

***n*-Bu₄NI-catalyzed selective dual amination of sp³ C–H bonds: oxidative domino synthesis of imidazo[1,5-*c*]quinazolines on a gram-scale**

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Electronic Supplementary Information

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General information

All commercial reagents and solvents were used without additional purification unless otherwise specified. Melting points were measured with an X-4 melting point apparatus (Bei Jing Taike Co., Ltd.) and were uncorrected. ¹H-NMR and ¹³C-NMR were determined in CDCl₃ on a Bruker DPX 300 MHz or a Bruker AVANCE III 400 MHz spectrometer at room temperature, respectively, and tetramethylsilane (TMS) served as an internal standard. Spin multiplicities are given as s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet) as well as brs (broad). Coupling constants (*J*) are given in hertz (Hz). ESI-MS was carried out on a LCMS-2020 (Shimadzu, Japan). HRMS were recorded on a LTQ-Orbitrap XL (Thermofisher, U.S.A.). All experiments were monitored by thin layer chromatography (TLC). TLC was performed on pre-coated silica gel plates (Qingdao Haiyang Chemical Co., Ltd).

Optimization of the reaction condition

Table S1 Screening of Reaction Conditions^a

Entry	XI	Oxidant (equiv)	Additive (equiv)	Solvent	Temp. (°C)	Time (h)	Yield ^b (%)	20 mol% XI / Oxidant Additive, Solvent Temperature, Time	
								1a	2a
1	<i>n</i> -Bu ₄ NI	5.5 M TBHP in decane (4)		DMSO	90	10	36		
2		5.5 M TBHP in decane (4)		DMSO	90	10	nd		
3	NIS	5.5 M TBHP in decane (4)		DMSO	90	10	26		
4	I ₂	5.5 M TBHP in decane (4)		DMSO	90	10	23		
5	PhI	5.5 M TBHP in decane (4)		DMSO	90	10	nd		
6	KI	5.5 M TBHP in decane (4)		DMSO	90	10	33		
7	<i>n</i> -Bu ₄ NI	1atm air		DMSO	90	10	nd		
8	<i>n</i> -Bu ₄ NI	30% Aq. H ₂ O ₂ (4)		DMSO	90	10	trace		
9	<i>n</i> -Bu ₄ NI	(<i>t</i> BuO) ₂ (4)		DMSO	90	10	nd		
10	<i>n</i> -Bu ₄ NI	K ₂ S ₂ O ₈ (4)		DMSO	90	10	messy		
11	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)		DMSO	90	10	37		
12	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	K ₂ CO ₃ (2)	DMSO	90	10	messy		
13	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (2)	DMSO	90	10	80		

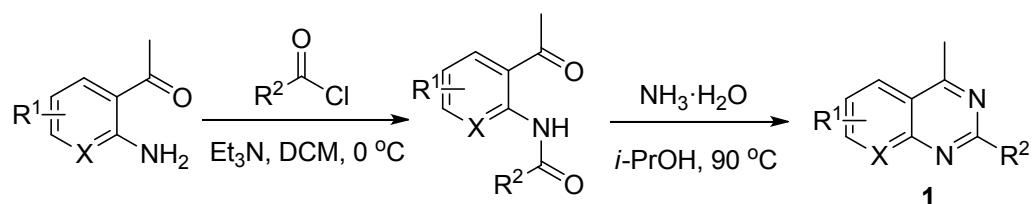
14	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CF ₃ COOH (2)	DMSO	90	10	messy
15	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	PhCOOH (2)	DMSO	90	10	72
16	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	PhCH ₂ COOH (2)	DMSO	90	10	78
17	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	<i>o</i> -C ₆ H ₄ (COOH) ₂ (2)	DMSO	90	10	47
18	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ CH ₂ COOH (2)	DMSO	90	10	65
19	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ (CH ₂) ₃ COOH (2)	DMSO	90	10	78
20	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	NaH ₂ PO ₄ ·2H ₂ O (2)	DMSO	90	10	67
21	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (2)	DMF	90	10	40
22	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (2)	DMA	90	10	46
23	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (2)	toluene	90	10	22
24	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (2)	CH ₃ CN	90	10	26
25	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (2)	dioxane	90	10	26
26	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (2)	DCE	90	10	23
27	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (2)	NMP	90	10	40
28	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (2)	H ₂ O	90	10	30
29	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (1)	DMSO	90	10	61
30	<i>n</i>-Bu₄NI	70% Aq. TBHP (4)	CH₃COOH (3)	DMSO	90	10	88
31	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (4)	DMSO	90	10	86
32	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (3)	DMSO	100	10	81
33	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (3)	DMSO	110	10	79
34	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (3)	DMSO	75	10	58
35	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (3)	DMSO	90	12	81

36	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (4)	CH ₃ COOH (3)	DMSO	90	15	81
37	<i>n</i> -Bu ₄ NI	70% Aq. TBHP (2)	CH ₃ COOH (3)	DMSO	90	10	65

^a Reaction conditions: **1a** (0.3 mmol), **2a** (0.6 mmol), XI (20 mol%), oxidant (indicated amount), additive (indicated amount), in a tested solvent (2 mL) at a selected temperature. nd = not detected. ^b Isolated yield.

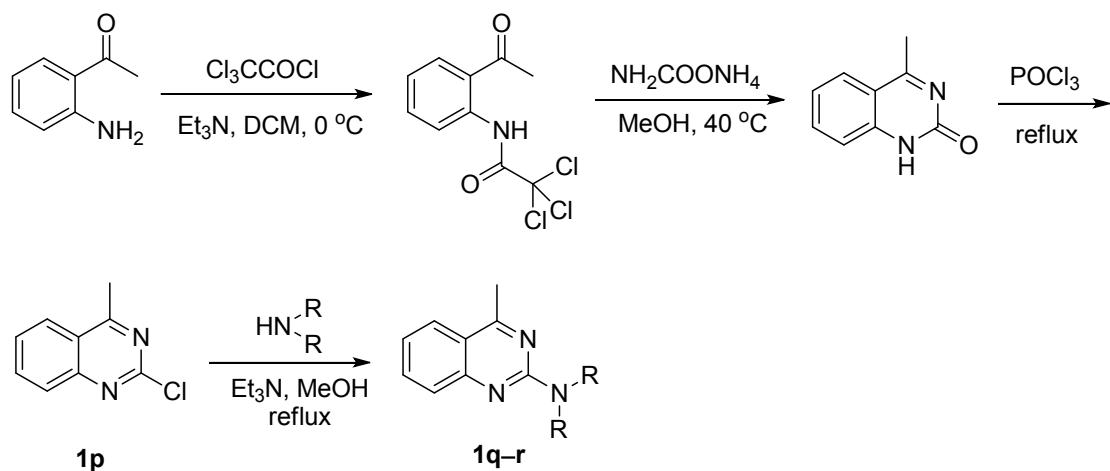
General procedure for the synthesis of substrates and products

General procedure for the synthesis of 4-methylquinazolines (**1a–o**, **1s** and **1t**):



To a solution of 2-aminoacetophenone derivatives (20 mmol) and triethylamine (3.3 mL, 1.2 equiv) in dichloromethane (DCM) (60 mL) cooled in an ice-water bath, chloride (1.5 equiv) was added dropwise. The progress of the reaction was monitored by TLC. Upon completion, the solution was washed with diluted hydrochloric acid, saturated NaHCO₃, brine, and dried over anhydrous Na₂SO₄. The organic phase was concentrated in vacuo to give amide as an intermediate without further purification. The amide, 25% ammonia water (20 mL) and isopropanol (20 mL) were added to a 250 mL sealed tube. The tube was located in a preheated 90 °C oil bath and stirred for 10 h. The reaction mixture was cooled to room temperature, washed with diluted hydrochloric acid, saturated NaHCO₃, brine, and dried over anhydrous Na₂SO₄, then concentrated in vacuo. The residue was then purified by chromatography on silica gel with an eluent of petroleum ether and ethyl acetate. Products were characterized by Mp, ¹H-, ¹³C-NMR and MS (ESI).

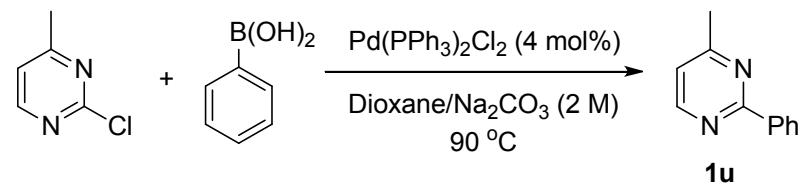
Procedure for the synthesis of 4-methylquinazolines (**1p–r**):



To a solution of 2-aminoacetophenone derivatives (20 mmol) and triethylamine (3.3 mL, 1.2 equiv) in dichloromethane (DCM) (60 mL) cooled in an ice-water bath, trichloroacetyl chloride (1.2 equiv) was added dropwise. The progress of the reaction was monitored by TLC. Upon completion, the solution

was washed with diluted hydrochloric acid, saturated NaHCO_3 , brine, and dried over anhydrous Na_2SO_4 . The organic phase was concentrated in vacuo to give amide as an intermediate without further purification. Ammonium carbamate (5 equiv) was added to a solution of amide in methanol (40 mL). The mixture was stirred at about 40 °C for 8 h. The excess ammonium carbamate was filtered. The organic phase was concentrated in vacuo and the gray residue was recrystallized from ethyl acetate/hexanes 1/3 (v/v) to give 4-methylquinazolin-2(1*H*)-one (76% yield for two steps). POCl_3 (5 mL) was added drop wise to 4-methylquinazolin-2(1*H*)-one (10 mmol) at 0 °C. The mixture was refluxed for 3 h. Excess POCl_3 was distilled off and the residue was cooled to room temperature and then added drop wise into crushed ice. The aqueous layer was extracted with ethyl acetate, washed with saturated NaHCO_3 , brine, and dried over anhydrous Na_2SO_4 , then concentrated in vacuo. The residue was then purified by chromatography on silica gel with an eluent of petroleum ether and ethyl acetate to give **1p** (48% yield). To a solution of **1p** (2 mmol) in methanol (5 mL), secondary amine (1.2 equiv) and triethylamine (4 equiv) were added. The mixture was refluxed for 3 h. The solvent was distilled off and the residue was then purified by chromatography on silica gel with an eluent of petroleum ether and ethyl acetate to give **1q** (87% yield) and **1r** (86% yield). Products were characterized by Mp, ¹H-, ¹³C-NMR and MS (ESI).

Procedure for the synthesis of 4-methyl-2-phenylpyrimidine (**1u**):

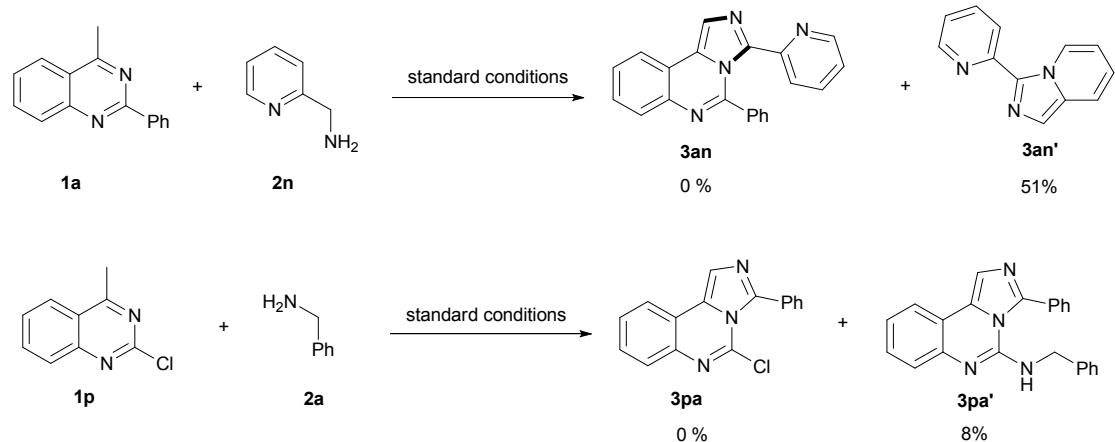


To a round-bottom flask was added 2-chloro-4-methylpyrimidine (2 mmol), arylboronic acid (2 equiv), $\text{PdCl}_2(\text{PPh}_3)_2$ (4 mol%) and Na_2CO_3 (2 M, 5 mL) in dioxane (5 mL). The reaction mixture was heated to 90 °C until the 2-chloro-4-methylpyrimidine was consumed completely. The heterogeneous aqueous was concentrated in vacuo and the residue was diluted with EtOAc, washed by brine. The organic layer was dried over anhydrous Na_2SO_4 , concentrated and then purified by chromatography on silica gel with an eluent of petroleum ether and ethyl acetate to give **1u** (100% yield).

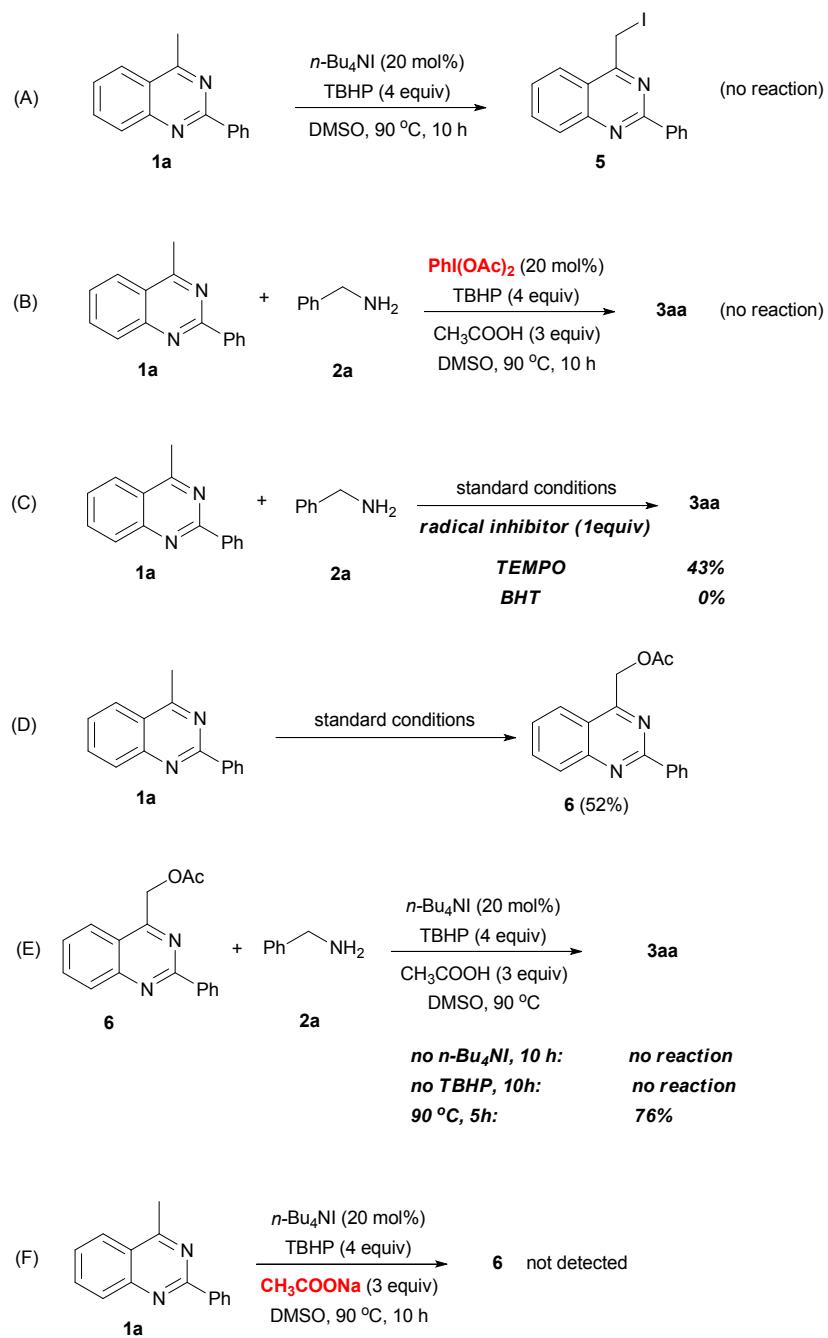
General procedure for the synthesis of substituted imidazo[1,5-*c*]quinazolines (**3**):

A mixture of 4-methylquinazoline **1** (0.3 mmol), benzylamine **2** or amino acid **4** (0.6 mmol), $n\text{-Bu}_4\text{NI}$ (0.06 mmol), TBHP (1.2 mmol, 70% in water) and acetic acid (0.9 mmol) in 2 mL DMSO was stirred in a Schlenk tube at 90 °C. After stirring for 10 h, the reaction mixture was cooled to the room temperature, and extracted by ethyl acetate (3×5 mL). The organic phase was then washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was then purified by chromatography on silica gel with an eluent of petroleum ether and ethyl acetate. Products were characterized by Mp, ¹H-, ¹³C-NMR and HRMS (ESI).

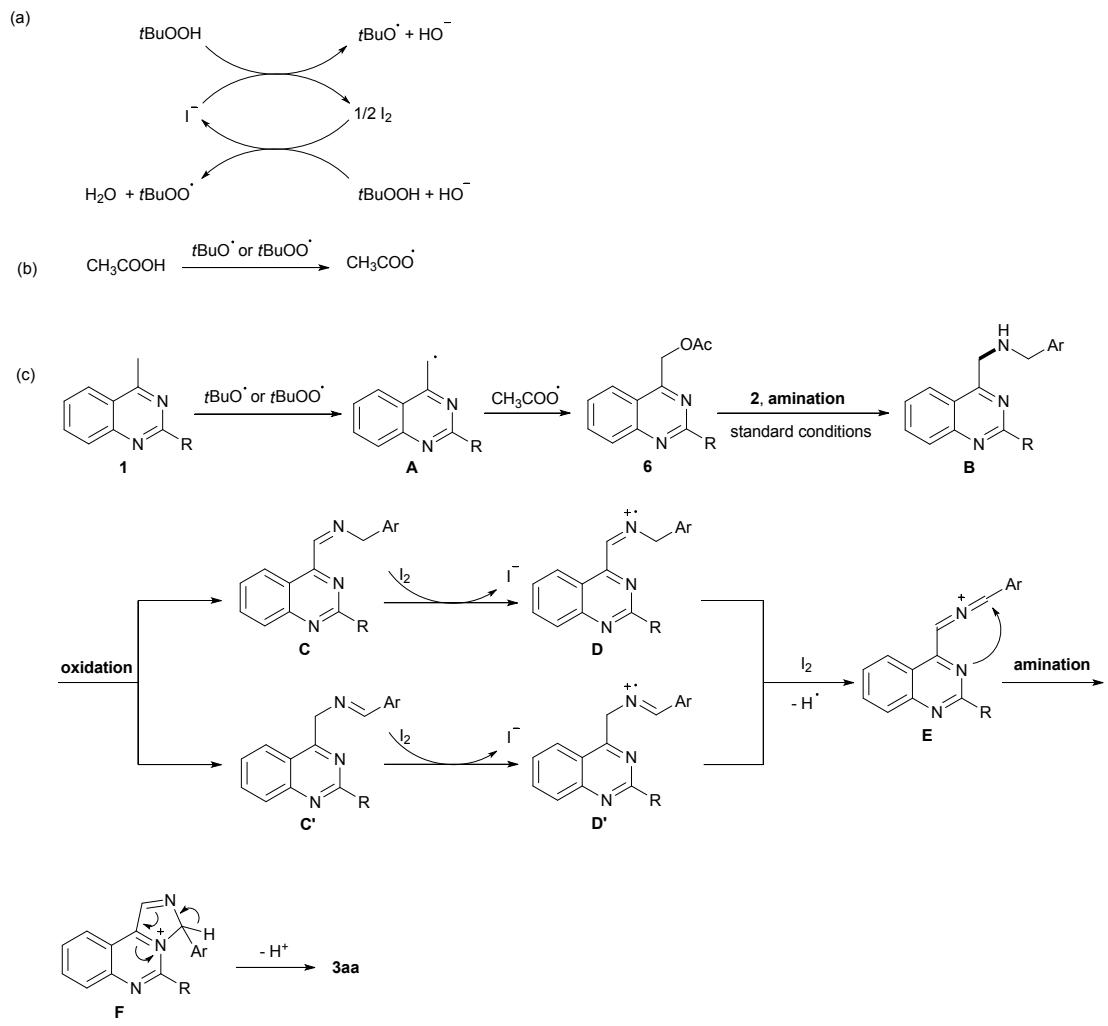
The failure examples:



Control experiments on the reaction mechanism

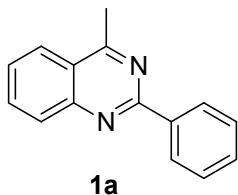


Scheme S1 Control reactions A–F.

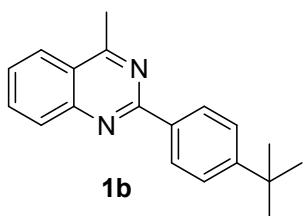


Scheme S2 Plausible reaction mechanism.

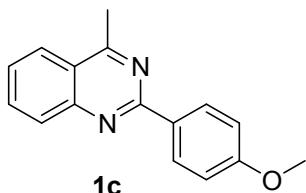
Substrate characterizations



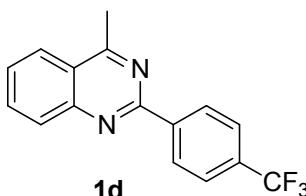
*4-Methyl-2-phenylquinazoline (1a)*¹. white solid, 76% yield for two steps, mp. 84 – 85 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.63 (dd, *J* = 7.9, 1.8 Hz, 2H), 8.09 (d, *J* = 8.3 Hz, 2H), 7.87 (ddd, *J* = 8.5, 6.9, 1.3 Hz, 1H), 7.64 – 7.45 (m, 4H), 3.02 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 168.1, 160.0, 150.2, 138.2, 133.4, 130.3, 129.1, 128.48, 128.52, 126.7, 124.8, 122.8, 21.9; MS (ESI): 221.00 [M+H]⁺.



