Efficient aerobic oxidative synthesis of 2-aryl quinazolines via benzyl C-H bond amination catalyzed by 4-hydroxy-TEMPO

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Electronic Supplementary Information

General:

All reagents were purchased from commercial suppliers and used without further purification unless otherwise noted. Flash chromatography was carried out with silica gel (200-300 mesh). Analytical TLC was performed with silica gel GF254 plates, and the products were visualized by UV detection. ^{1}H NMR and ^{13}C NMR (400 MHz or 300 MHz and 100 MHz or 75 MHz, respectively) spectra were recorded in $CDCl_3$. Chemical shifts (δ) are reported in ppm using TMS as internal standard and spin-spin coupling constants (*J*) are given in Hz. Low resolution EI-MS spectra and ESI-MS were measured on an HP 5988A spectrometer by direct inlet at 70 eV and Bruker Daltonics Esquire6000, respectively. The high resolution mass spectra (HRMS) were measured on a Bruker Daltonics APEX II 47e spectrometer by ESI.

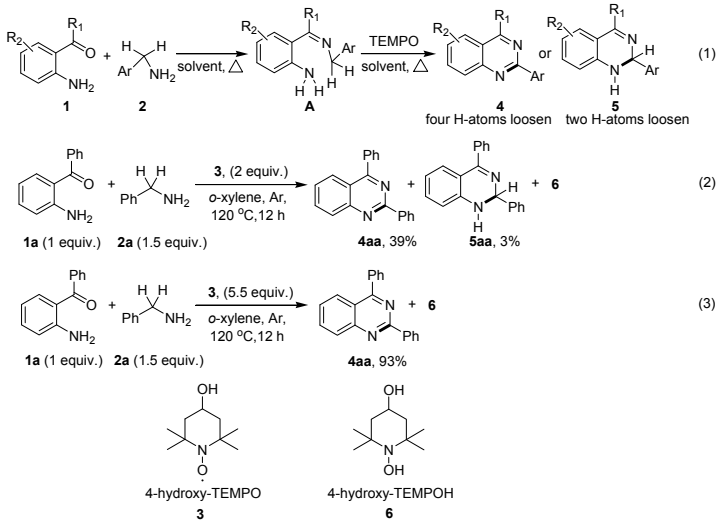
The starting materials 2-aminophenyl-2,5-dimethylphenylmethanone (**1b**)[1], 2-aminophenyl-4-bromophenylmethanone (**1c**)[2], 2-aminophenyl-4-methoxyphenyl-methanone (**1d**)[2], 2-amino-5-bromophenyl-phenylmethanone (**1e**)[3], 1-(2-amino-phenyl)propan-1-one (**1f**)[2], 1-(2-aminophenyl)pentan-1-one (**1g**)[2], 1-(2-amino-phenyl)-2-methylpropan-1-one (**1h**) [2], 1-(2-aminophenyl)-2,2-dimethylpropan-1-one (**1i**)[2], 2-amino-5-nitrobenzaldehyde (**1k**) [4], methyl 4-amino-3-formyl- benzoate (**1l**) [5], and methyl 3-amino-4-formylbenzoate (**1m**) [5] were prepared according to literature methods. The purity of these materials was confirmed by spectroscopic analysis and the spectroscopic data matches the previously reported literature values.

General experimental procedure:

Oxidative synthesis of quinazoline 4 (Scheme ESI1 and entry 1 in Table ESI2): A mixture of 2-aminobenzophenone **1a** (197 mg, 1 mmol), benzylamine **2a** (160 mg, 1.5 mmol) and 4-hydroxy-TEMPO (947 mg, 5.5 mmol) was placed in a 10 mL Schlenck tube in *o*-xylene (0.3 mL) and stirred at 120 °C under argon atmosphere for 12 h. When the starting materials were consumed completely monitored by TLC, oxygen was purged into the reaction mixture for 30 minutes at 120 °C to recover the oxidant **3**. Then the reaction mixture was isolated by silica gel column chromatography to give the product **4aa** as a white crystalline solid (R_f = 0.3, hexane/ethyl acetate, 80:1; 262 mg; 93%) and the recovered oxidant **3** in 85% yield (R_f = 0.3, hexane/ethyl acetate, 3:1). The identity and purity of the product was confirmed by ^{1}H and ^{13}C NMR spectroscopic analysis.

Aerobic oxidative synthesis of quinazoline 4 (entry 1 in Table 2): A mixture of 2-aminobenzophenone **1a** (197 mg, 1 mmol), benzyl amine **2a** (321 mg, 3 mmol) and 4-hydroxy-TEMPO (34 mg, 0.20 mmol, 20 mol%) was placed in a 10 mL three necked flask in *o*-xylene (0.3 mL) and stirred at 140 ^{o}C under oxygen atmosphere for 13 h. When the starting materials were consumed completely monitored by TLC, the reaction mixture was isolated by silica gel column chromatography (R_f = 0.3, hexane/ethyl acetate, 80:1) to give product as a white crystalline solid (257 mg; 91%). The identity and purity of the product was confirmed by ^{1}H and ^{13}C NMR spectroscopic analysis.

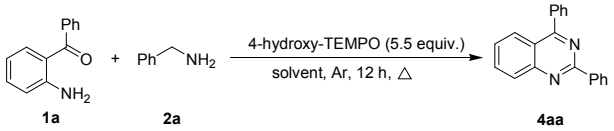
Oxidative synthesis of quinazolines using stoichiometric 4-hydroxy-TEMPO



Scheme ESI-1 4-Hydroxy-TEMPO-mediated benzyl C-H bond amination and synthesis of quinazolines.

The study was initiated by treating a mixture of 2-aminobenzophenone **1a** (1 equiv.) and benzylamine **2a** (1.5 equiv.) in *o*-xylene with a stoichiometric 4-hydroxy-TEMPO **3** at 120 ^{o}C under argon atmosphere. We envisioned that after 2-aminobenzaldehydes and 2-aminobenzoketones condense with arylmethanamines, the product imines A would undergo a tandem benzyl C-H oxidation/intramolecular amination process by oxidation by TEMPO and would be transformed to heterocyclic products (Scheme ESI-1). As expected, the desired reaction took place, leading to the formation of the product 2,4-diphenylquinazoline **4aa**. When 2 equivalent (insufficient) of **3** were used, 2,4-diphenylquinazoline **4aa** was obtained in 39 % yield, along with a small amount of 1,2-dihydro-2,4-diphenylquinazoline **5aa** (in 3% yield) and the recovered starting material (Scheme ESI-1, eq. 2). The conversion was complete when the amount of **3** was raised to 5.5 equivalents, and the product **4aa** was generated in 93% yield (Scheme ESI-1, eq. 3). Obviously compound **5aa** is the reaction intermediate and it is much more reactive than compound **A** with **3**. Therefore, the loss of the second two hydrogen atoms from compound **5aa** to **3** is a kinetically rapid process.

Table ESI-1 Optimization on the tandem oxidative synthesis of 2-aryl quinazoline using 4-hydroxy-TEMPO as the oxidant [a]

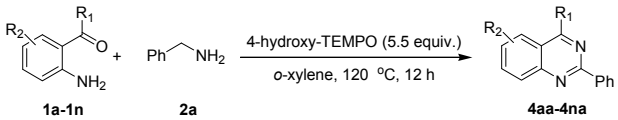


1a 2a 4aa

Entry	Solvent	T/°C	Yield [b] (%)
1	MeCN	80	0[c]
2	Benzne	80	trace[c]
3	Ethyl acetate	80	0[c]
4	*t*-Butanol	120	trace[c]
5	Tolune	100	71
6	*o*-Xylene	120	93
7	*o*-Xylene	120	93[d]
8	*o*-Xylene	120	92[e]
9	*o*-Xylene	120	65[f]

[a] 2-Aminobenzophenone (**1a**; 1 mmol), benzylamine (**2a**; 1.5 mmol, 1.5 equiv.) and 4-hydroxy-TEMPO (5.5 mmol, 5.5 equiv.) were dissolved in solvent (0.3 mL) in a 10 mL Schlenck tube and stirred for 12 h under Ar at different temperatures. [b] Yield of isolated product after purification by silica gel column chromatography. [c] TLC analysis. [d] TEMPO used instead of 4-hydroxy-TEMPO. [e] 4-methoxy-TEMPO used instead of 4-hydroxy-TEMPO. [f] 3 mL solvent used.

Table ESI-2 Tandem oxidative synthesis of 2-aryl quinazolines using 4-hydroxy-TEMPO as the oxidant [a]



1a-1n 2a 4aa-4na

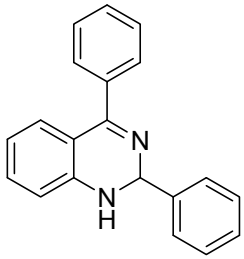
Entry	Product	R^1	R^2	Yield [b] (%)
1		Ph (**1a**)	H	93 (**4aa**)
2		2,5-di-MePh (**1b**)	H	73 (**4ba**)
3		4-Br-C_6H_4 (**1c**)	H	93 (**4ca**)
4		4-$MeOC_6H_4$ (**1d**)	H	91 (**4da**)
5		Ph (**1e**)	6-Br	93(**4ea**)
6		Ethyl (**1f**)	H	85 (**4fa**)
7	(**4aa-4ia**)	*n*-Butyl (**1g**)	H	88 (**4ga**)
8		*i*-Pr (**1h**)	H	80 (**4ha**)
9		*s*-Butyl (**1i**)	H	90 (**4ia**)
10		H (**1j**)	6,8-di-Br	83 (**4ja**)
11		H (**1k**)	6-NO_2	80 (**4ka**)
12		H (**1l**)	6-CO_2CH_3	83 (**4la**)
13	(**4ja-4na**)	H (**1m**)	7-CO_2CH_3	81 (**4ma**)
14		H (**1n**)	H	80 (**4na**)

[a] 2-aminobenzoketone or 2-aminobenzaldehyde (**1**; 1 mmol), benzylamine (**2**, 1.5 mmol, 1.5 equiv.) and 4-hydroxy-TEMPO (5.5 mmol, 5.5 equiv.) were dissolved in *o*-xylene (0.3 mL) in a 10 mL Shlenck tube and stirred under Ar for 12 h at 120 °C. [b] Yield of isolated product after purification by silica gel column chromatography.

Studies on the intermediate 5

a) Isolation and identify of the intermediate1,2-dihydro-2,4-diphenylquinazoline **5aa**

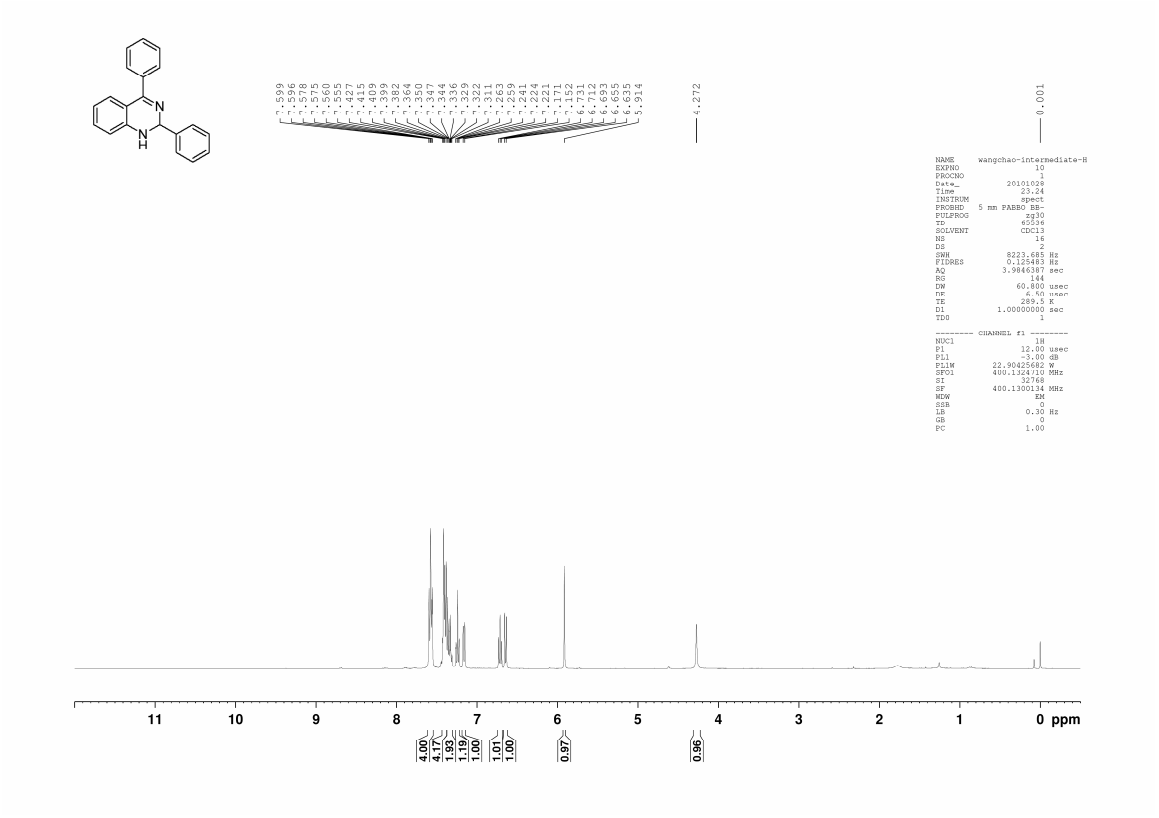
2-aminobenzophenone **1a** (197 mg, 1 mmol), 4-hydroxy-TEMPO (344 mg, 2 mmol), benzyl amine **2a** (160 mg, 1.5 mmol) and *o*-xylene (0.3 mL) were added to a Schlenk tube. Then the reaction vessel was flushed with Ar three times and was stirred at 120 ^{o}C for 12 h. The reaction mixture was purified by flash column chromatography to give the corresponding products1,2-dihydro-2,4-diphenylquinazoline **5aa** 10 mg (in 3 % yield) and 2,4-diphenylquinazoline **4aa** 110 mg (in 39 % yield). The identity and purity of the product was confirmed by ^{1}H and ^{13}C NMR spectroscopic analysis and matches the literature report[6].

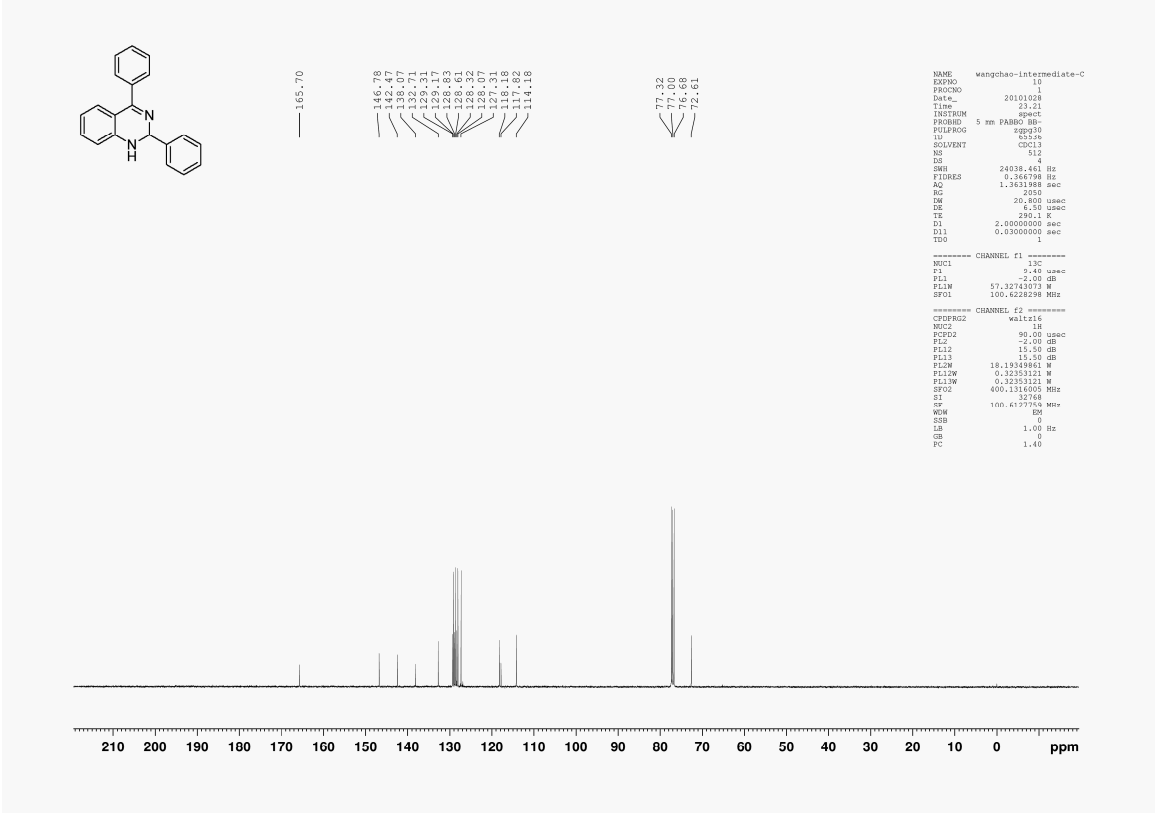


1,2-dihydro-2,4-diphenylquinazoline 5aa

Yellow solid, m.p. 51-53 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.27 (brs, 1H, N*H*), 5.91 (s, 1H), 6.64 (d, *J* = 8.0 Hz, 1H), 6.71 (t, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.24 (t, *J* = 8.0 Hz, 1H), 7.26-7.38 (m, 2H), 7.40-7.43 (m, 4H), 7.55-7.60 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 72.6, 114.2, 117.8, 118.2, 127.3, 128.1, 128.3, 128.6, 128.8, 129.2, 129.3, 132.7, 138.1, 142.5, 146.8, 165.7. ESI-MS *m/z*: 285.2 ($M+H^+$).

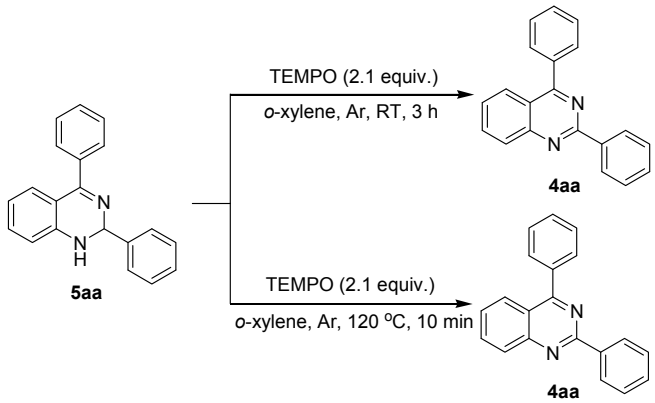
b) ^{1}H and ^{13}C spectra of intermediate1,2-dihydro-2,4-diphenylquinazoline 5aa





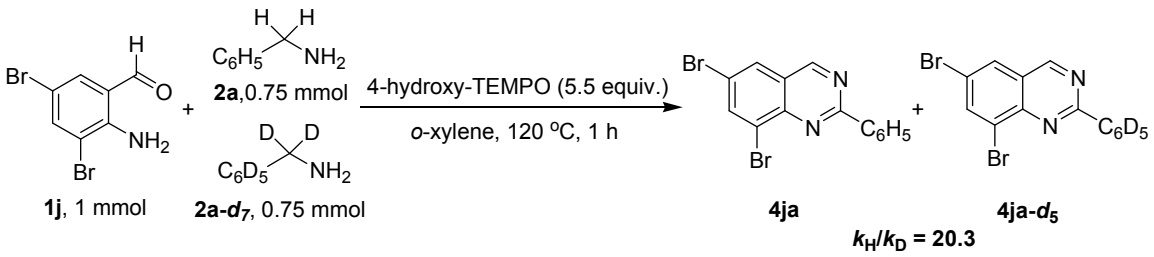
c) Oxidation of 1,2-dihydro-2,4-diphenylquinazoline 5aa with TEMPO

1,2-dihydro-2,4-diphenylquinazoline **5aa** (57 mg, 0.2 mmol), TEMPO (72 mg, 0.42 mmol) and *o*-xylene (0.2 mL) were added to a Schlenk tube. Then the reaction vessel was flushed with Ar three times and stirred for 3 h at room temperature or 10 minutes at 120 ^{o}C. The reaction mixture was purified by flash column chromatography to give 2,4-diphenylquinazoline **4aa** nearly quantitative.



Scheme ESI-2 Oxidation of 1,2-dihydro-2,4-diphenylquinazoline 5aa with TEMPO

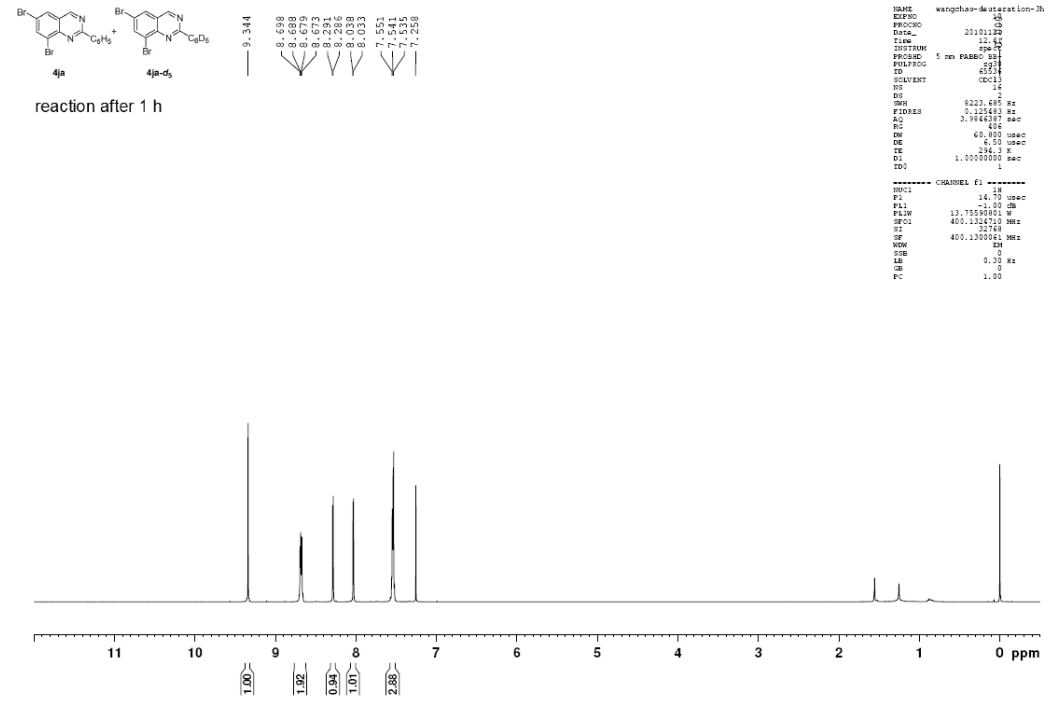
Studies on the kinetic isotope effects.

