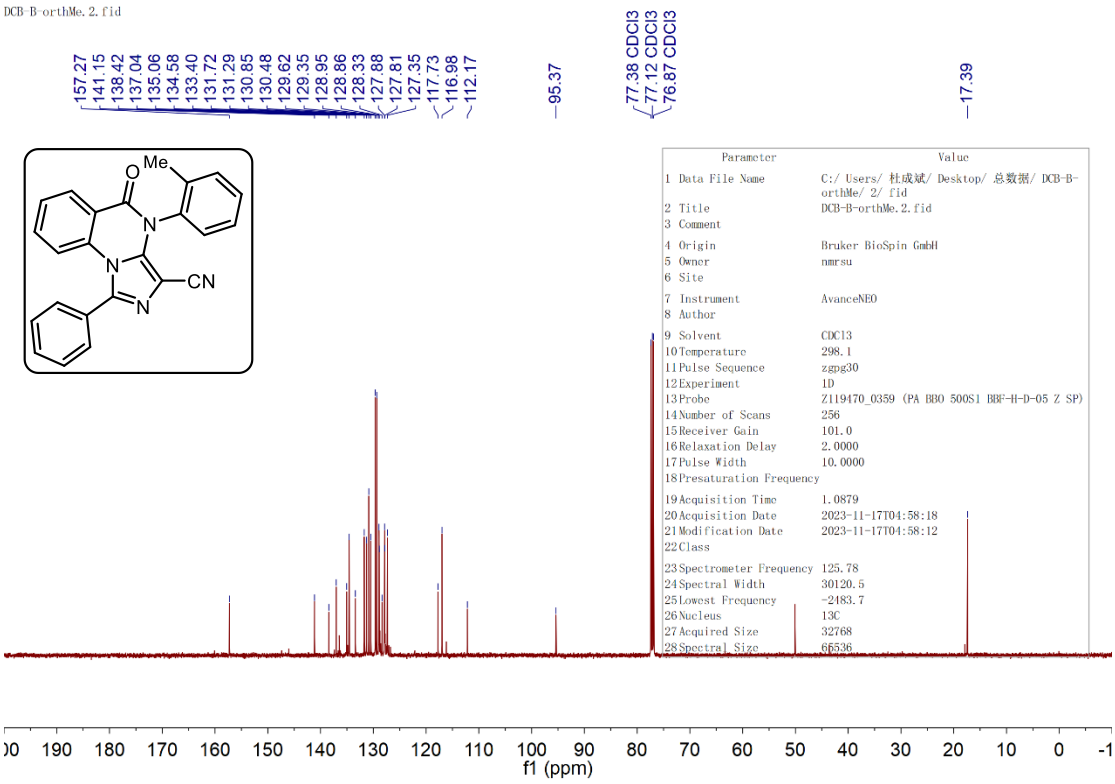
4-(4-bromophenyl)-5-oxo-1-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4la)