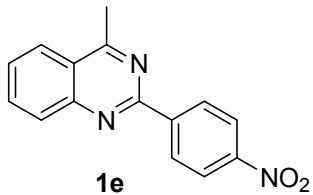
2-(4-(Tert-butyl)phenyl)-4-methylquinazoline (1b). colorless oil, 91% yield for two steps. ¹H NMR (300 MHz, CDCl₃) δ 8.65 – 8.43 (m, 2H), 8.08 (d, *J* = 8.4 Hz, 2H), 7.85 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.62 – 7.50 (m, 3H), 3.01 (s, 3H), 1.39 (s, 9H); ¹³C NMR (75 MHz, CDCl₃) δ 167.9, 160.1, 153.5, 150.3, 135.6, 133.2, 129.0, 128.3, 126.5, 125.4, 124.8, 122.8, 34.8, 31.3, 21.9; MS (ESI): 277.15 [M+H]⁺; HRMS (ESI) m/z calcd for C₁₉H₂₁N₂ [M+H]⁺ 277.1699, found 277.1696.



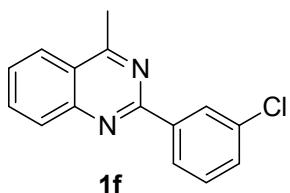
*2-(4-Methoxyphenyl)-4-methylquinazoline (1c)*¹. white solid, 80% yield for two steps, mp. 112 – 113 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.69 – 8.46 (m, 2H), 8.14 – 7.98 (m, 2H), 7.83 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.54 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.11 – 6.97 (m, 2H), 3.90 (s, 3H), 2.99 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 168.0, 161.6, 159.9, 150.3, 133.4, 130.9, 130.1, 128.9, 126.3, 124.9, 122.6, 113.8, 55.3, 21.9; MS (ESI): 251.10 [M+H]⁺.



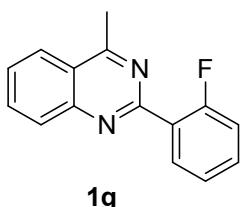
*4-Methyl-2-(4-(trifluoromethyl)phenyl)quinazoline (1d)*². white solid, 95% yield for two steps, mp. 86 – 87 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.75 (d, *J* = 8.1 Hz, 2H), 8.20 – 8.03 (m, 2H), 7.90 (ddd, *J* = 8.5, 6.9, 1.3 Hz, 1H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.63 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 3.03 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.5, 158.6, 150.2, 141.6, 133.7, 131.8 (q, *J*_{C-F} = 32.2 Hz), 129.3, 128.8, 127.4, 125.4 (q, *J*_{C-F} = 3.8 Hz), 125.0, 124.3 (d, *J*_{C-F} = 272.2 Hz), 123.2, 21.9; MS (ESI): 289.05 [M+H]⁺.



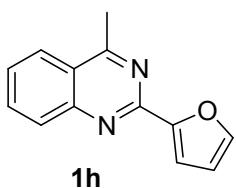
*4-Methyl-2-(4-nitrophenyl)quinazoline (1e)*³. yellow solid, 38% yield for two steps, mp. 171 – 172 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.79 (d, *J* = 8.7 Hz, 2H), 8.33 (d, *J* = 8.7 Hz, 2H), 8.10 (t, *J* = 8.1 Hz, 2H), 7.91 (t, *J* = 7.6 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 3.03 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 168.6, 158.0, 150.9, 150.1, 150.0, 135.6, 133.6, 129.1, 127.2, 124.8, 123.1, 123.0, 21.8; MS (ESI): 266.00 [M+H]⁺.



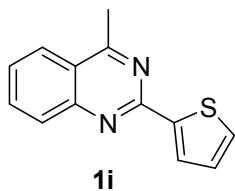
*2-(3-Chlorophenyl)-4-methylquinazoline (1f)*⁴. yellow solid, 64% yield for two steps, mp. 106 – 107 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.65 – 8.61 (m, 1H), 8.55 – 8.47 (m, 1H), 8.13 – 8.03 (m, 2H), 7.87 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.60 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.47 – 7.43 (m, 2H), 3.01 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 168.4, 158.7, 150.2, 140.1, 134.6, 133.6, 130.2, 129.7, 129.2, 128.5, 127.1, 126.5, 124.9, 123.1, 21.9; MS (ESI): 255.05 [M+H]⁺.



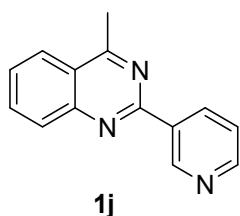
2-(2-Fluorophenyl)-4-methylquinazoline (1g). white solid, 57% yield for two steps, mp. 63 – 64 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.18 – 8.06 (m, 3H), 7.90 (t, *J* = 7.8 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.52 – 7.39 (m, 1H), 7.36 – 7.14 (m, 2H), 3.03 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 168.3, 162.7, 159.4, 158.9 (d, *J*_{C-F} = 3.9 Hz), 150.0, 133.6, 132.0, 131.2 (d, *J*_{C-F} = 8.5 Hz), 129.1, 127.4, 124.8, 124.1 (d, *J*_{C-F} = 3.4 Hz), 122.5, 116.7 (d, *J*_{C-F} = 22.3 Hz), 21.8; MS (ESI): 239.00 [M+H]⁺; HRMS (ESI) m/z calcd for C₁₅H₁₂FN₂ [M+H]⁺ 239.0979, found 239.0983.



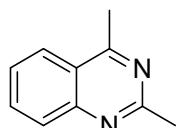
*2-(Furan-2-yl)-4-methylquinazoline (1h)*⁵. white solid, 93% yield for two steps, mp. 82 – 83 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.13 – 8.00 (m, 2H), 7.84 (ddd, *J* = 8.5, 7.0, 1.3 Hz, 1H), 7.68 (dd, *J* = 1.7, 0.8 Hz, 1H), 7.55 (ddd, *J* = 8.1, 7.0, 1.0 Hz, 1H), 7.45 (dd, *J* = 3.4, 0.8 Hz, 1H), 6.60 (dd, *J* = 3.4, 1.8 Hz, 1H), 2.97 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 168.6, 153.2, 152.6, 149.8, 145.0, 133.7, 128.8, 126.8, 124.9, 122.7, 113.7, 112.1, 21.8; MS (ESI): 211.05 [M+H]⁺.



*4-Methyl-2-(thiophen-2-yl)quinazoline (1i)*⁶. white solid, 89% yield for two steps, mp. 86 – 87 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.15 (dd, $J = 3.7, 1.2$ Hz, 1H), 8.07 – 7.94 (m, 2H), 7.82 (ddd, $J = 8.4, 6.9, 1.4$ Hz, 1H), 7.57 – 7.44 (m, 2H), 7.18 (dd, $J = 5.0, 3.7$ Hz, 1H), 2.96 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 168.3, 156.9, 150.1, 144.1, 133.6, 129.6, 128.9, 128.7, 128.2, 126.5, 125.0, 122.7, 21.8; MS (ESI): 227.05 [M+H]⁺.

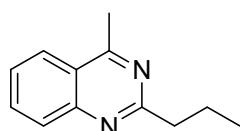


*4-Methyl-2-(pyridin-3-yl)quinazoline (1j)*⁴. yellow solid, 71% yield for two steps, mp. 107 – 109 °C. ^1H NMR (300 MHz, CDCl_3) δ 9.81 (s, 1H), 8.88 (d, $J = 7.9$ Hz, 1H), 8.72 (d, $J = 3.6$ Hz, 1H), 8.10 (t, $J = 8.7$ Hz, 2H), 7.89 (t, $J = 7.6$ Hz, 1H), 7.62 (t, $J = 7.5$ Hz, 1H), 7.45 (dd, $J = 7.8, 4.9$ Hz, 1H), 3.03 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 168.1, 157.9, 150.5, 149.9, 149.8, 135.4, 133.4, 128.8, 127.0, 124.7, 122.8, 122.7, 21.7; MS (ESI): 222.00 [M+H]⁺.



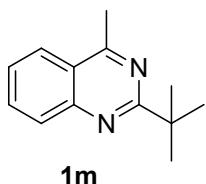
1k

*2,4-Dimethylquinazoline (1k)*⁷. yellow oil, 45% yield for two steps. ^1H NMR (300 MHz, CDCl_3) δ 8.06 (d, $J = 8.3$ Hz, 1H), 7.94 (d, $J = 8.4$ Hz, 1H), 7.87 – 7.80 (m, 1H), 7.57 (t, $J = 7.6$ Hz, 1H), 2.93 (s, 3H), 2.85 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.0, 163.4, 149.8, 133.5, 128.1, 126.5, 124.8, 122.1, 26.3, 21.6; MS (ESI): 159.00 [M+H]⁺.

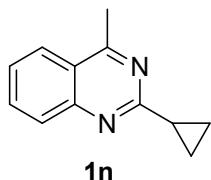


1l

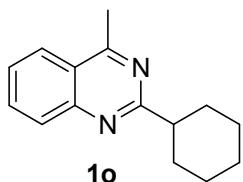
*4-Methyl-2-propylquinazoline (1l)*⁷. colorless oil, 73% yield for two steps. ^1H NMR (400 MHz, CDCl_3) δ 8.06 (d, $J = 8.3$ Hz, 1H), 7.96 (d, $J = 8.4$ Hz, 1H), 7.83 (t, $J = 7.7$ Hz, 1H), 7.56 (t, $J = 7.6$ Hz, 1H), 3.08 – 3.01 (m, 2H), 2.93 (s, 3H), 2.01 – 1.86 (m, 2H), 1.05 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.1, 166.8, 149.9, 133.5, 128.5, 126.6, 124.9, 122.5, 42.0, 22.4, 21.7, 14.1; MS (ESI): 187.10 [M+H]⁺.



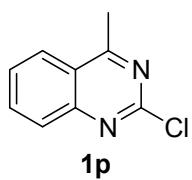
*2-(Tert-butyl)-4-methylquinazoline (1m)*⁸. white solid, 93% yield for two steps, mp. 49 – 50 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.07 – 8.00 (m, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.80 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.53 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 2.92 (s, 3H), 1.50 (s, 9H); ¹³C NMR (75 MHz, CDCl₃) δ 172.6, 167.2, 149.7, 132.7, 128.8, 126.2, 124.6, 122.1, 39.3, 29.5, 21.8; MS (ESI): 201.10 [M+H]⁺.



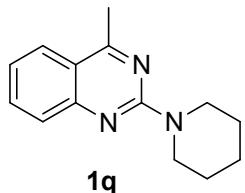
2-Cyclopropyl-4-methylquinazoline (1n). yellow solid, 92% yield for two steps, mp. 55 – 57 °C. ¹H NMR (300 MHz, CDCl₃) δ 7.90 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.71 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.47 – 7.35 (m, 1H), 2.79 (s, 3H), 2.30 (tt, *J* = 8.2, 4.8 Hz, 1H), 1.31 – 1.11 (m, 2H), 1.13 – 0.94 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 167.8, 167.3, 149.9, 133.2, 128.0, 125.8, 124.8, 122.5, 21.7, 18.4, 10.3; MS (ESI): 185.10 [M+H]⁺; HRMS (ESI) m/z calcd for C₁₂H₁₃N₂ [M+H]⁺ 185.1073 , found 185.1073.



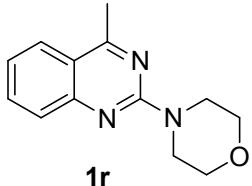
*2-Cyclohexyl-4-methylquinazoline (1o)*³. yellow solid, 66% yield for two steps, mp. 46 – 48 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.08 – 8.00 (m, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.81 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.54 (ddd, *J* = 8.2, 6.9, 1.1 Hz, 1H), 3.04 – 2.95 (m, 1H), 2.92 (s, 3H), 2.08 – 2.04 (m, 2H), 1.95 – 1.67 (m, 5H), 1.57 – 1.31 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.0, 167.8, 150.0, 133.1, 128.6, 126.3, 124.8, 122.6, 47.9, 31.9, 26.4, 26.0, 21.7; MS (ESI): 227.15 [M+H]⁺.



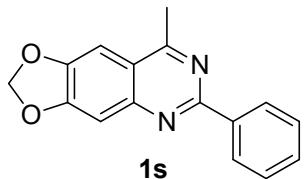
*2-Chloro-4-methylquinazoline (1p)*⁹. yellow solid, 48% yield, mp. 110 – 112 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.09 (d, *J* = 8.4 Hz, 1H), 8.01 – 7.86 (m, 2H), 7.65 (ddd, *J* = 8.2, 6.7, 1.4 Hz, 1H), 2.96 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 172.1, 156.8, 151.4, 134.9, 128.2, 127.9, 125.3, 122.8, 21.7; MS (ESI): 179.10 [M+H]⁺.



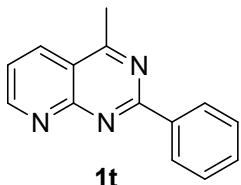
*4-Methyl-2-(piperidin-1-yl)quinazoline (**1q**)¹⁰. yellow solid, 87% yield, mp. 74 – 75 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.79 (dd, *J* = 8.2, 0.7 Hz, 1H), 7.59 (ddd, *J* = 8.1, 6.7, 1.4 Hz, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.14 (ddd, *J* = 8.1, 6.7, 1.4 Hz, 1H), 4.14 – 3.51 (m, 4H), 2.75 (s, 3H), 1.75 – 1.57 (dt, *J* = 9.3, 3.8 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 168.6, 158.6, 152.2, 133.3, 126.1, 125.2, 121.6, 118.7, 44.9, 26.0, 25.0, 21.9; MS (ESI): 228.15 [M+H]⁺.*



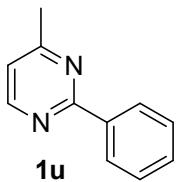
*4-(4-Methylquinazolin-2-yl)morpholine (**1r**)¹⁰. yellow solid, 86% yield, mp. 48 – 50 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.84 (dd, *J* = 8.2, 0.8 Hz, 1H), 7.63 (ddd, *J* = 8.2, 6.7, 1.4 Hz, 1H), 7.57 (d, *J* = 8.2 Hz, 1H), 7.21 (ddd, *J* = 8.1, 6.7, 1.3 Hz, 1H), 4.06 – 3.89 (m, 4H), 3.85 – 3.70 (m, 4H), 2.78 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.0, 158.5, 151.9, 133.6, 126.3, 125.3, 122.4, 119.2, 67.1, 44.5, 21.9; MS (ESI): 230.15 [M+H]⁺.*



*8-Methyl-6-phenyl-[1,3]dioxolo[4,5-g]quinazoline (**1s**)¹. white solid, 21% yield for two steps, mp. 185 – 187 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.63 – 8.44 (m, 2H), 7.56 – 7.39 (m, 3H), 7.29 (s, 1H), 7.23 (s, 1H), 6.09 (s, 2H), 2.85 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 165.2, 159.2, 153.4, 149.8, 147.9, 138.4, 130.0, 128.5, 128.2, 119.6, 105.4, 102.1, 100.3, 22.2; MS (ESI): 265.10 [M+H]⁺.*

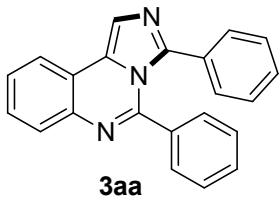


*4-Methyl-2-phenylpyrido[2,3-d]pyrimidine (**1t**)*. red solid, 70% yield for two steps, mp. 97 – 99 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.21 (dd, *J* = 4.3, 1.9 Hz, 1H), 8.81 – 8.65 (m, 2H), 8.44 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.64 – 7.44 (m, 4H), 3.02 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 163.5, 158.6, 157.6, 137.4, 134.4, 131.2, 129.2, 128.5, 122.3, 117.6, 21.6; HRMS (ESI) m/z calcd for C₁₄H₁₂N₃ [M+H]⁺ 222.1026, found 222.1021.

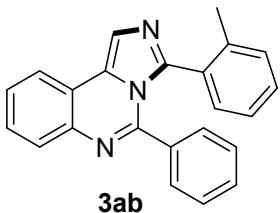


*4-Methyl-2-phenylpyrimidine (**1u**)¹¹. yellow oil, 100% yield. ¹H NMR (300 MHz, CDCl₃) δ 8.64 (d, *J* = 5.1 Hz, 1H), 8.50 – 8.32 (m, 2H), 7.57 – 7.39 (m, 3H), 7.04 (d, *J* = 5.0 Hz, 1H), 2.59 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 167.3, 164.4, 156.8, 137.8, 130.5, 128.5, 128.2, 118.6, 24.4; MS (ESI): 171.10 [M+H]⁺.*

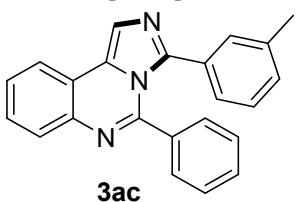
Product and intermediate 6 characterizations



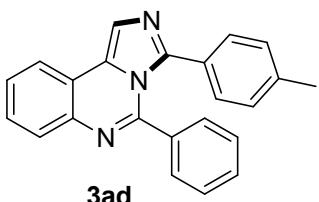
3,5-Diphenylimidazo[1,5-c]quinazoline (3aa). yellow solid, 88% yield, mp. 142 – 145 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.13 – 8.05 (m, 1H), 8.04 (s, 1H), 7.95 – 7.88 (m, 1H), 7.60 – 7.53 (m, 2H), 7.34 (d, J = 7.4 Hz, 2H), 7.23 – 6.97 (m, 8H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.2, 142.7, 138.1, 133.8, 131.4, 130.3, 129.9, 129.2, 128.6, 128.5, 128.2, 128.0, 127.7, 127.4, 121.7, 120.6, 119.3; HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{16}\text{N}_3$ $[\text{M}+\text{H}]^+$ 322.1339, found 322.1338.



5-Phenyl-3-(o-tolyl)imidazo[1,5-c]quinazoline (3ab). yellow solid, 83% yield, mp. 146 – 148 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.12 – 8.06 (m, 1H), 8.05 (s, 1H), 7.94 – 7.86 (m, 1H), 7.63 – 7.49 (m, 2H), 7.35 – 7.27 (m, 2H), 7.19 – 7.10 (m, 1H), 7.08 – 6.93 (m, 4H), 6.92 – 6.84 (m, 2H), 2.06 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.4, 141.6, 138.0, 137.0, 133.1, 131.6, 130.8, 129.7, 129.6, 129.5, 128.8, 128.5, 128.4, 128.2, 127.3, 125.1, 121.7, 120.3, 119.4, 20.1; HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{18}\text{N}_3$ $[\text{M}+\text{H}]^+$ 336.1495, found 336.1495.

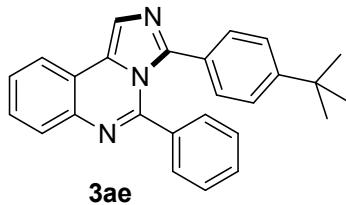


5-Phenyl-3-(m-tolyl)imidazo[1,5-c]quinazoline (3ac). yellow solid, 75% yield, mp. 193 – 196 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.11 – 8.03 (m, 1H), 8.01 (s, 1H), 7.96 – 7.84 (m, 1H), 7.62 – 7.48 (m, 2H), 7.40 – 7.30 (m, 2H), 7.24 – 7.15 (m, 1H), 7.12 – 6.87 (m, 5H), 6.83 (s, 1H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.3, 142.8, 138.1, 136.9, 133.9, 131.2, 130.2, 129.8, 128.8, 128.40, 128.37, 128.1, 127.6, 127.5, 126.3, 121.7, 120.6, 119.3, 20.9; HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{18}\text{N}_3$ $[\text{M}+\text{H}]^+$ 336.1495, found 336.1492.

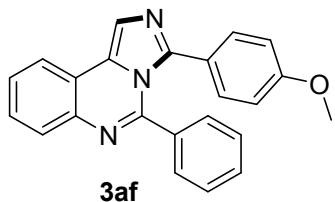


5-Phenyl-3-(p-tolyl)imidazo[1,5-c]quinazoline (3ad). white solid, 71% yield, mp. 204 – 206 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.11 – 8.03 (m, 1H), 8.01 (s, 1H), 7.93 – 7.85 (m, 1H), 7.61 – 7.48 (m, 2H), 7.36 – 7.29 (m, 2H), 7.21 (t, J = 7.4 Hz, 1H), 7.07 (t, J = 7.6 Hz, 2H), 7.00 (d, J = 8.1 Hz, 2H), 6.82 (d, J = 8.0 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.4, 142.9, 138.1, 138.0, 133.9, 130.1,

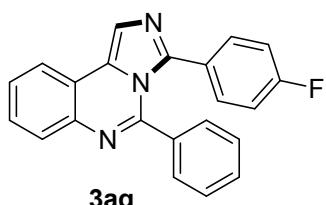
129.6, 129.0, 128.7, 128.6, 128.41, 128.36, 128.2, 128.1, 127.7, 121.7, 120.6, 119.4, 21.2; HRMS (ESI) m/z calcd for $C_{23}H_{18}N_3$ [M+H]⁺ 336.1495, found 336.1496.