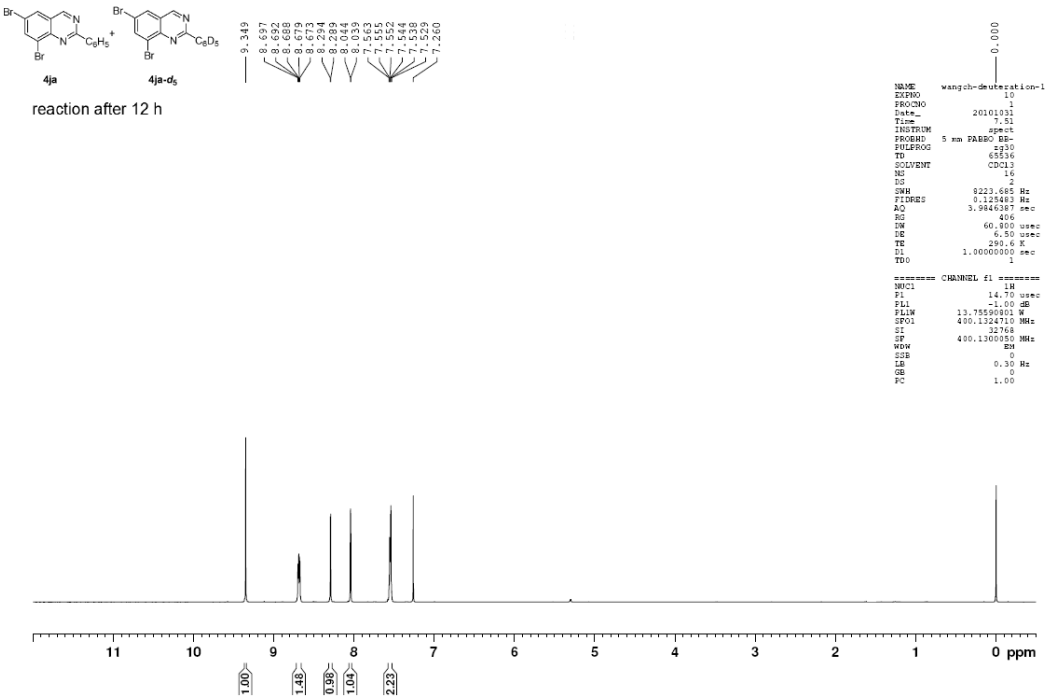


Scheme ESI-3 The kinetic isotope effects (KIE) experiment.

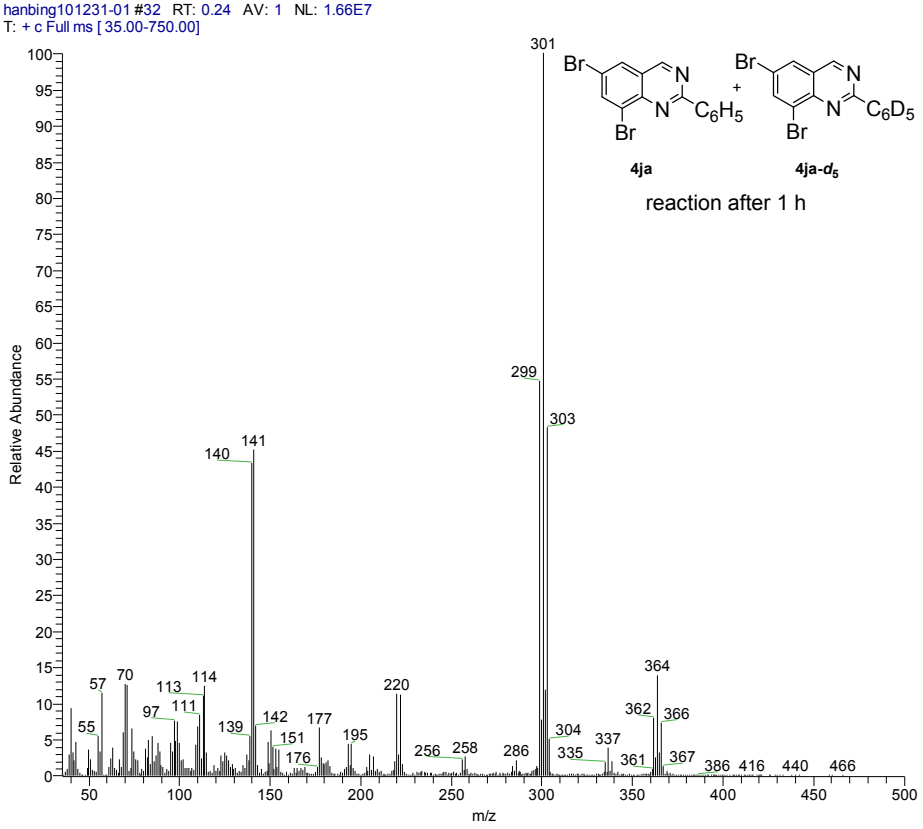
To a Schlenk tube were added 2-amino-3,5-dibromobenzaldehyde **1j** (279 mg, 1 mmol), 4-hydroxy- TEMPO (5.5 mmol), *o*-xylene (0.3 mL), and the reaction vessel was flushed with Ar three times, followed by the addition of benzyl amine **2a** (80 mg, 0.75 mmol), and benzyl amine-d_7 **2a-*d*$_7$** (84 mg, 0.75 mmol). The reaction mixture was stirred at 120 ^{o}C for 1 h (about ~18 % conversion). The reaction mixture was purified by flash column chromatography to give the corresponding mixed products **4ja** and **4ja-*d*$_5$**. The molar ratio of two products is determined by ^{1}H NMR analysis and abundant peak of Mass Spectra.

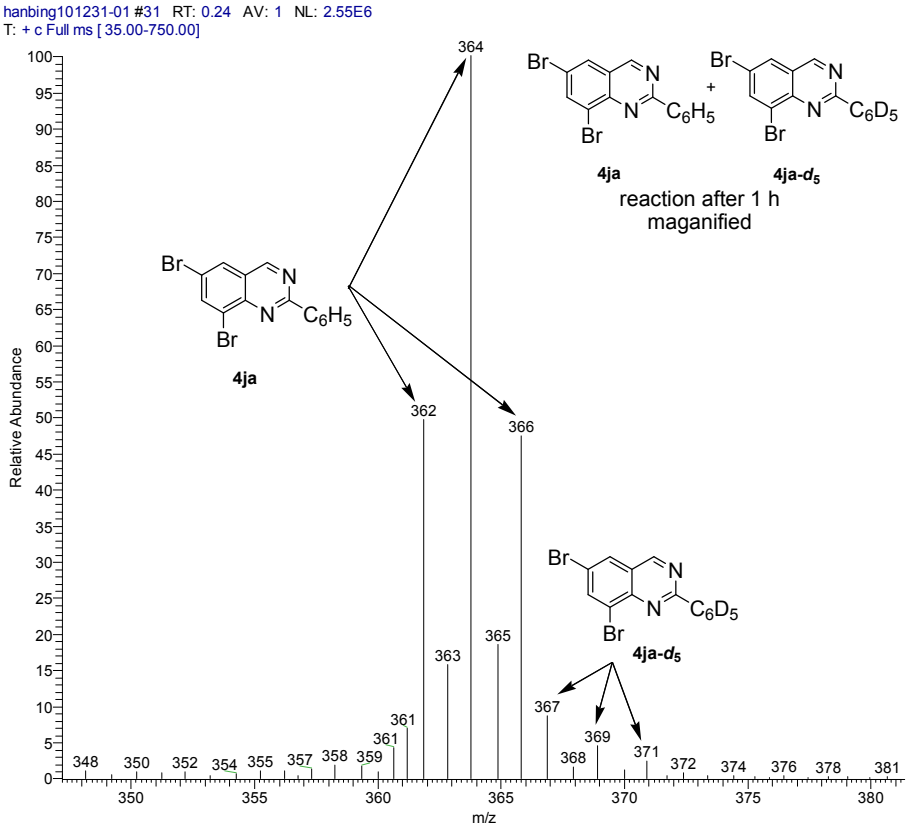
a) ^{1}H spectrum of the kinetic isotope effects.

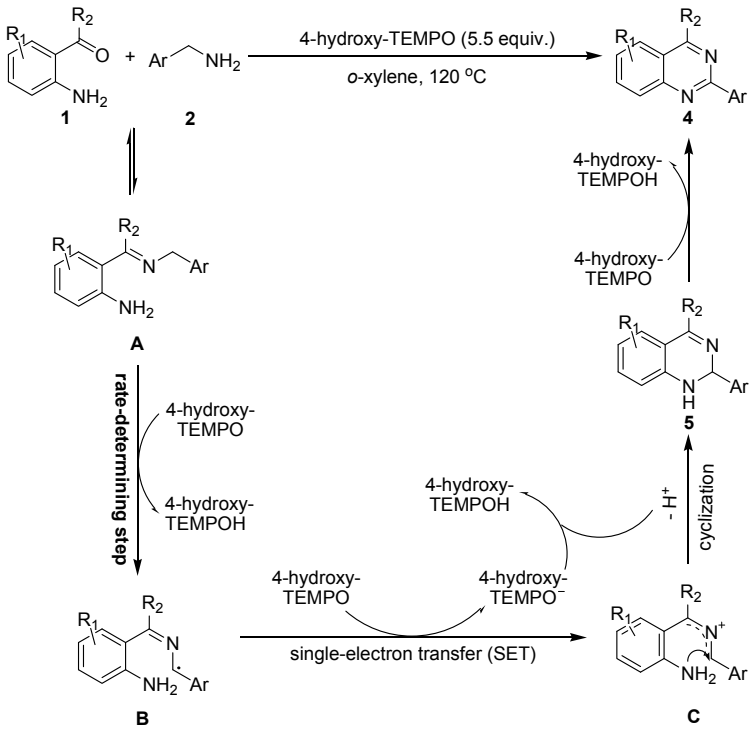




b) EI-Mass Spectra of the kinetic isotope effects.



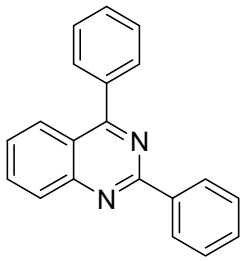




Scheme ESI-4 A plausible mechanism for the tandem oxidative synthesis of 2-aryl quinazolines using 4-hydroxy-TEMPO as the oxidant.

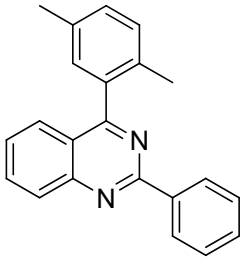
Analytical data for compounds 4aa-4lc

2,4-diphenylquinazoline (4aa) *(Entry 1 in Table 2)*



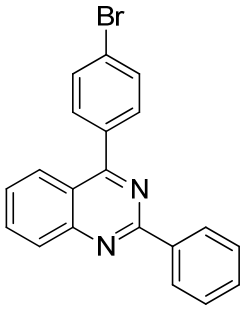
Colorless solid, m.p. 117-119 °C (lit.[6] 116-117 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.54 (m, 4H), 7.58-7.62 (m, 3H), 7.85-7.89 (m, 3H), 8.12 (d, *J* = 8.4 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 8.70 (d, *J* = 8 Hz, *J* = 1.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 121.6, 126.9, 128.4, 128.6, 129.1, 129.8, 130.1, 130.4, 133.4, 137.6, 138.2, 151.9, 160.1, 168.2. MS *m/z* (relative intensity, %): 283 (M+1, 12.6), 282 (M, 65.0), 281 (M-1, 100), 203 (7.9), 178 (8.1), 149 (10.0), 77 (6.3), 40 (16.4); column chromatography was performed on silica gel (R_f = 0.3, hexane/ethyl acetate, 80:1).

4-(2,5-dimethylphenyl)-2-phenylquinazoline (4ba) *(Entry 2 in Table 2)*



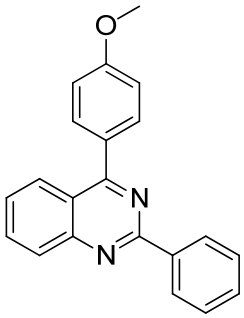
Colorless solid, m.p. 116-117 °C (lit.[7] 114-116 °C). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.16 (s, 3H), 2.40 (s, 3H), 7.22-7.30 (m, 3H), 7.45-7.54 (m, 4H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.84-7.89 (m, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 8.65-8.68 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.5, 21.0, 122.6, 126.9, 127.1, 128.5, 128.7, 129.0, 129.9, 130.1, 130.4, 130.6, 133.2, 133.6, 135.1, 136.8, 138.3, 151.4, 160.3, 170.0. MS *m/z* (relative intensity, %): 311 (M+1, 8.4), 310 (M, 45.5), 309 (M-1, 100), 294 (23.7), 149 (12.0), 97 (12.1), 57 (17.8), 40 (44.8); column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 80:1).

4-(4-bromophenyl)-2-phenylquinazoline (4ca) *(Entry 3 in Table 2)*



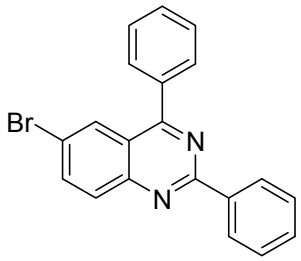
Colorless solid, m.p. 155-157 °C (lit.[7] 154-156 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.57 (m, 4H), 7.72-7.78 (m, 4H), 7.86-7.91 (m, 1H), 8.06 (d, *J* = 7.6 Hz, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 8.67 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 2H). ^{13}C NMR (100 MHz, CDCl3) δ 121.4, 124.6, 126.5, 127.2, 128.5, 128.6, 129.3, 130.6, 131.7, 131.8, 133.7, 136.5, 138.0, 152.0, 160.2, 167.0. MS *m/z* (relative intensity, %): 362 (M+2, 71.6), 360 (M, 76.2), 281 (100), 40 (52.6); column chromatography was performed on silica gel (hexane/ethyl acetate, 80:1).

4-(4-methoxyphenyl)-2-phenylquinazoline (4da) *(Entry 4 in Table 2)*



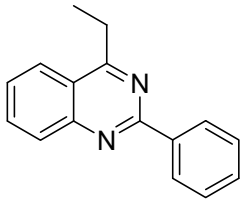
Colorless solid, m.p. 131-133 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.93 (s, 3H), 7.12 (m, 2H), 7.47-7.56 (m, 4H), 7.85-7.91 (m, 3H), 8.13-8.18 (m, 2H), 8.70 (dd, *J* = 7.6 Hz, *J* = 1.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 114.0, 121.6, 126.8, 127.0, 128.4, 128.6, 129.1, 130.2, 130.4, 131.8, 133.3, 138.3, 152.0, 160.1, 161.2, 167.7. MS *m/z* (relative intensity, %): 313 (M+1, 18.1), 312 (M, 88.0), 311 (M-1, 100), 281 (44.2), 268 (20.9), 149 (20.9). HRMS calc. $C_{21}H_{16}N_2O+H^+$: 313.1335, found: 313.1330; column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 60:1).

6-bromo-2,4-diphenylquinazoline (4ea) *(Entry 5 in Table 2)*



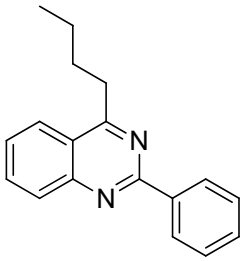
Colorless solid, m.p. 210-211 °C (lit.[7] 209-211 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.55 (m, 3H), 7.60-7.62 (m, 3H), 7.84-7.87 (m, 2H), 7.93 (dd, *J* = 8.4 Hz, *J* = 8.8 Hz, *J* = 2.0 Hz, 1H), 8.02 (d, *J* = 8.8 Hz, 1H), 8.25 (dd, *J* = 2.0 Hz, 1H), 8.65-8.68 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 120.6, 122.7, 128.6, 128.67, 128.74, 129.1, 130.0, 130.2, 130.8, 130.9, 137.0, 137.1, 137.7, 150.7, 160.5, 167.4. MS *m/z* (relative intensity, %): 362 (M+2, 30.2), 361 (M+1, 32.5), 360 (M, 30.4), 359 (26.2), 281 (70.3), 149 (58.9), 83 (77.4), 57 (100), 43 (97.1); column chromatography was performed on silica gel (R_f = 0.2, hexane/dichloromethane, 4:1).

4-ethyl-2-phenylquinazoline (4fa) *(Entry 6 in Table 2)*



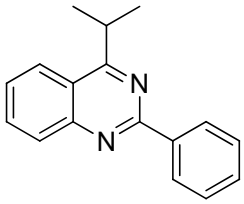
Colorless solid, m.p. 45-46 °C (lit.[8] 44-46 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.52 (t, *J* = 7.2 Hz, 3H), 3.33 (q, *J* = 7.2 Hz, 2H), 7.46-7.54 (m, 4H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.84 (ddd, *J* = 8.4 Hz, *J* = 8.0 Hz, *J* = 1.2 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H),7.80 (t, *J* = 8.4 Hz, 1H), 8.05 (d, *J* = 8.4 Hz, 2H),8.65 (dd, *J* = 8.4 Hz, *J* = 1.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 12.3, 27.7, 122.3, 124.4, 126.7, 128.4, 128.6, 129.4, 130.3, 133.1, 138.5, 150.6, 160.1, 172.0. ESI-MS *m/z*: 235.1 ($M+H^+$); column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 60:1).

4-butyl-2-phenylquinazoline (4ga) *(Entry 7 in Table 2)*



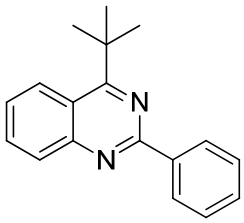
Colorless solid, m.p. 47-49 °C (lit.[7] 45-47 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.03 (t, *J* = 7.2 Hz, 3H), 1.49-1.59 (m, 2H), 1.93-2.00 (m, 2H), 3.34 (t, *J* = 7.6 Hz, 2H), 7.47-7.59 (m, 4H), 7.85 (t, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 8.64 (dd, *J* = 8.0 Hz, *J* = 1.2 Hz, 2H).^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 22.8, 30.6, 34.3, 122.5, 124.6, 126.7, 128.47, 128.54, 129.4, 130.3, 133.2, 138.5, 150.7, 160.1, 171.5. ESI-MS *m/z* (relative intensity, %): 263.2 ($M+H^+$); column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 60:1).

4-isopropyl-2-phenylquinazoline (4ha) *(Entry 8 in Table 2)*



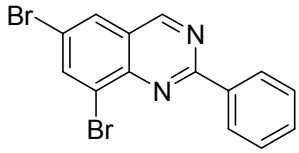
Colorless solid, m.p. 65-67 °C (lit.[7] 64-66 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.50 (d, *J* = 6.8 Hz, 6H), 3.89-3.99 (m, 1H), 7.46-7.57 (m, 4H), 7.80-7.84 (m, 1H), 7.82 (t, *J* = 7.2 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 8.68 (dd, *J* = 8 Hz, *J* = 1.2 Hz ,2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.8, 31.2, 121.7, 124.1, 126.6, 128.4, 128.6, 129.6, 130.3, 133.0, 138.6, 151.0, 160.0, 175.4. ESI-MS *m/z* (relative intensity, %): 249.2 ($M+H^+$); column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 60:1).

4-tert-butyl-2-phenylquinazoline (4ia) *(Entry 9 in Table 2)*



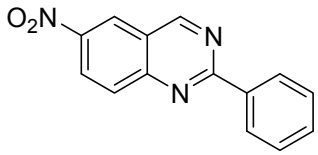
Colorless solid, m.p. 69-71 °C (lit.[7] 70-72 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.71 (s, 9H), 7.46-7.54 (m, 4H), 7.76-7.80 (m, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 8.42 (m, *J* = 8.4 Hz, 1H), 8.68 (dd, *J* = 8 Hz, *J* = 1.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.6, 40.5, 121.5, 125.6, 126.5, 128.4, 128.5, 130.3, 130.4, 132.2, 138.6, 152.0, 158.8, 176.3. MS *m/z* (relative intensity, %): 231 (28.9), 229 (89.3), 166 (12.2), 92 (22.6), 63 (100); column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 60:1).

6,8-dibromo-2-phenylquinazoline (4ja) *(Entry 11 in Table 2)*



Yellow solid, m.p. 151-153 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (m, 3H), 8.01 (d, *J* = 2.0 Hz, 1H), 8.28 (d, *J* = 2.0 Hz, 1H), 8.68 (m, 2H), 9.33 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 120.2, 125.0, 125.5, 128.71, 128.75, 128.9, 131.3, 137.1, 140.1, 147.0, 159.8, 161.8. EI-MS *m/z* (relative intensity, %): 366 (M+4, 49.0), 364 (M+2, 100), 362 (M, 55.2), 256 (16.8), 177 (41.3), 74 (14.5), 40 (78.8). HRMS calc. $C_{14}H_8Br_2N_2$+H^+: 362.9127, found: 362.9122; column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 40:1).

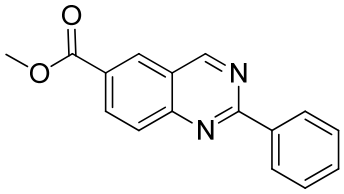
6-nitro-2-phenylquinazoline (4ka) *(Entry 12 in Table 2)*



Pale yellow solid, m.p. 217-219 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.59 (m, 3H), 8.20 (d, *J* = 2.0 Hz, 3H), 8.63-8.68 (m, 3H), 8.28 (d, *J* = 2.0 Hz, 1H), 8.68 (m, 2H), 9.34

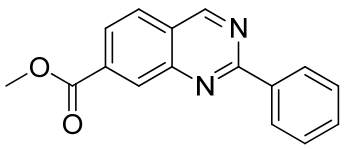
(s, 1H), 8.20 (d, *J* = 9.2 Hz, 1H), 8.63-8.68 (m, 3H), 8.86 (d, *J* = 2.4 Hz, 1H), 9.63 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 122.3, 124.1, 127.5, 128.9, 129.3, 130.7, 132.0, 137.0, 145.7, 153.2, 162.3, 164.0. MS *m/z* (relative intensity, %): 252 (M+1, 11.6), 251 (M, 100), 250 (M-1, 7.3), 205 (21.8), 178 (54.6), 44 (55.4), 42 (72.0). HRMS calc. $C_{14}H_9N_3O_2$+H^+: 252.0768, found: 252.0765; column chromatography was performed on silica gel (R_f = 0.2, hexane/dichloromethane, 2:1).

methyl 2-phenylquinazoline-6-carboxylate (4la) *(Entry 13 in Table 2)*



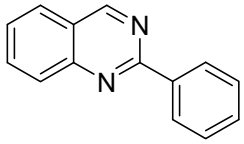
Colorless solid, m.p. 193-194 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.02 (s, 3H), 7.54-7.55 (m, 3H), 8.11 (d, *J* = 8.8 Hz, 1H), 8.48 (dd, *J* = 8.8 Hz, *J* = 1.6 Hz, 1H), 8.63-8.68 (m, 3H), 9.55 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 52.6, 122.7, 128.6, 128.7, 128.8, 128.9, 130.1, 131.2, 133.5, 137.5, 152.7, 161.6, 162.6, 165.9. MS *m/z* (relative intensity, %): 265 (M+1, 16.5), 264 (M, 100), 263 (M-1, 13.6), 233 (52.8), 178 (15.7), 103 (17.8), 40 (66.3). HRMS calc. $C_{16}H_{12}N_2O_2$+H^+: 265.0972, found: 265.0972; column chromatography was performed on silica gel (R_f = 0.3, hexane/ethyl acetate, 20:1).

methyl 2-phenylquinazoline-7-carboxylate (4ma) *(Entry 14 in Table 2)*



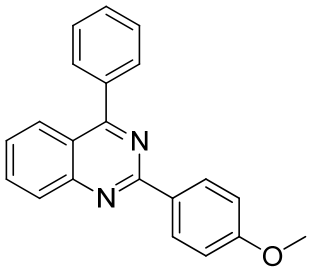
Colorless solid, m.p. 170-171 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.02 (s, 3H), 7.50-7.57 (m, 3H), 7.94 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 8.7 Hz, 1H), 8.60-8.63 (m, 2H), 8.76 (s, 1H), 9.49 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 52.7, 125.2, 126.7, 127.3, 128.6, 130.9, 131.1, 135.0, 137.5, 150.3, 160.5, 161.7, 166.1. MS *m/z* (relative intensity, %): 265 (M+1, 17.5), 264 (M, 100), 263 (M-1, 18.5), 233 (40.7), 85 (46.4), 71 (60.4), 57 (70.7), 40 (54.8). HRMS calc. $C_{16}H_{12}N_2O_2$+H^+: 265.0972, found: 265.0968; column chromatography was performed on silica gel (R_f = 0.3, hexane/ethyl acetate, 20:1).