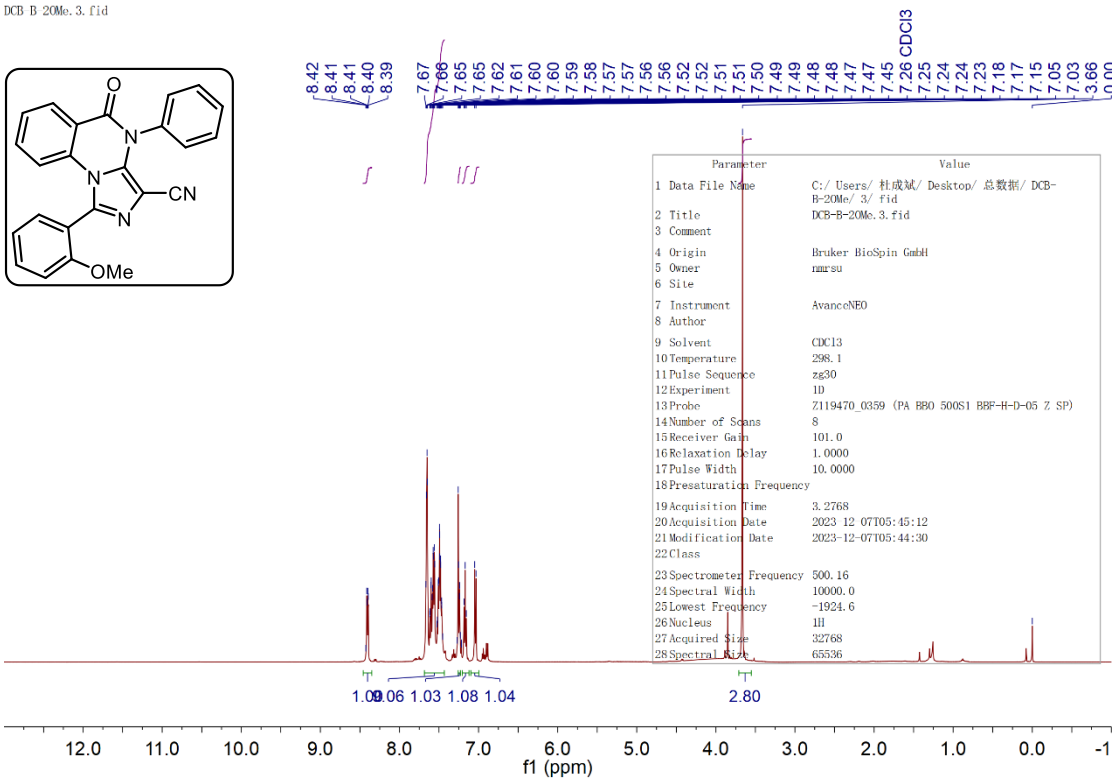


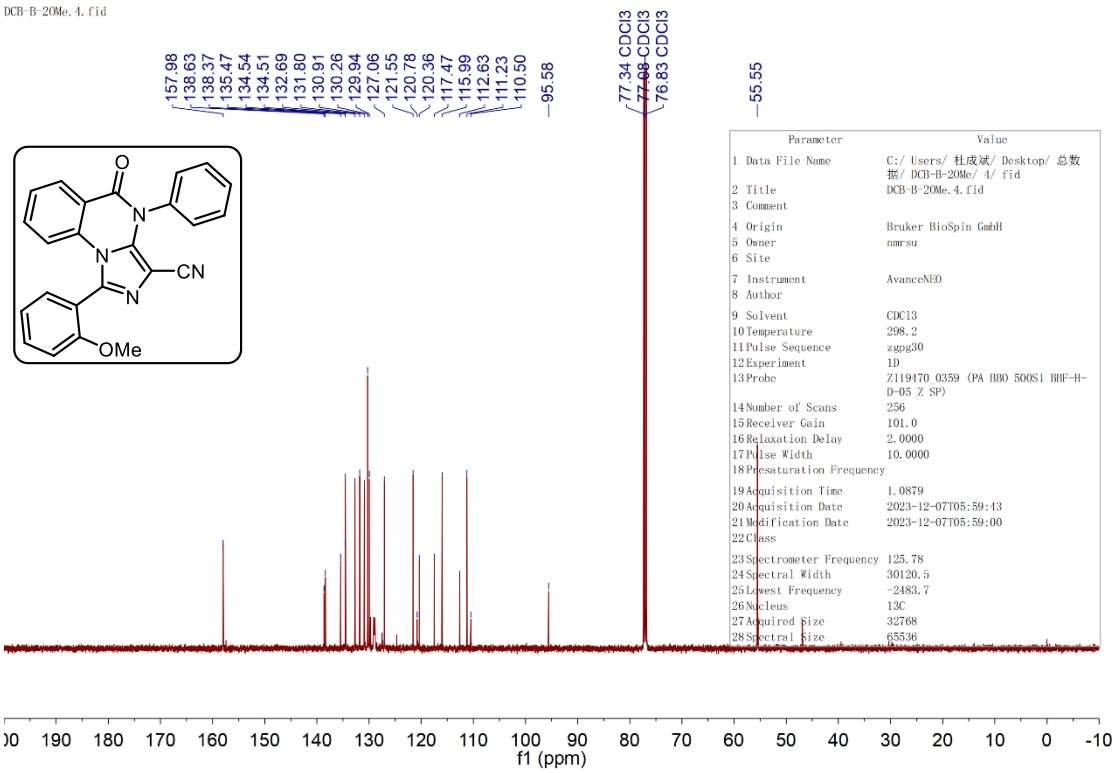
5-oxo-1-phenyl-4-(o-tolyl)-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ma)