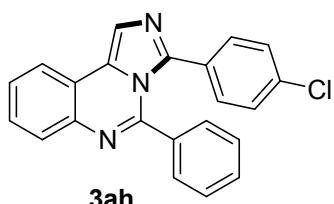
3-(4-(Tert-butyl)phenyl)-5-phenylimidazo[1,5-c]quinazoline (3ae). yellow solid, 76% yield, mp. 188 – 189 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.12 – 8.04 (m, 1H), 8.02 (s, 1H), 7.97 – 7.87 (m, 1H), 7.61 – 7.50 (m, 2H), 7.32 – 7.26 (m, 2H), 7.19 – 7.10 (m, 1H), 7.07 – 6.98 (m, 6H), 1.24 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 151.1, 146.4, 142.9, 138.1, 133.8, 130.1, 129.6, 128.9, 128.7, 128.5, 128.44, 128.37, 128.2, 127.6, 124.4, 121.7, 120.6, 119.5, 34.5, 31.2; HRMS (ESI) m/z calcd for $C_{26}H_{24}N_3$ [M+H]⁺ 378.1965, found 378.1968.



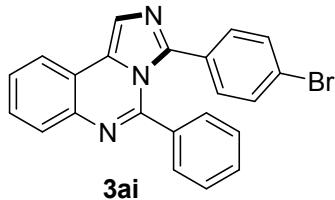
3-(4-Methoxyphenyl)-5-phenylimidazo[1,5-c]quinazoline (3af). yellow solid, 75% yield, mp. 189 – 190 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.12 – 8.02 (m, 1H), 8.00 (s, 1H), 7.94 – 7.85 (m, 1H), 7.61 – 7.49 (m, 2H), 7.33 (d, *J* = 7.2 Hz, 2H), 7.22 (d, *J* = 7.4 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 2H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.55 (d, *J* = 8.7 Hz, 2H), 3.73 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.4, 146.3, 142.6, 138.0, 133.8, 130.5, 130.0, 129.8, 128.8, 128.4, 128.3, 128.2, 127.7, 124.0, 121.7, 120.5, 119.4, 113.0, 55.3; HRMS (ESI) m/z calcd for $C_{23}H_{18}N_3O$ [M+H]⁺ 352.1444, found 352.1446.



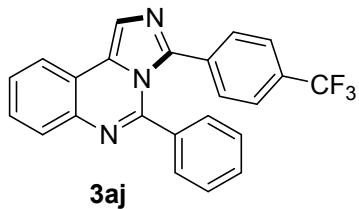
3-(4-Fluorophenyl)-5-phenylimidazo[1,5-c]quinazoline (3ag). yellow solid, 85% yield, mp. 180 – 182 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.12 – 8.04 (m, 1H), 8.02 (s, 1H), 7.95 – 7.86 (m, 1H), 7.62 – 7.51 (m, 2H), 7.37 – 7.30 (m, 2H), 7.29 – 7.21 (m, 1H), 7.17 – 7.05 (m, 4H), 6.78 – 6.64 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 162.4 (d, *J*_{C-F} = 249.1 Hz), 146.0, 141.6, 138.1, 133.7, 131.0 (d, *J*_{C-F} = 8.5 Hz), 130.4, 130.1, 128.8, 128.6, 128.3, 127.9, 127.8 (d, *J*_{C-F} = 3.4 Hz), 121.8, 120.7, 119.3, 114.5 (d, *J*_{C-F} = 22.0 Hz); HRMS (ESI) m/z calcd for $C_{22}H_{15}FN_3$ [M+H]⁺ 340.1245, found 340.1245.



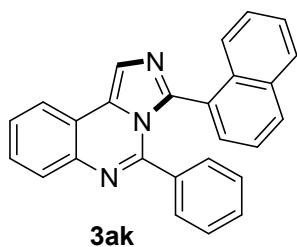
*3-(4-Chlorophenyl)-5-phenylimidazo[1,5-*c*]quinazoline (3ah)*. yellow solid, 76% yield, mp. 196 – 197 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.14 – 8.05 (m, 1H), 8.02 (s, 1H), 7.96 – 7.87 (m, 1H), 7.62 – 7.49 (m, 2H), 7.37 – 7.24 (m, 3H), 7.13 (t, J = 7.6 Hz, 2H), 7.09 – 6.96 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.9, 141.4, 138.1, 134.1, 133.6, 130.5, 130.3, 130.1, 130.0, 128.7, 128.62, 128.58, 128.2, 127.9, 127.6, 121.8, 120.8, 119.2; HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{15}\text{ClN}_3$ [$\text{M}+\text{H}]^+$ 356.0949, found 356.0948.



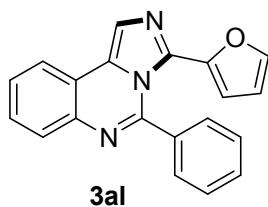
*3-(4-Bromophenyl)-5-phenylimidazo[1,5-*c*]quinazoline (3ai)*. yellow solid, 80% yield, mp. 185 – 188 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.11 – 8.04 (m, 1H), 8.02 (s, 1H), 7.96 – 7.88 (m, 1H), 7.62 – 7.51 (m, 2H), 7.36 – 7.27 (m, 3H), 7.21 – 7.06 (m, 4H), 7.04 – 6.91 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.9, 141.5, 138.1, 133.7, 130.58, 130.55, 130.47, 130.1, 128.8, 128.7, 128.6, 128.3, 128.0, 122.4, 121.8, 120.9, 119.2; HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{15}\text{BrN}_3$ [$\text{M}+\text{H}]^+$ 400.0444, found 400.0441.



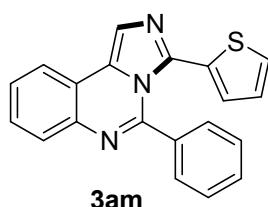
*5-Phenyl-3-(4-(trifluoromethyl)phenyl)imidazo[1,5-*c*]quinazoline (3aj)*. yellow solid, 77% yield, mp. 170 – 173 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.13 – 8.07 (m, 1H), 8.06 (s, 1H), 7.96 – 7.89 (m, 1H), 7.63 – 7.54 (m, 2H), 7.35 – 7.27 (m, 4H), 7.25 – 7.19 (m, 3H), 7.13 – 7.05 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.7, 141.0, 138.2, 135.0, 133.6, 130.9, 130.2, 129.8 (dd, $J_{\text{C}-\text{F}} = 65.2, 32.6$ Hz), 129.4, 128.8, 128.71, 128.65, 128.3, 128.0, 124.2 (q, $J_{\text{C}-\text{F}} = 3.7$ Hz), 123.8 (d, $J_{\text{C}-\text{F}} = 272.2$ Hz), 121.9, 121.0, 119.1; HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{15}\text{F}_3\text{N}_3$ [$\text{M}+\text{H}]^+$ 390.1213, found 390.1215.



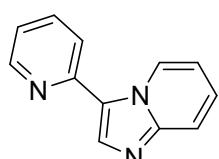
*3-(Naphthalen-1-yl)-5-phenylimidazo[1,5-*c*]quinazoline (3ak)*. yellow solid, 90% yield, mp. 83 – 86 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.21 – 8.06 (m, 2H), 7.97 – 7.83 (m, 1H), 7.72 – 7.53 (m, 4H), 7.51 – 7.44 (m, 1H), 7.44 – 7.33 (m, 2H), 7.28 – 7.23 (m, 1H), 7.21 – 7.12 (m, 1H), 7.01 (brs, 2H), 6.90 – 6.82 (m, 1H), 6.65 (brs, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.5, 140.8, 138.2, 133.11, 133.06, 132.2, 130.0, 129.3, 129.23, 129.21, 128.61, 128.60, 128.4, 128.1, 127.7, 126.6, 125.9, 125.3, 124.5, 121.8, 120.7, 119.5; HRMS (ESI) m/z calcd for $\text{C}_{26}\text{H}_{18}\text{N}_3$ [$\text{M}+\text{H}]^+$ 372.1495, found 372.1493.



3-(Furan-2-yl)-5-phenylimidazo[1,5-c]quinazoline (3al). yellow oil, 62% yield. ^1H NMR (300 MHz, CDCl_3) δ 8.09 – 8.02 (m, 1H), 8.01 (s, 1H), 7.95 – 7.87 (m, 1H), 7.61 – 7.52 (m, 2H), 7.52 – 7.44 (m, 2H), 7.39 – 7.31 (m, 1H), 7.30 – 7.20 (m, 2H), 6.86 (dd, J = 1.8, 0.8 Hz, 1H), 6.49 (dd, J = 3.4, 0.7 Hz, 1H), 6.19 (dd, J = 3.4, 1.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.1, 144.0, 143.4, 138.2, 134.1, 133.4, 130.4, 129.8, 128.8, 128.6, 128.3, 127.9, 127.7, 121.8, 121.0, 118.9, 112.0, 110.9; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{14}\text{N}_3\text{O}$ [M+H] $^+$ 312.1131, found 312.1131.

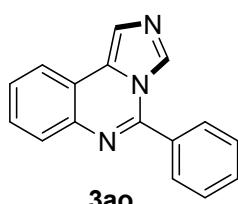


5-Phenyl-3-(thiophen-2-yl)imidazo[1,5-c]quinazoline (3am). yellow solid, 76% yield, mp. 129 – 131 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.14 – 8.04 (m, 1H), 8.03 (s, 1H), 7.97 – 7.84 (m, 1H), 7.66 – 7.51 (m, 2H), 7.47 – 7.40 (m, 2H), 7.35 – 7.27 (m, 1H), 7.25 – 7.16 (m, 3H), 6.58 (dd, J = 5.1, 3.7 Hz, 1H), 6.33 (dd, J = 3.7, 1.1 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.0, 138.1, 136.2, 133.9, 132.2, 130.5, 130.1, 129.9, 128.64, 128.59, 128.3, 128.2, 127.9, 127.0, 126.8, 121.8, 121.1, 119.1; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{14}\text{N}_3\text{S}$ [M+H] $^+$ 328.0903, found 328.0906.



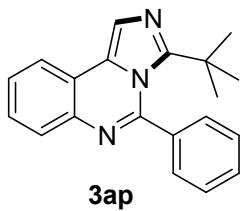
3an'

*3-(Pyridin-2-yl)imidazo[1,2-a]pyridine (3an')*¹². yellow solid, 51% yield, mp. 68 – 70 °C. ^1H NMR (300 MHz, CDCl_3) δ 9.96 (d, J = 7.3 Hz, 1H), 8.63 (d, J = 4.3 Hz, 1H), 8.35 (d, J = 8.1 Hz, 1H), 7.77 (td, J = 8.0, 1.7 Hz, 1H), 7.59 (s, 1H), 7.53 (d, J = 9.0 Hz, 1H), 7.19 (dd, J = 6.4, 5.0 Hz, 1H), 6.86 (dd, J = 8.5, 6.8 Hz, 1H), 6.73 (t, J = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 151.2, 148.1, 136.5, 135.4, 132.9, 126.0, 121.7, 121.6, 121.0, 120.1, 118.0, 113.5; MS (ESI): 196.05 [M+H] $^+$.

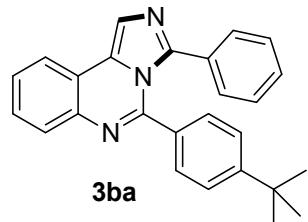


5-Phenylimidazo[1,5-c]quinazoline (3ao). yellow solid, 23% yield, mp. 140 – 142 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.27 (s, 1H), 8.04 – 7.96 (m, 1H), 7.95 – 7.87 (m, 3H), 7.86 (s, 1H), 7.66 – 7.58 (m, 3H), 7.57 – 7.47 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.4, 138.5, 133.0, 131.4, 130.1, 129.3,

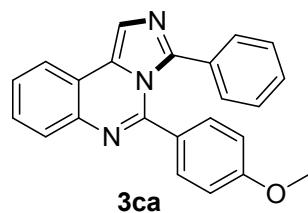
128.7, 128.6, 128.5, 122.1, 121.1, 119.0; HRMS (ESI) m/z calcd for $C_{16}H_{12}N_3$ [M+H]⁺ 246.1026, found 246.1027.



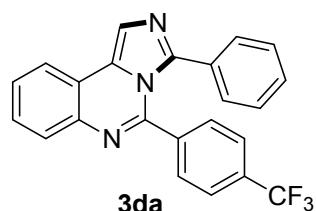
3-(Tert-butyl)-5-phenylimidazo[1,5-c]quinazoline (3ap). yellow solid, 83% yield, mp. 109 – 112 °C. ¹H NMR (300 MHz, CDCl₃) δ 7.97 – 7.88 (m, 1H), 7.83 – 7.73 (m, 2H), 7.67 – 7.59 (m, 2H), 7.56 – 7.39 (m, 5H), 1.14 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 152.1, 147.1, 138.5, 137.4, 131.2, 130.4, 128.8, 128.6, 128.2, 128.1, 127.6, 121.3, 119.8, 118.7, 35.9, 31.1; HRMS (ESI) m/z calcd for $C_{20}H_{20}N_3$ [M+H]⁺ 302.1652, found 302.1651.



5-(4-(Tert-butyl)phenyl)-3-phenylimidazo[1,5-c]quinazoline (3ba). white solid, 96% yield, mp. 176 – 179 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.10 – 8.04 (m, 1H), 8.02 (s, 1H), 7.96 – 7.86 (m, 1H), 7.61 – 7.50 (m, 2H), 7.24 – 7.18 (m, 2H), 7.13 – 7.04 (m, 5H), 7.03 – 6.93 (m, 2H), 1.22 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 153.2, 146.4, 142.7, 138.2, 131.7, 130.8, 130.3, 129.3, 128.4, 128.3, 128.2, 127.8, 127.3, 124.7, 121.7, 120.5, 119.3, 34.6, 31.1; HRMS (ESI) m/z calcd for $C_{26}H_{24}N_3$ [M+H]⁺ 378.1965, found 378.1965.

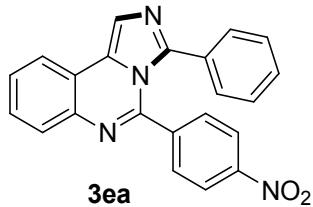


5-(4-Methoxyphenyl)-3-phenylimidazo[1,5-c]quinazoline (3ca). yellow solid, 97% yield, mp. 146 – 148 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.12 – 8.03 (m, 1H), 8.01 (s, 1H), 7.94 – 7.82 (m, 1H), 7.60 – 7.48 (m, 2H), 7.30 – 7.23 (m, 2H), 7.19 – 7.10 (m, 3H), 7.10 – 7.02 (m, 2H), 6.68 – 6.43 (m, 2H), 3.72 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 160.9, 146.0, 142.7, 138.3, 131.7, 130.4, 130.3, 129.3, 128.4, 128.2, 128.0, 127.9, 127.4, 126.2, 121.7, 120.6, 119.2, 113.1, 55.4; HRMS (ESI) m/z calcd for $C_{23}H_{18}N_3O$ [M+H]⁺ 352.1444, found 352.1443.

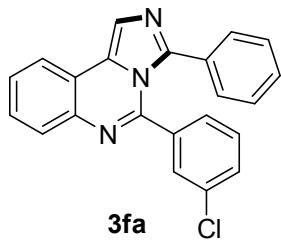


3-Phenyl-5-(4-(trifluoromethyl)phenyl)imidazo[1,5-c]quinazoline (3da). yellow solid, 79% yield,

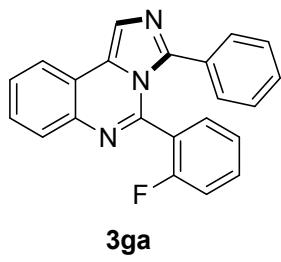
mp. 219 – 222 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.15 – 8.06 (m, 1H), 8.05 (s, 1H), 7.94 – 7.87 (m, 1H), 7.65 – 7.52 (m, 2H), 7.43 (d, $J = 8.1$ Hz, 2H), 7.32 (d, $J = 8.2$ Hz, 2H), 7.19 – 7.11 (m, 1H), 7.11 – 6.97 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 144.7, 142.3, 137.9, 137.1, 131.7 (dd, $J_{\text{C}-\text{F}} = 66.4, 33.6$ Hz), 131.2, 130.2, 129.3, 129.1, 129.0, 128.7, 128.5, 128.4, 127.7, 124.6 (q, $J_{\text{C}-\text{F}} = 3.7$ Hz), 123.5 (d, $J_{\text{C}-\text{F}} = 272.4$ Hz), 121.9, 120.9, 119.5; HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{15}\text{F}_3\text{N}_3$ [M+H] $^+$ 390.1213, found 390.1214.



5-(4-Nitrophenyl)-3-phenylimidazo[1,5-c]quinazoline (3ea). yellow solid, 80% yield, mp. 251 – 254 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.15 – 8.07 (m, 1H), 8.07 (s, 1H), 7.98 – 7.86 (m, 3H), 7.67 – 7.55 (m, 2H), 7.54 – 7.47 (m, 2H), 7.19 – 7.10 (m, 3H), 7.10 – 7.01 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.0, 143.8, 142.1, 139.7, 137.8, 131.0, 130.1, 129.7, 129.3, 129.2, 128.8, 128.7, 128.4, 127.8, 122.7, 121.9, 121.1, 119.4; HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{15}\text{N}_4\text{O}_2$ [M+H] $^+$ 367.1190, found 367.1189.

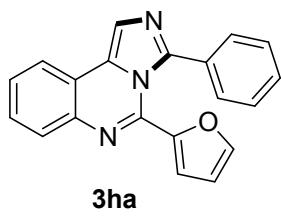


5-(3-Chlorophenyl)-3-phenylimidazo[1,5-c]quinazoline (3fa). yellow solid, 90% yield, mp. 185 – 188 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.12 – 8.05 (m, 1H), 8.03 (s, 1H), 7.93 – 7.83 (m, 1H), 7.67 – 7.49 (m, 2H), 7.32 (t, $J = 1.8$ Hz, 1H), 7.26 – 7.06 (m, 7H), 7.01 (t, $J = 7.9$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 144.7, 142.4, 137.9, 135.3, 133.9, 131.3, 130.2, 130.0, 129.1, 129.0, 128.8, 128.6, 128.5, 128.3, 127.7, 126.9, 121.8, 120.8, 119.4; HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{15}\text{ClN}_3$ [M+H] $^+$ 356.0949, found 356.0949.



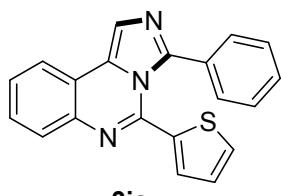
3ga

5-(2-Fluorophenyl)-3-phenylimidazo[1,5-c]quinazoline (3ga). yellow solid, 98% yield, mp. 185 – 187 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.13 – 8.05 (m, 1H), 8.01 (s, 1H), 7.95 – 7.86 (m, 1H), 7.65 – 7.48 (m, 3H), 7.23 – 6.98 (m, 7H), 6.58 – 6.46 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.1 (d, $J_{\text{C}-\text{F}} = 250.1$ Hz), 142.8, 141.8, 137.8, 132.3 (d, $J_{\text{C}-\text{F}} = 8.3$ Hz), 130.48 (d, $J_{\text{C}-\text{F}} = 2.6$ Hz), 130.46, 129.7, 129.5, 128.9, 128.5, 128.3, 127.1, 124.3 (d, $J_{\text{C}-\text{F}} = 3.3$ Hz), 123.1 (d, $J_{\text{C}-\text{F}} = 14.5$ Hz), 121.9, 120.5, 119.7, 115.3 (d, $J_{\text{C}-\text{F}} = 20.6$ Hz); HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{15}\text{FN}_3$ [M+H] $^+$ 340.1245, found 340.1242.



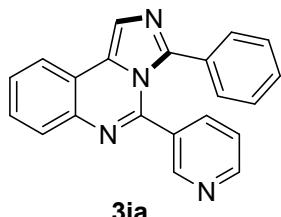
3ha

5-(Furan-2-yl)-3-phenylimidazo[1,5-c]quinazoline (3ha). yellow solid, 94% yield, mp. 220 – 222 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.09 – 8.01 (m, 1H), 8.00 (s, 1H), 7.93 – 7.83 (m, 1H), 7.61 – 7.48 (m, 2H), 7.44 – 7.32 (m, 2H), 7.30 – 7.17 (m, 3H), 6.93 – 6.86 (m, 1H), 6.86 – 6.78 (m, 1H), 6.26 (dd, J = 3.5, 1.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.7, 143.8, 143.0, 137.7, 137.0, 131.9, 130.3, 128.7, 128.5, 128.2, 128.1, 127.93, 127.85, 121.8, 120.8, 119.5, 114.6, 111.5; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{14}\text{N}_3\text{O}$ [M+H]⁺ 312.1131, found 312.1129.



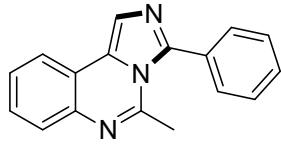
3ia

3-Phenyl-5-(thiophen-2-yl)imidazo[1,5-c]quinazoline (3ia). yellow solid, 76% yield, mp. 213 – 216 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.12 – 7.99 (m, 2H), 7.94 – 7.83 (m, 1H), 7.65 – 7.47 (m, 2H), 7.34 – 7.25 (m, 3H), 7.24 – 7.10 (m, 3H), 6.68 (dd, J = 3.8, 1.1 Hz, 1H), 6.57 (dd, J = 5.0, 3.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 142.7, 140.5, 138.0, 134.7, 132.0, 131.1, 130.7, 128.6, 128.51, 128.50, 128.3, 128.1, 127.7, 126.6, 121.7, 120.9, 119.2; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{14}\text{N}_3\text{S}$ [M+H]⁺ 328.0903, found 328.0897.