2-phenylquinazoline (4na) *(Entry 15 in Table 2)*



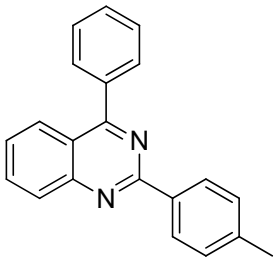
White grey solid, m.p. 97-98 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48- 7.56 (m, 3H), 7.60 (ddd, *J* = 8.0 Hz, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H),7.87-7.93 (m, 1H), 8.08 (dd, *J* = 8.4 Hz, *J* = 1.2 Hz, 1H), 8.62 (dd, *J* = 8.0 Hz, *J* = 2.0 Hz, 2H), 8.70 (d, *J* = 2.4 Hz, 1H), 9.46 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 123.5, 127.0, 127.1, 128.52, 128.54, 130.5, 134.0, 138.0, 150.7, 160.4, 161.0. EI-MS *m/z* (relative intensity, %): 207 (M+1, 17.7), 206 (M, 100), 205 (M-1, 35.0), 179 (54.4), 103 (18.5), 76 (15.2). HRMS calc. $C_{14}H_{10}N_2$+H^+: 207.0917, found: 207.0918; column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 30:1).

2-(4-methoxyphenyl)-4-phenylquinazoline (4ab) *(Entry 1 in Table 3)*



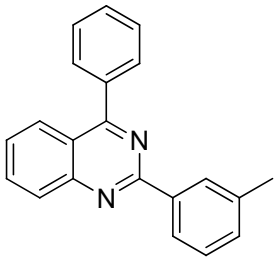
Colorless solid, m.p. 159-160 °C (lit.[7] 158-160 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.89 (s, 3H), 7.03 (d, *J* = 9.2 Hz, 2H), 7.51 (ddd, *J* = 8.4 Hz, *J* = 7.6 Hz, *J* = 1.0 Hz, 1H), 7.57-7.62 (m, 3H), 7.83-7.89 (m, 3H), 8.10 (t, *J* = 8.0 Hz, 2H), 8.65 (d, *J* = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, CDCl3) δ 55.3, 113.8, 121.3, 126.4, 126.9, 128.4, 128.9, 129.8, 130.1, 130.2, 130.9, 133.3, 137.7, 152.0, 160.0, 161.7, 168.0. MS *m/z* (relative intensity, %): 313 (M+1, 20.4), 312 (M, 100), 311 (M-1, 86.9), 281 (40.1), 178 (21.6), 149 (21.3), 77 (11.7), 43 (34.1); column chromatography was performed on silica gel (R_f = 0.3, hexane/dichloromethane, 2:1).

4-phenyl-2-p-tolylquinazoline (4ac) *(Entry 2 in Table 3)*



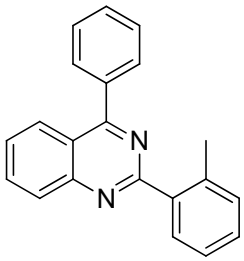
Colorless solid, m.p. 165-167 °C (lit.[7] 166-168 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.44 (s, 3H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.51 (ddd, *J* = 8.0 Hz, *J* = 7.2 Hz, *J* = 1.0 Hz, 1H), 7.57-7.61 (m, 3H), 7.84-7.89 (m, 3H), 8.10 (dd, *J* = 8.4 Hz, *J* = 1.0 Hz, 1H), 8.30 (d, *J* = 8.8 Hz, 1H), 8.59 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, CDCl3) δ 21.5, 121.6, 126.7, 127.0, 128.5, 128.6, 129.1, 129.3, 129.8, 130.2, 133.4, 135.5, 137.8, 140.7, 152.0, 160.3, 168.2. MS *m/z* (relative intensity, %): 297 (M+1, 16.7), 296 (M, 72.3), 295 (M-1, 100), 209 (31.4), 178 (20.0), 149 (60.1), 77 (14.5), 43 (35.1); column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 100:1).

4-phenyl-2-m-tolylquinazoline (4ad) *(Entry 3 in Table 3)*



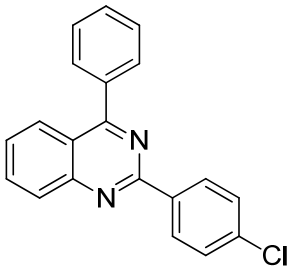
Colorless solid, m.p. 113-115 °C (lit.[7]115-117 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.48 (s, 3H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.51 (ddd, *J* = 8.4 Hz, *J* = 8.0 Hz, *J* = 1.2 Hz, 1H), 7.58-7.62 (m, 3H), 7.85-7.89 (m, 3H), 8.11 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 8.49 (d, *J* = 8.0 Hz, 1H), 8.50 (s, 1H). ^{13}C NMR (100 MHz, CDCl3) δ 21.5, 121.6, 125.9, 126.9, 127.0, 128.4, 128.5, 129.10, 129.13, 129.9, 130.2, 131.3, 133.5. 137.7, 138.1, 152.0, 160.4, 168.3. MS *m/z* (relative intensity, %): 297 (M+1, 7.5), 296 (M, 42.7), 295 (M-1, 70.6), 209 (91.9), 195 (100); column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 100:1).

4-phenyl-2-o-tolylquinazoline (4ae) *(Entry 4 in Table 3)*



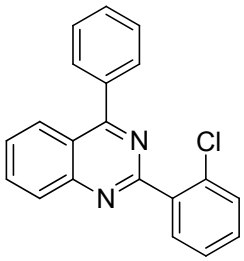
Colorless solid, m.p. 73-75 °C (lit.[7] 72-74 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.67 (s, 3H), 7.31-7.36 (m, 3H), 7.57-7.62 (m, 4H), 7.84-7.87 (m, 2H), 7.89-7.93 (m, 1H), 7.94-7.99 (m, 1H), 8.17 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 121.0, 125.9, 126.9, 127.2, 128.5, 129.1, 129.2, 129.9, 130.1, 130.7, 131.2, 133.6, 137.4, 137.5, 138.8, 151.6, 163.4, 168.0. MS *m/z* (relative intensity, %): 297 (M+1, 13.8), 296 (M, 75.1), 295 (M-1, 100), 218 (12.3), 147 (21.8); column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 80:1).

2-(4-chlorophenyl)-4-phenylquinazoline (4af) *(Entry 5 in Table 3)*



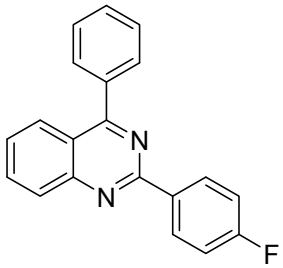
Colorless solid, m.p. 191-193 °C (lit.[7] 190-192 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.50 (m, 2H), 7.53-7.61(m, 4H), 7.85-7.91 (m, 3H), 8.11-8.14 (m, 2H), 8.63-8.66 (t, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, CDCl3) δ 121.7, 127.0, 127.2, 128.5, 128.7, 129.1, 130.0, 130.1, 133.6, 136.68, 136.70, 137.5, 151.9, 159.2, 168.4. EI-MS *m/z* (relative intensity, %): 318 (M+2, 20.7), 317 (M+1, 42.9), 316 (M, 65.5), 315 (M-1, 99.1), 177 (21.6), 83 (20.2), 43 (44.4), 40 (100); column chromatography was performed on silica gel (R_f = 0.3, hexane/ethyl acetate, 50:1).

2-(2-chlorophenyl)-4-phenylquinazoline (4ag) *(Entry 6 in Table 3)*



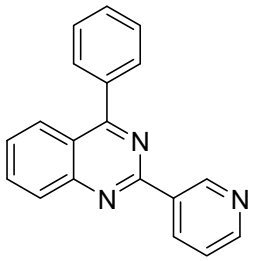
Yellow solid, m.p. 93-94 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.43 (m, 2H), 7.51-7.66 (m, 5H), 7.86-7.97 (m, 4H), 8.20 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 121.3, 126.8, 127.0, 127.7, 128.6, 129.1, 130.0, 130.2, 130.5, 131.8, 133.1, 133.8, 137.2, 138.4, 151.5, 161.3, 168.2. MS *m/z* (relative intensity, %): 318 (M+2, 25.0), 316 (M, 73.0), 315 (M-1, 100), 203 (15.2), 40 (86.4). HRMS calc. $C_{20}H_{13}ClN_2$+H^+: 317.0840, found: 317.0836; column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 60:1).

2-(4-fluorophenyl)-4-phenylquinazoline (4ah) *(Entry 7 in Table 3)*



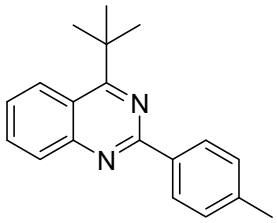
Colorless solid, m.p. 153-155 °C (lit.[7] 153-157 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (dd, *J* = 8.4 Hz, *J* = 9.2 Hz, 1H), 7.56 (dd, *J* = 8.0 Hz, *J* = 7.2 Hz, 3H), 7.85-7.90 (m, 3H), 8.11 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 8.70 (d, *J* = 8.8 Hz, 1H), 8.71 (d, *J* = 8.8 Hz, 1H),. ^{13}C NMR (100 MHz, CDCl3) δ 115.2, 115.4, 121.5, 126.93, 126.94, 128.5, 129.0, 129.9, 130.1, 130.7, 130.8, 133.5, 134.3, 134.4, 137.5, 151.9, 159.2, 163.3, 165.8, 168.3. MS *m/z* (relative intensity, %): 301 (M+1, 11.5), 300 (M, 70.2), 299 (M-1, 100), 203 (9.9), 150 (7.0), 84 (7.4), 42 (12.6); column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 60:1).

4-phenyl-2-(pyridin-3-yl)quinazoline (4ai) *(Entry 8 in Table 3)*



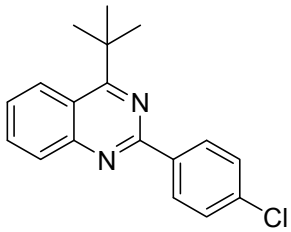
Colorless solid, m.p. 158-160 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (s, 1H), 7.57-7.62 (m, 4H), 7.88-7.94 (m, 3H), 8.16 (m, 2H), 8.75 (s, 1H), 8.93 (d, *J* = 8.0 Hz, 1H), 9.90 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 121.9, 123.3, 127.1, 127.5, 128.6, 129.2, 130.1, 130.2, 133.8, 135.8, 137.4, 150.4, 151.1, 151.9, 158.4, 168.6. EI-MS *m/z* (relative intensity, %): 283 (M, 11.0), 282 (M-1, 18.9), 205 (33.2), 149 (100), 121 (87.8), 91 (72.1), 70 (65.7), 57 (64.7). HRMS calc. $C_{19}H_{13}N_3$+H^+: 284.1182, found: 284.1180; column chromatography was performed on silica gel (R_f = 0.3, hexane/ethyl acetate, 10:1).

4-tert-butyl-2-p-tolylquinazoline (4ic) *(Entry 9 in Table 3)*



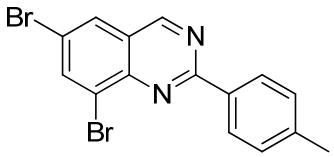
Colorless solid, mp. 74-75 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.71 (s, 9H), 2.44 (s, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.48-7.52 (m, 1H), 7.76-7.80 (m, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 8.41 (d, *J* = 8.4 Hz, 1H), 8.56 (d, *J* = 8.0Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.5, 30.6, 40.5, 121.4, 125.3, 126.5, 128.5, 129.2, 130.2, 132.2, 136.9, 140.5, 152.0, 158.9, 176.2. ESI-MS *m/z*: 277.3 (M+1). HRMS calc.$C_{19}H_{20}N_2$+H^+: 277.1699, found: 277.1695; column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 80:1).

4-tert-butyl-2-(4-chlorophenyl)quinazoline (4if) *(Entry 10 in Table 3)*



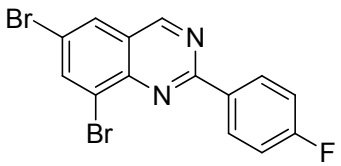
Colorless solid, m.p. 89-91 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.71 (s, 9H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.81 (t, *J* = 7.6 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 8.44 (d, *J* = 8.4Hz, 1H), 8.62 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.6, 40.6, 121.6, 125.8, 126.5, 128.6, 129.9, 130.3, 132.4, 136.5, 137.1, 152.0, 157.9, 176.5. ESI-MS *m/z*: 297.3 (M+1). HRMS calc.$C_{18}H_{17}ClN_2$+H^+: 297.1153, found: 297.1147; column chromatography was performed on silica gel (R_f = 0.2, hexane/ethyl acetate, 60:1).

6,8-dibromo-2-p-tolylquinazoline (4jc) *(Entry 11 in Table 3)*



Yellow solid, m.p. 193-195 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ2.44 (s, 3H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.99 (d, *J* = 2.0 Hz, 1H), 8.26 (d, *J* = 2.0 Hz, 1H), 8.55 (d, *J* = 8.0 Hz, 2H), 9.30 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 21.6, 119.8, 124.9, 125.4, 128.7, 128.9, 129.5, 134.4, 140.0, 141.7, 147.0, 159.7, 162.0. EI-MS *m/z* (relative intensity, %): 380 (M+4, 5.5), 378 (M+2, 11.9), 376 (M, 7.2), 281 (19.8), 149 (38.8), 44 (100). HRMS calc. $C_{15}H_{10}Br_2N_2$+H^+: 376.9283, found: 376.9287; column chromatography was performed on silica gel (R_f = 0.3, hexane/ethyl acetate, 40:1).

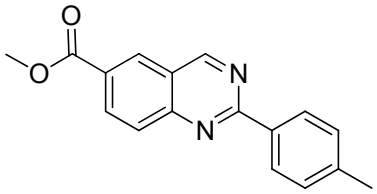
6,8-dibromo-2-(4-fluorophenyl)quinazoline (4jh) *(Entry 12 in Table 3)*



Yellow solid, m.p. 213-215 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (t, *J* = 8.8 Hz, 2H),

8.03 (d, *J* = 2.0 Hz, 1H), 8.28 (d, *J* = 2.0 Hz, 1H), 8.67-8.71 (m, 2H), 9.32 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 115.6, 115.9, 120.2, 125.0, 125.4, 128.8, 131.1, 131.2, 133.35, 133.38, 140.2, 147.1, 159.9, 161.0, 163.9, 166.4. EI-MS *m/z* (relative intensity, %): 384 (M+4, 49.8), 382 (M+2, 100), 380 (M, 50.8), 355 (26.9), 195 (39.1), 149 (62.7), 57 (53.4). HRMS calc. $C_{14}H_7Br_2FN_2+H^+$: 380.9033, found: 380.9035; column chromatography was performed on silica gel (R_f = 0.3, hexane/ethyl acetate, 40:1).

methyl 2-p-tolylquinazoline-6-carboxylate (4lc) *(Entry 13 in Table 3)*



Pale yellow solid, m.p. 155-157 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.45 (s, 3H), 4.01 (s, 3H), 7.35 (d, *J* = 8.0 Hz, 2H), 8.09 (d, *J* = 8.0 Hz, 2H), 8.46 (dd, *J* = 8.8 Hz, *J* = 2.0 Hz, 1H), 8.53 (d, *J* = 8.0, 2H), 8.65 (d, *J* = 2.0 Hz, 1H), 9.52 (s, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 52.5, 122.6, 128.4, 128.8, 129.5, 130.2, 133.4, 134.8, 141.6, 152.7, 161.6, 162.7, 165.9. MS *m/z* (relative intensity, %): 279 (M+1, 18.0), 278 (M, 100), 277 (M-1, 20.0), 247 (41.4), 192 (10.0), 109 (14.7), 40 (5.6). HRMS calc. $C_{17}H_{14}N_2O_2+H^+$: 279.1128, found: 279.1123; column chromatography was performed on silica gel (R_f = 0.3, hexane/ethyl acetate, 20:1).

Reference:

1 D. G. Kawkins, O. Meth-Cohn, *J. Chem. Soc., Perkin Trans. 1*, 1983, 2077.

2 C. M. Counceller, C. C. Eichman, B. C. Wray, J. P. Stambuli, *Org. Lett.*, 2008, **10**, 1021.

3 S. Atechian, N. Nock, R. D. Norcross, H. Ratni, A. W. Thomas, J. Verron, R. Masciadri, *Tetrahedron*, 2007, **63**, 2811.

4 M. P. Hutt, F. A. Mackeller, *J. Heterocyclic Chem.*, 1984, **21**, 349.

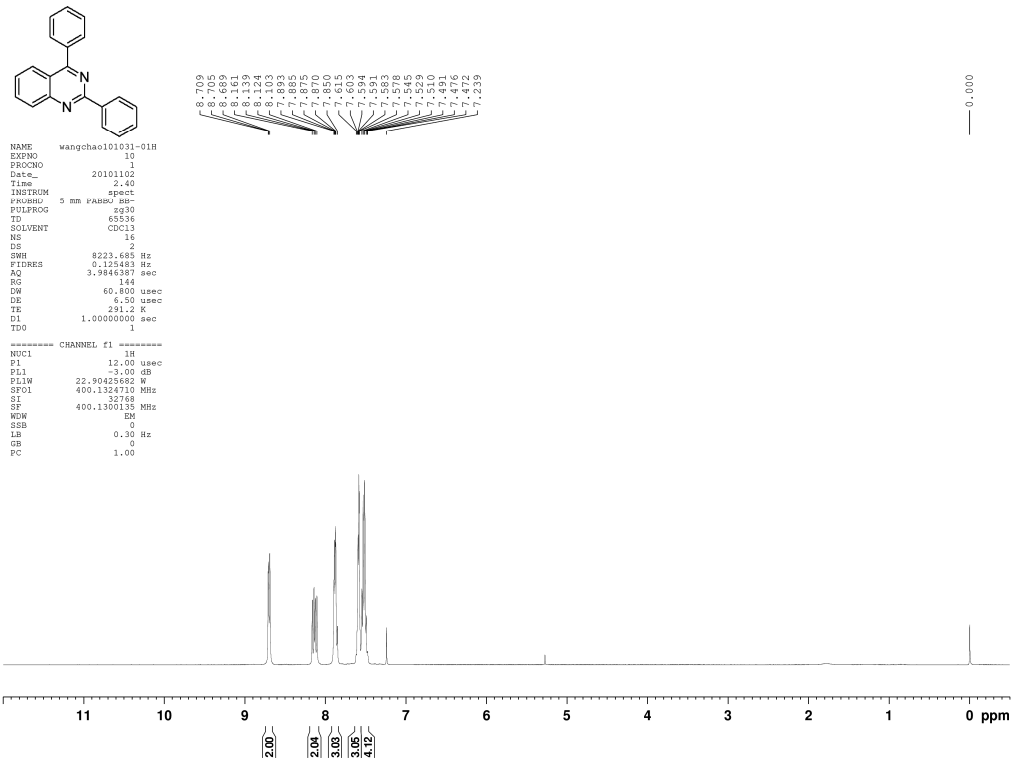
5 C. Zhang, C. K. De, R. Mal, D. Seidel, *J. Am. Chem. Soc.*, 2008, **130**, 416.

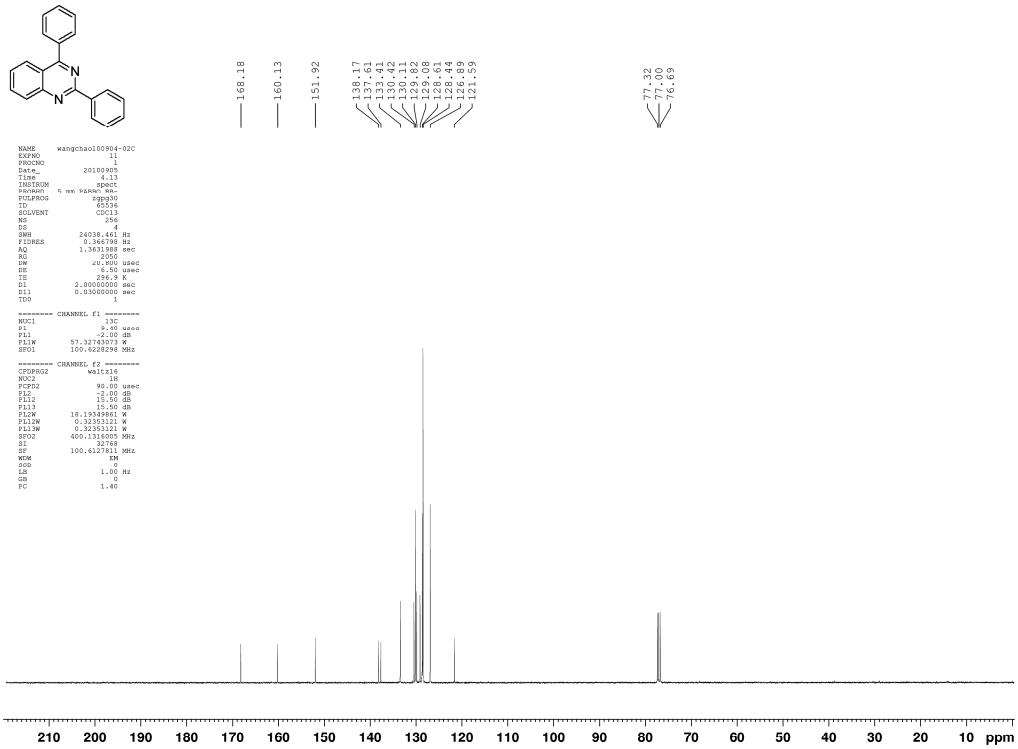
6 J. Bergman, A. Brynolf, B. Elman, E. Vuorinen, *Tetrahedron*, 1986, **42**, 3697.