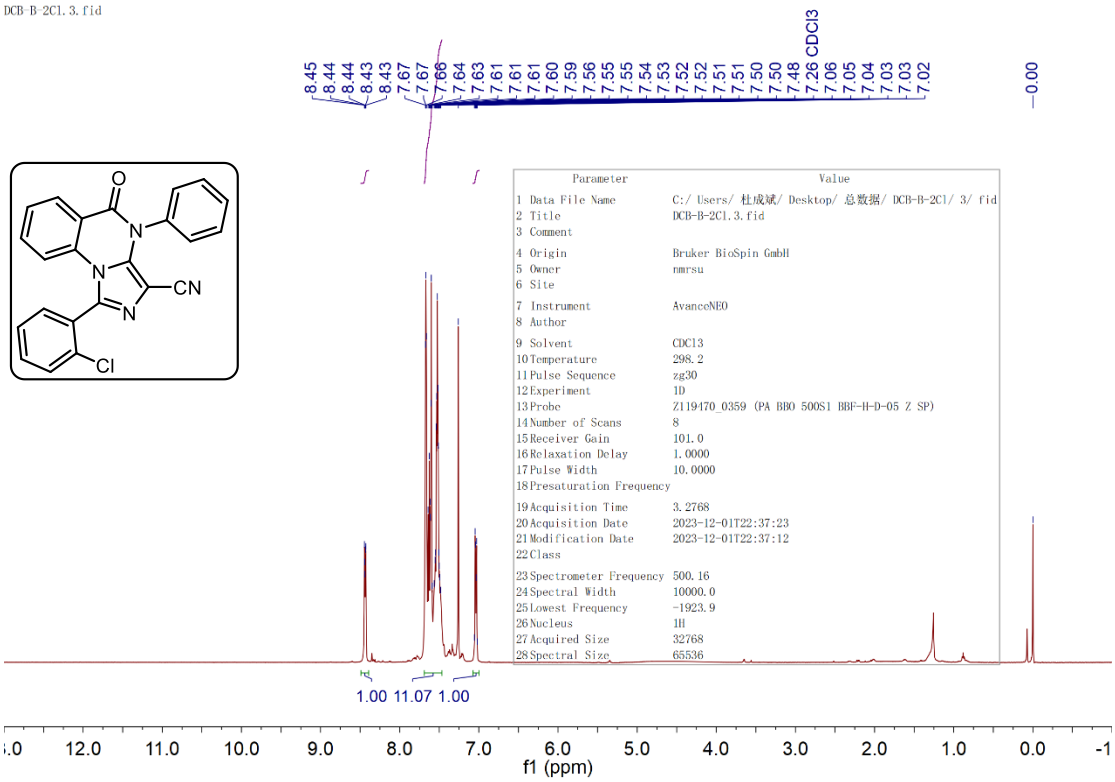


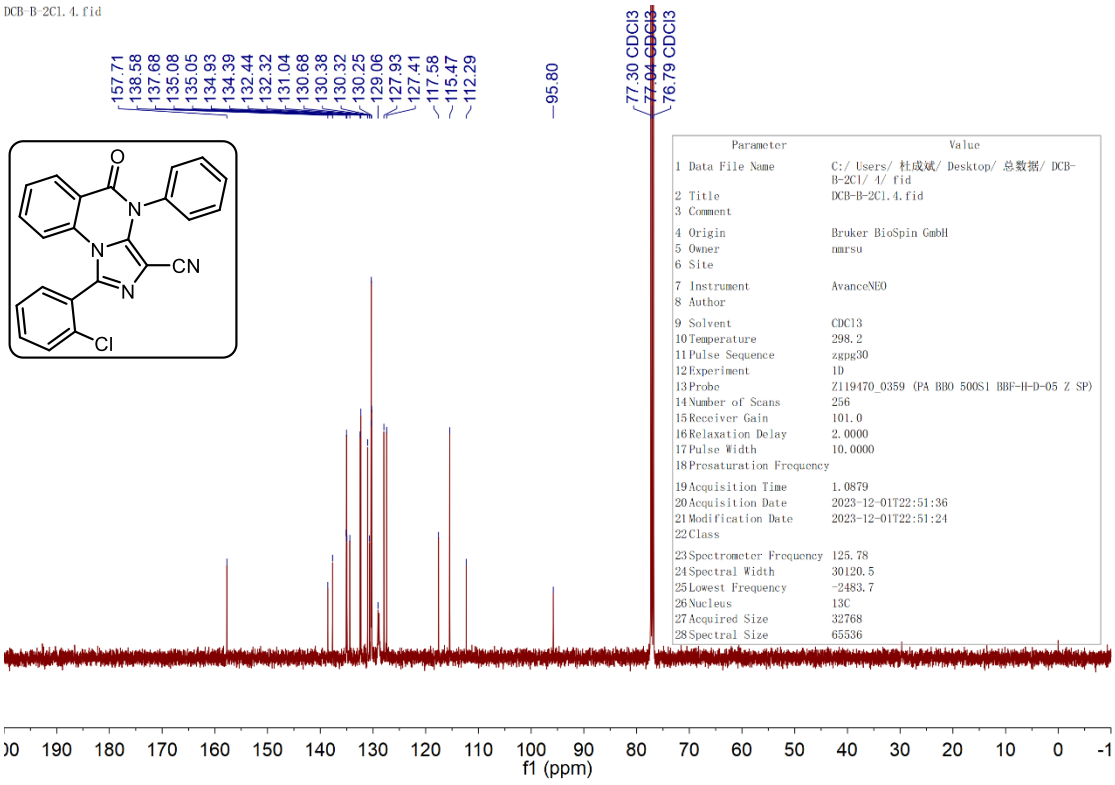
1-(2-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ab)



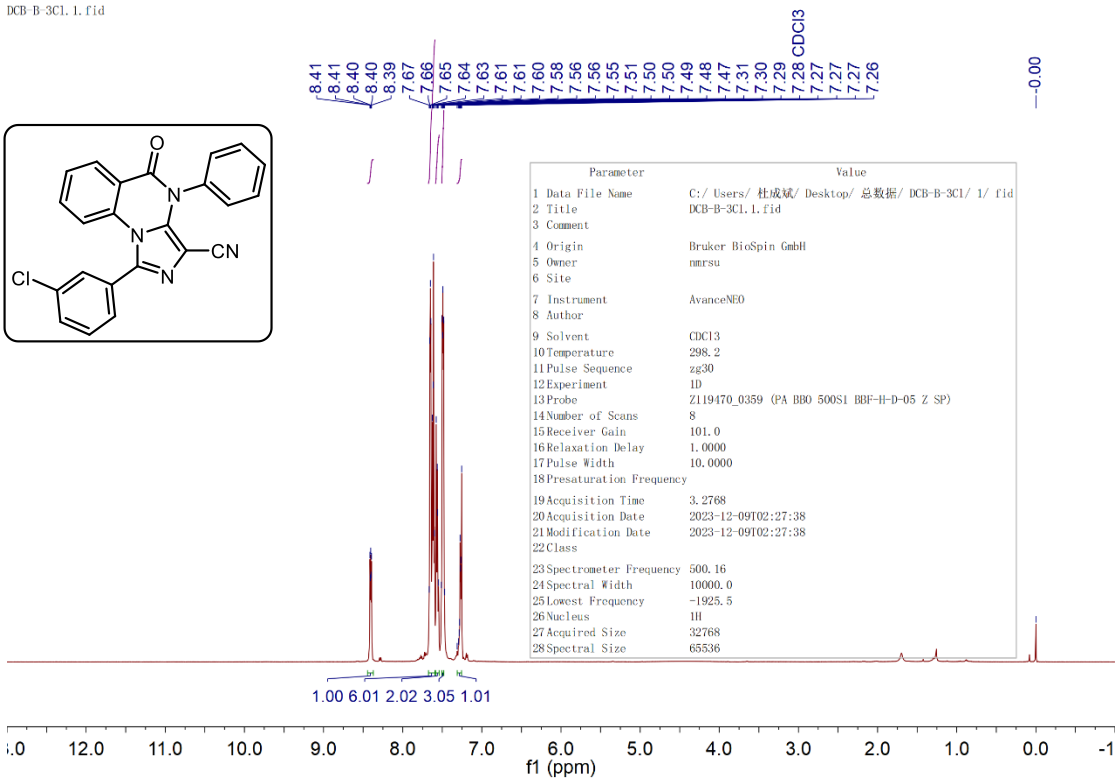


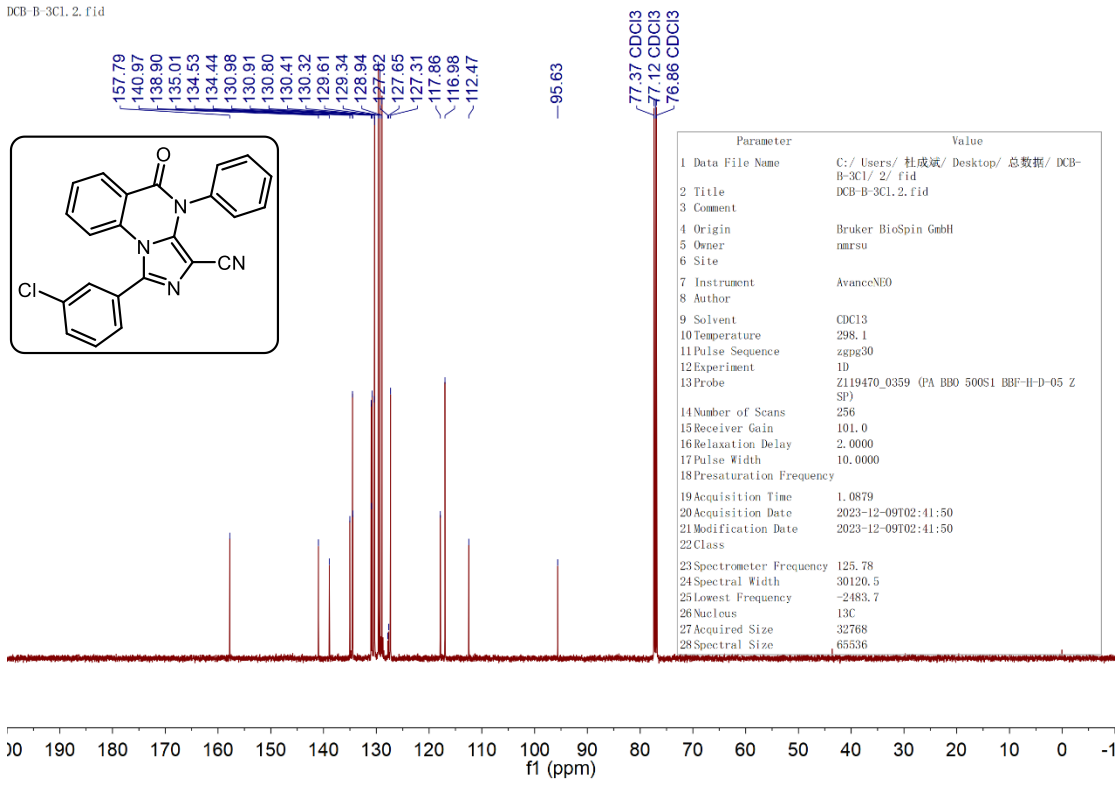
1-(2-chlorophenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ac)