3ja

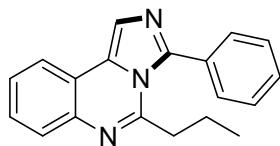
3-Phenyl-5-(pyridin-3-yl)imidazo[1,5-c]quinazoline (3ja). yellow solid, 98% yield, mp. 204 – 206 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.68 (d, J = 1.8 Hz, 1H), 8.42 (dd, J = 4.9, 1.5 Hz, 1H), 8.12 – 8.05 (m, 1H), 8.04 (s, 1H), 7.97 – 7.85 (m, 1H), 7.66 – 7.54 (m, 2H), 7.54 – 7.46 (m, 1H), 7.21 – 7.04 (m, 5H), 6.94 (dd, J = 7.9, 4.9 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 150.4, 149.3, 143.4, 142.2, 137.9, 135.5, 130.9, 130.13, 130.10, 129.6, 129.0, 128.7, 128.6, 128.3, 127.9, 122.1, 121.8, 120.9, 119.4; HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{15}\text{N}_4$ [M+H]⁺ 323.1291, found 323.1287.



3ka

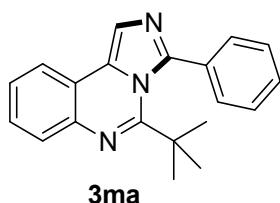
5-Methyl-3-phenylimidazo[1,5-c]quinazoline (3ka). white solid, 76% yield, mp. 154 – 155 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.01 – 7.90 (m, 1H), 7.85 (s, 1H), 7.78 – 7.68 (m, 1H), 7.60 – 7.53 (m, 2H), 7.53 – 7.41 (m, 5H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.0, 141.9, 137.7, 132.8, 130.7,

129.7, 129.3, 128.4, 128.1, 127.9, 127.3, 121.7, 119.9, 119.5, 24.7; HRMS (ESI) m/z calcd for C₁₇H₁₄N₃ [M+H]⁺ 260.1182, found 260.1179.



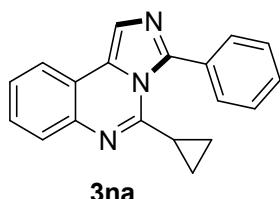
3a

3-Phenyl-5-propylimidazo[1,5-c]quinazoline (3a). yellow solid, 55% yield, mp. 78 – 81 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.00 – 7.94 (m, 1H), 7.87 (s, 1H), 7.78 – 7.71 (m, 1H), 7.60 – 7.42 (m, 7H), 2.74 – 2.47 (m, 2H), 1.65 – 1.52 (m, 2H), 0.63 (t, J = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 148.2, 141.6, 137.7, 133.0, 130.4, 129.6, 129.5, 128.3, 128.1, 127.8, 127.5, 121.6, 120.0, 119.3, 37.3, 20.4, 13.4; HRMS (ESI) m/z calcd for C₁₉H₁₈N₃ [M+H]⁺ 288.1495, found 288.1495.



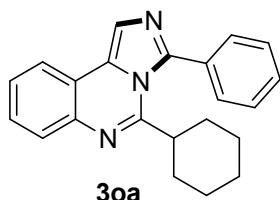
3ma

5-(Tert-butyl)-3-phenylimidazo[1,5-c]quinazoline (3ma). yellow oil, 91% yield. ¹H NMR (300 MHz, CDCl₃) δ 7.99 – 7.85 (m, 2H), 7.80 – 7.70 (m, 1H), 7.60 – 7.51 (m, 2H), 7.51 – 7.35 (m, 5H), 1.25 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 154.3, 143.1, 137.0, 135.3, 131.8, 131.0, 129.4, 128.2, 128.1, 127.9, 127.5, 121.1, 120.7, 119.2, 40.2, 30.0; HRMS (ESI) m/z calcd for C₂₀H₂₀N₃ [M+H]⁺ 302.1652, found 302.1651.



3na

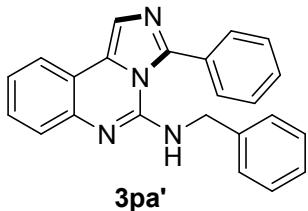
5-Cyclopropyl-3-phenylimidazo[1,5-c]quinazoline (3na). yellow solid, 91% yield, mp. 112 – 114 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.09 – 7.91 (m, 1H), 7.88 (s, 1H), 7.70 – 7.62 (m, 3H), 7.51 – 7.41 (m, 5H), 1.74 (tt, J = 8.1, 4.9 Hz, 1H), 1.42 – 1.31 (m, 2H), 0.83 – 0.70 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 149.2, 141.8, 137.8, 133.1, 130.3, 129.7, 129.3, 128.2, 128.0, 127.3, 127.2, 121.6, 120.1, 119.1, 15.6, 10.8; HRMS (ESI) m/z calcd for C₁₉H₁₆N₃ [M+H]⁺ 286.1339, found 286.1339.



3oa

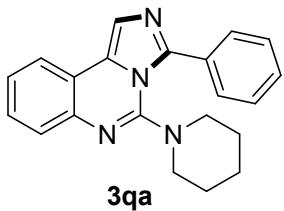
5-Cyclohexyl-3-phenylimidazo[1,5-c]quinazoline (3oa). white solid, 87% yield, mp. 153 – 156 °C. ¹H NMR (300 MHz, CDCl₃) δ 8.00 – 7.94 (m, 1H), 7.89 (s, 1H), 7.81 – 7.73 (m, 1H), 7.60 – 7.43 (m, 7H), 2.88 – 2.72 (m, 1H), 1.82 – 1.71 (m, 2H), 1.67 – 1.42 (m, 5H), 1.22 – 1.03 (m, 1H), 0.75 – 0.51

(m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 152.1, 141.3, 137.8, 133.6, 130.2, 129.7, 129.5, 128.21, 128.19, 127.7, 127.6, 121.6, 119.9, 119.3, 40.7, 30.9, 25.7, 25.6; HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{22}\text{N}_3$ [$\text{M}+\text{H}]^+$ 328.1808, found 328.1809.



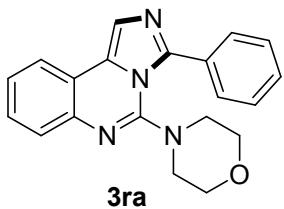
3pa'

N-Benzyl-3-phenylimidazo[1,5-*c*]quinazolin-5-amine (**3pa'**). yellow solid, 8% yield, mp. 33 – 35 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, $J = 7.7$ Hz, 1H), 7.82 (s, 1H), 7.63 – 7.54 (m, 3H), 7.49 – 7.34 (m, 5H), 7.32 – 7.21 (m, 3H), 7.13 – 7.05 (m, 2H), 5.12 (brs, 1H), 4.64 (d, $J = 5.0$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 141.3, 139.9, 139.5, 137.4, 131.2, 131.1, 130.5, 130.1, 128.57, 128.56, 127.7, 127.5, 125.1, 123.9, 121.8, 120.1, 116.6, 45.8; HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{19}\text{N}_4$ [$\text{M}+\text{H}]^+$ 351.1604, found 351.1603.



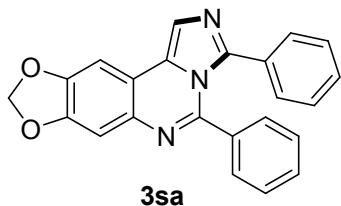
3qa

3-Phenyl-5-(piperidin-1-yl)imidazo[1,5-*c*]quinazoline (**3qa**). yellow solid, 37% yield, mp. 163 – 165 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.93 (dd, $J = 7.8, 1.1$ Hz, 1H), 7.88 (s, 1H), 7.73 – 7.63 (m, 3H), 7.49 – 7.40 (m, 4H), 7.37 (td, $J = 7.7, 1.1$ Hz, 1H), 3.33 (brs, 2H), 2.72 (brs, 2H), 1.36 (brs, 4H), 0.71 (brs, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.8, 142.3, 139.2, 131.8, 131.6, 130.5, 128.7, 128.3, 127.3, 126.4, 125.7, 121.6, 120.9, 118.3, 50.5, 24.0, 23.7; HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{21}\text{N}_4$ [$\text{M}+\text{H}]^+$ 329.1761, found 329.1763.



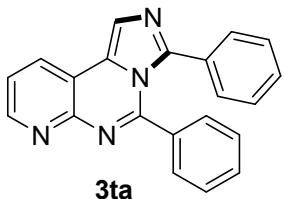
3ra

4-(3-Phenylimidazo[1,5-*c*]quinazolin-5-yl)morpholine (**3ra**). yellow solid, 48% yield, mp. 173 – 175 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.94 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.90 (s, 1H), 7.75 – 7.64 (m, 3H), 7.52 – 7.43 (m, 4H), 7.40 (td, $J = 7.6, 1.3$ Hz, 1H), 3.80 – 2.50 (m, 8H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.7, 141.9, 138.8, 131.8, 131.6, 130.5, 129.1, 128.5, 127.5, 126.6, 126.2, 121.7, 121.1, 118.4, 64.9, 49.7; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{19}\text{N}_4\text{O}$ [$\text{M}+\text{H}]^+$ 331.1553, found 331.1552.

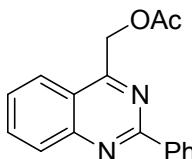


3sa

3,5-Diphenyl-[1,3]dioxolo[4,5-g]imidazo[1,5-c]quinazoline (3sa). yellow solid, 35% yield, mp. 201 – 203 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.87 (s, 1H), 7.39 (s, 1H), 7.32 – 7.28 (m, 3H), 7.18 (t, J = 7.5 Hz, 1H), 7.13 – 6.97 (m, 7H), 6.10 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.6, 148.4, 144.5, 141.6, 134.2, 133.8, 131.5, 130.8, 129.7, 129.1, 128.6, 127.9, 127.7, 127.4, 119.2, 114.4, 107.2, 101.9, 99.9; HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{16}\text{N}_3\text{O}_2$ [M+H] $^+$ 366.1237, found 366.1234.



3,5-Diphenylimidazo[1,5-c]pyrido[3,2-e]pyrimidine (3ta). yellow solid, 69% yield, mp. 220 – 223 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.81 (d, J = 3.2 Hz, 1H), 8.40 (d, J = 6.6 Hz, 1H), 8.09 (s, 1H), 7.50 (dd, J = 7.8, 4.7 Hz, 1H), 7.42 (d, J = 7.4 Hz, 2H), 7.22 – 7.11 (m, 4H), 7.10 – 6.98 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 150.1, 149.6, 149.3, 143.4, 133.0, 131.0, 130.49, 130.48, 129.8, 129.1, 129.0, 128.4, 127.55, 127.52, 123.3, 122.2, 114.7; HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{15}\text{N}_4$ [M+H] $^+$ 323.1291, found 323.1290.



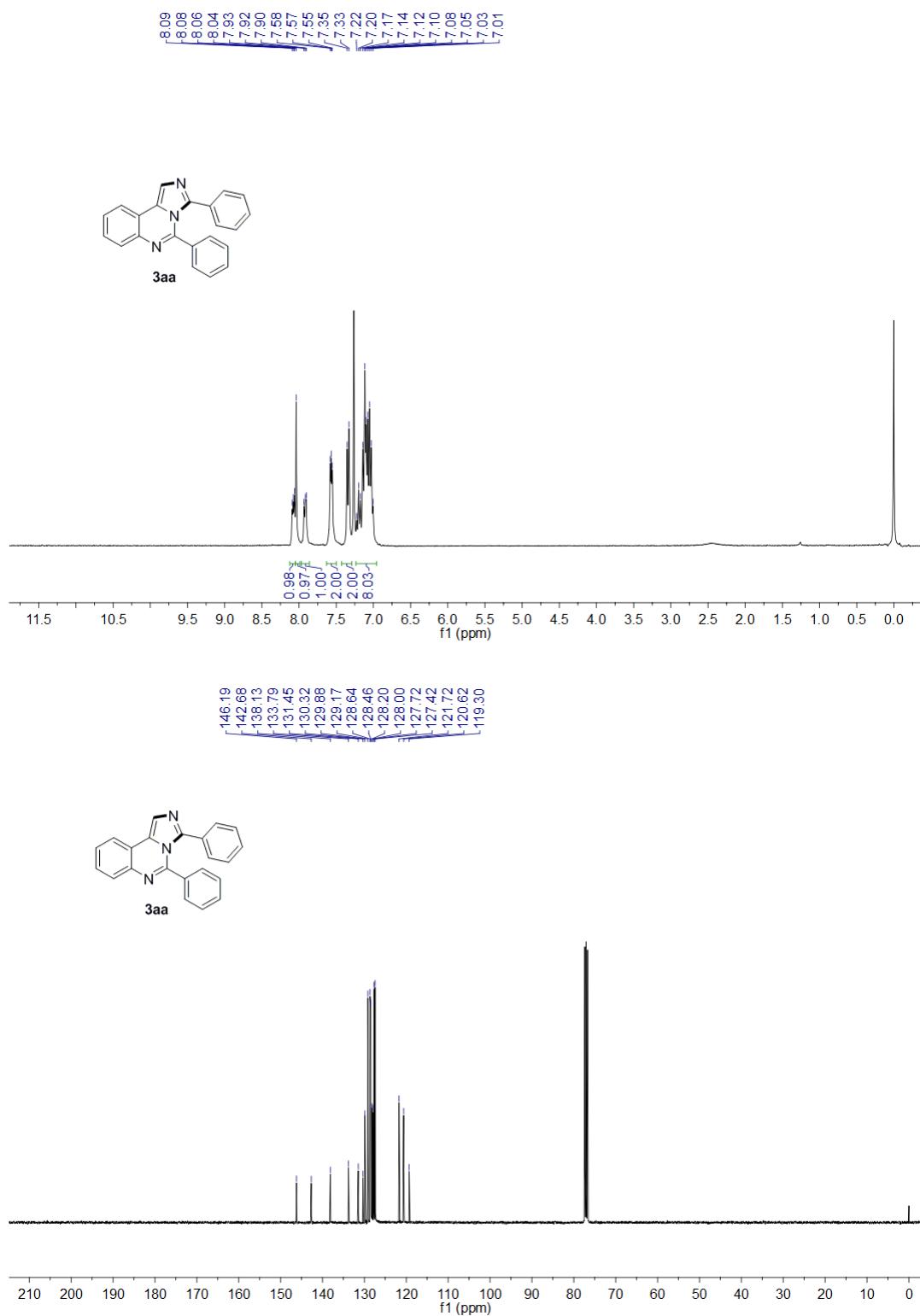
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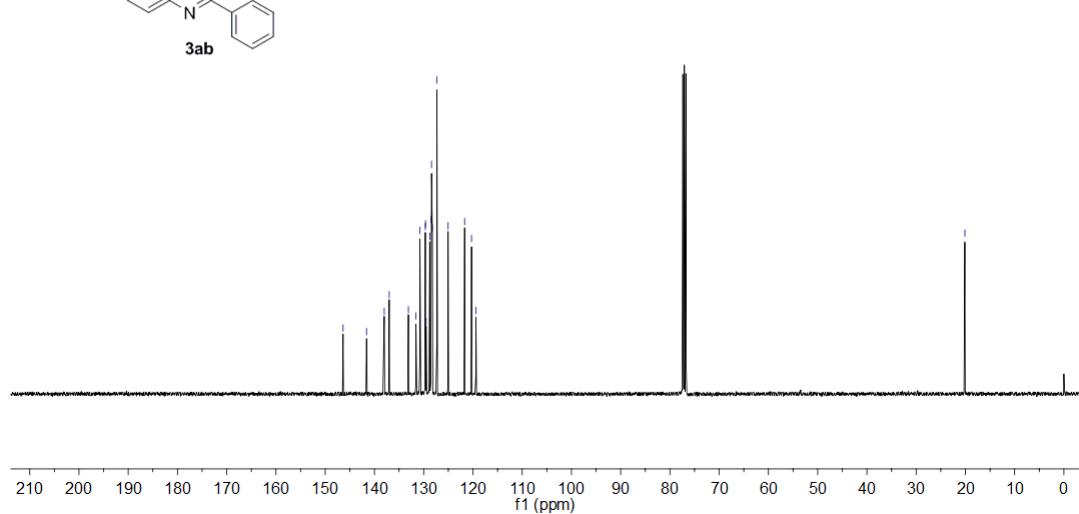
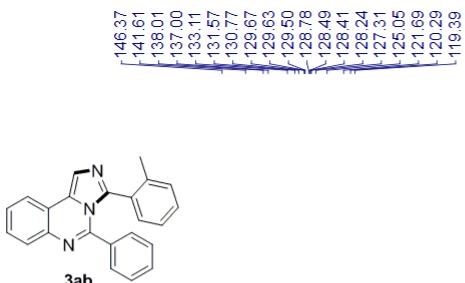
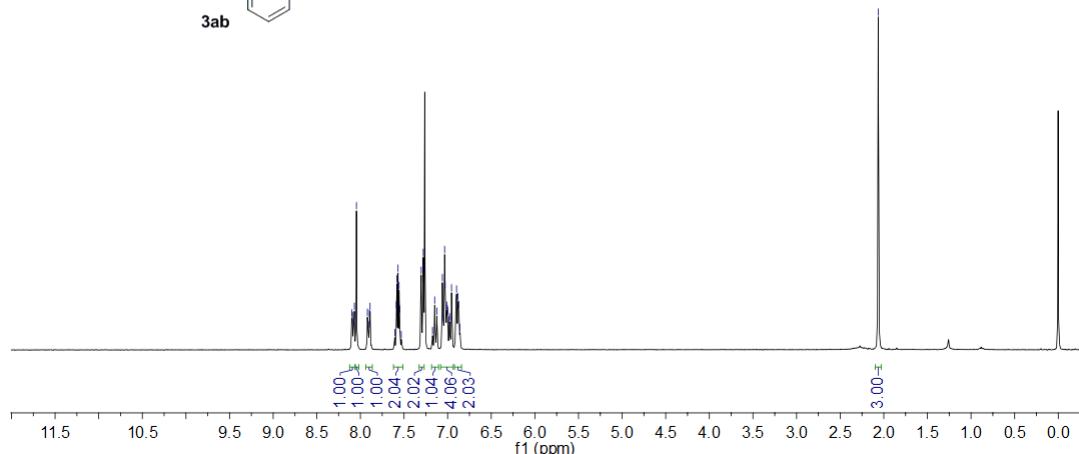
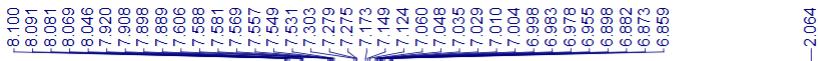
(2-Phenylquinazolin-4-yl)methyl acetate (6). yellow solid, 52% yield, mp. 87 – 90 °C. ^1H NMR (300 MHz, CDCl_3) δ 8.68 – 8.56 (m, 2H), 8.12 (d, J = 8.4 Hz, 1H), 8.08 – 7.99 (m, 1H), 7.89 (ddd, J = 8.4, 6.9, 1.4 Hz, 1H), 7.60 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.57 – 7.48 (m, 3H), 5.77 (s, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.6, 163.6, 160.1, 151.1, 137.8, 133.9, 130.7, 129.5, 128.6, 127.4, 123.8, 121.3, 64.2, 20.9; MS (ESI): 279.05 [M+H] $^+$; HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{15}\text{N}_2\text{O}_2$ [M+H] $^+$ 279.1128, found 279.1127.