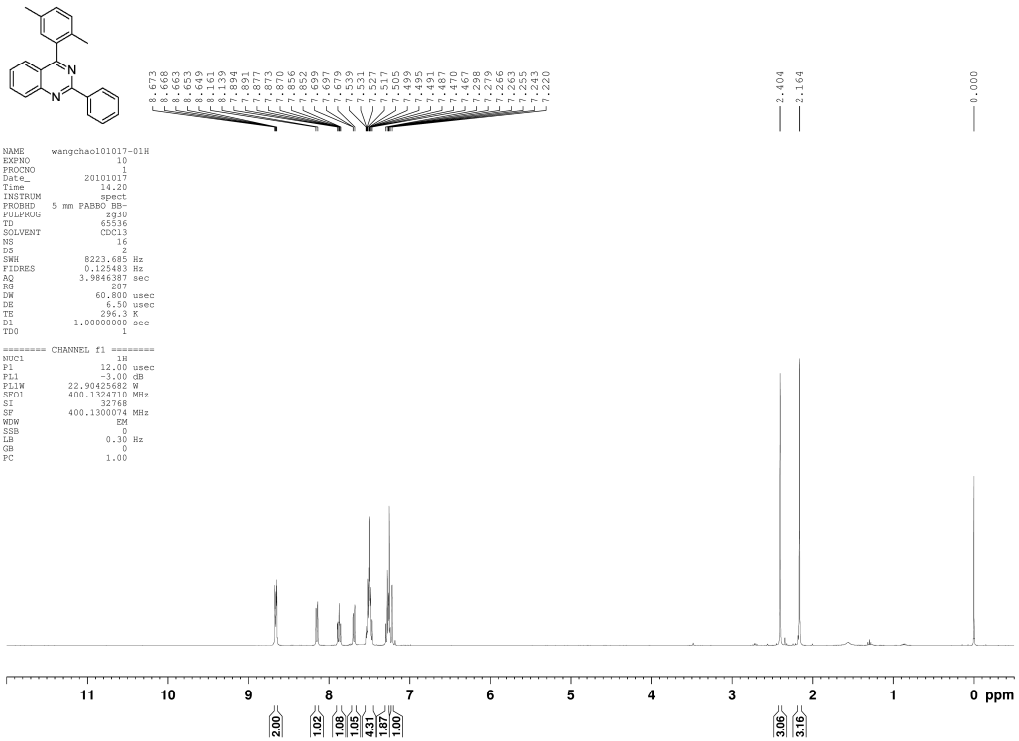
7 J. Zhang, D. Zhu, C. Yu, C. Wan, Z. Wang, *Org. Lett.*, 2010, **12**, 2841.

8 Y. Tamura, M. W. Chun, G. Nishida, S. Kwon, M. Ikeda, *Chem. Pharm. Bull.*, 1978, **26**, 2866.

^{1}H and ^{13}C spectra



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FIDRES 0.125483 Hz
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DE 6.50 usec
TE 296.3 K
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TD0 1
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SFO1 400.1324710 MHz
SI 32768
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WDW EM
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LB 0.30 Hz
GB 0
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9
8
7
6
5
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1.07
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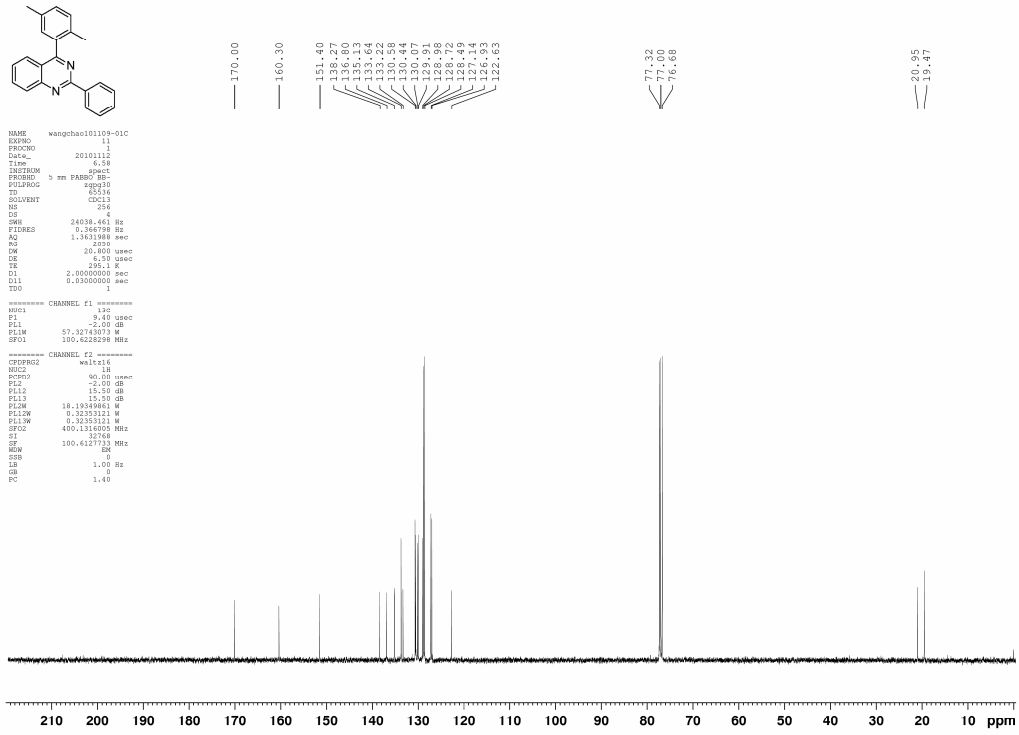
3.06
3.16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TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
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P1 9.40 usec
PL1 -2.00 dB
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SFO1 100.6228298 MHz
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PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127753 MHz
WDW EM
SSB 0
LB 1.00 Hz
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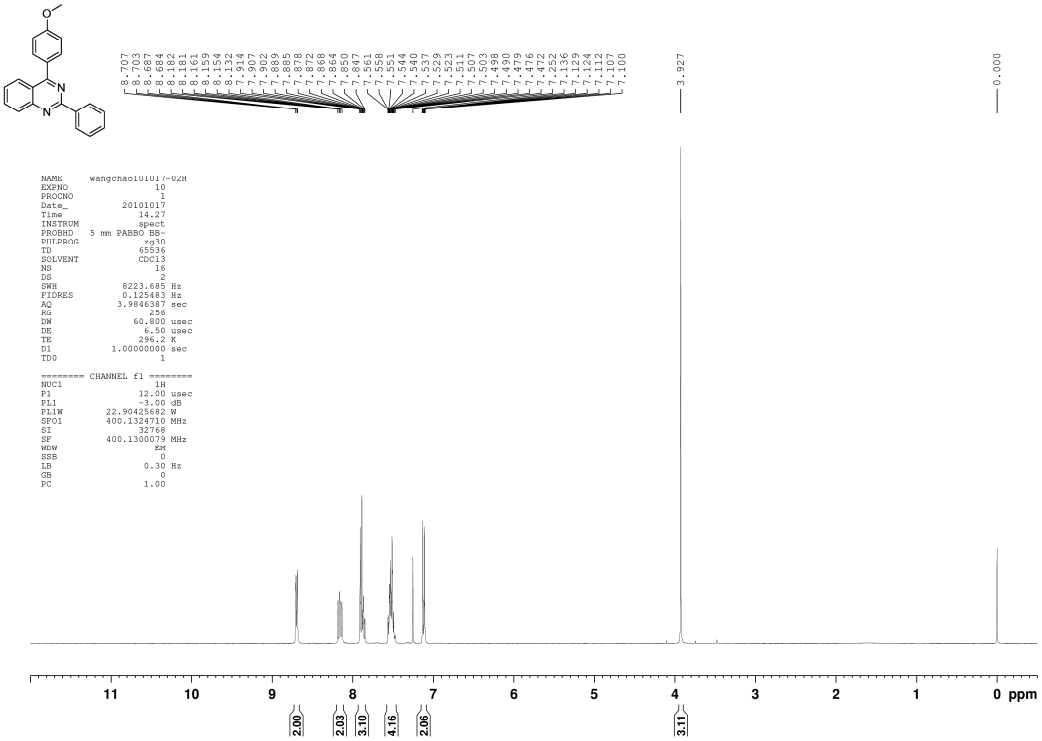
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TE 296.2 K
D1 1.00000000 sec
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PL1 -3.00 dB
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SFO1 400.1324710 MHz
SI 32768
SF 400.1300079 MHz
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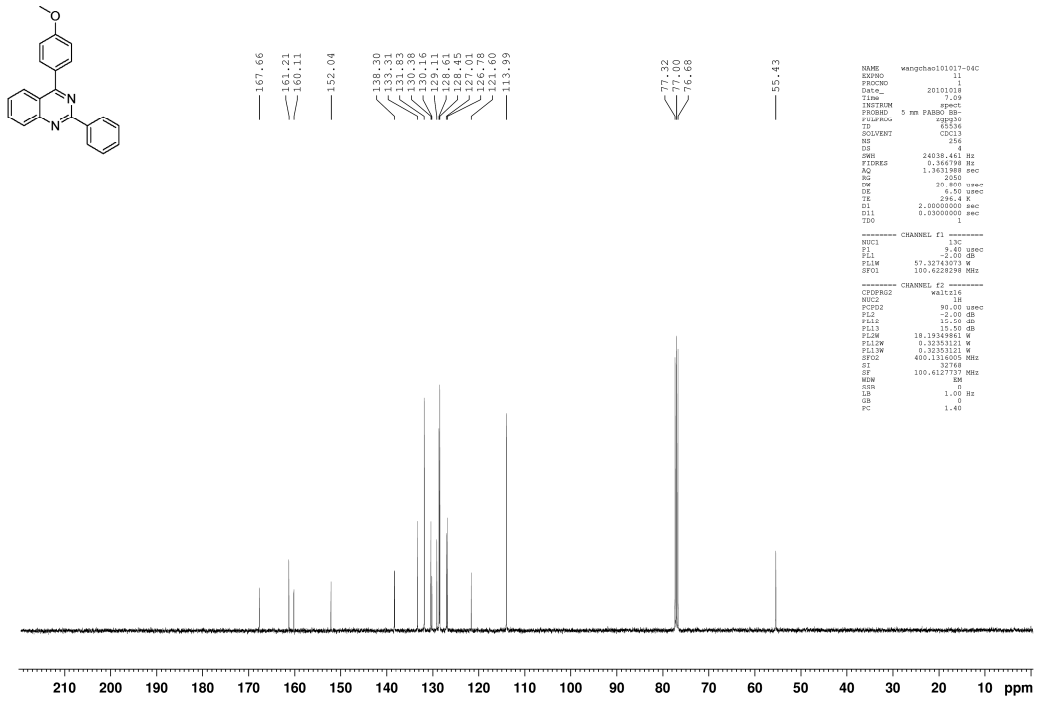
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Time 7.09
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TE 296.4 K
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NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
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WDW EM
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PC 1.40
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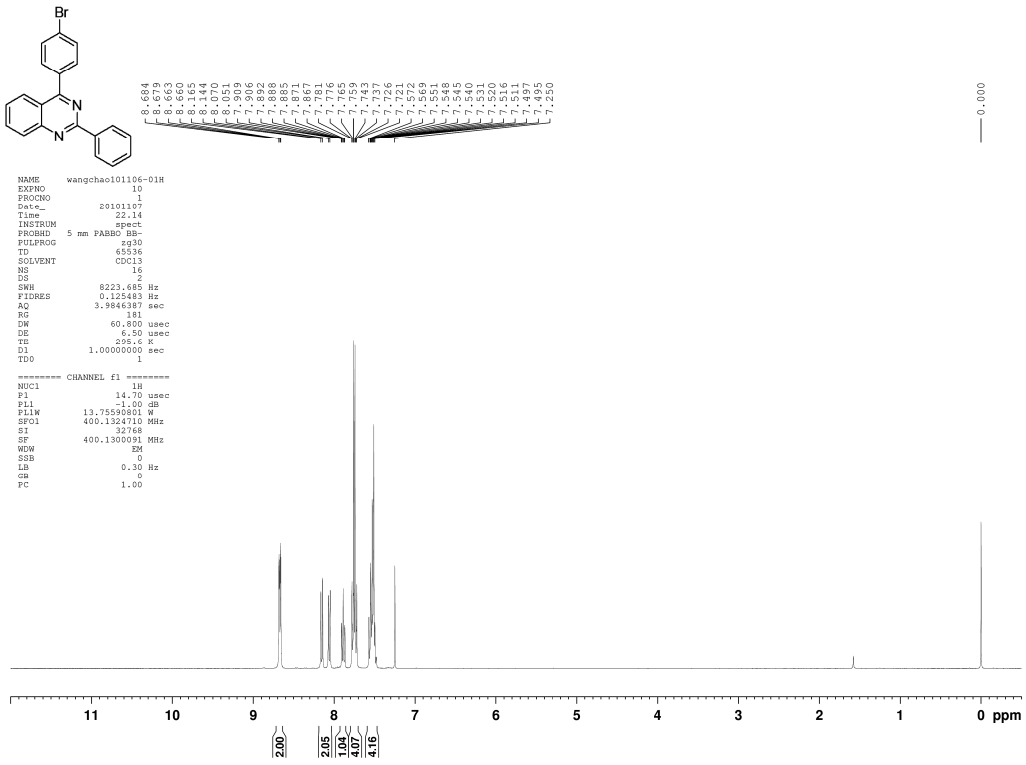
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FIDRES 0.125483 Hz
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DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
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SFO1 400.1324710 MHz
SI 32768
SF 400.1300091 MHz
WDW EM
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PC 1.00
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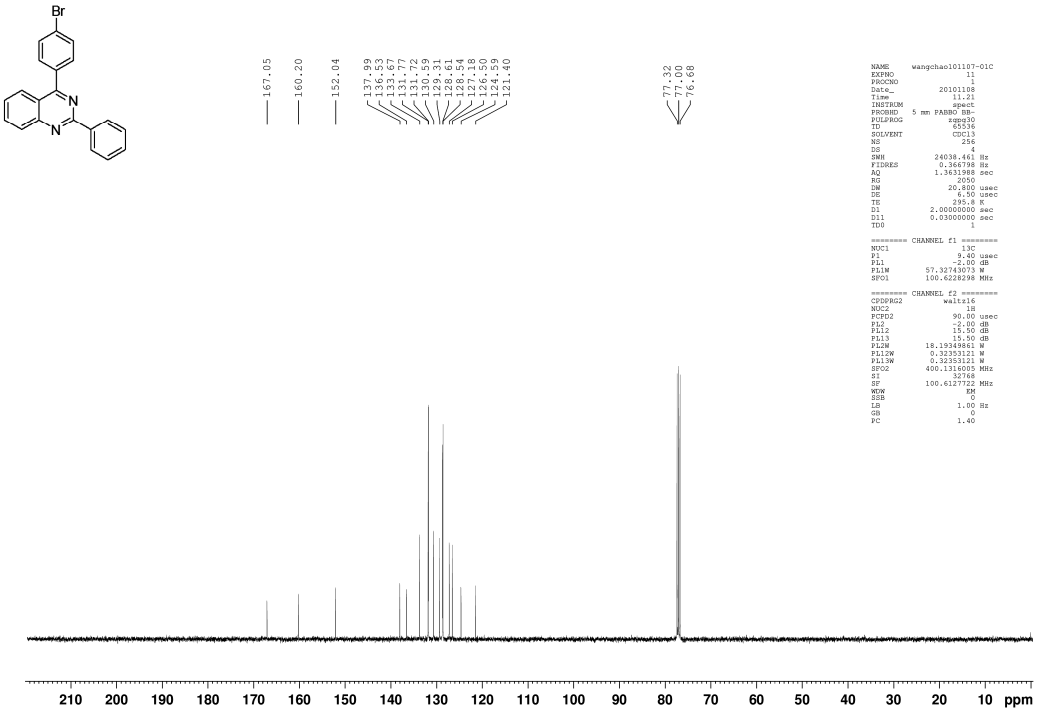
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EXPNO 11
PROCNO 1
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Time 11.21
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PULPROG zgpg30
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SOLVENT CDCl3
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FIDRES 0.366798 Hz
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RG 2050
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
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P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210
200
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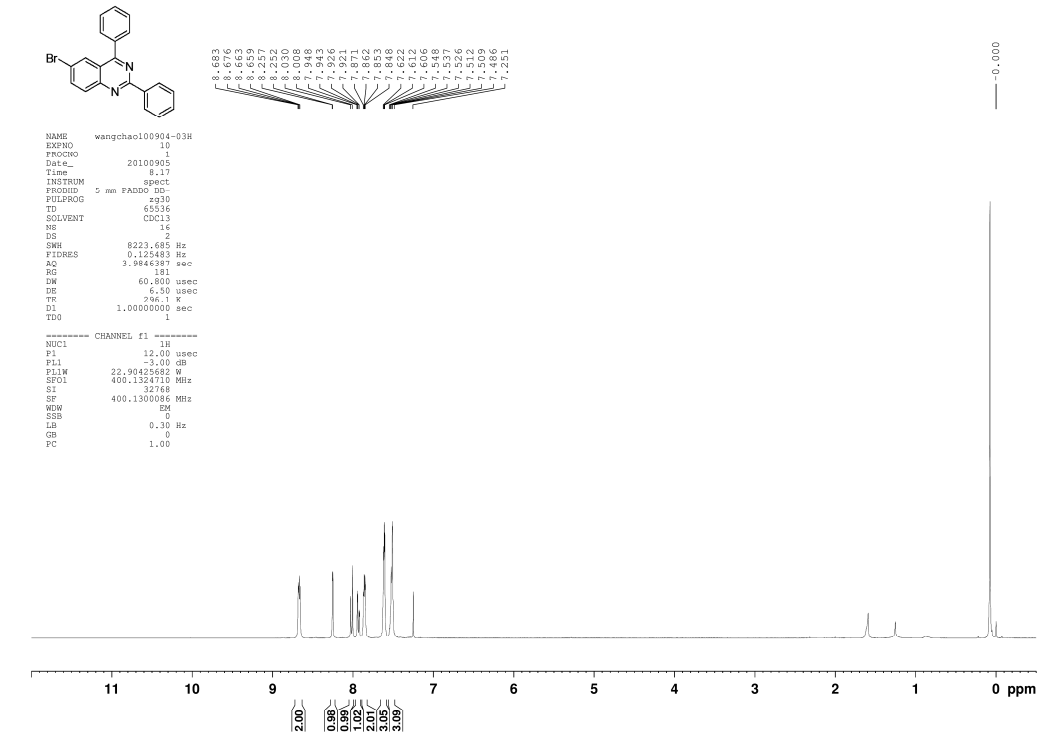
20
10 ppm

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TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8223.685 Hz
FIDRES                 0.125483 Hz
AQ                     3.9846387 sec
RG                          181
DW                       60.800 usec
DE                        6.50 usec
TE                       296.1 K
D1                  1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       12.00 usec
PL1                      -3.00 dB
PL1W                22.90425682 W
SFO1                400.1324710 MHz
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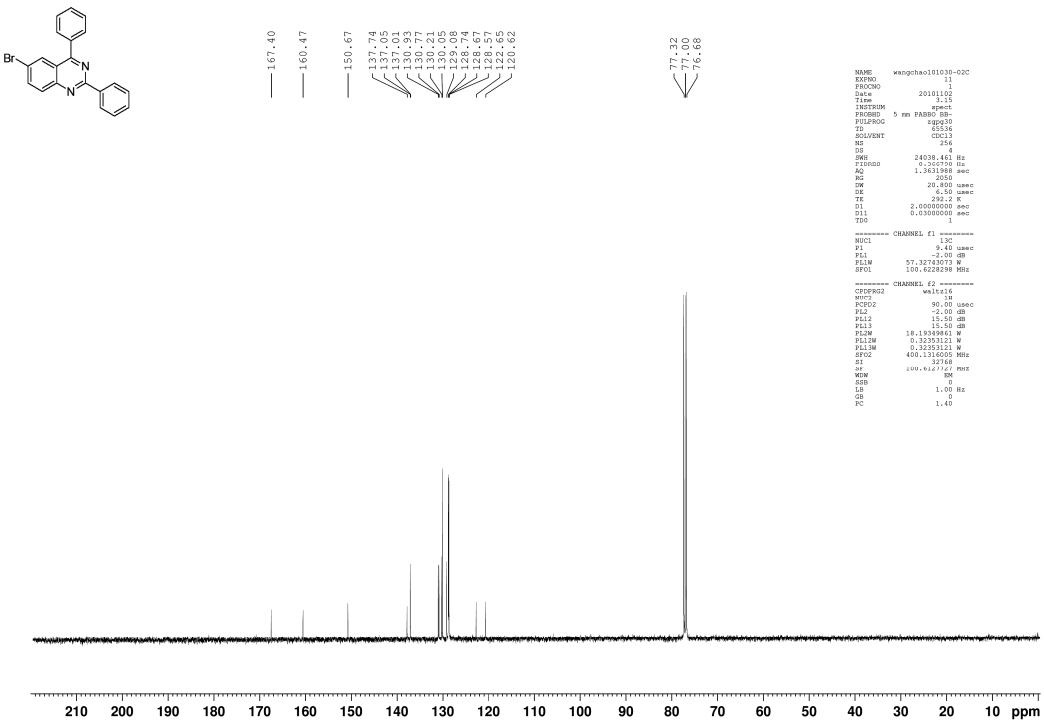