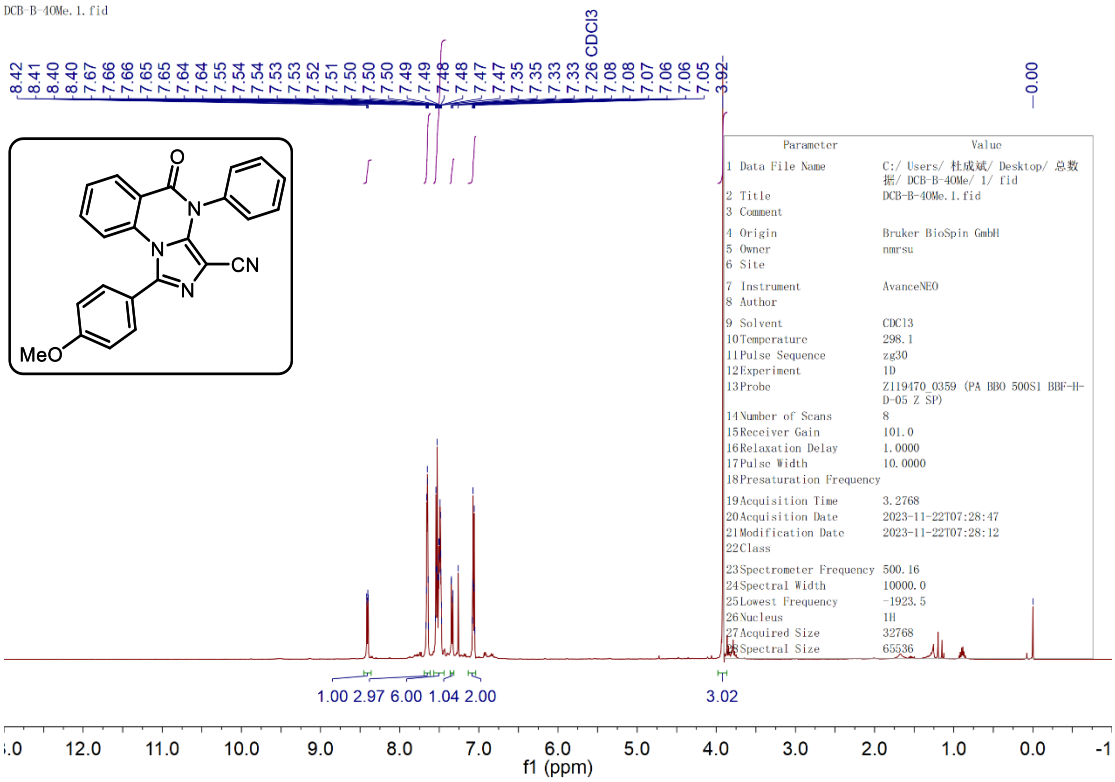


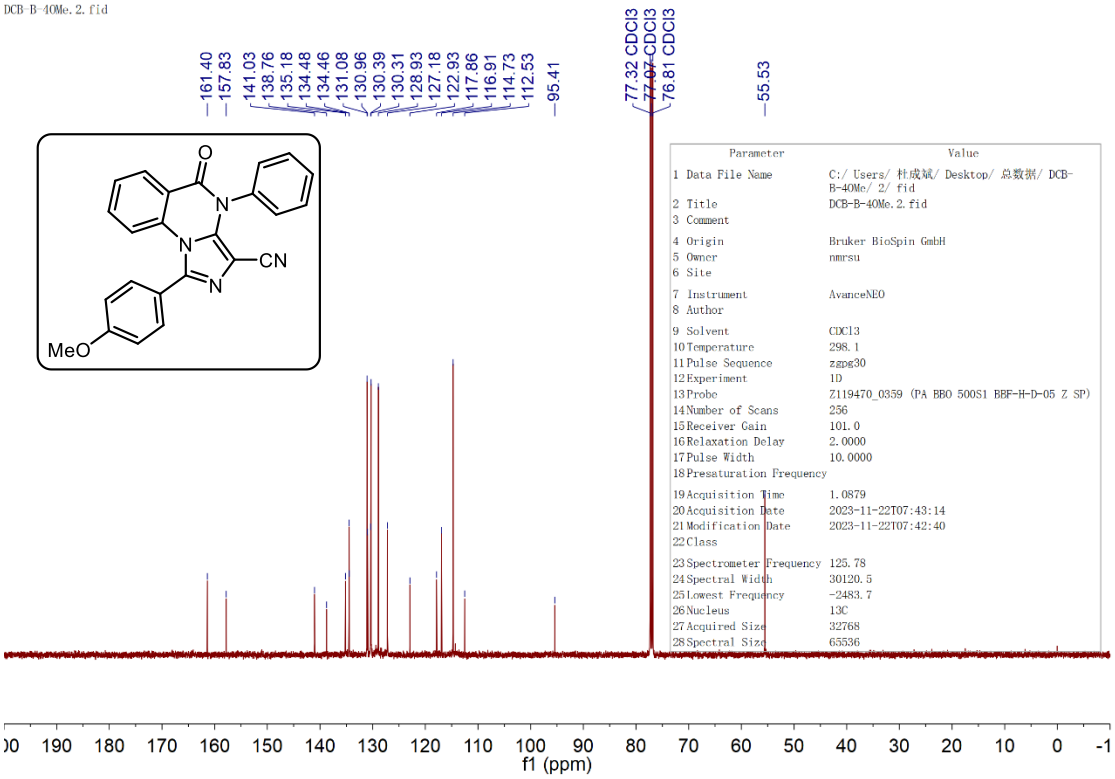
1-(3-chlorophenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ad)