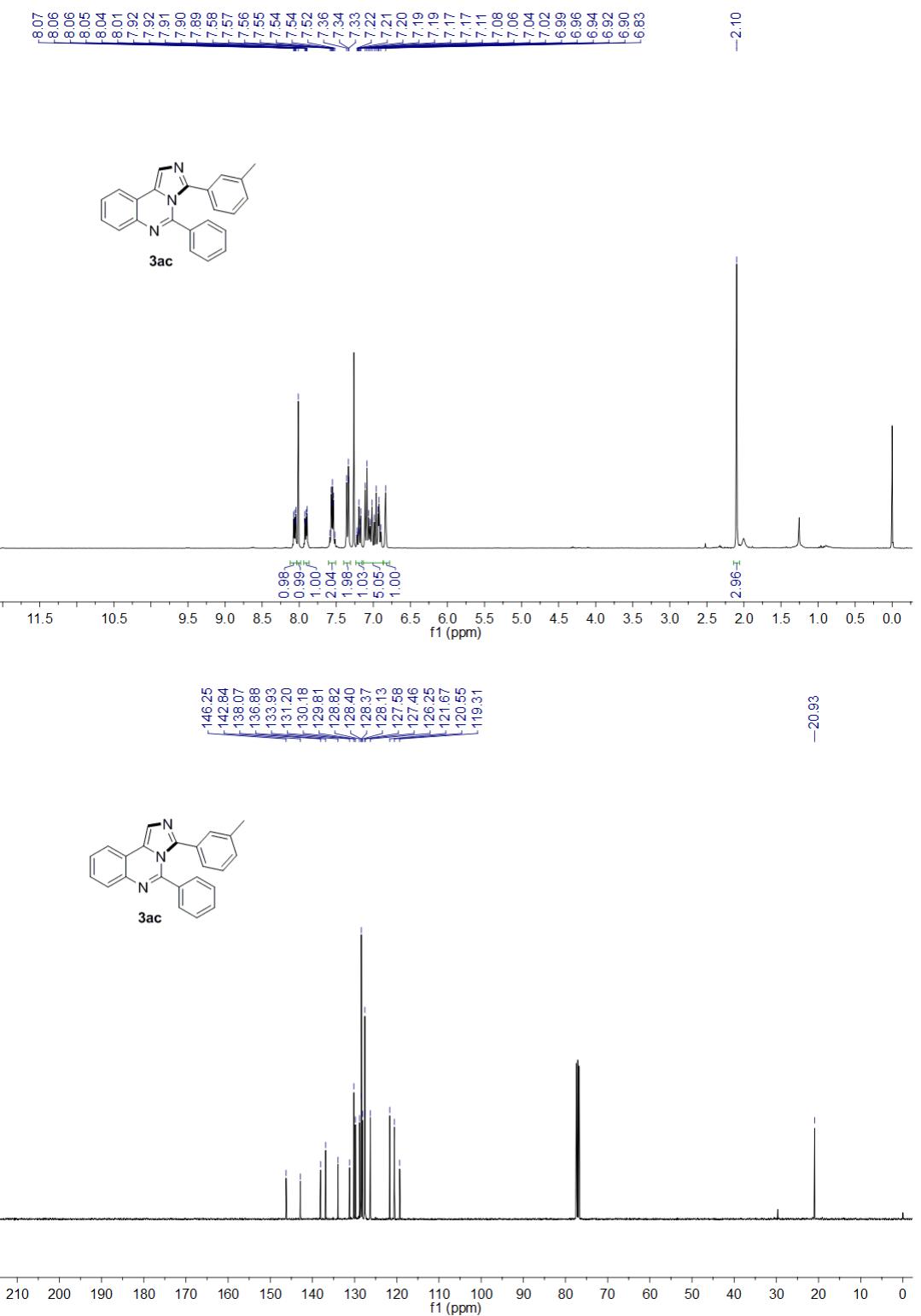
References

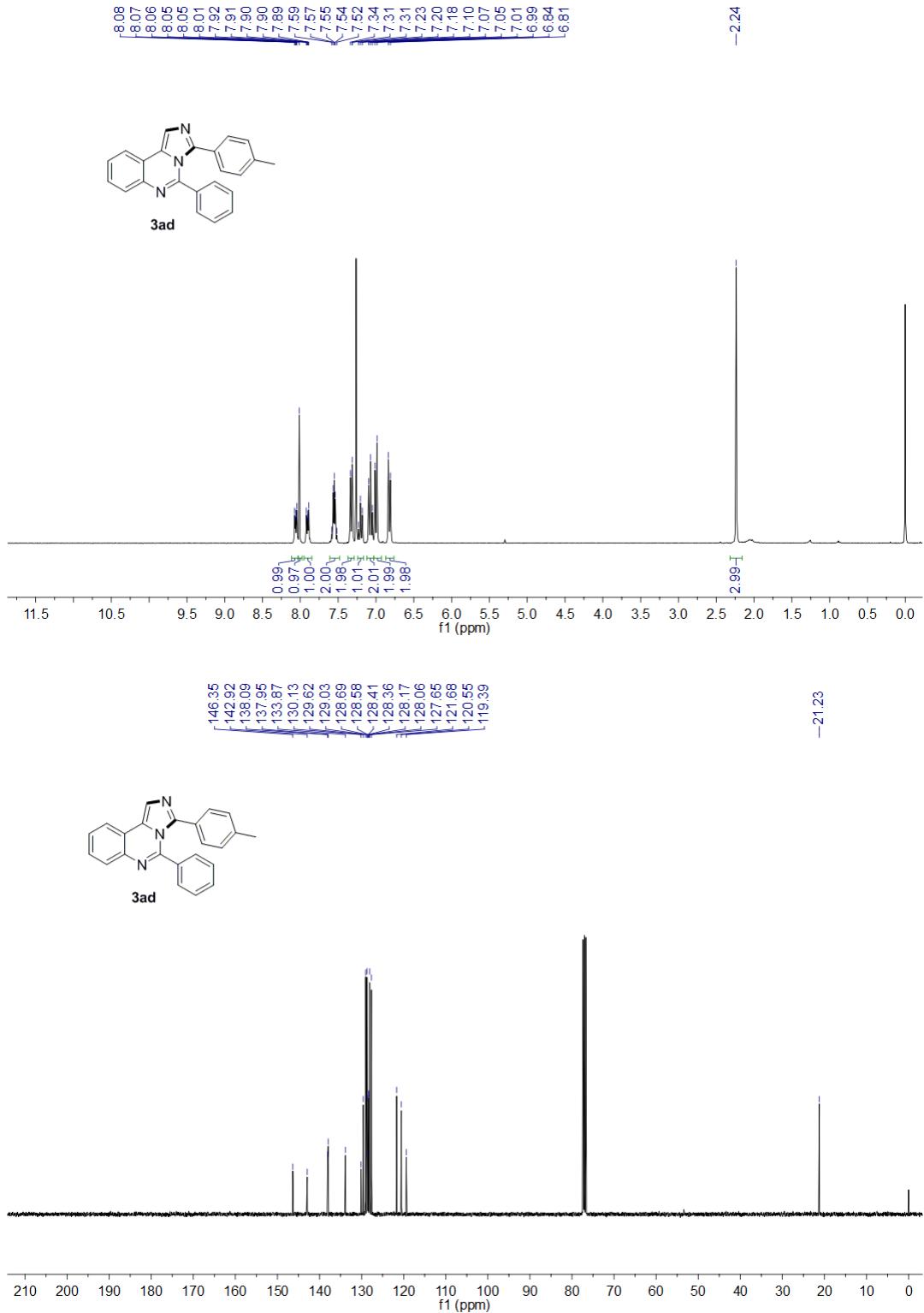
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Spectral copies of ^1H - and ^{13}C -NMR of products and intermediate 6

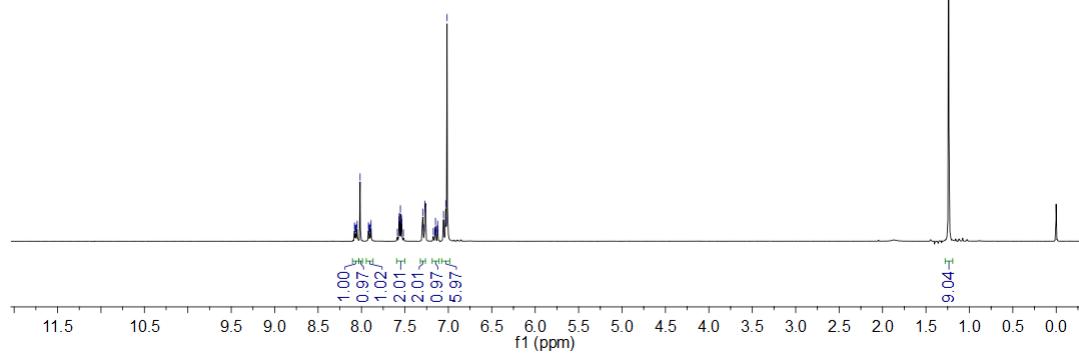
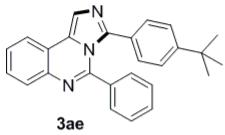




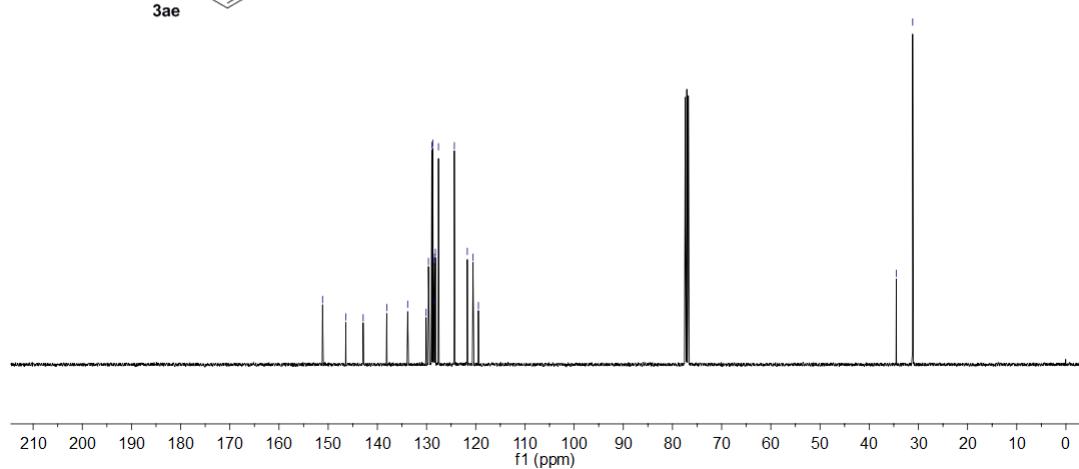
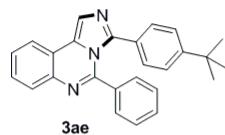


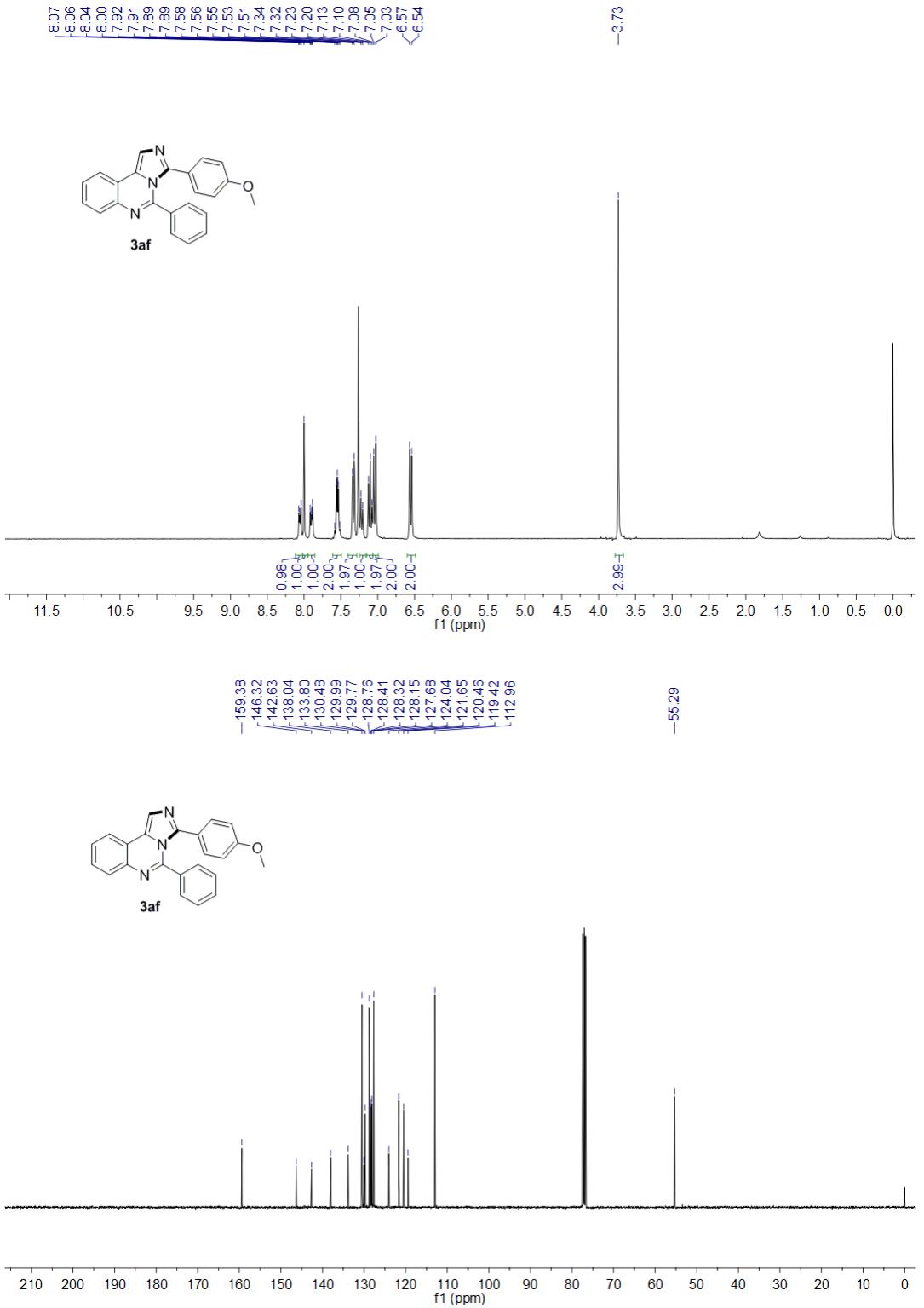


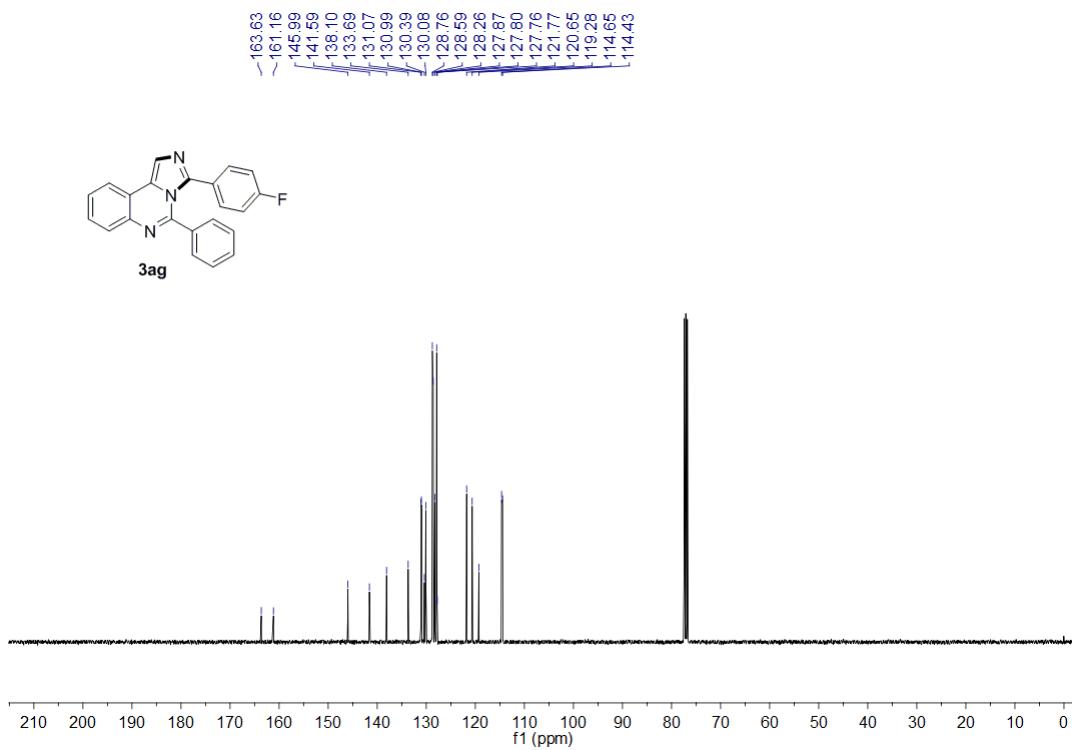
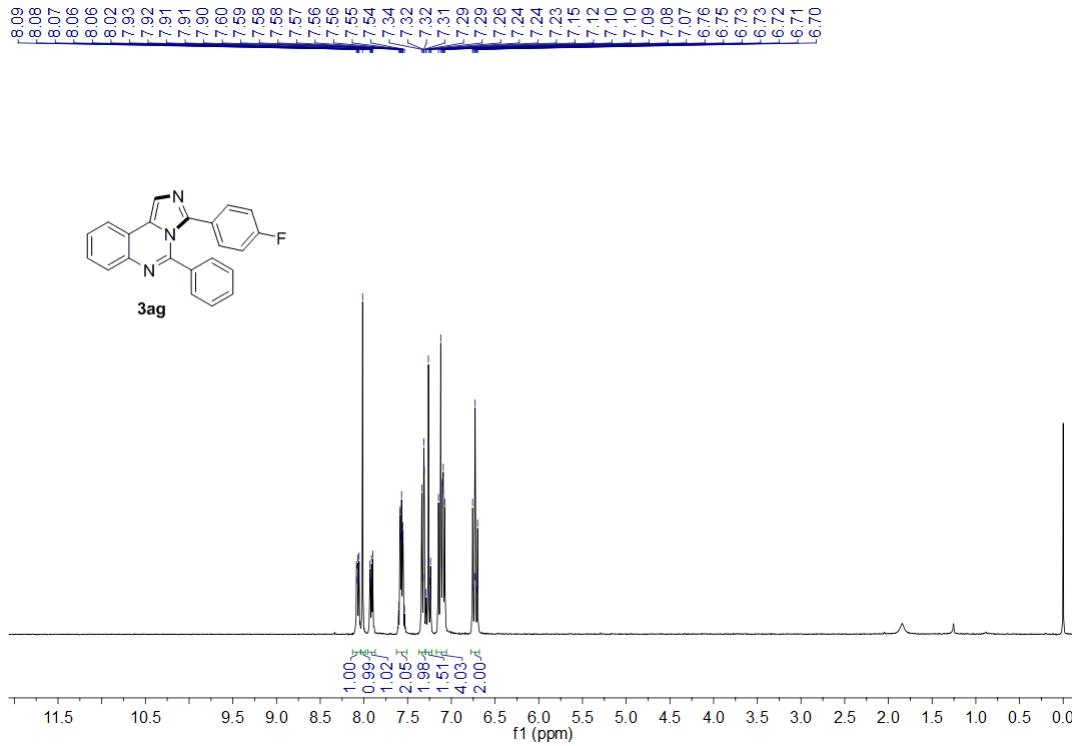
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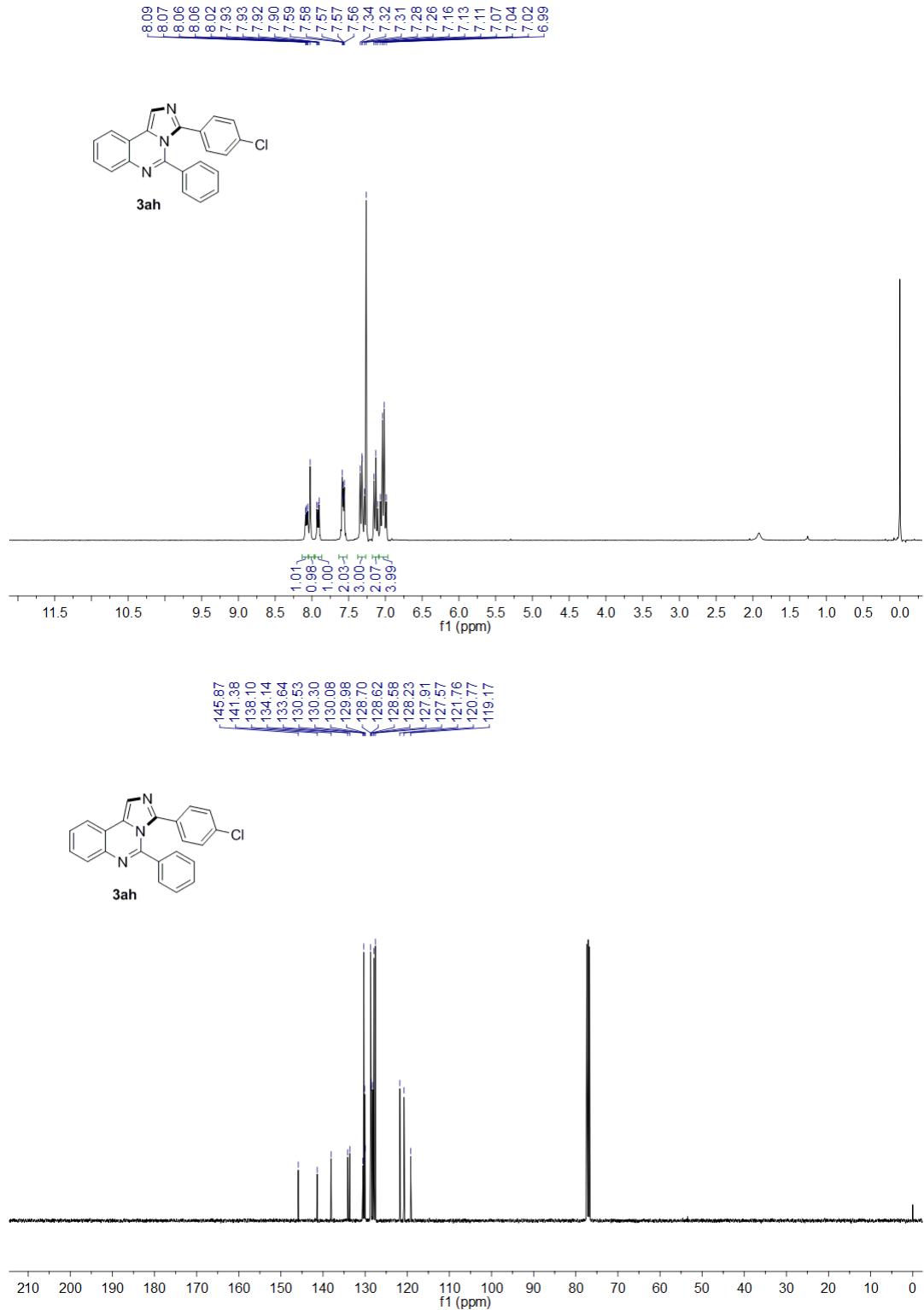