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SOLVENT                   CDCl3
NS                          256
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.366790 Hz
AQ                     1.3631988 sec
RG                         2050
DW                       20.800 usec
DE                        6.50 usec
TE                       292.2 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         13C
P1                        9.40 usec
PL1                      -2.00 dB
PL1W                57.32743073 W
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
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NUC2                         1H
PCPD2                    90.00 usec
PL2                      -2.00 dB
PL12                     15.50 dB
PL13                     15.50 dB
PL2W                18.19349841 W
PL12W                0.32353121 W
PL13W                0.32353121 W
SFO2                400.1316005 MHz
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SF                  100.6147677 MHz
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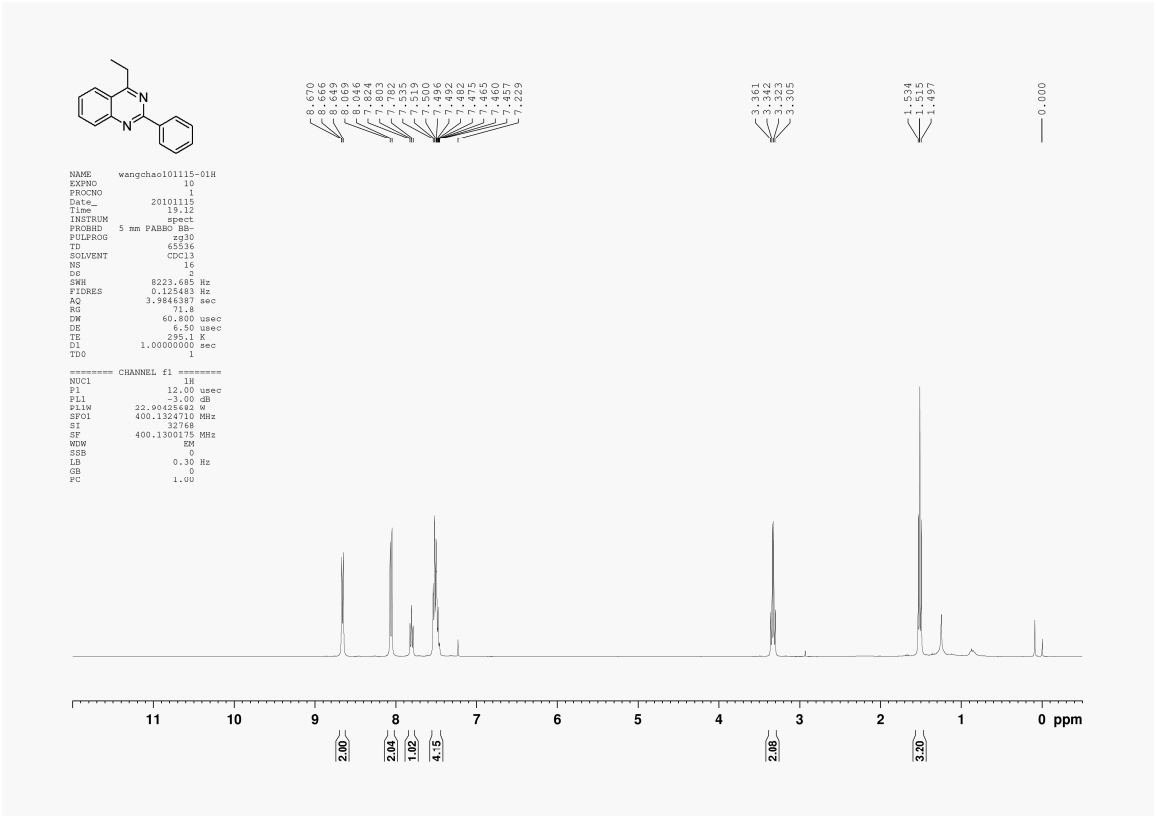
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11
10
9
8
7
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5
4
3
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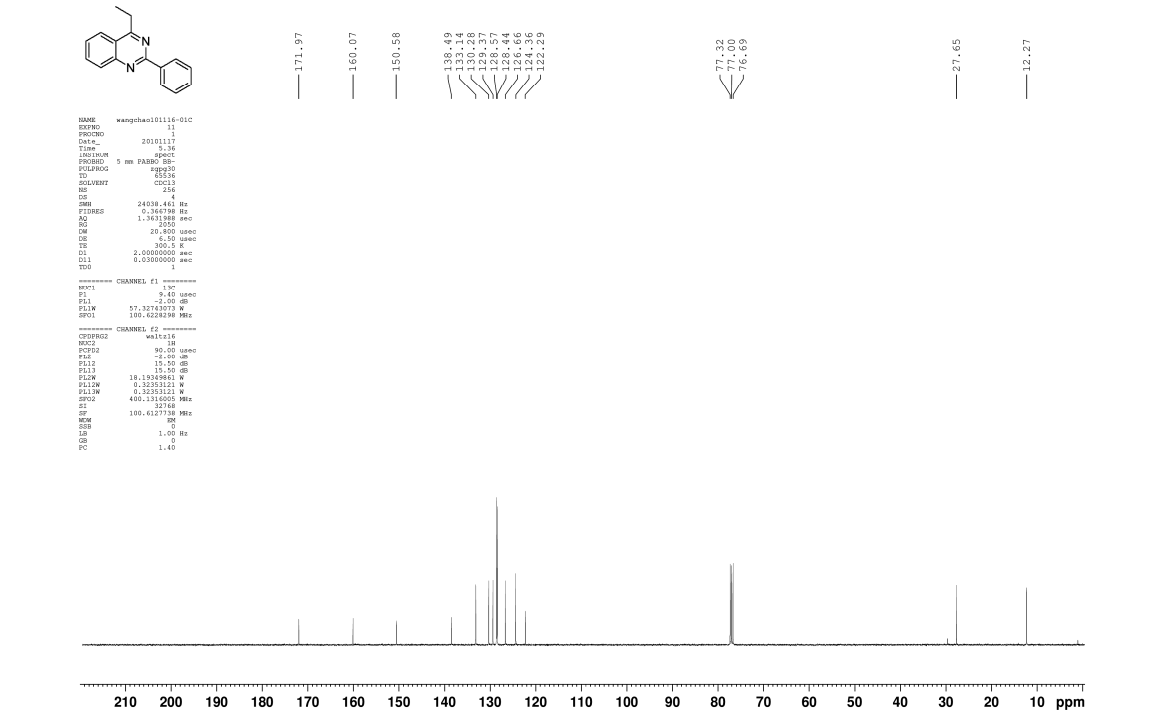
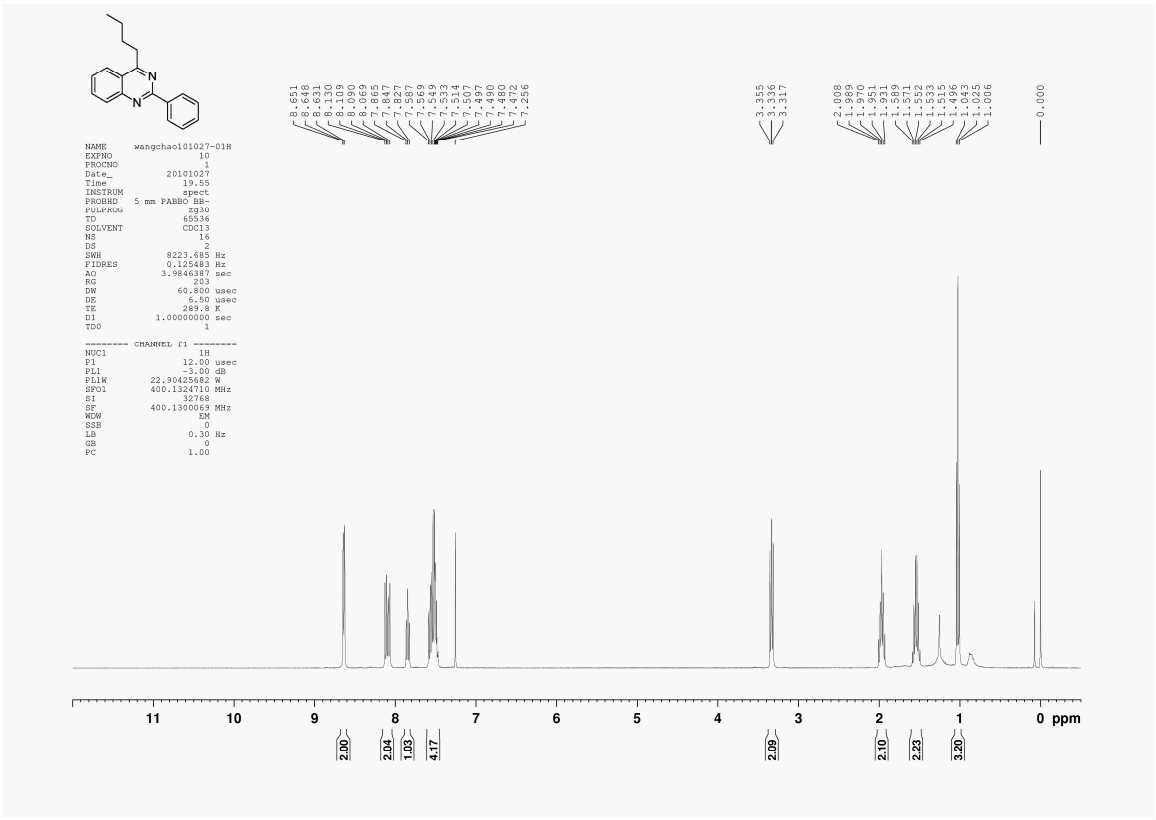
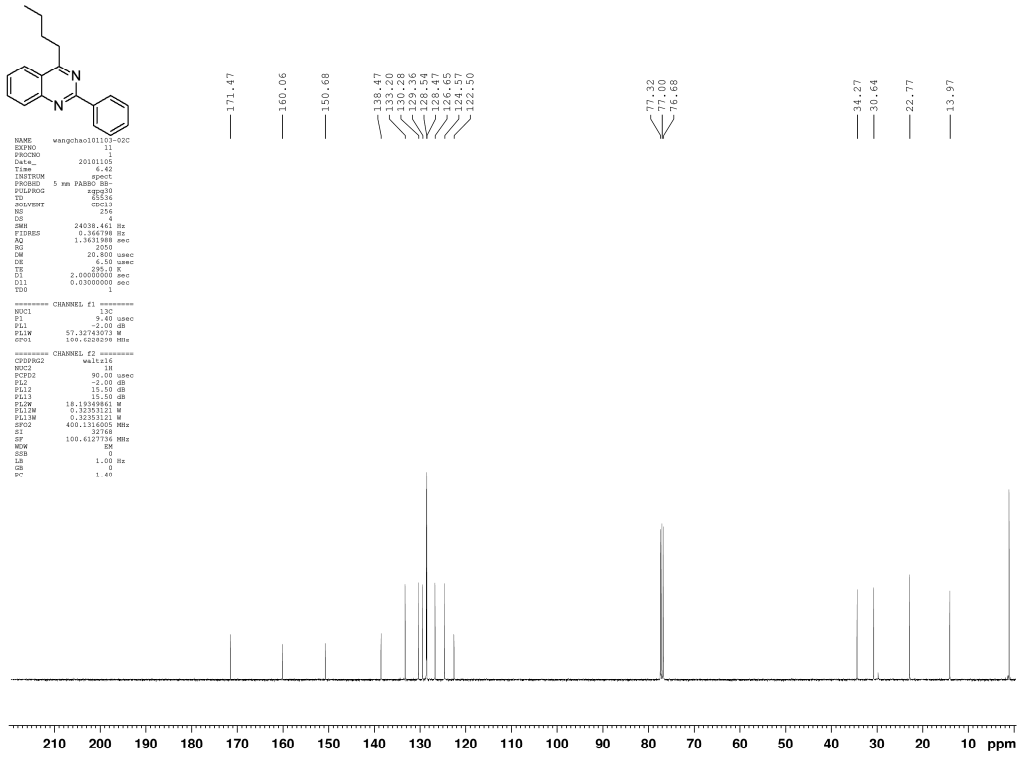
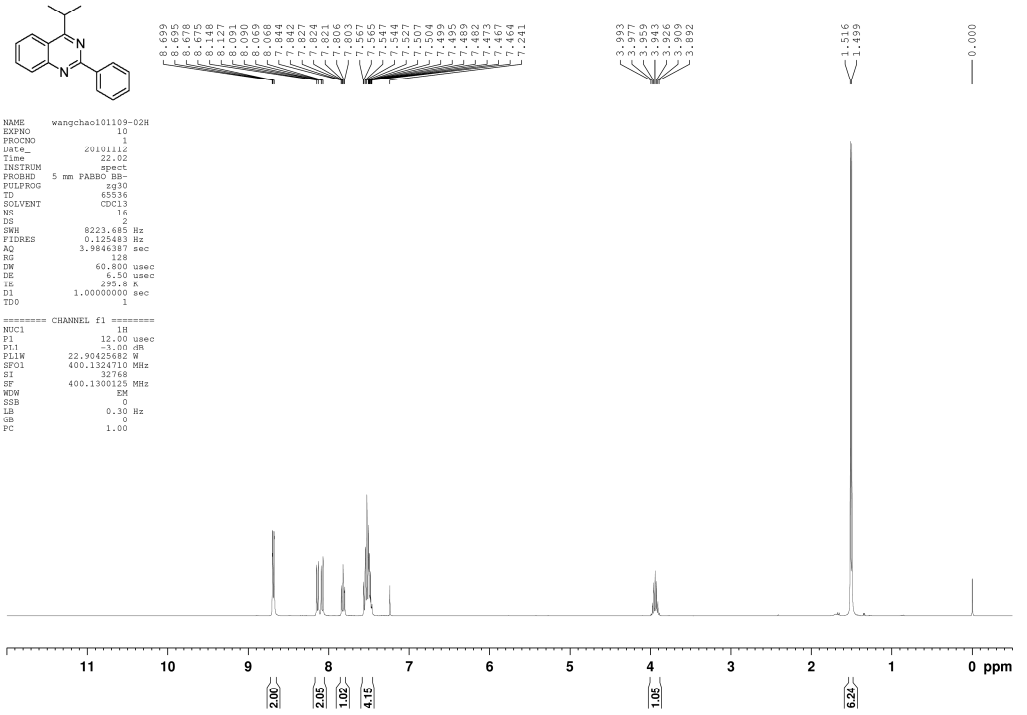
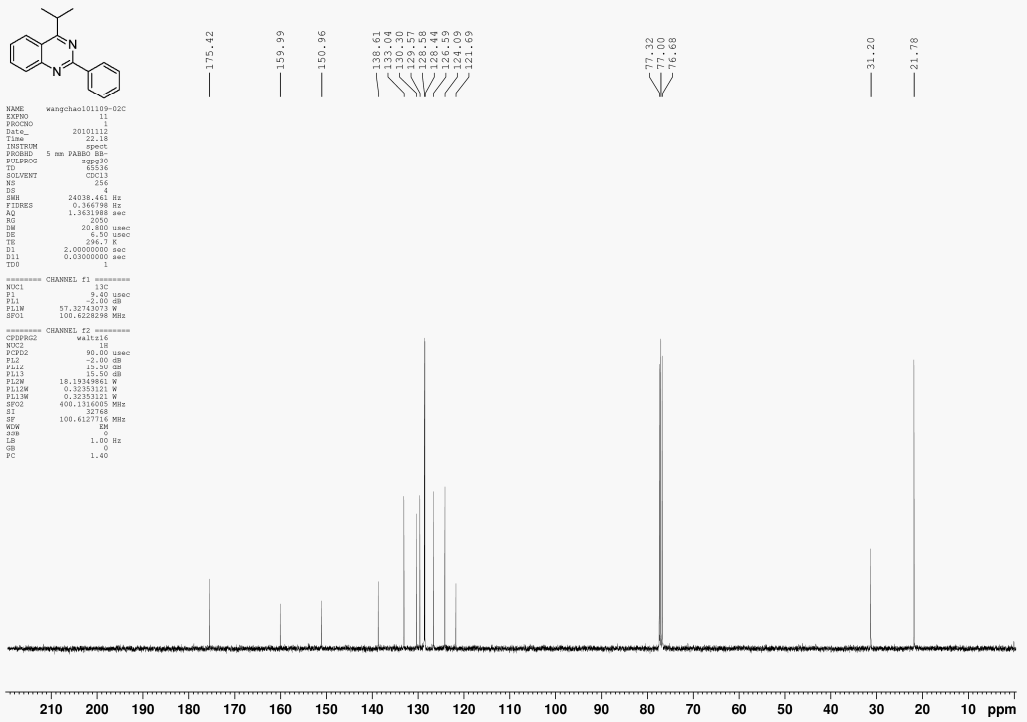
1.02
4.15
2.08
3.20

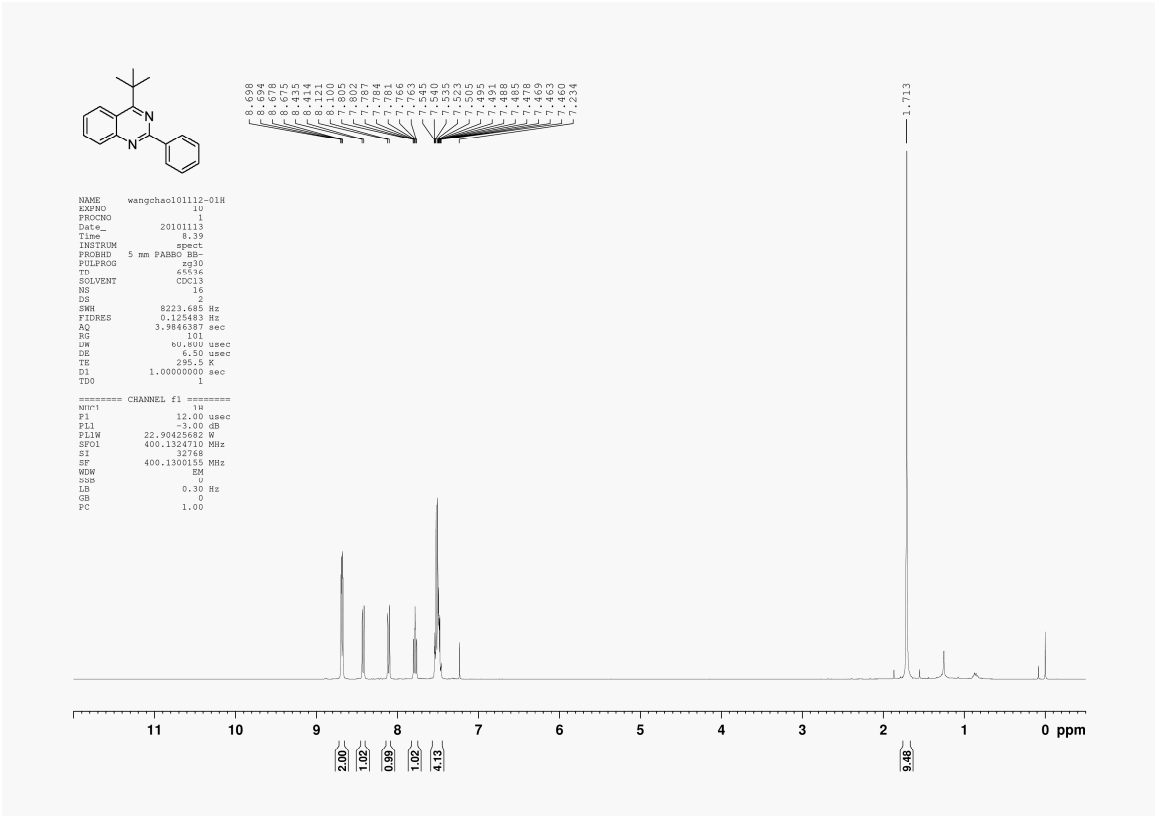

171.97
160.07
150.58
138.49
133.14
130.28
129.37
128.57
128.44
125.66
124.36
122.29
77.32
77.00
76.69
27.65
12.27
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

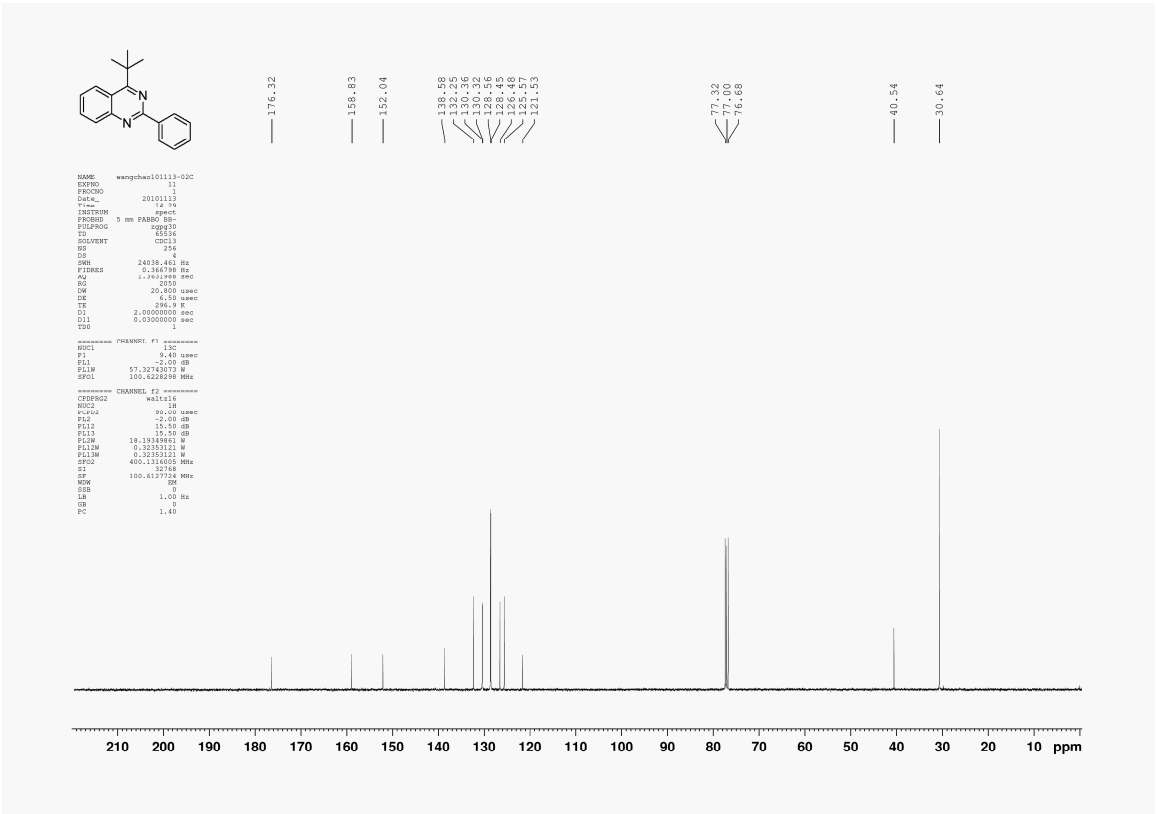

8.651
8.648
8.631
8.130
8.109
8.090
8.069
7.865
7.847
7.827
7.587
7.569
7.549
7.533
7.514
7.507
7.497
7.480
7.472
7.256
3.355
3.336
3.317
2.008
1.989
1.970
1.951
1.931
1.589
1.571
1.552
1.533
1.515
1.496
1.483
1.025
1.006
0.000
NAME wangchao101027-01H
EXPNO 10
PROCNO 1
Date_ 20101027
Time 19.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 289.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
PL1W 22.90425682 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00 2.04 1.03 4.17 2.09 2.10 2.23 3.20

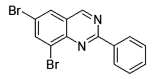

171.47
160.06
150.68
138.47
133.20
130.28
130.06
128.54
128.47
126.65
124.57
122.50
77.32
77.00
76.68
34.27
30.64
22.77
13.97
NAME wangchao101103-02C
EXPNO 11
PROCNO 1
Date_ 20101105
Time 6.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT cdcl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

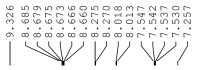

8.699
8.695
8.678
8.675
8.148
8.127
8.091
8.090
8.068
8.068
7.844
7.842
7.827
7.824
7.821
7.806
7.803
7.567
7.565
7.547
7.544
7.527
7.507
7.504
7.499
7.485
7.483
7.482
7.473
7.467
7.464
7.241
3.993
3.977
3.959
3.943
3.926
3.909
3.892
1.516
1.499
0.000
NAME wangchao101109-02H
EXPNO 10
PROCNO 1
Date_ 20101112
Time 22.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
IE 295.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
PL1W 22.90425682 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.05
1.02
4.15
1.05
6.24


175.42
159.99
150.96
138.61
133.04
130.30
129.57
128.88
128.44
126.59
124.09
121.69
77.32
77.00
76.68
31.20
21.78
NAME wangchao101109-02C
EXPNO 11
PROCNO 1
Date_ 20101112
Time 22.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 -1.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

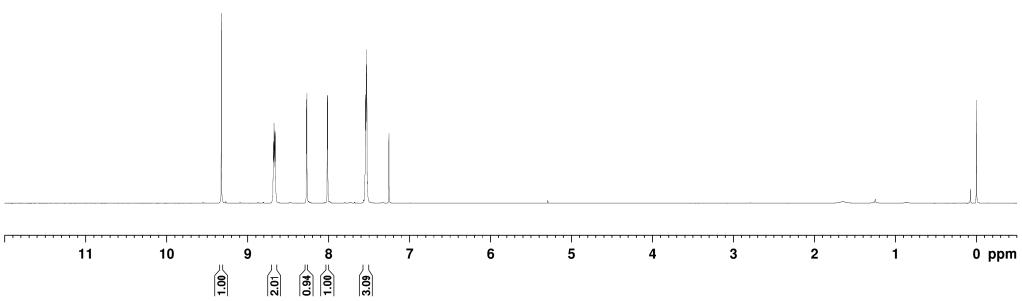

8.698
8.694
8.678
8.675
8.435
8.434
8.121
8.100
7.805
7.802
7.784
7.781
7.766
7.763
7.545
7.540
7.530
7.523
7.505
7.495
7.491
7.488
7.485
7.478
7.469
7.463
7.460
7.234
1.713
NAME wangchao101112-01H
EXPNO 10
PROCNO 1
Date_ 20101113
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 101
DW 60.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
PL1W 22.90425682 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300155 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.02
0.99
1.02
4.13
9.48

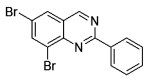

176.32
158.83
152.04
138.58
132.25
130.36
129.32
128.56
128.45
126.48
125.57
121.53
77.32
77.00
76.68
40.54
30.64
NAME wangchao101113-02C
EXPNO 11
PROCNO 1
Date_ 20101113
Time 12.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127724 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm