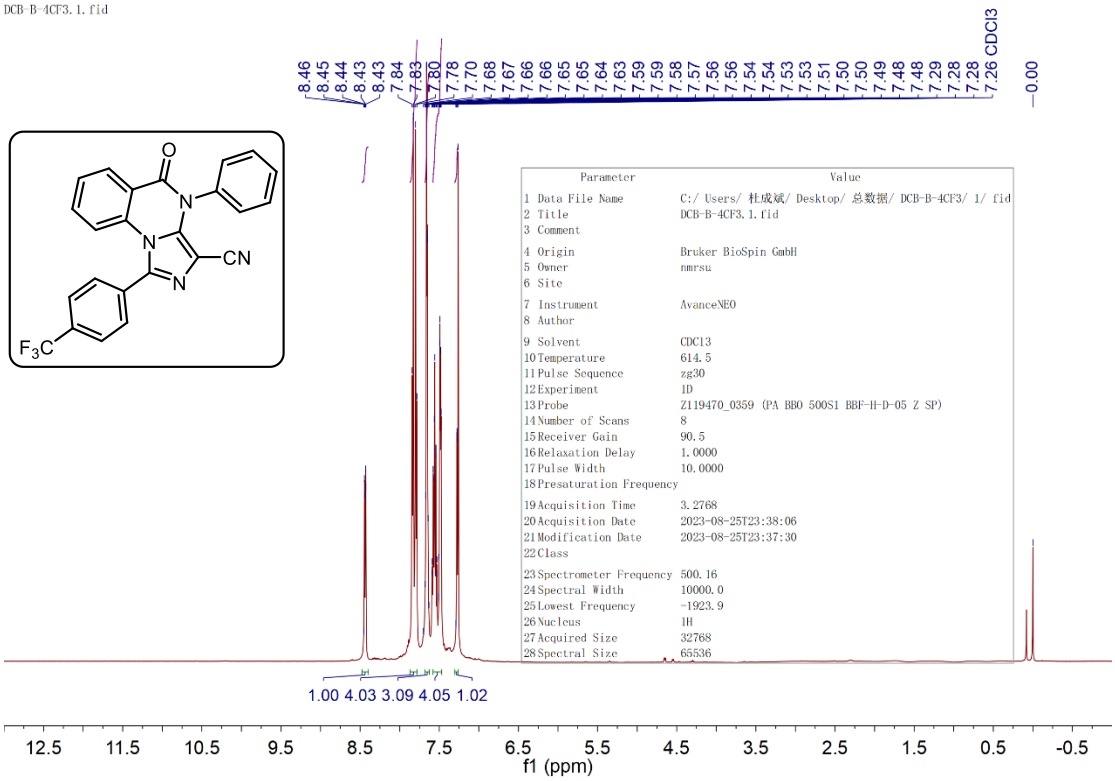


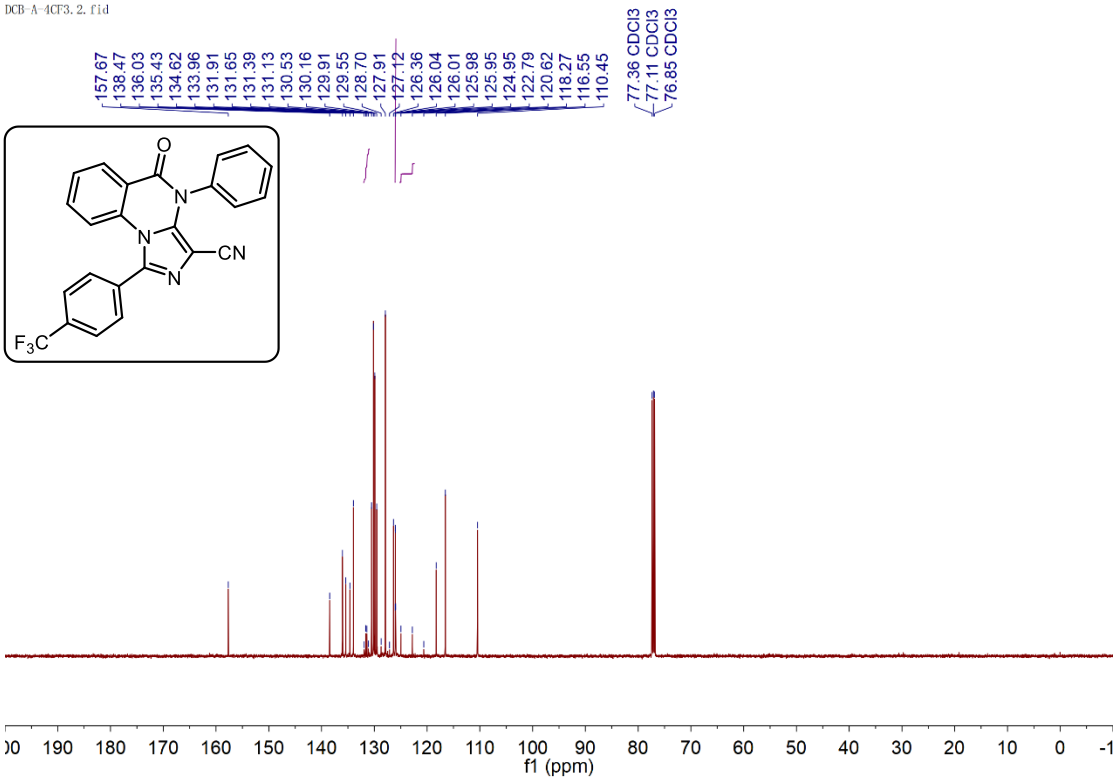
1-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ae)





5-oxo-4-phenyl-1-(4-(trifluoromethyl)phenyl)-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4af)





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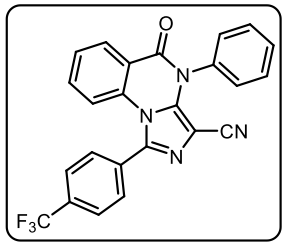