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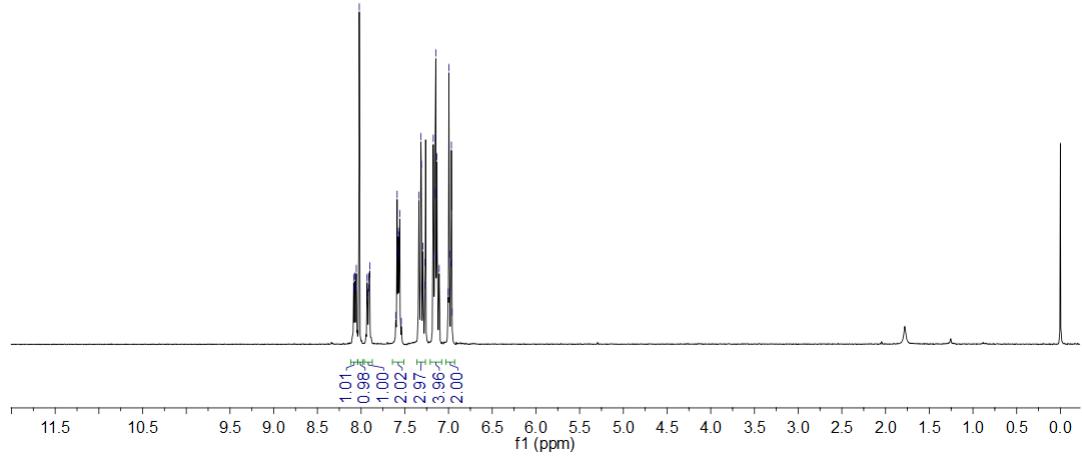




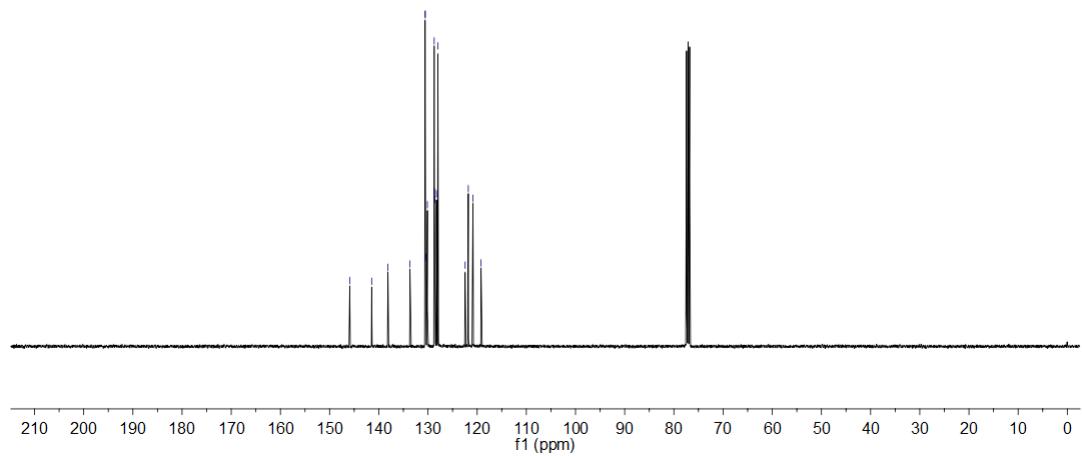
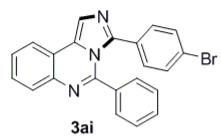


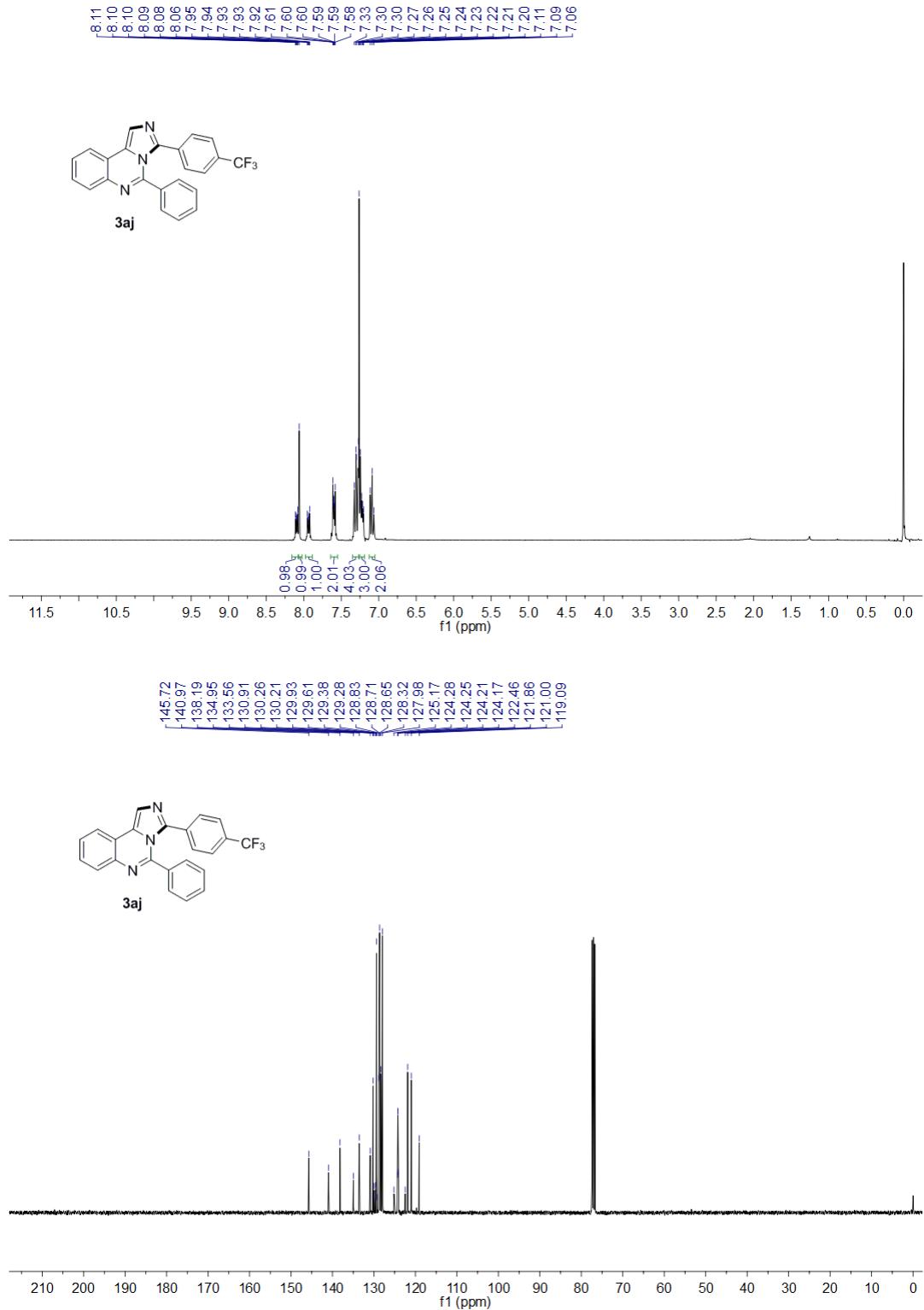


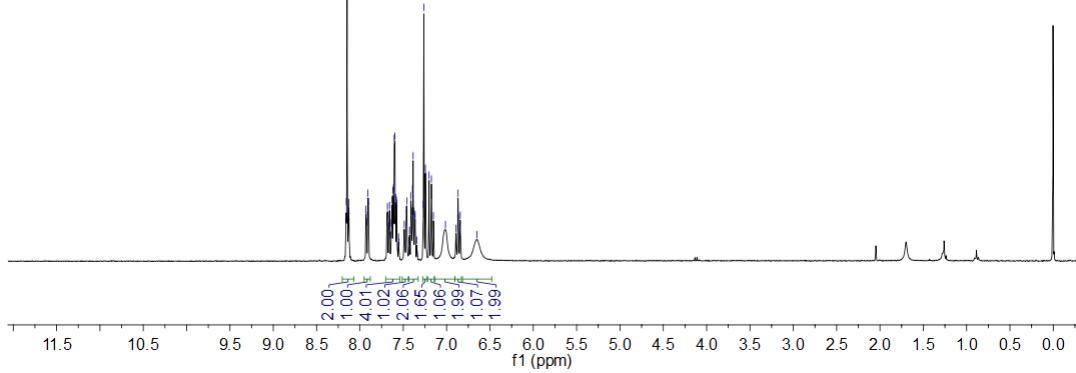
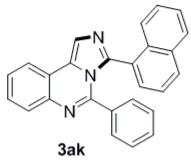
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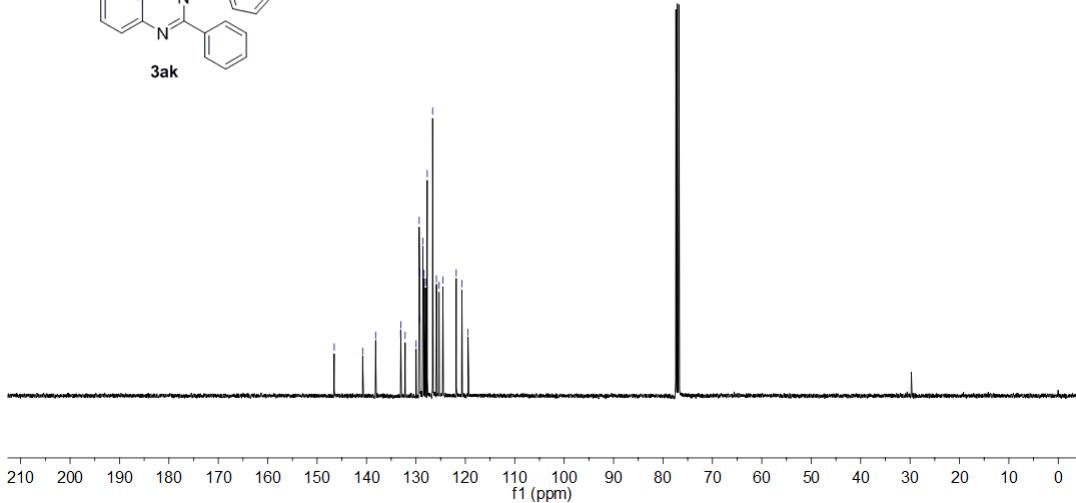
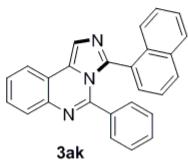
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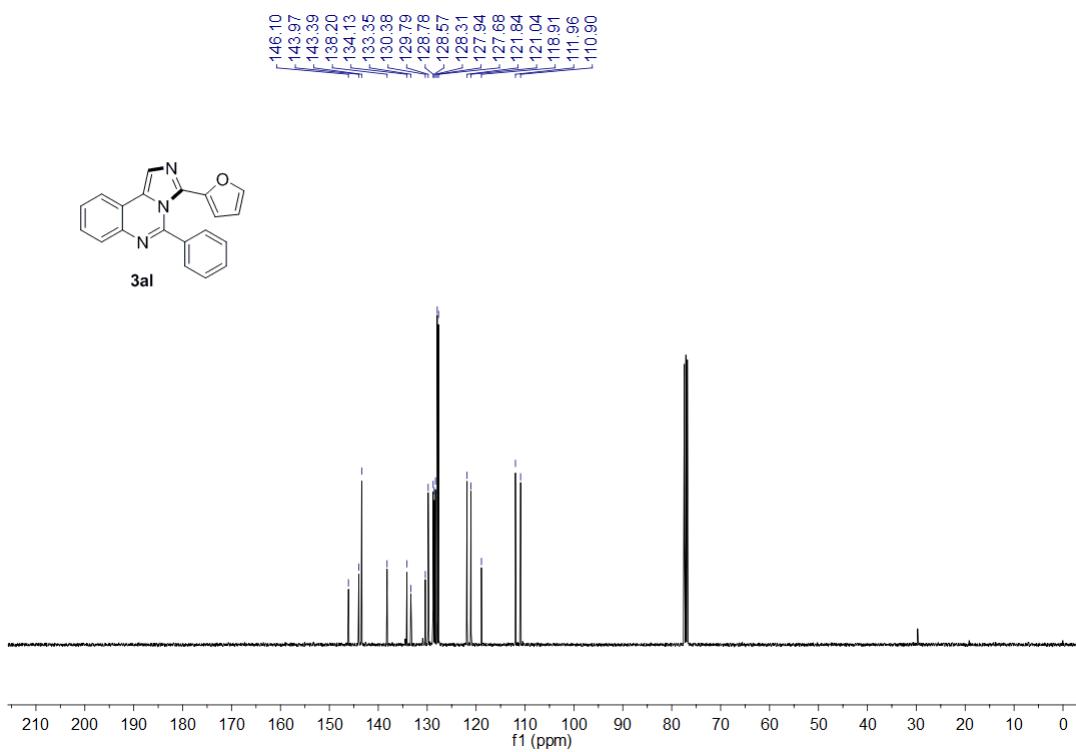
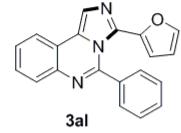


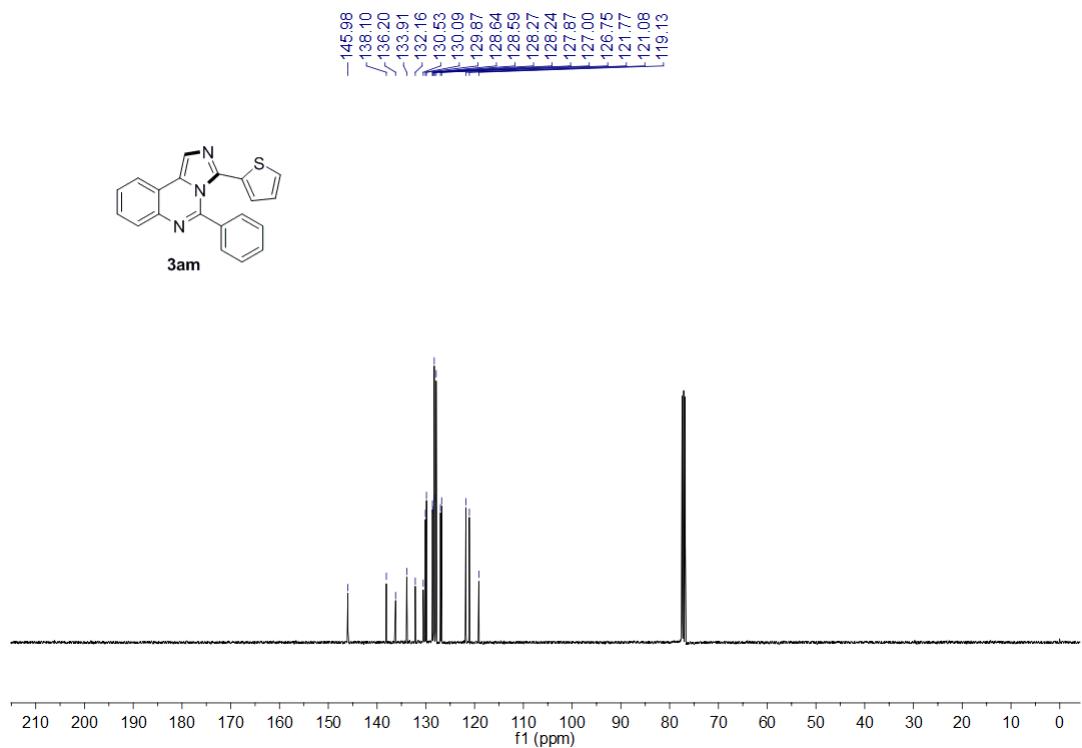
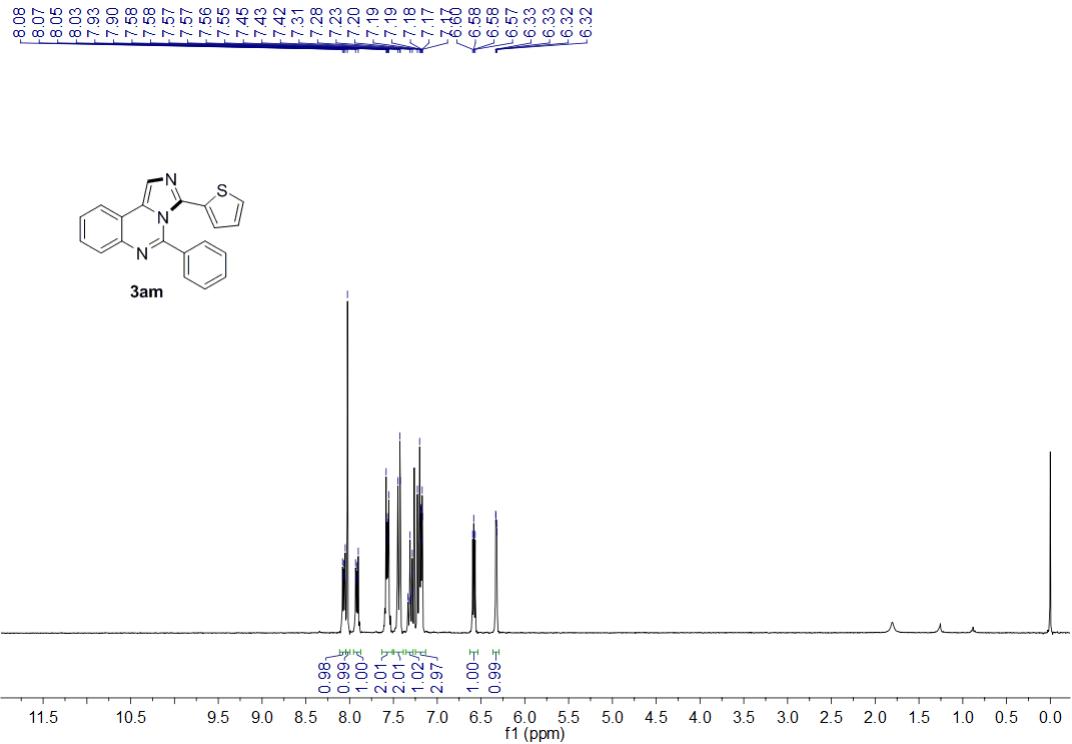




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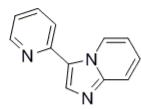




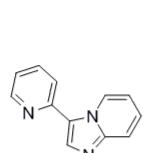
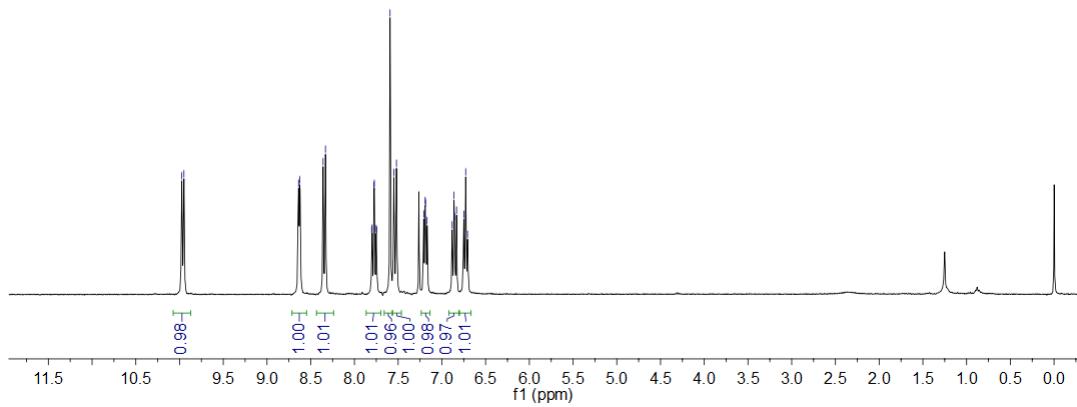


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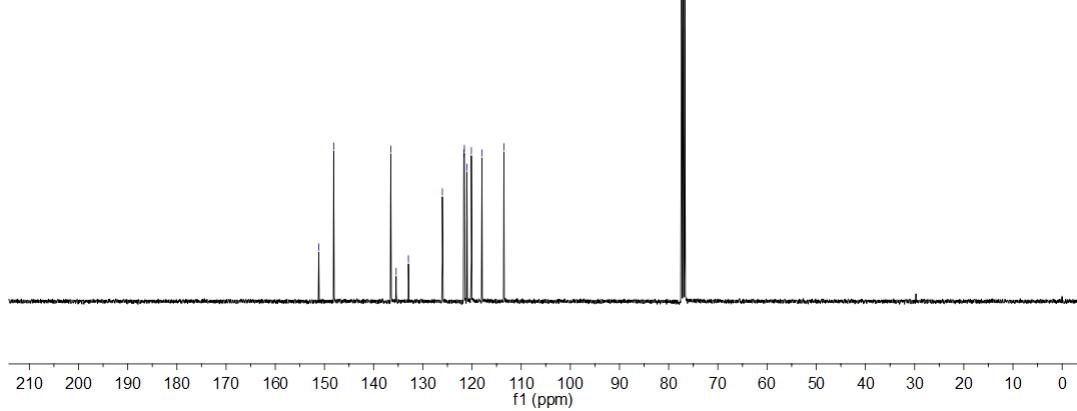


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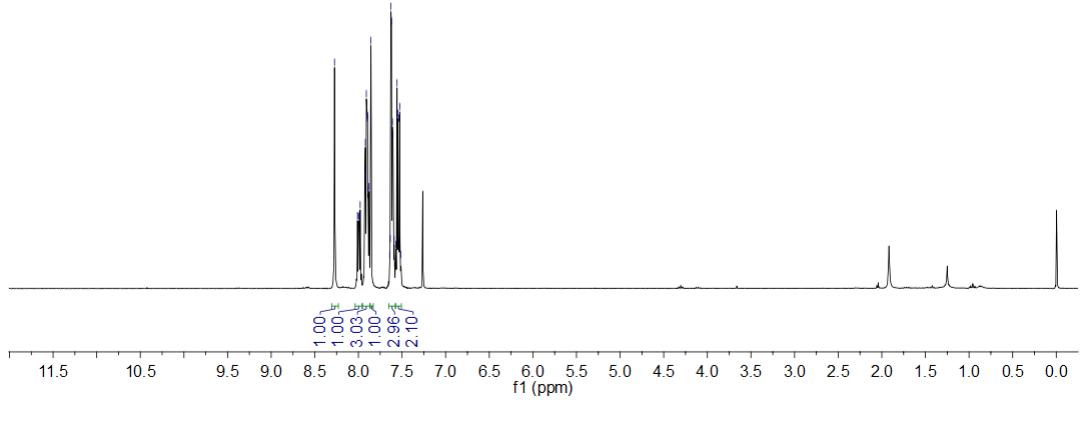
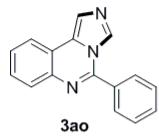