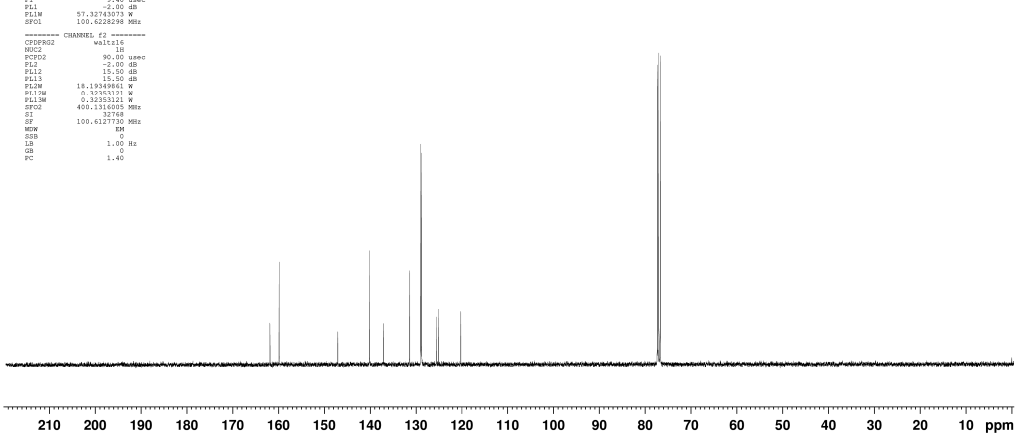


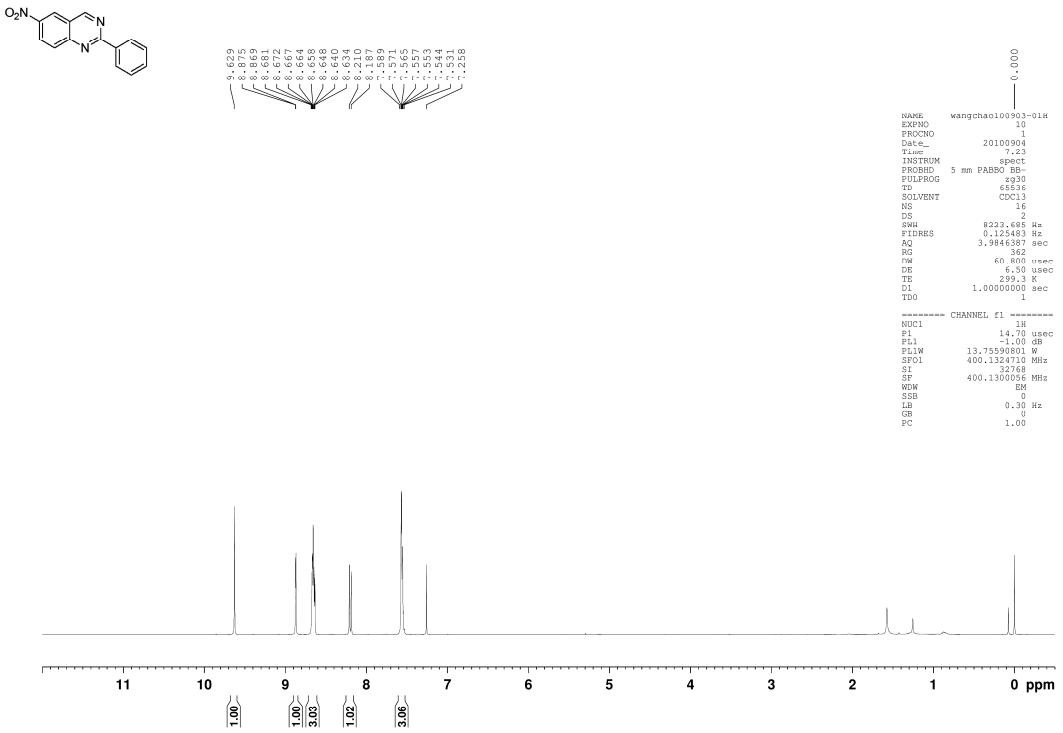

```
NAME        wanqchao101029-01H
EXPNO                       10
PROCNO                       1
Date_                 20101030
Time                     17.24
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                          16
DS                           2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                         256
DW                    60.800 usec
DE                     6.50 usec
TE                     292.1 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.00 usec
PL1                     -3.00 dB
PL1W               22.90425682 W
SFO1               400.1324710 MHz
SI                        32768
SF                 400.1300062 MHz
WDW                          EM
SSB                           0
LB                     0.30 Hz
GB                            0
PC                         1.00
```

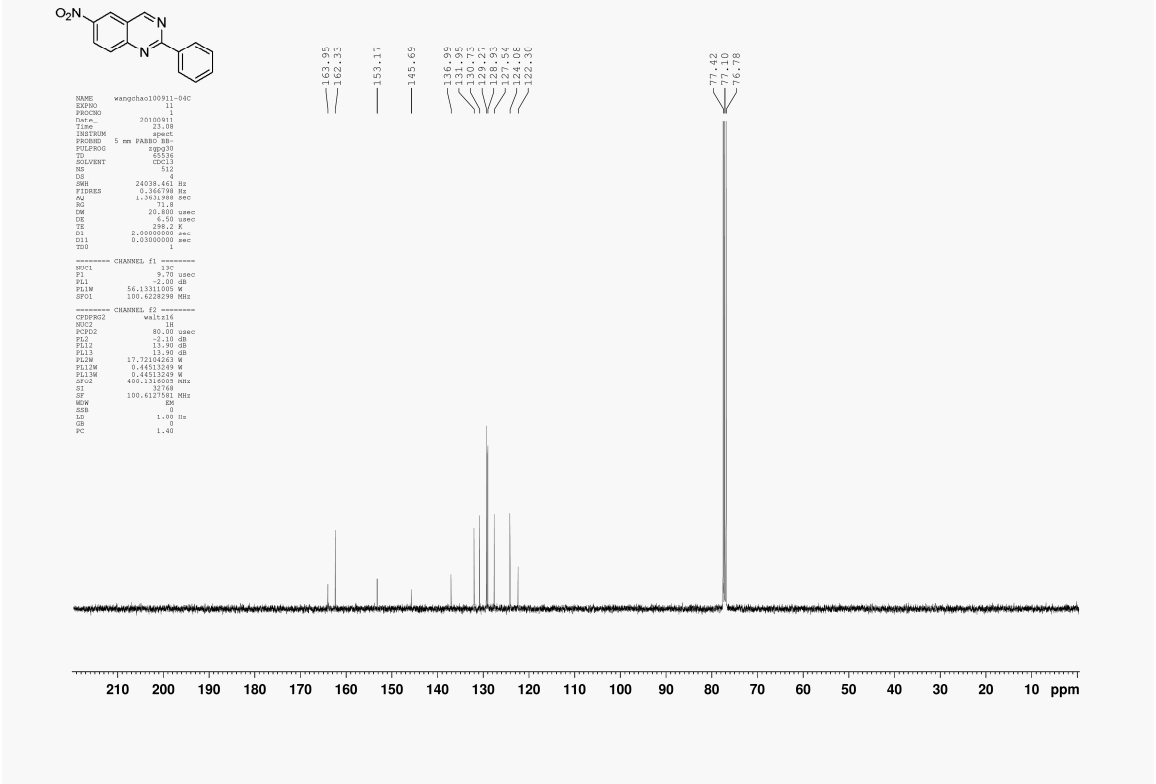


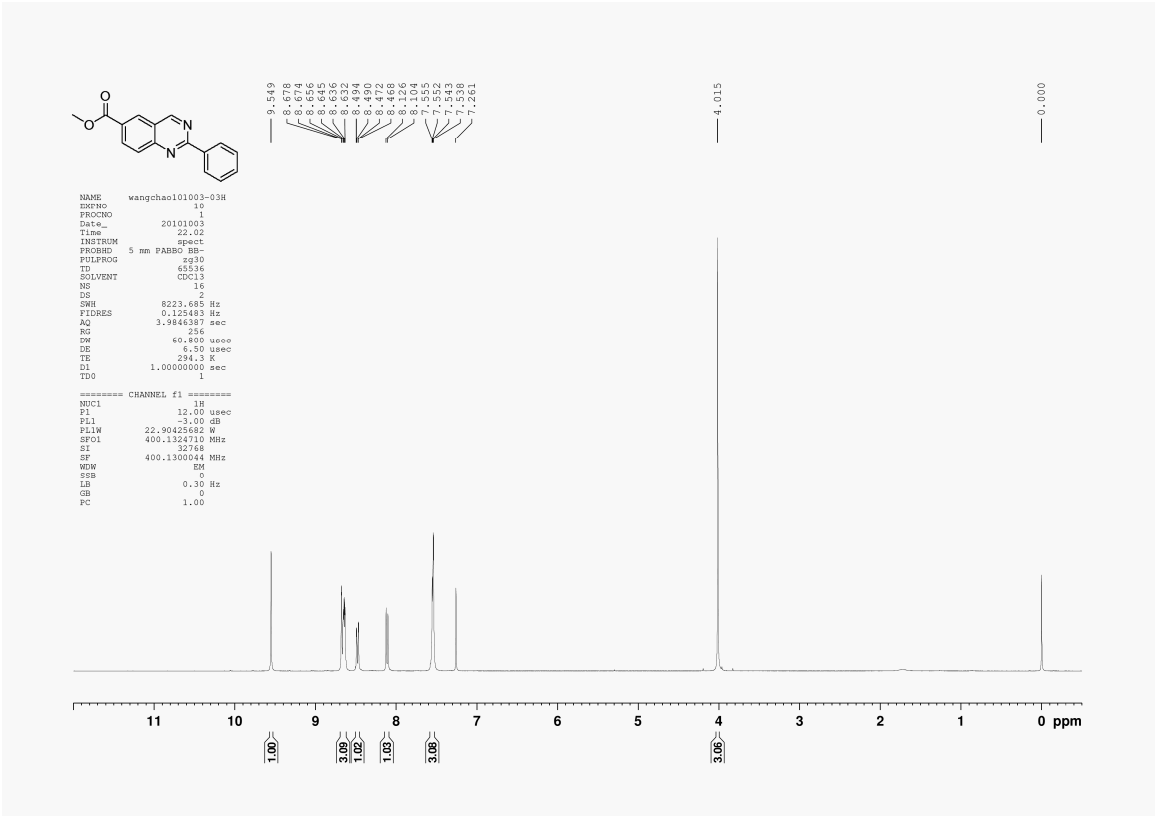


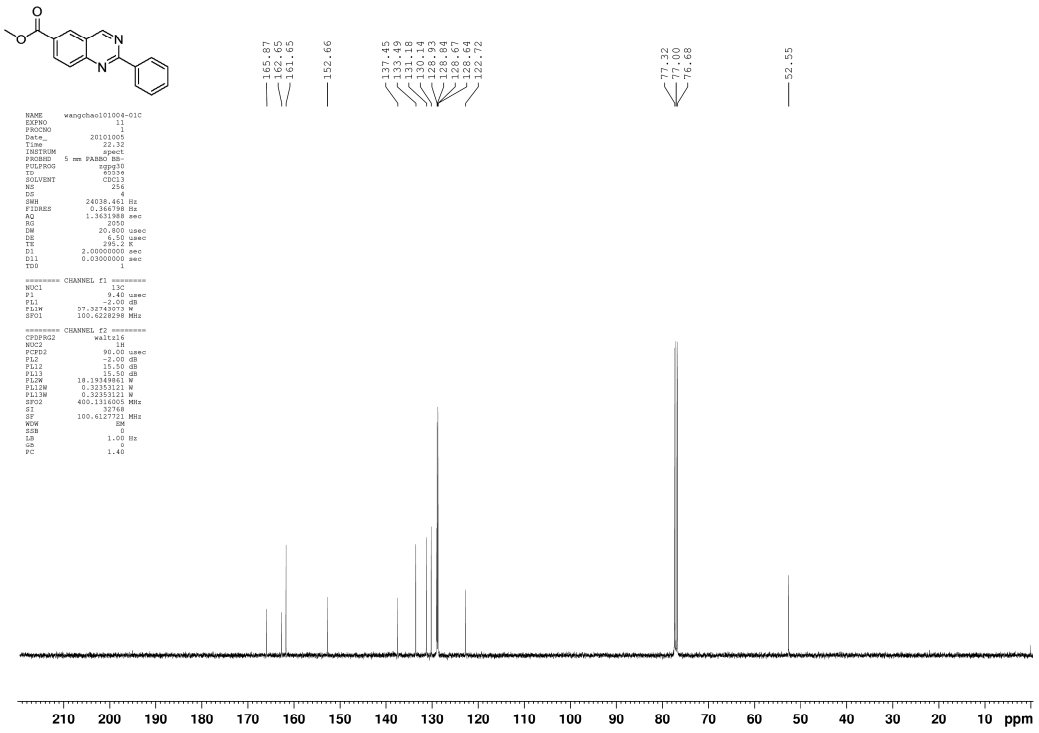

```
NAME        wanqchao101028-01C
EXPNO                       11
PROCNO                       1
Date_                 20101029
Time                     18.22
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        4096
DS                           4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                        2050
DW                    20.800 usec
DE                     6.50 usec
TE                     292.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                      9.40 usec
PL1                    -2.00 dB
PL1W               57.32745073 W
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  90.00 usec
PL2                    -2.00 dB
PL12                   15.50 dB
PL13                   15.50 dB
PL2W               18.19349961 W
PL12W               0.32353121 W
PL13W               0.32353121 W
SFO2               400.1316005 MHz
SI                        32768
SF                 100.6127730 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                         1.40
```

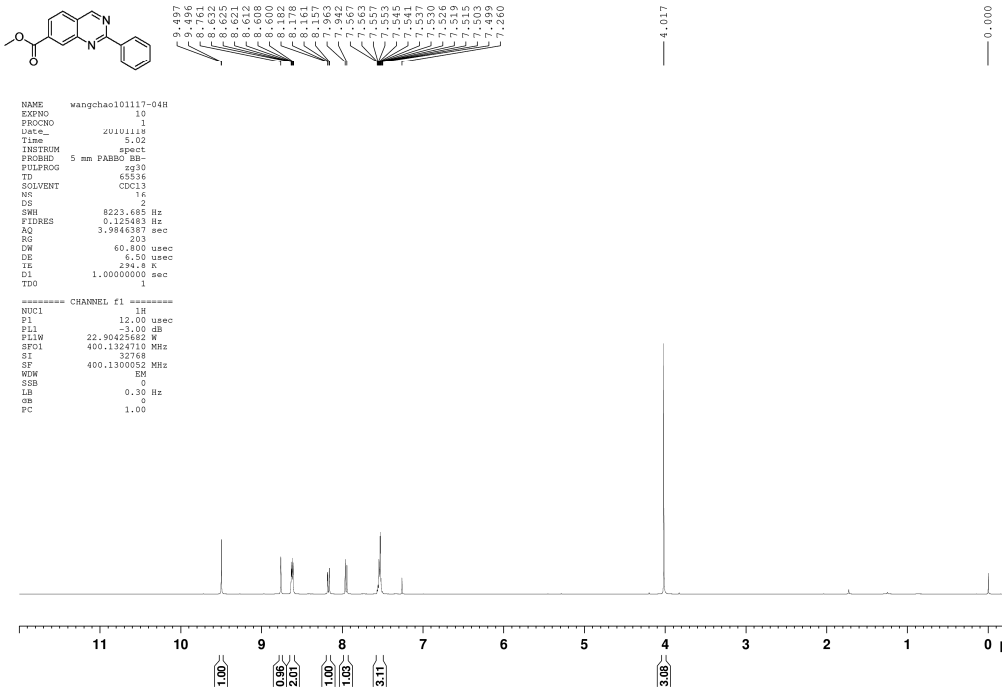


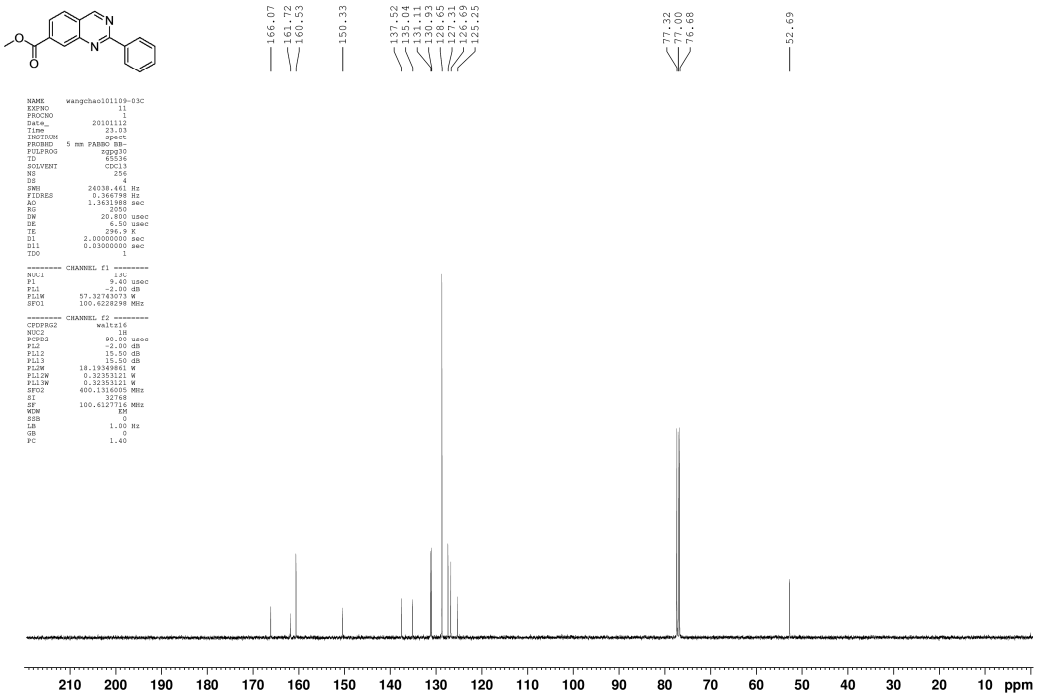

9.629
8.875
8.869
8.651
8.672
8.667
8.664
8.658
8.648
8.640
8.634
8.210
8.187
7.589
7.571
7.565
7.557
7.553
7.544
7.531
7.258
0.000
NAME wangchao100903-01H
EXPNO 10
PROCNO 1
Date_ 20100904
Time 7.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 362
DW 60.800 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 -1.00 dB
PL1W 13.75590801 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.00
3.03
1.02
3.06

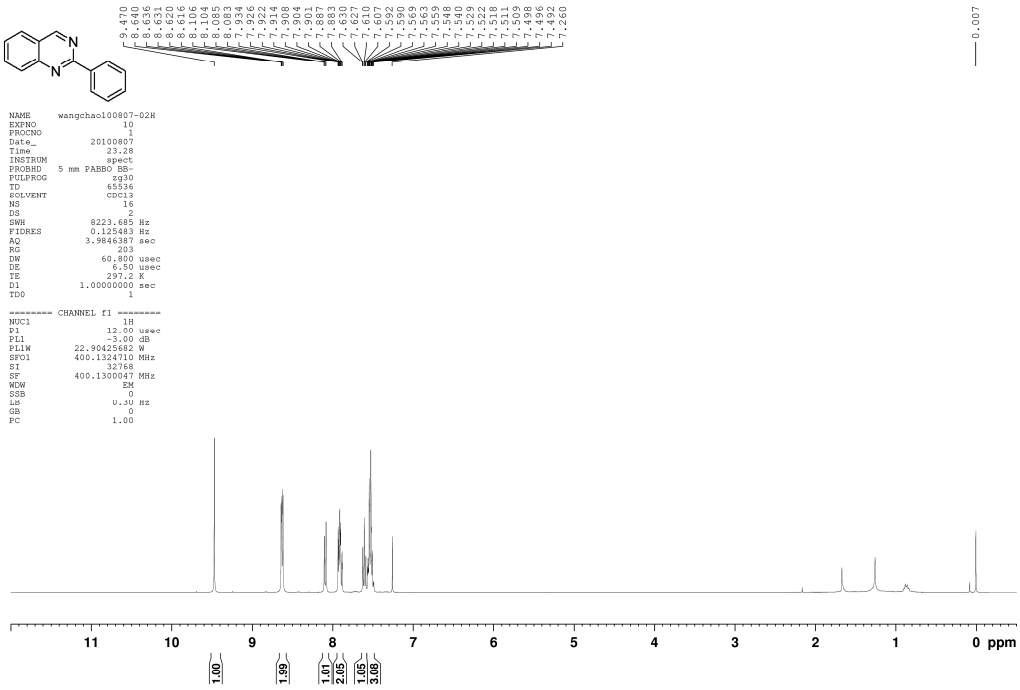

163.95
162.33
153.11
145.65
136.99
131.95
130.73
129.21
128.93
127.54
125.45
122.30
77.42
77.10
76.78
NAME wangchao100911-04C
EXPNO 11
PROCNO 1
Date_ 20100911
Time 23.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 71.8
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.10 dB
PL12 13.90 dB
PL13 13.90 dB
PL2W 17.72104263 W
PL12W 0.44513249 W
PL13W 0.44513249 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127581 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

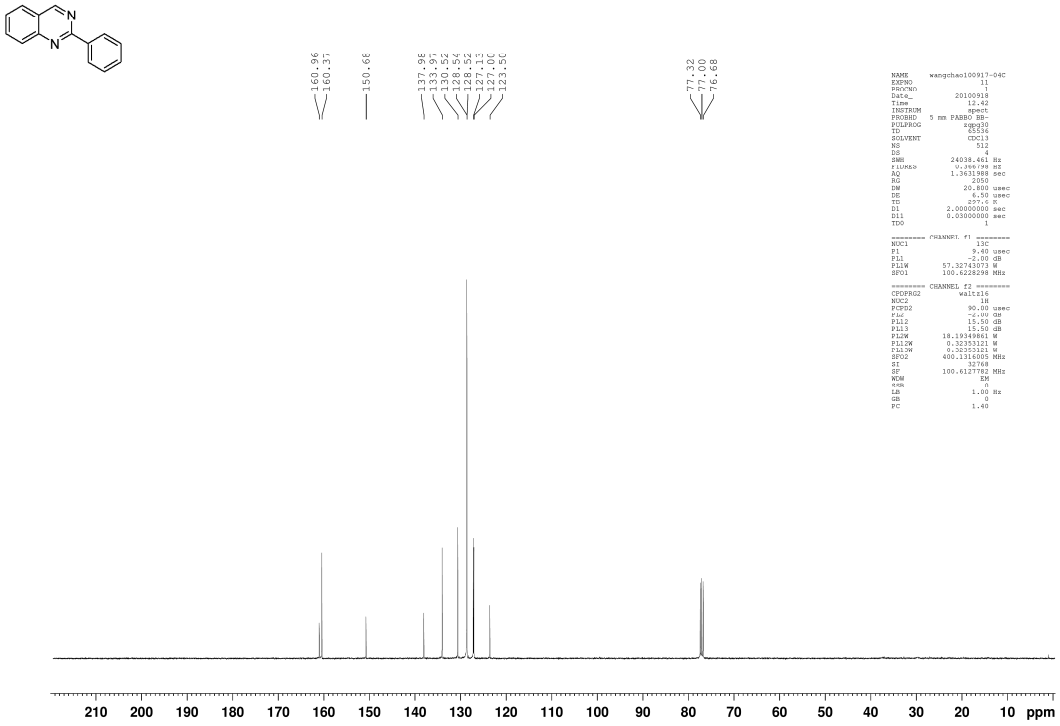

9.549
8.678
8.674
8.656
8.655
8.636
8.632
8.494
8.490
8.472
8.468
8.126
8.104
7.555
7.552
7.533
7.530
7.261
4.015
0.000
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
3.09
1.02
1.03
3.08
3.06