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5 Owner	nmrsu
6 Site	
7 Instrument	AvanceNEO
8 Author	
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11 Pulse Sequence	zgig
12 Experiment	1D
13 Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
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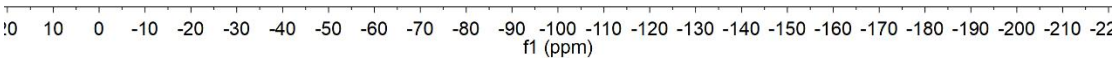
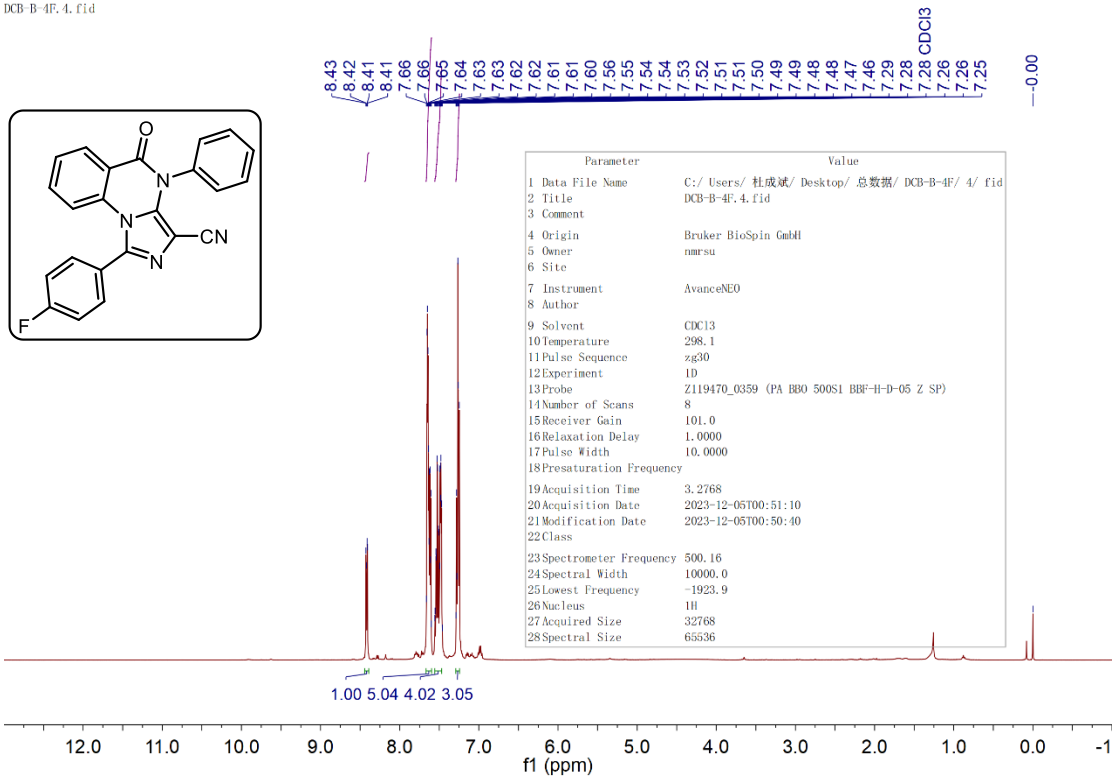
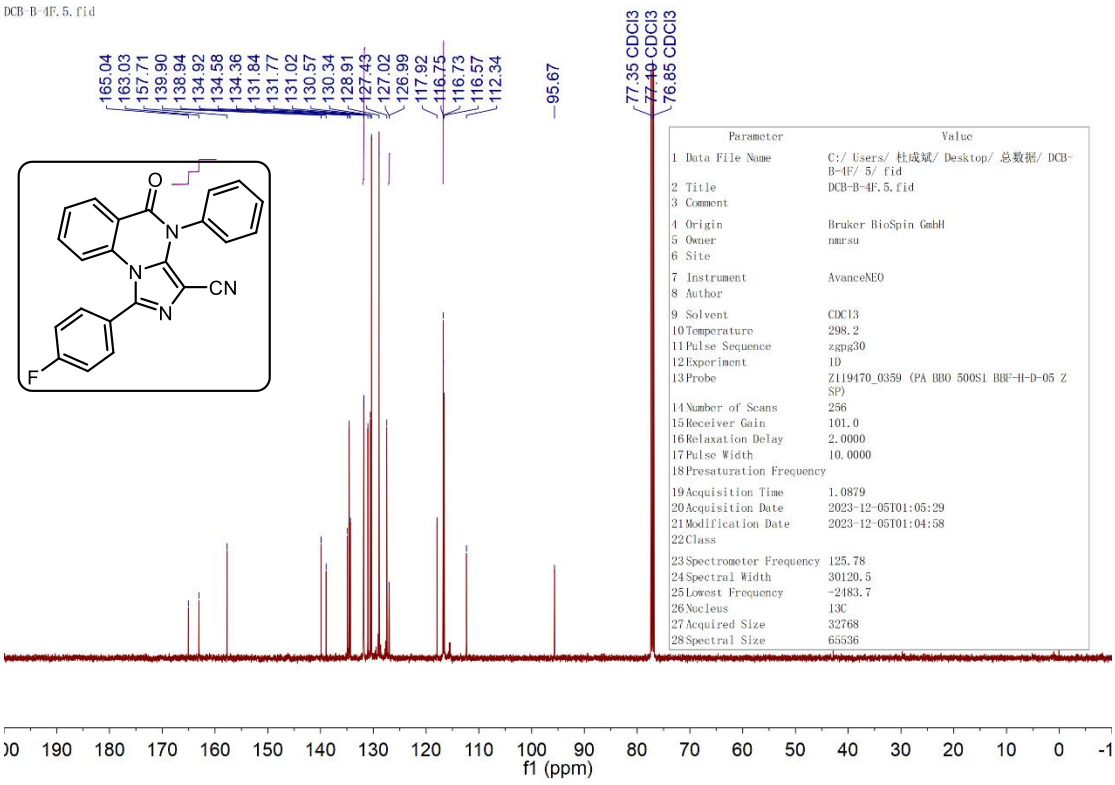