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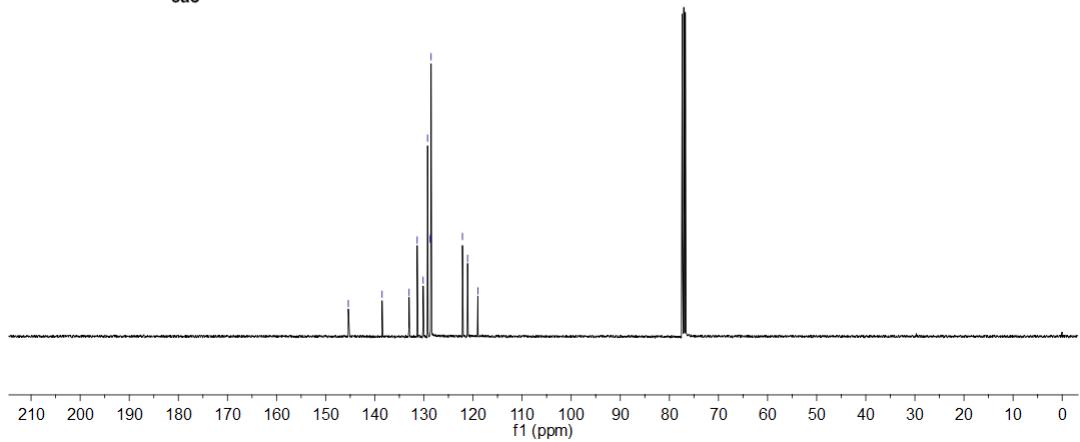
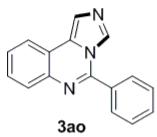
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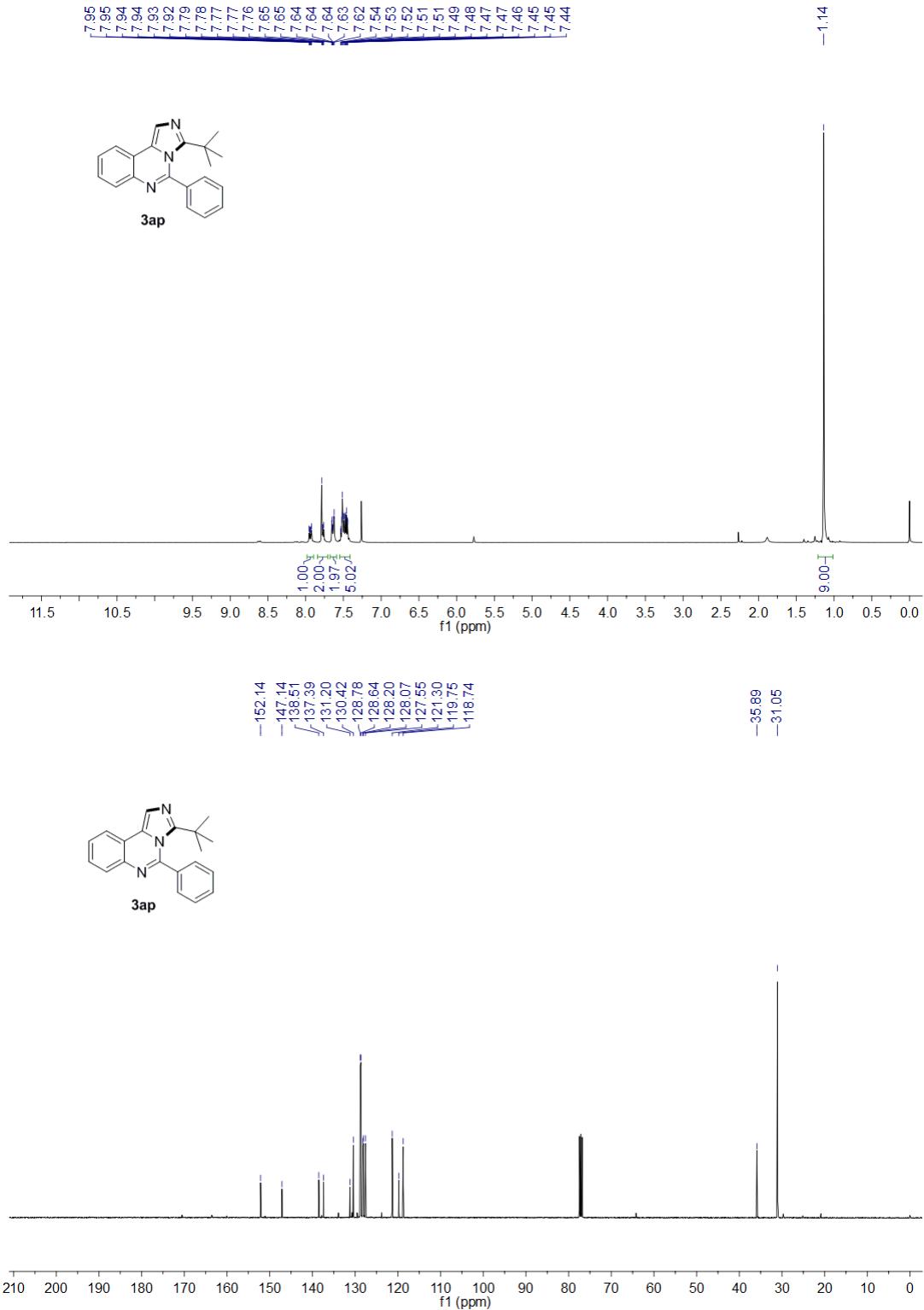


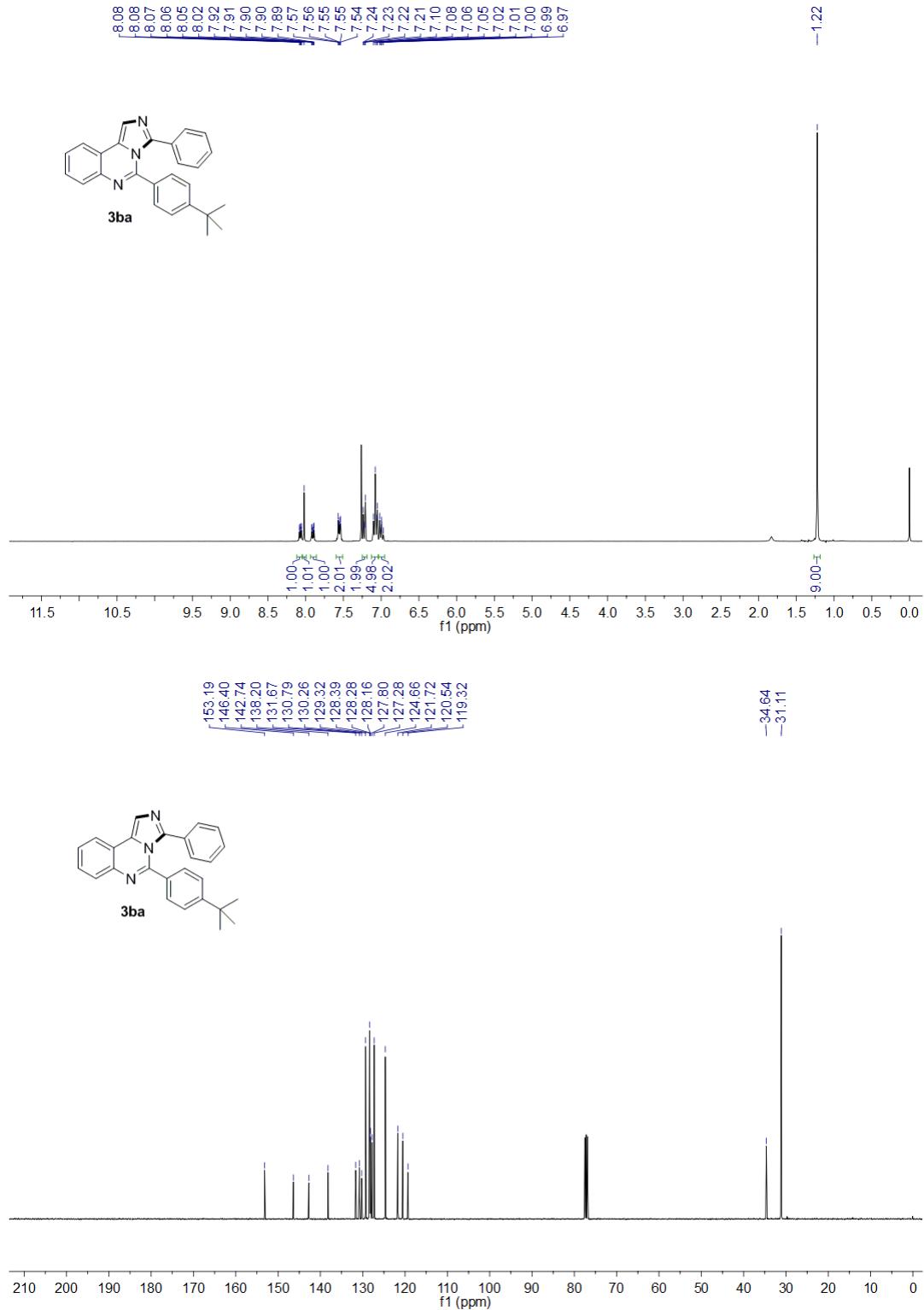
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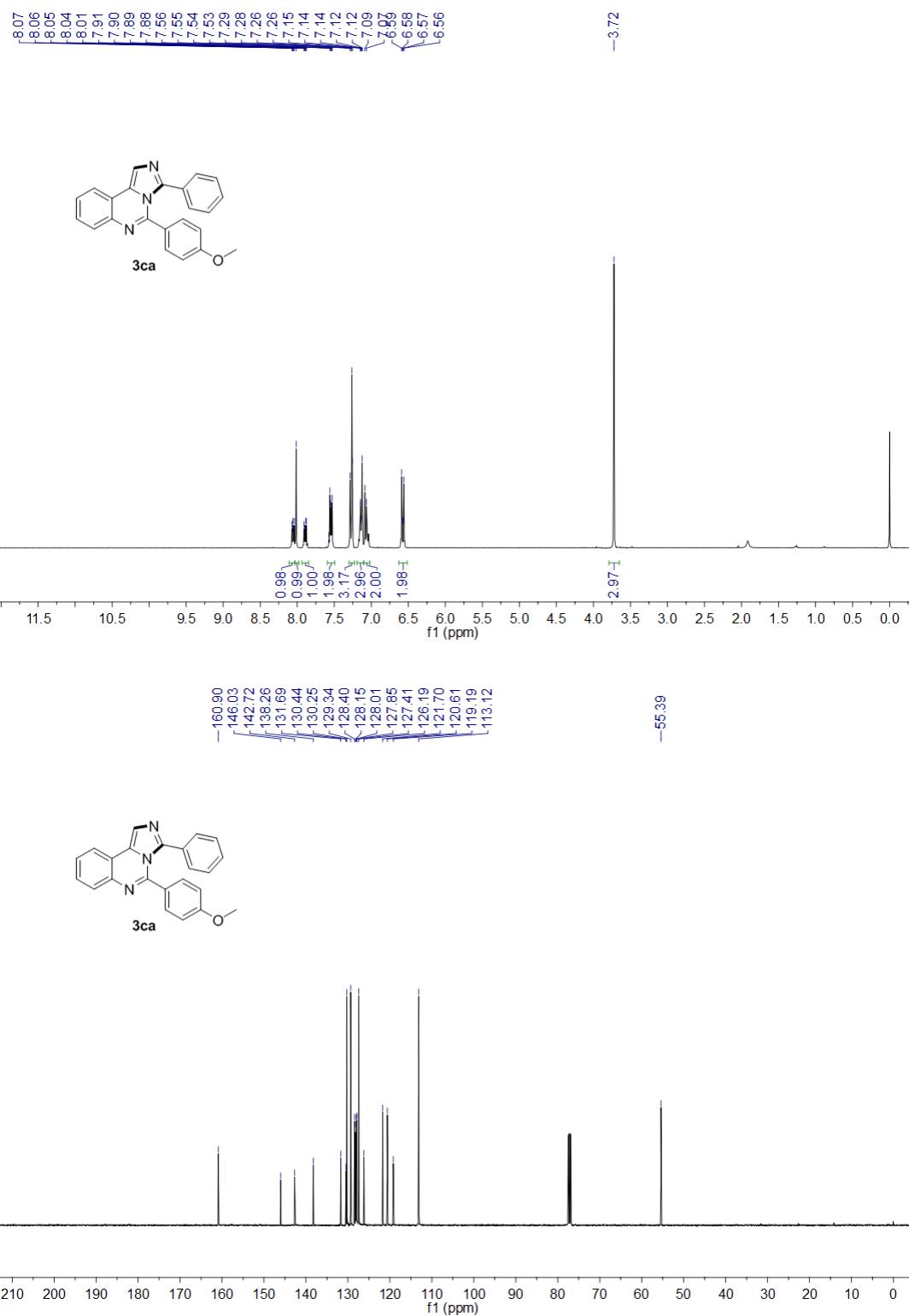


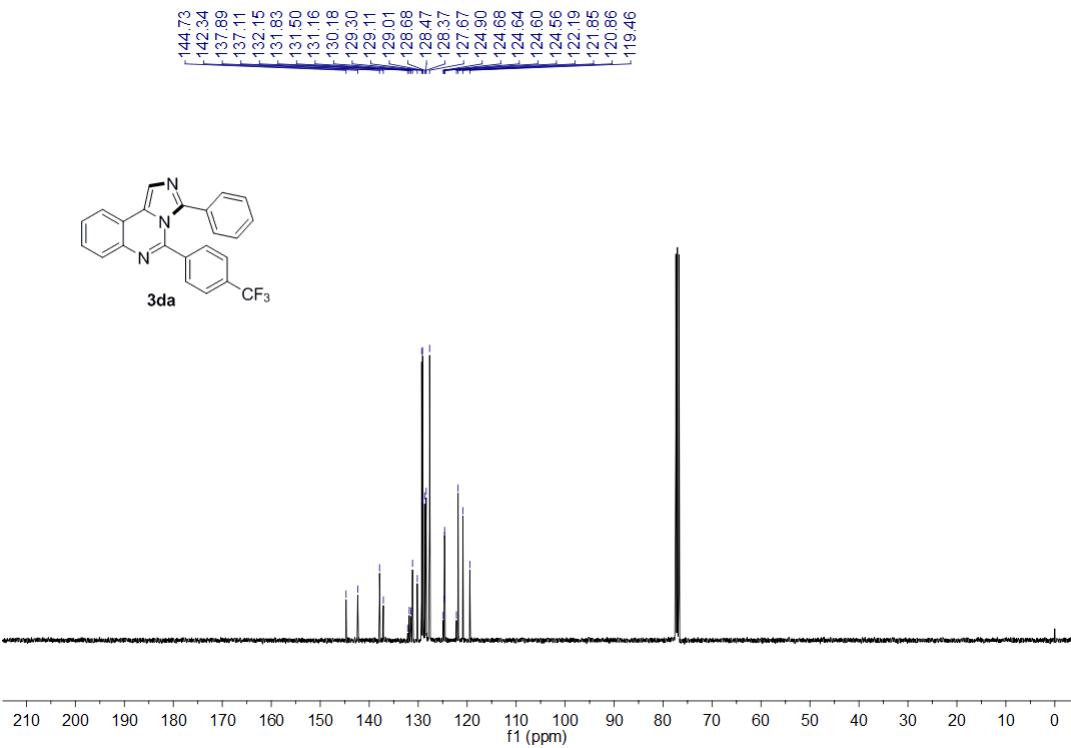
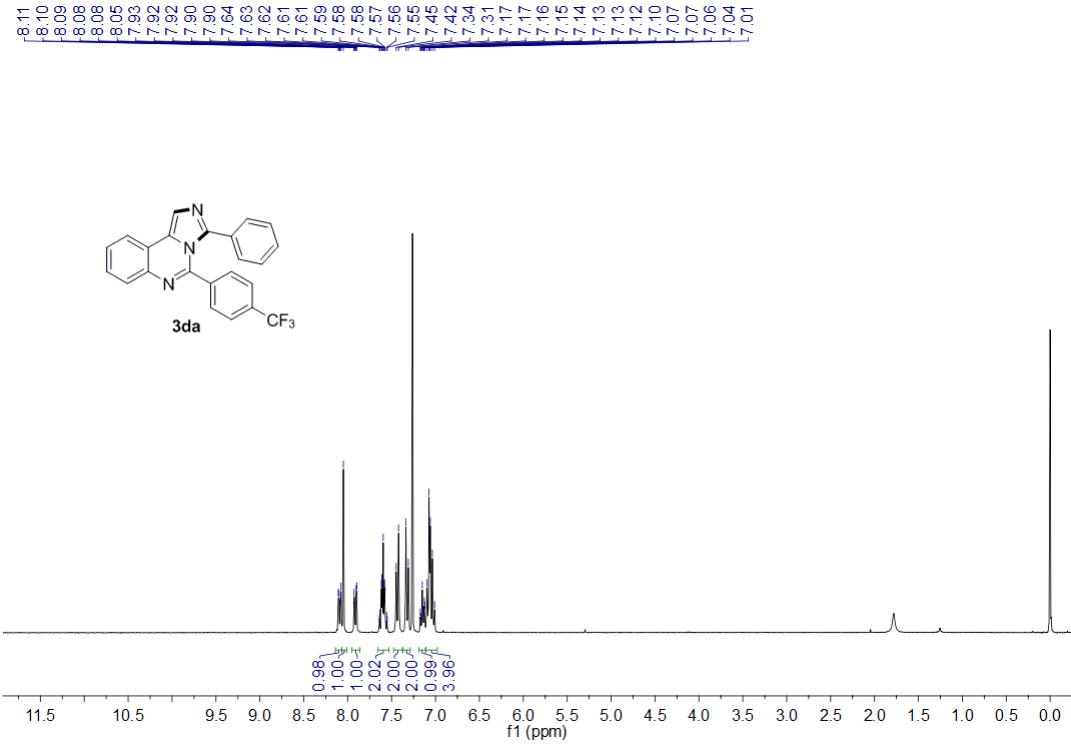
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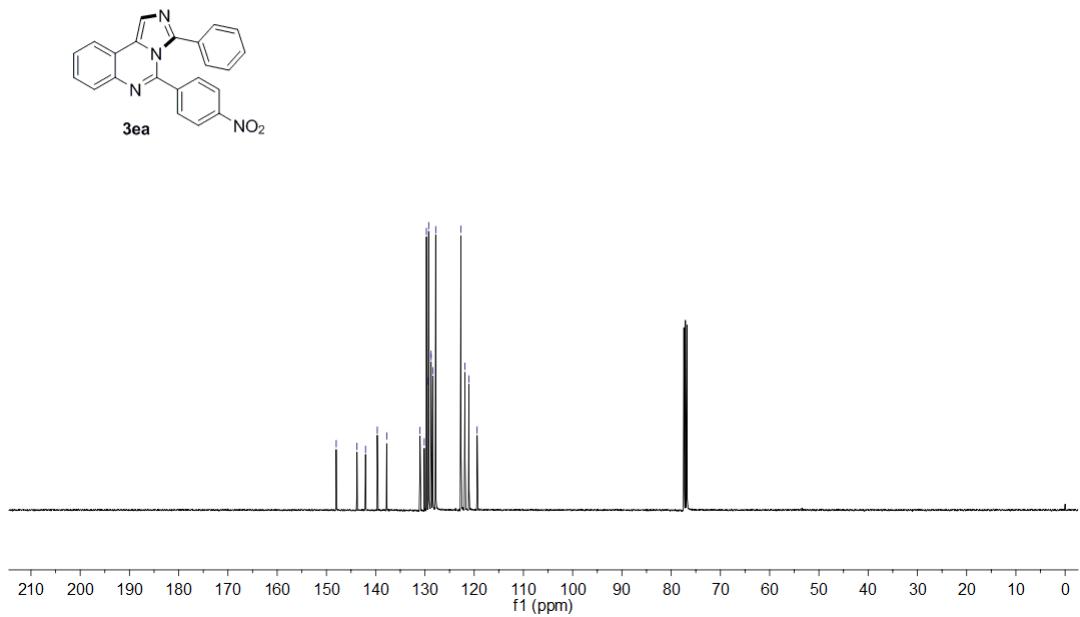
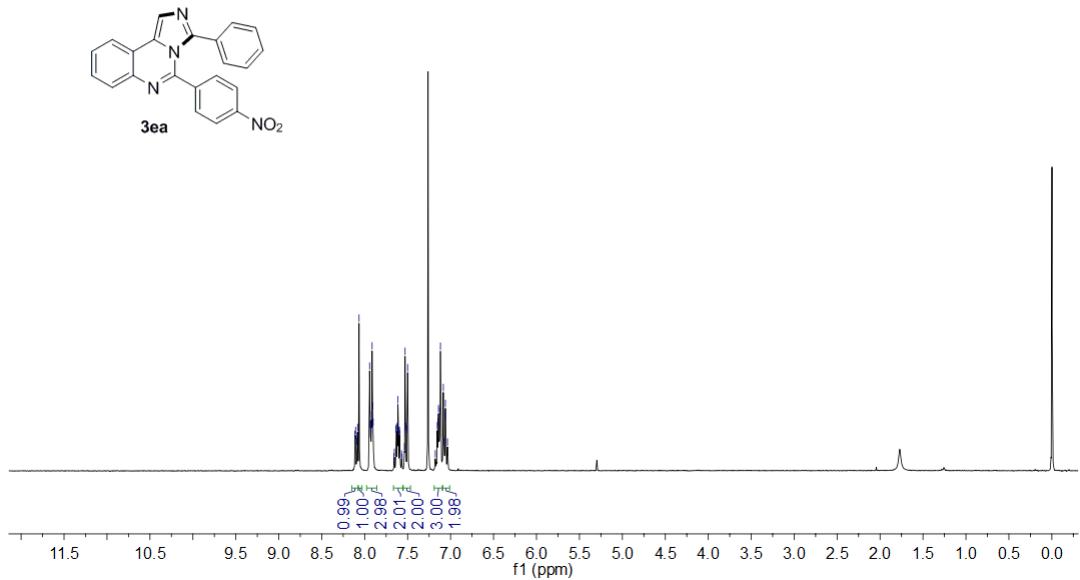