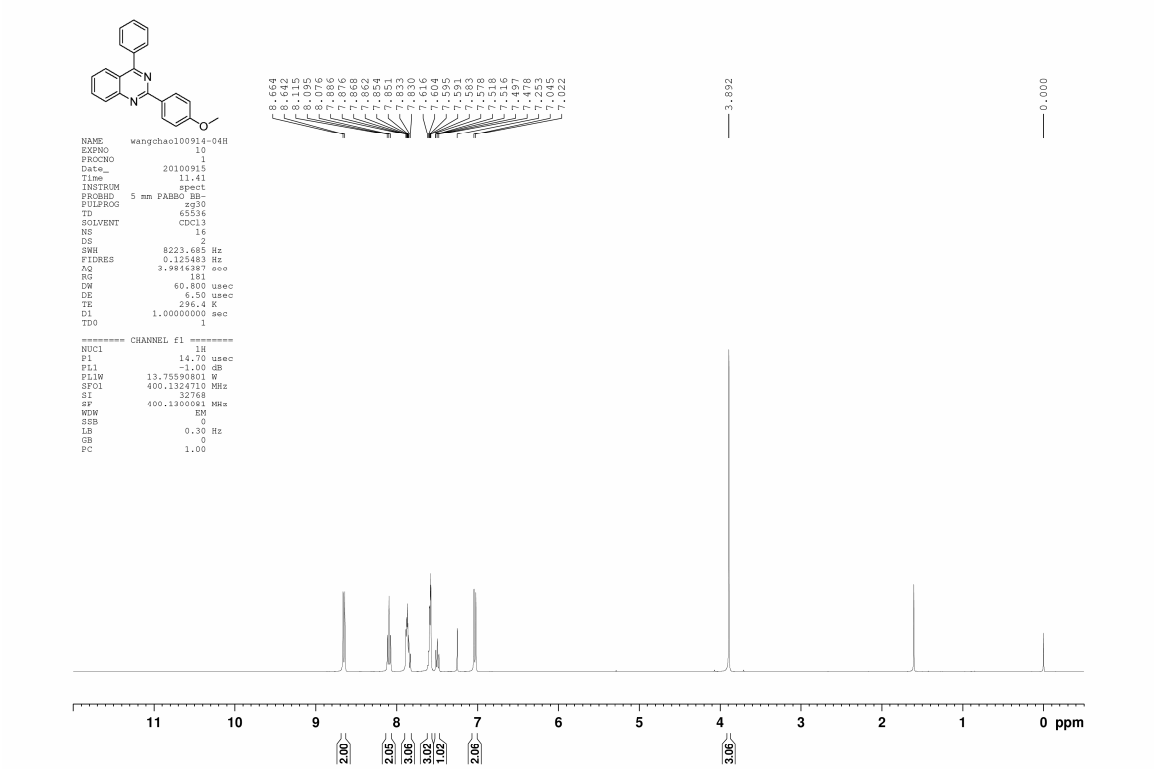

165.87
162.65
161.65
152.66
137.45
133.49
131.18
130.14
128.93
128.84
128.67
128.64
122.72
77.32
77.00
76.68
52.55
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

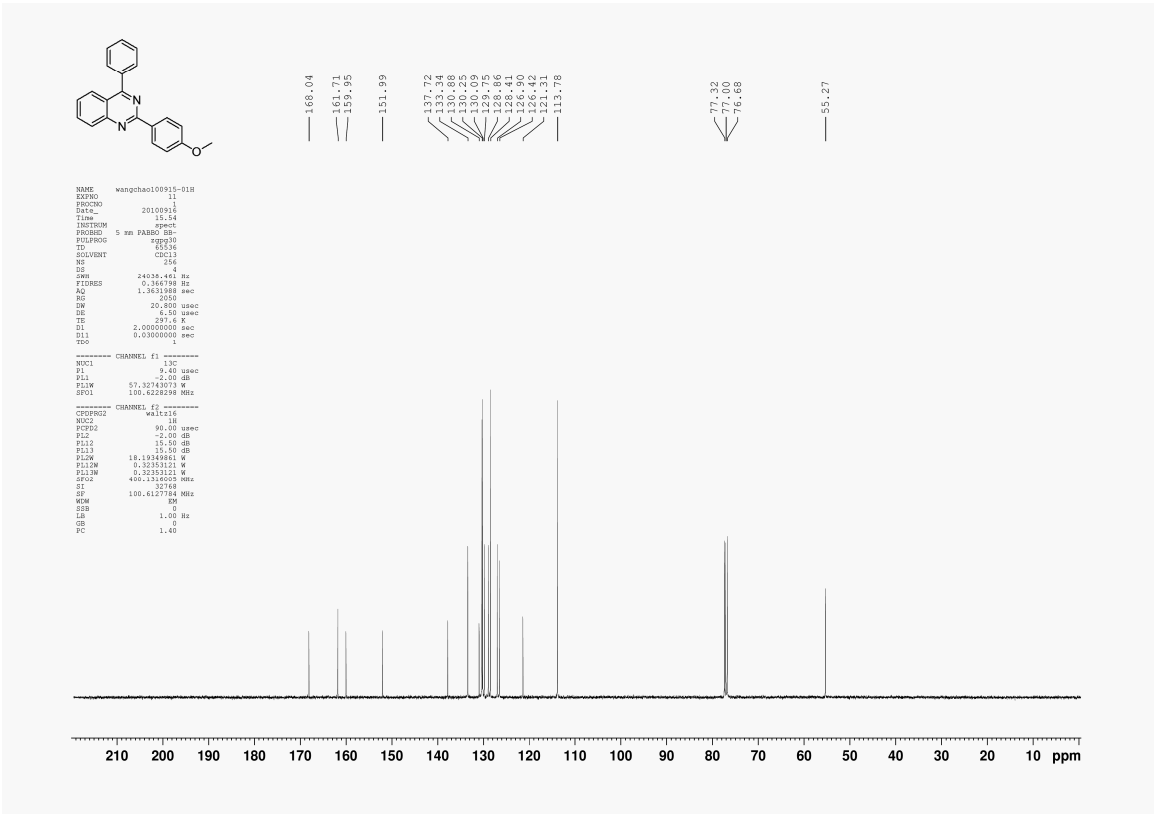

9.497
9.496
8.761
8.622
8.625
8.621
8.612
8.608
8.600
8.182
8.178
8.161
8.157
7.963
7.962
7.567
7.563
7.557
7.553
7.545
7.541
7.537
7.530
7.526
7.519
7.515
7.503
7.499
7.260
4.017
0.000
NAME wangchao101117-04H
EXPNO 10
PROCNO 1
Date_ 20101118
Time 5.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
PL1W 22.90425682 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 0.96 2.01 1.00 1.03 3.11 3.08

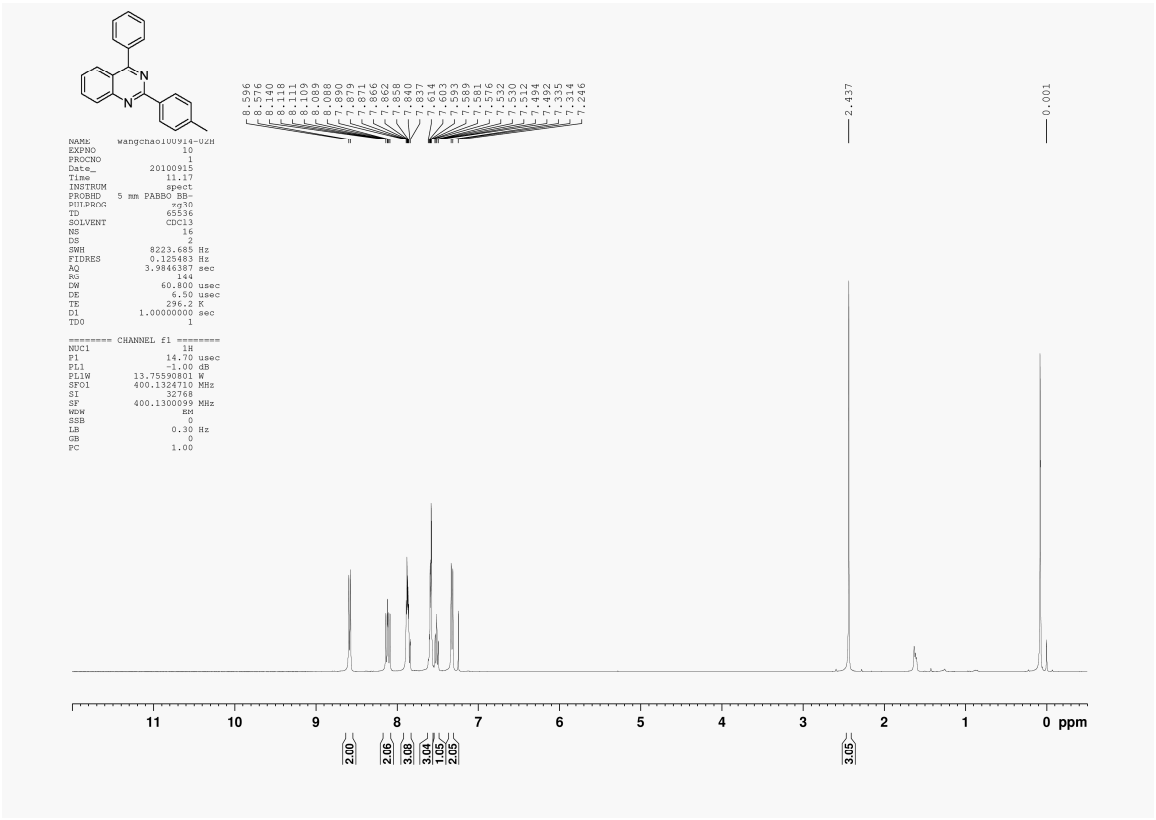

166.07
161.72
160.53
150.33
137.52
135.04
131.11
130.83
128.65
127.31
126.69
125.25
77.32
77.00
76.68
52.69
NAME wangchao101109-03C
EXPNO 11
PROCNO 1
Date_ 20101112
Time 23.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 26038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

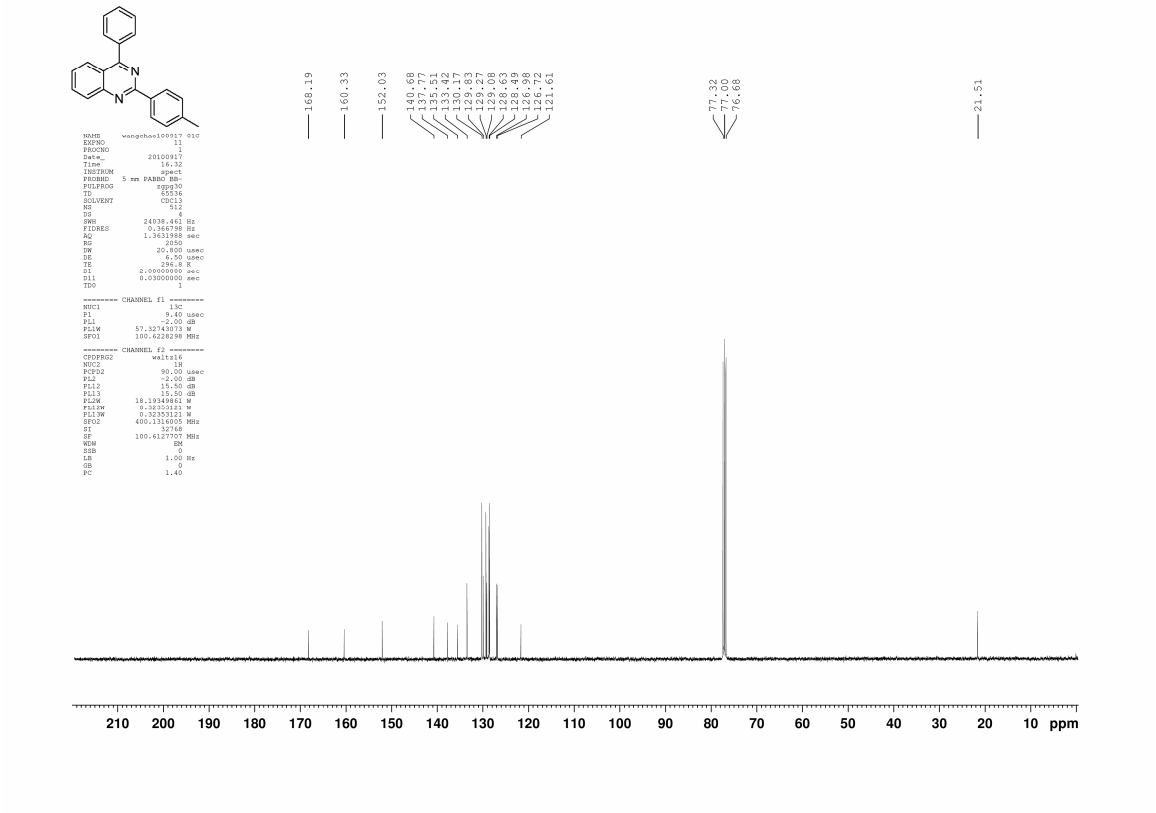

9.470
8.640
8.636
8.631
8.620
8.616
8.106
8.104
8.085
8.083
7.934
7.926
7.922
7.914
7.908
7.904
7.901
7.887
7.883
7.630
7.627
7.610
7.607
7.592
7.590
7.589
7.563
7.559
7.548
7.540
7.529
7.522
7.518
7.511
7.509
7.498
7.496
7.492
7.260
0.007
NAME wangchao100807-02H
EXPNO 10
PROCNO 1
Date_ 20100807
Time 23.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
PL1W 22.90425682 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.59
1.01
2.05
1.05
3.08

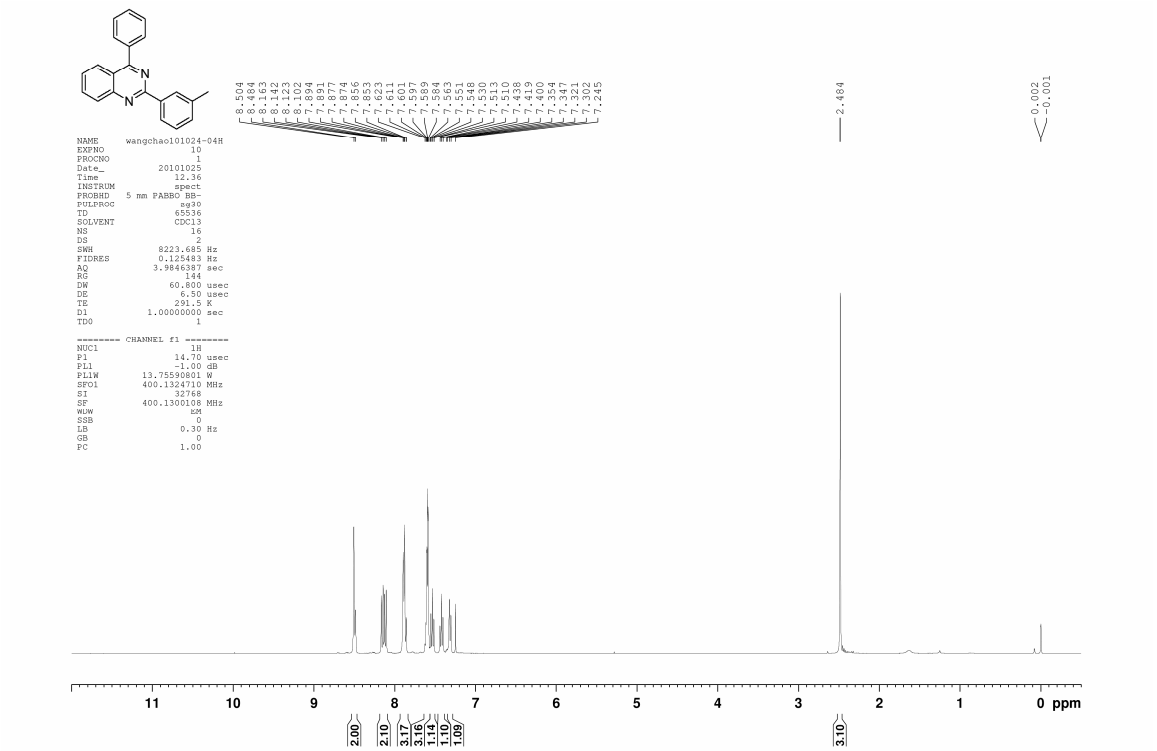

160.96
160.37
150.68
137.98
133.97
130.52
128.54
127.51
127.11
127.00
123.50
77.32
77.00
76.68
NAME wangchao100917-04C
EXPNO 11
PROCNO 1
Date_ 20100918
Time 12.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -6.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127782 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

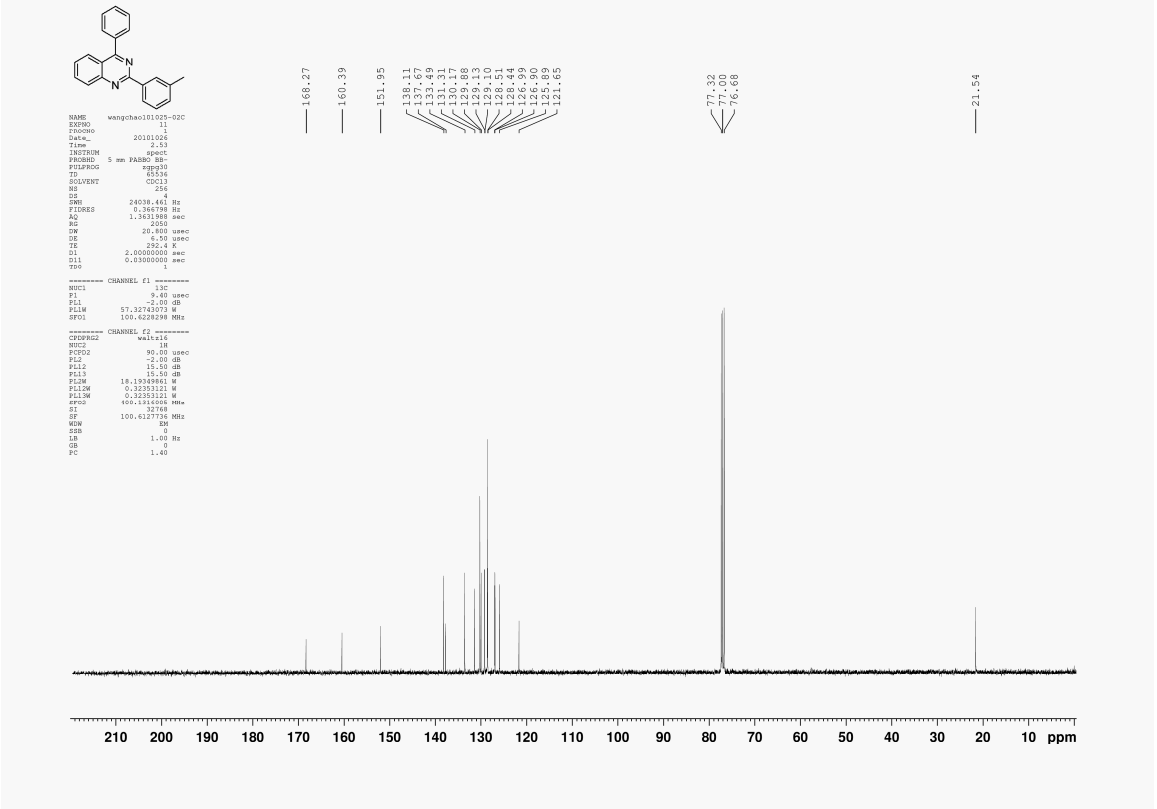

8.664
8.642
8.155
8.076
7.886
7.876
7.868
7.862
7.854
7.851
7.833
7.830
7.616
7.604
7.595
7.591
7.583
7.578
7.518
7.515
7.497
7.478
7.253
7.045
7.022
3.892
0.000
NAME wangchao100914-04H
EXPNO 10
PROCNO 1
Date_ 20100915
Time 11.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9816387 sec
RG 181
DW 60.800 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 -1.00 dB
PL1W 13.75590801 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00 2.05 3.06 3.02 1.02 2.05 3.06

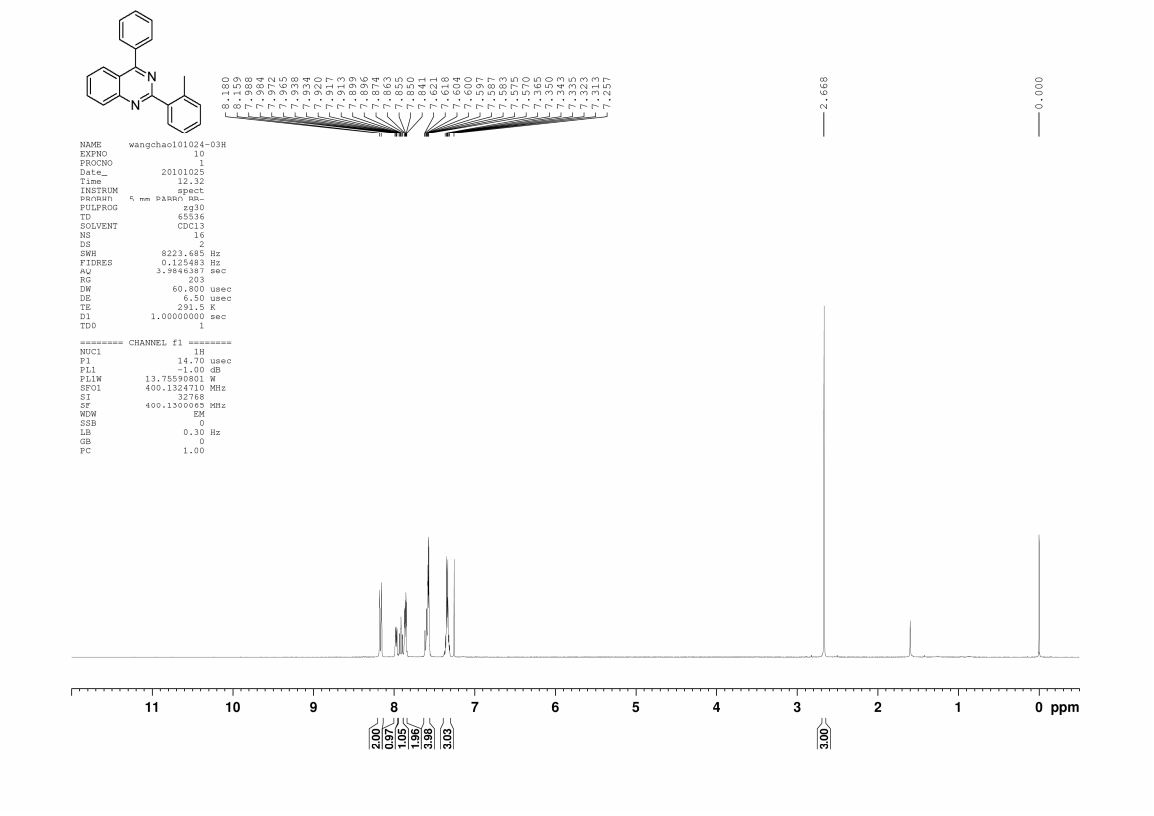

168.04
161.71
159.05
151.99
137.72
133.34
130.88
130.25
130.09
129.75
128.86
128.41
126.90
126.42
121.31
113.78
77.32
77.00
76.68
55.27
NAME wangchao100915-01H
EXPNO 11
PROCNO 1
Date_ 20100916
Time 15.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127784 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.596
8.576
8.140
8.118
8.111
8.109
8.089
8.088
7.990
7.979
7.971
7.966
7.862
7.858
7.840
7.837
7.614
7.603
7.593
7.589
7.581
7.576
7.532
7.530
7.512
7.494
7.492
7.345
7.314
7.246
2.437
0.001
11
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.06
3.08
3.04
1.05
2.05
3.05