1-(4-fluorophenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ag)





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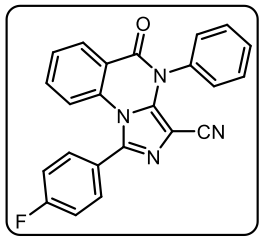

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5 Owner	nmrsu
6 Site	
7 Instrument	AvanceNEO
8 Author	
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10 Temperature	0.0
11 Pulse Sequence	zgig
12 Experiment	1D
13 Probe	Z119470_0359 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	15.0000
18 Presaturation Frequency	
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22 Class	
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27 Acquired Size	65536
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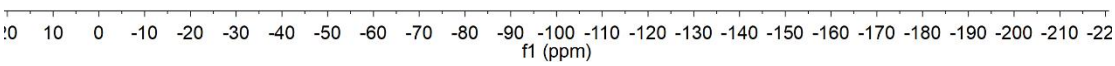
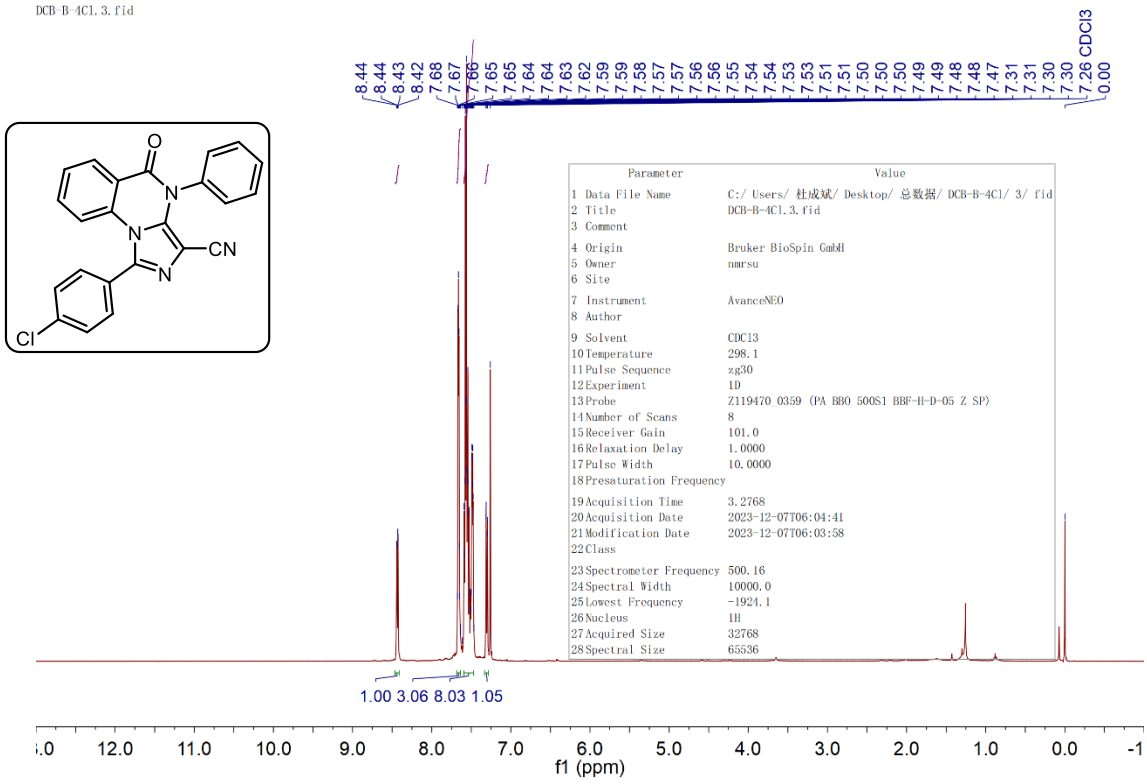
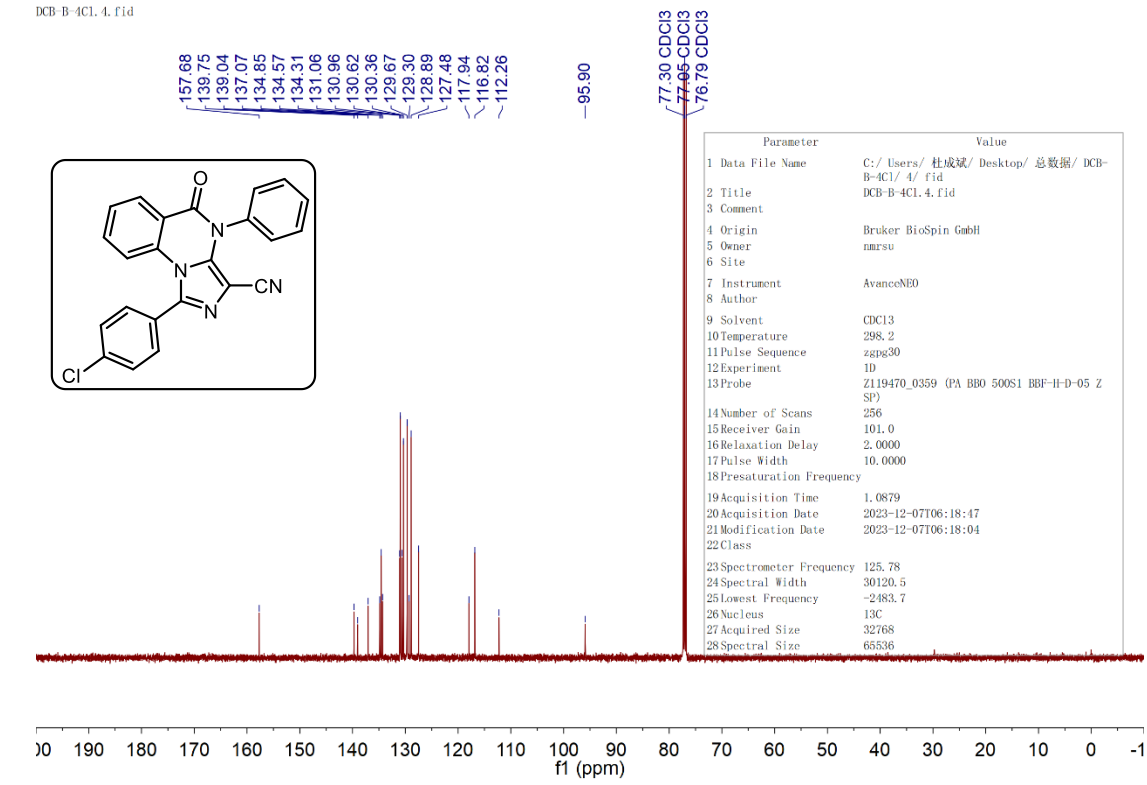
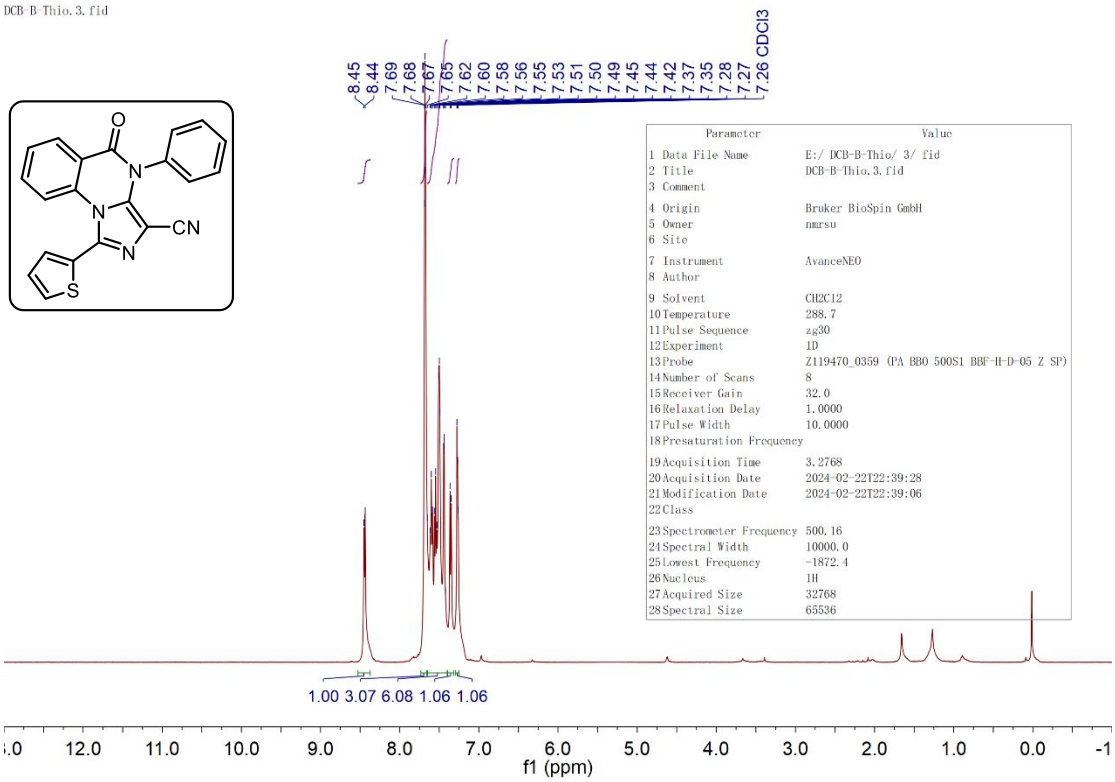