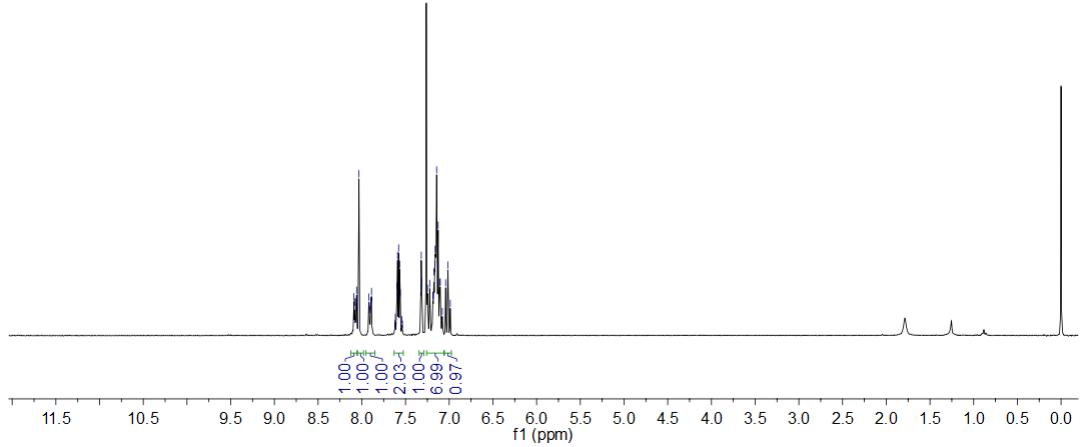
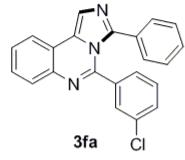




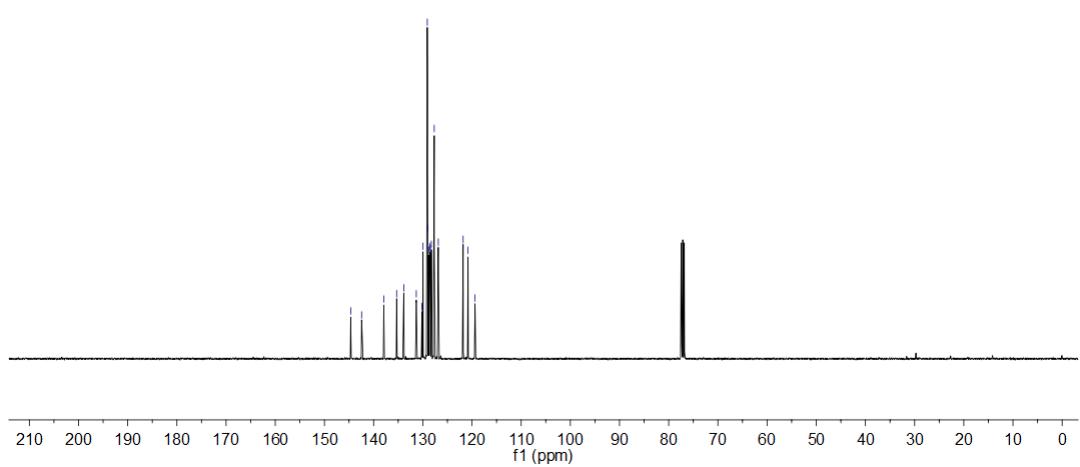


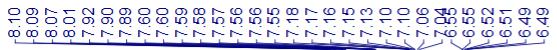


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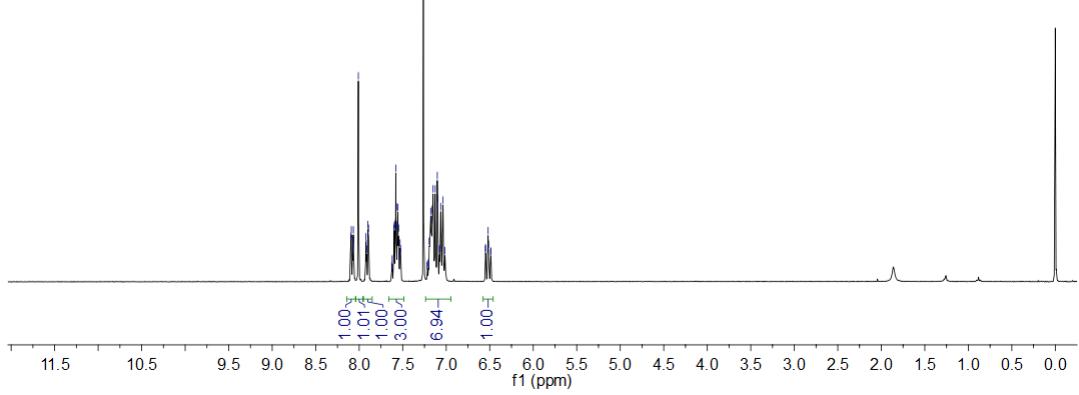


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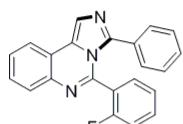




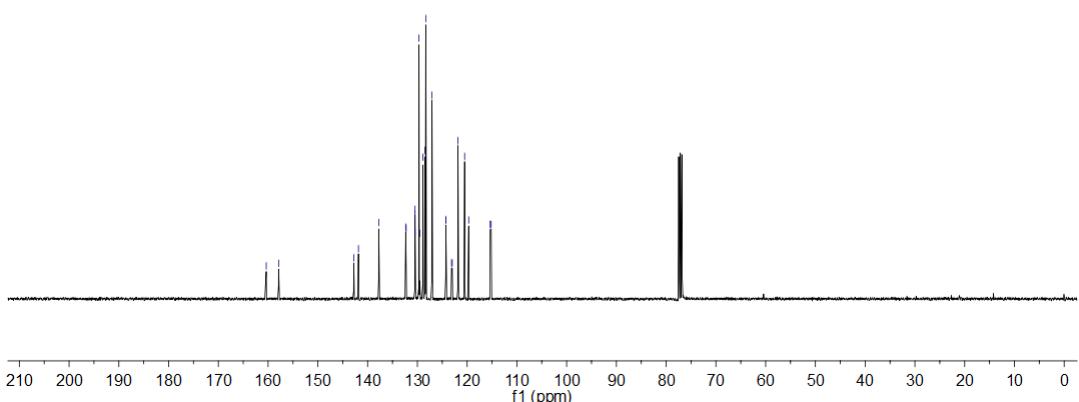
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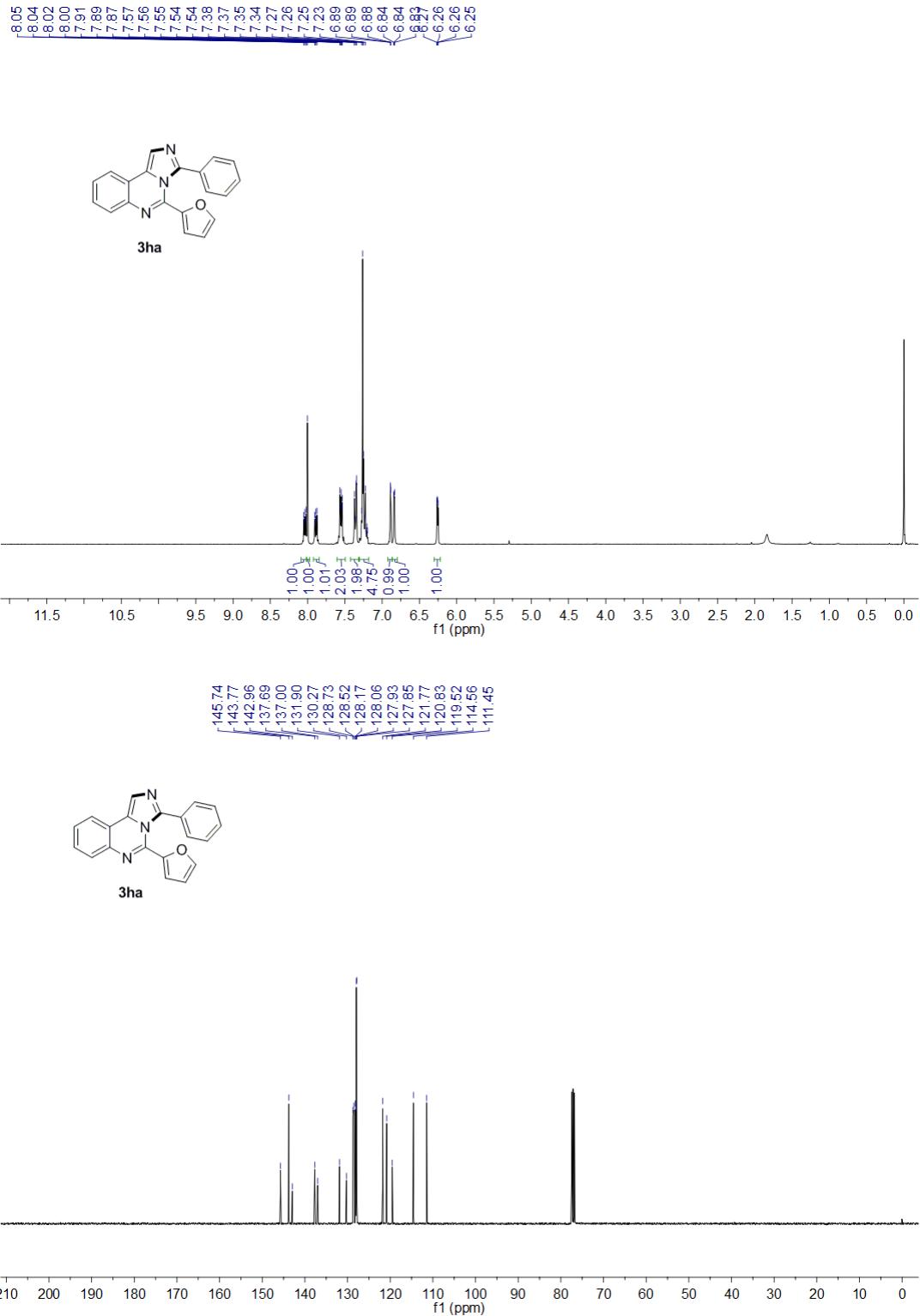


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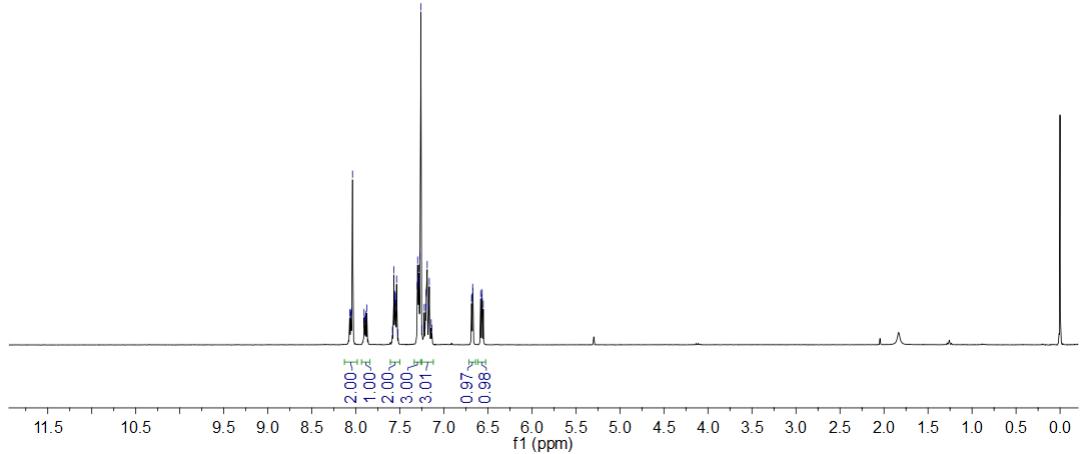
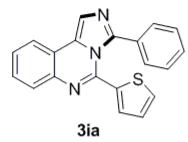


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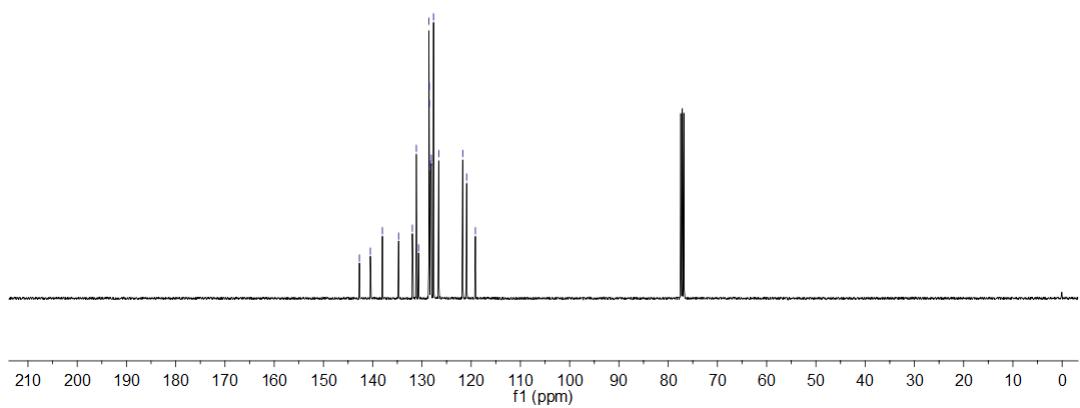
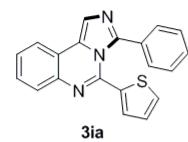




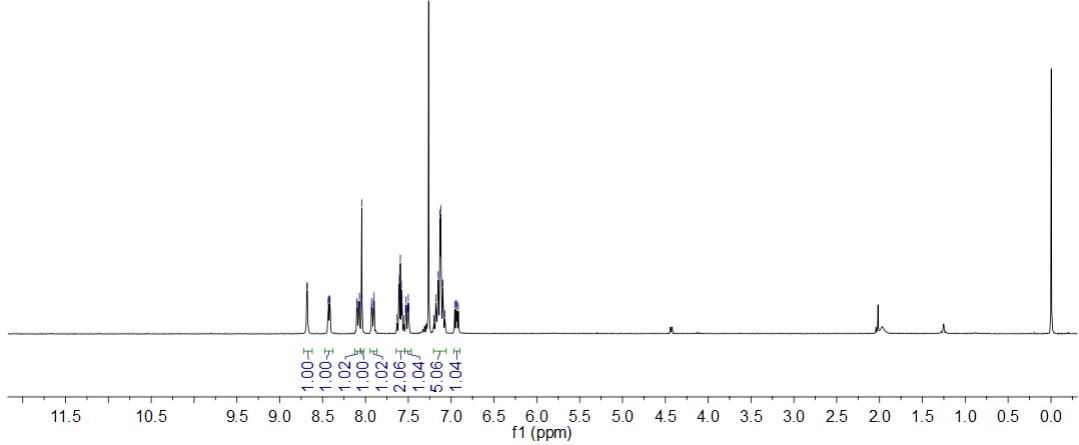
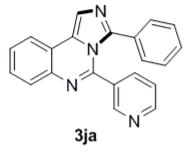
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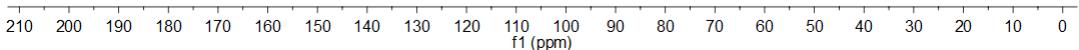
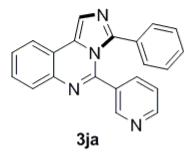
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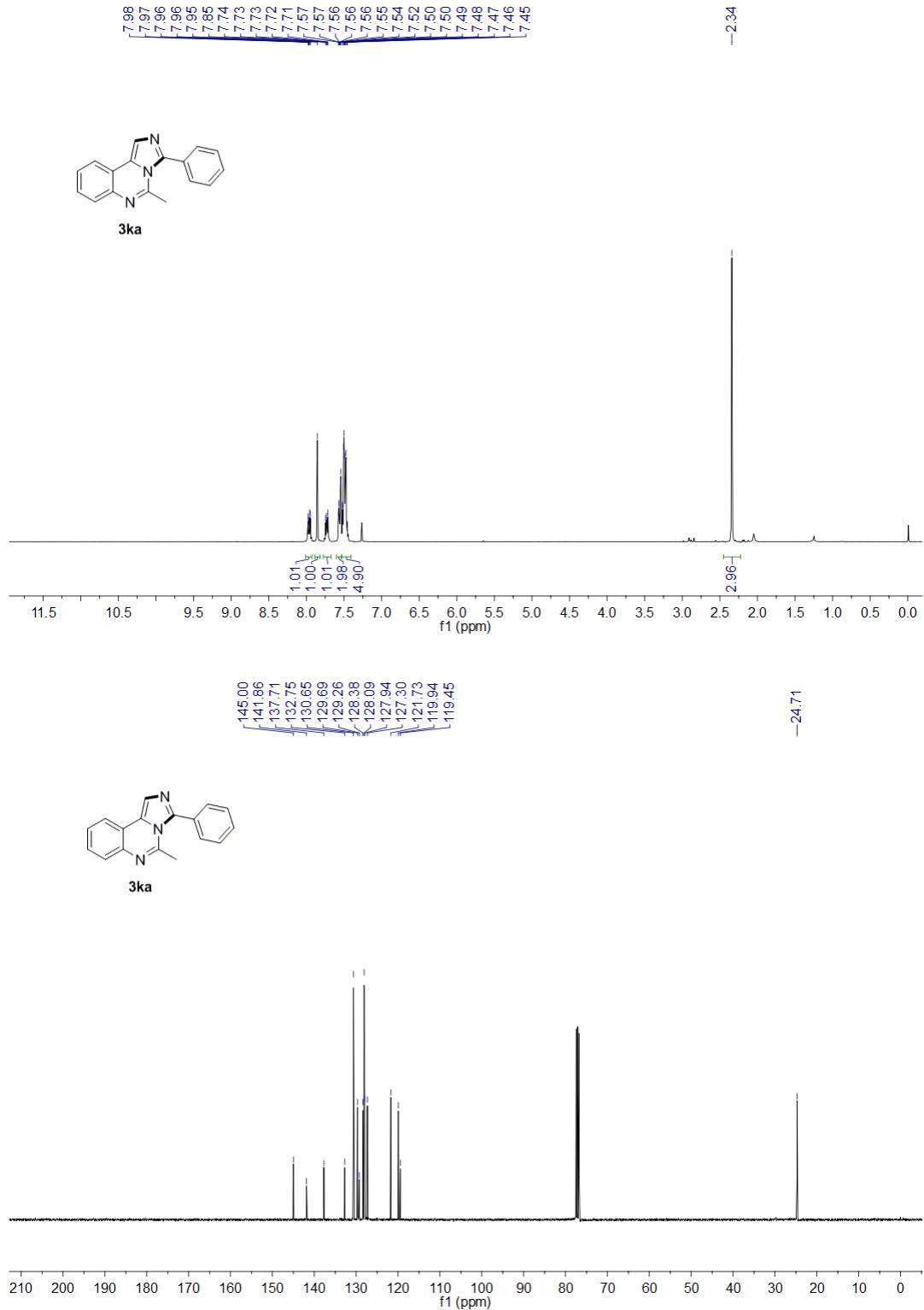


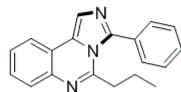
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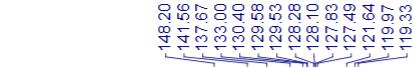
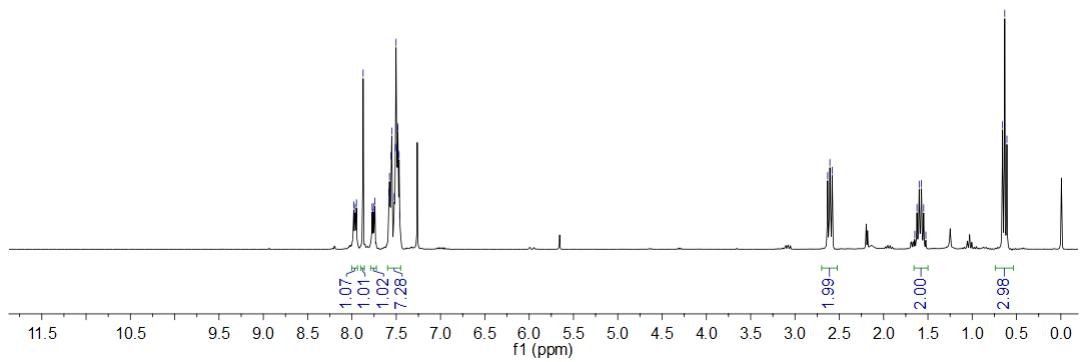
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121.83
120.88
119.36







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-37.30
-20.35
-13.39