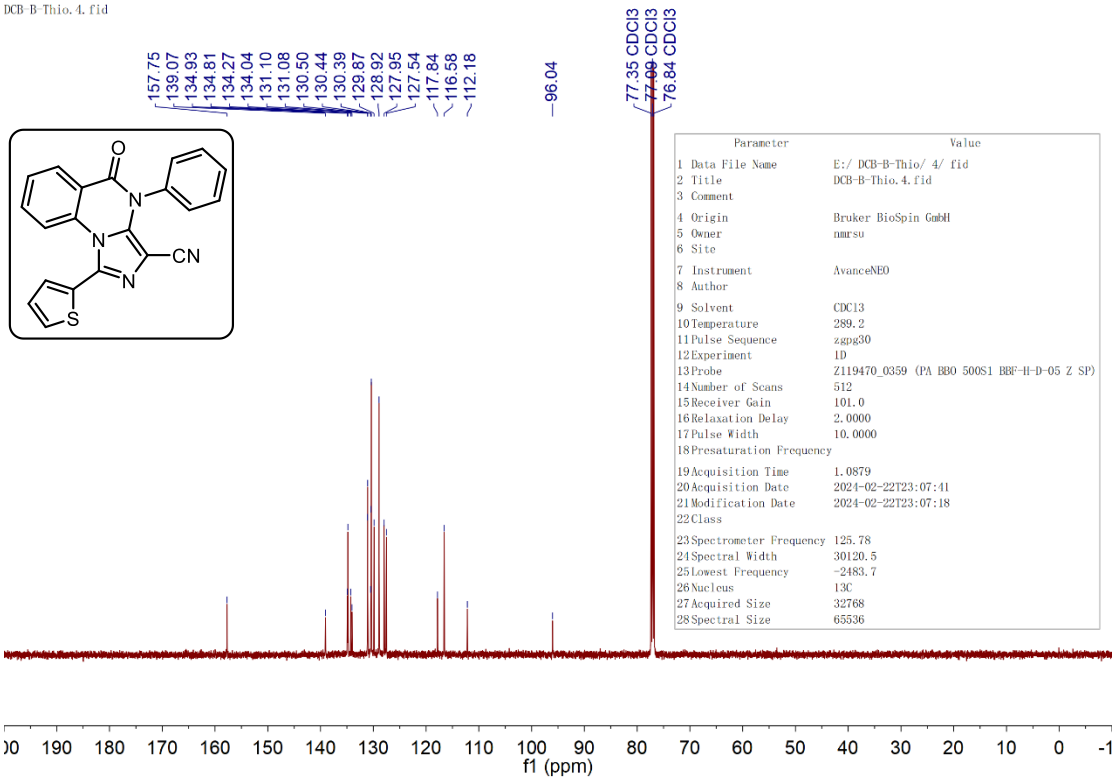
1-(4-chlorophenyl)-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ah)





5-oxo-4-phenyl-1-(thiophen-2-yl)-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4ai)





1-benzyl-5-oxo-4-phenyl-4,5-dihydroimidazo[1,5-a]quinazoline-3-carbonitrile (4aj)