168.19
160.33
152.03
140.68
137.77
135.51
133.42
130.17
129.83
129.27
128.08
128.03
128.49
126.98
126.72
121.61
77.32
77.00
76.68
21.51
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

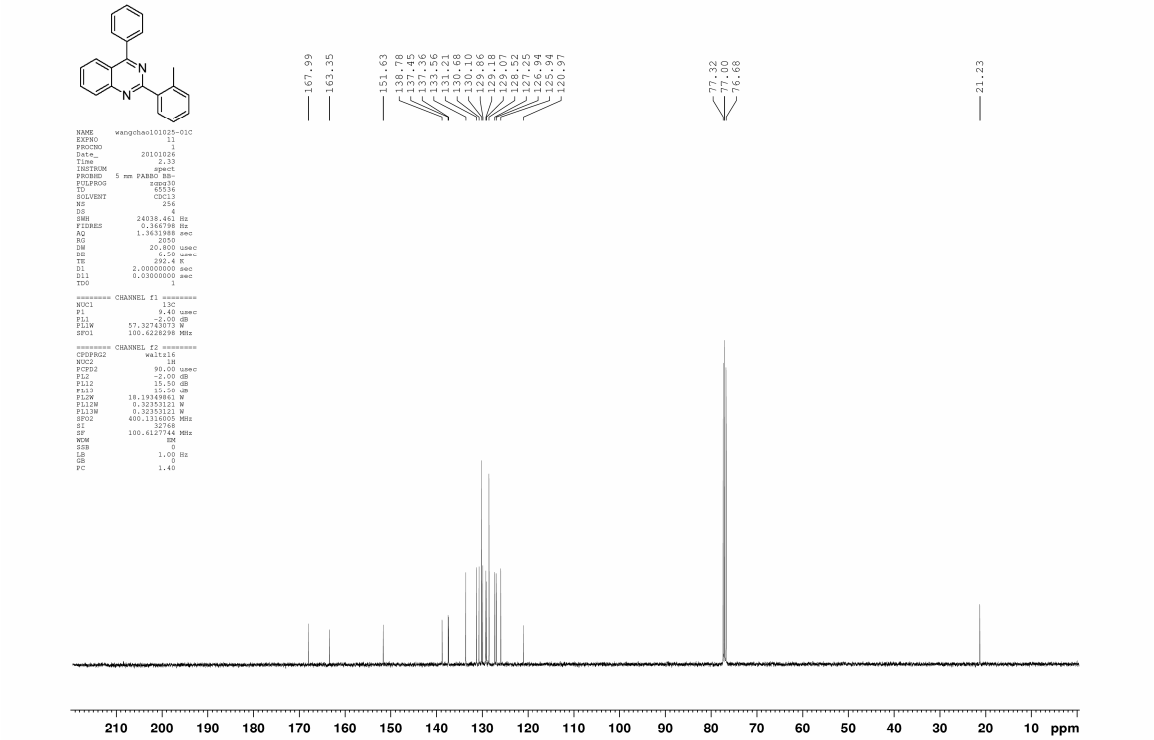

8.504
8.484
8.165
8.142
8.123
8.102
7.894
7.891
7.877
7.874
7.856
7.853
7.623
7.611
7.601
7.597
7.589
7.584
7.563
7.551
7.548
7.530
7.513
7.510
7.438
7.419
7.400
7.354
7.347
7.321
7.302
7.245
2.464
0.002
-0.001
11
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.10
3.17
3.16
1.14
1.10
1.09
3.10


168.27
160.39
151.95
138.11
137.67
133.49
131.31
130.17
129.88
129.13
128.10
128.51
128.44
126.99
126.90
121.89
121.65
77.32
77.00
76.68
21.54
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm



NAME wangchao101024-03H
EXPNO 10
PROCNO 1
Date_ 20101025
Time 12.32
INSTRUM spect
PROBHD 5 mm PABBO BA-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 291.5 K
D1 1.00000000 sec
TD0 1

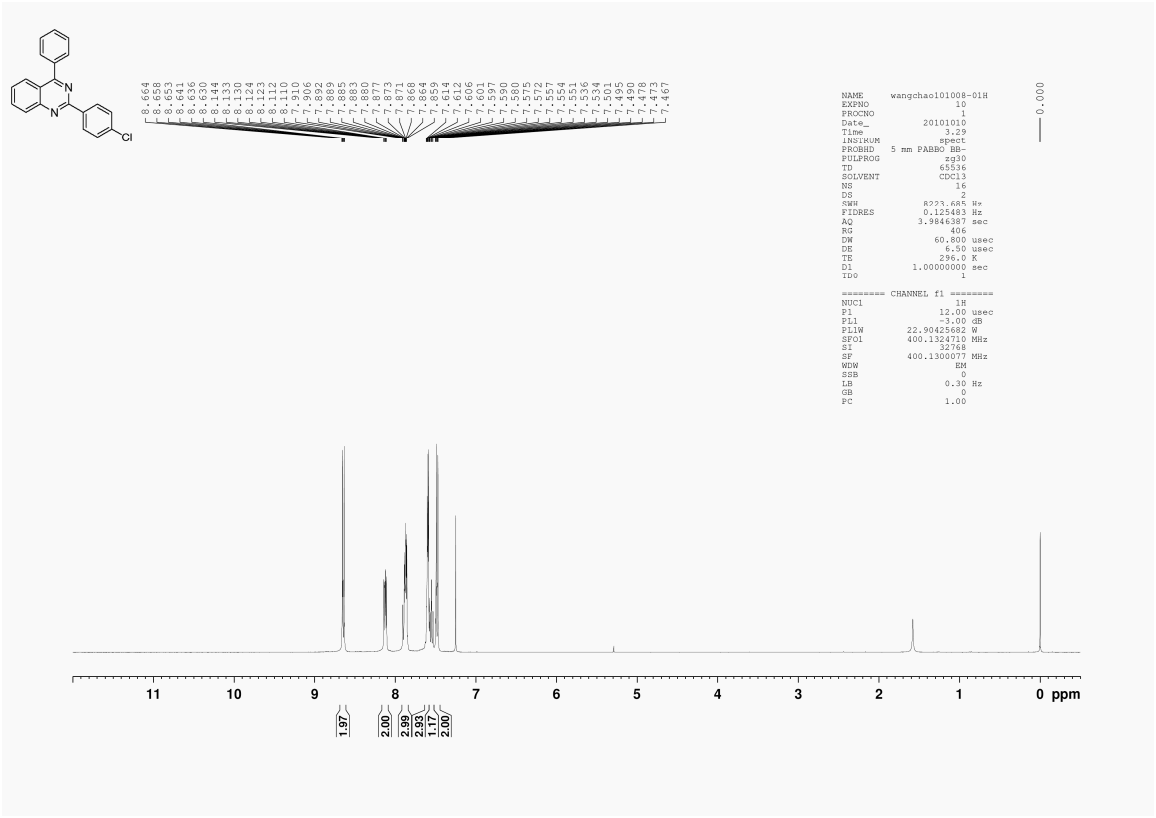
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 -1.00 dB
PL1W 13.75590801 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

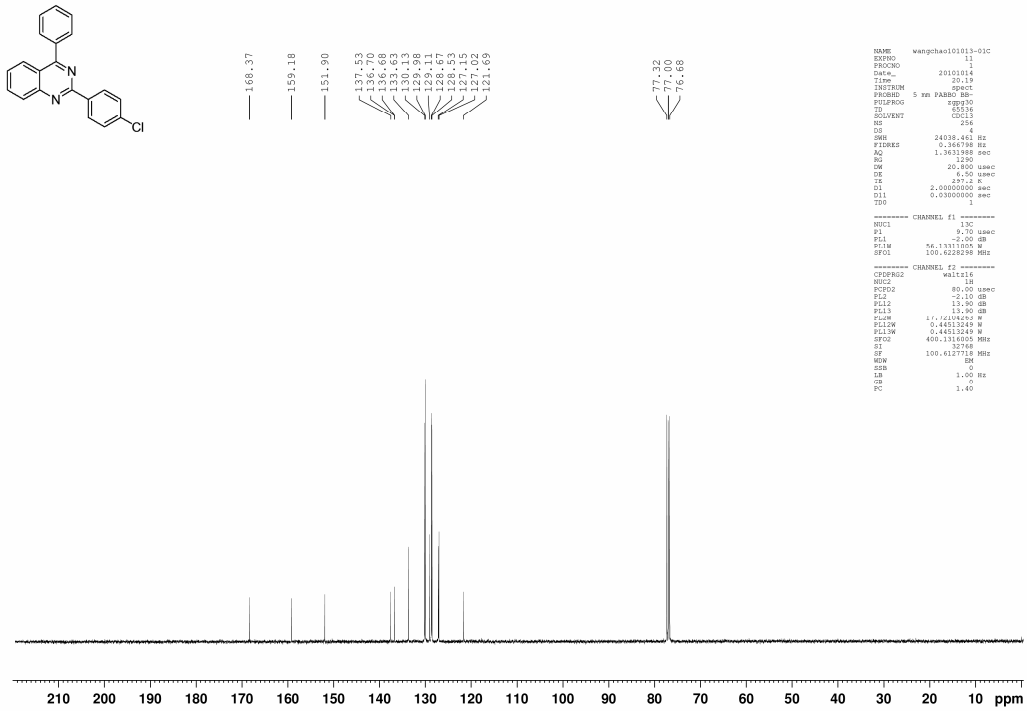


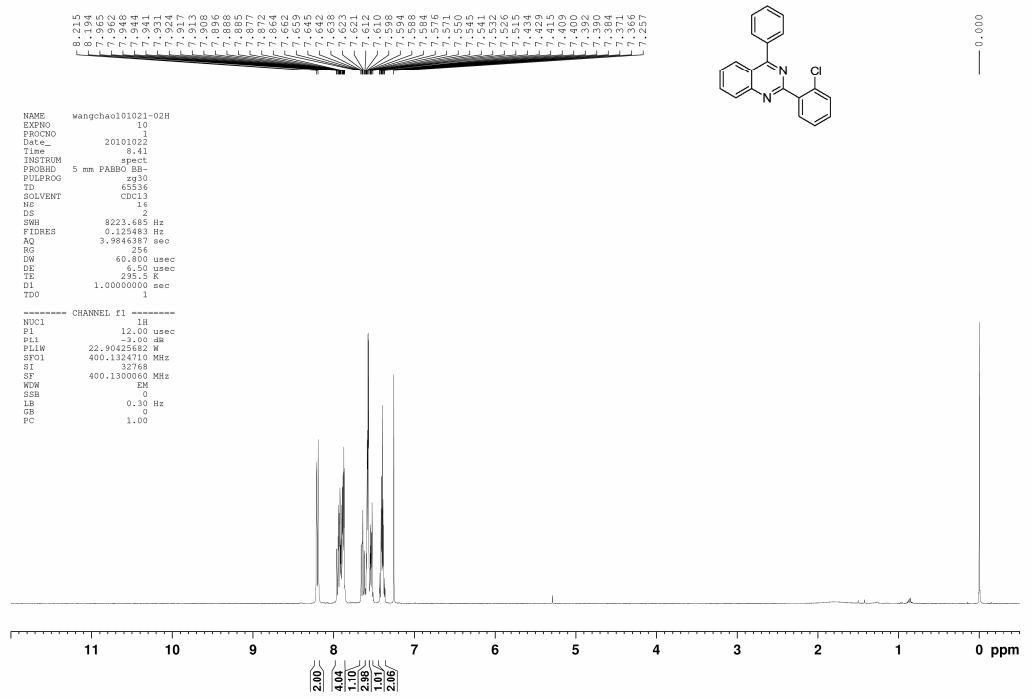
NAME wangchao101025-01C
EXPNO 11
PROCNO 1
Date_ 20101026
Time 2.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 292.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

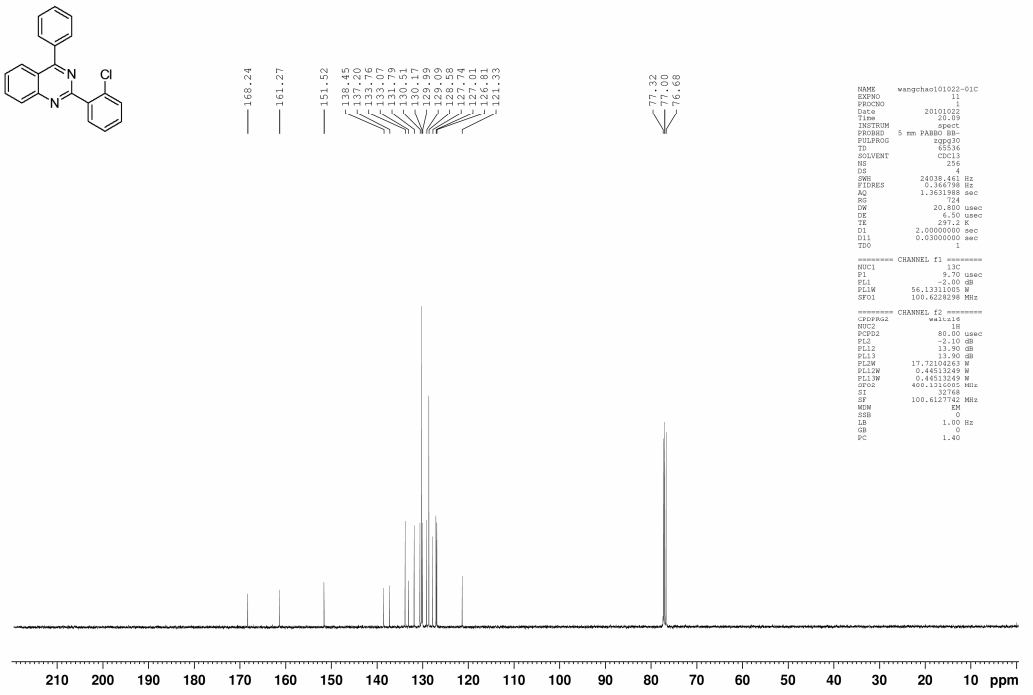
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz

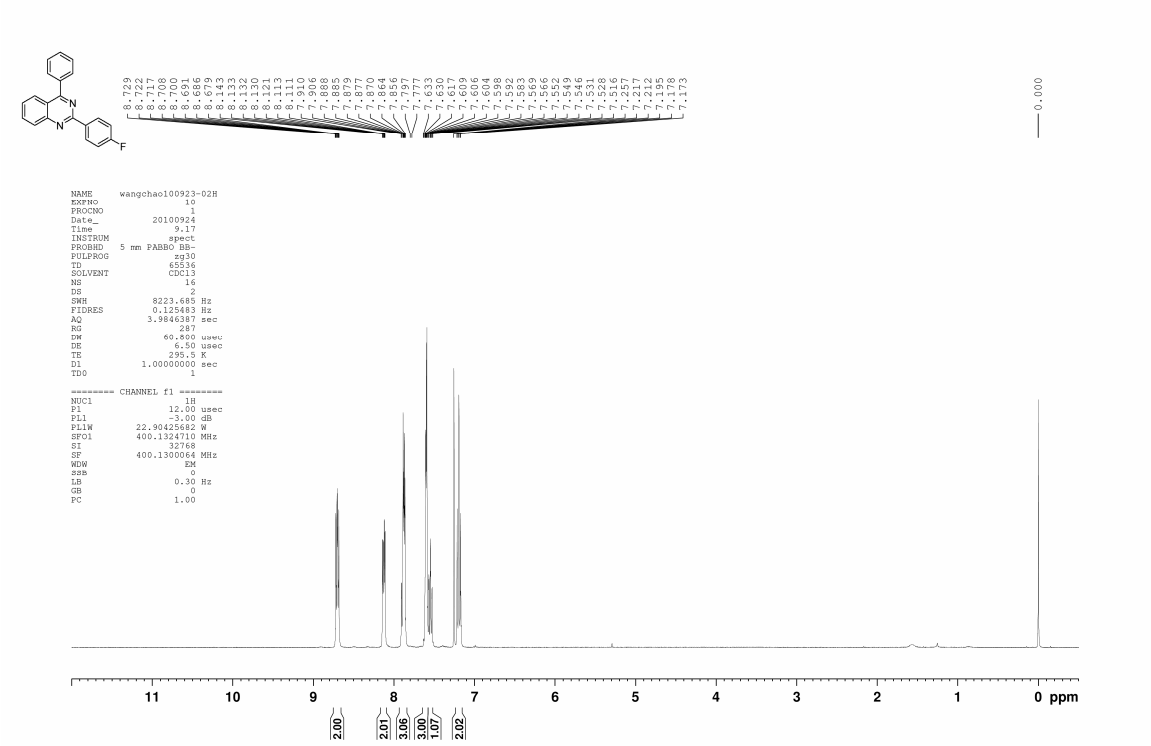
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127744 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

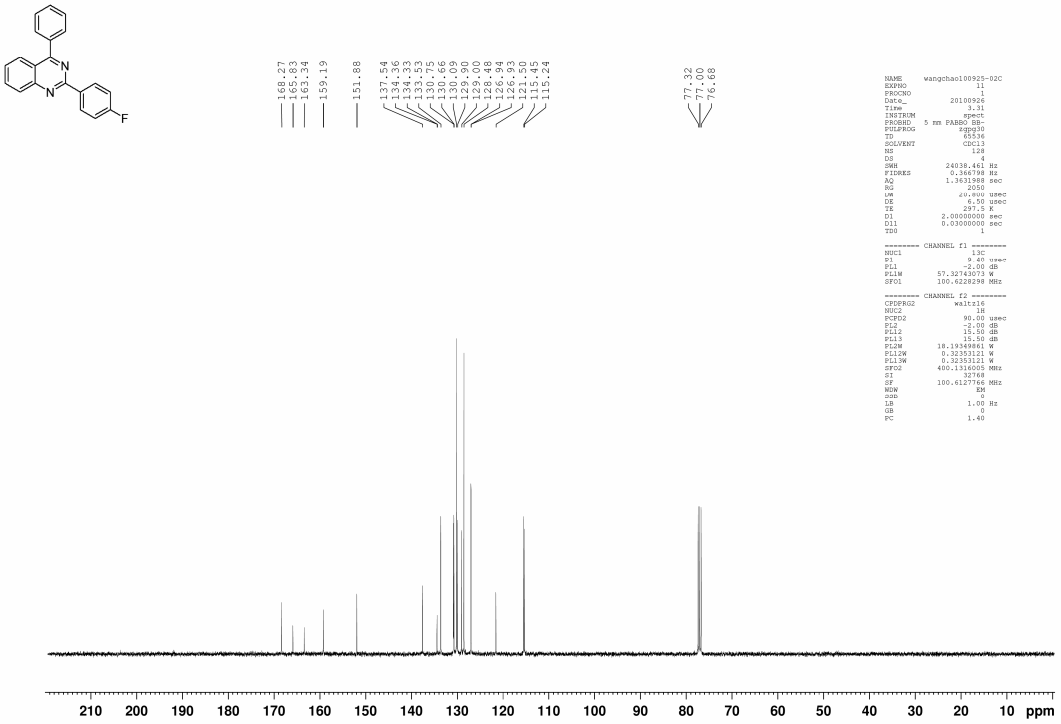

8.664
8.658
8.653
8.641
8.636
8.630
8.144
8.133
8.130
8.124
8.123
8.112
8.110
7.910
7.906
7.892
7.889
7.885
7.883
7.880
7.877
7.873
7.871
7.868
7.864
7.859
7.614
7.612
7.606
7.601
7.597
7.580
7.580
7.575
7.572
7.557
7.554
7.551
7.536
7.534
7.501
7.495
7.490
7.478
7.473
7.467
NAME wangchao101008-01H
EXPNO 10
PROCNO 1
Date_ 20101010
Time 3.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 406
DW 60.800 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
PL1W 22.90425682 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0.000
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.97
2.00
2.99
2.83
1.17
2.00

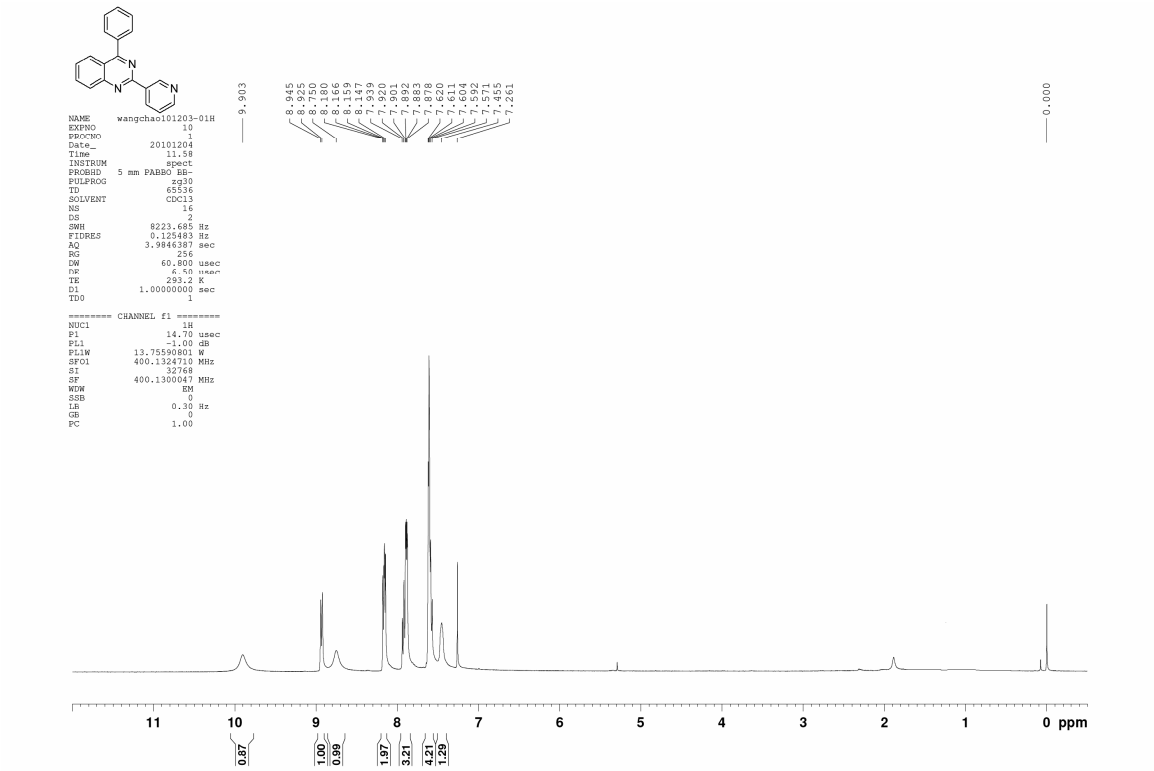

168.37
159.18
151.90
137.53
136.70
136.68
133.63
130.13
130.08
129.11
128.67
128.53
127.15
127.02
121.09
77.32
77.00
76.68
NAME wangchao101013-01C
EXPNO 11
PROCNO 1
Date_ 20101014
Time 20.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 1290
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.10 dB
PL12 13.90 dB
PL13 13.90 dB
PL2W 17.72104263 W
PL12W 0.44513249 W
PL13W 0.44513249 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127718 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

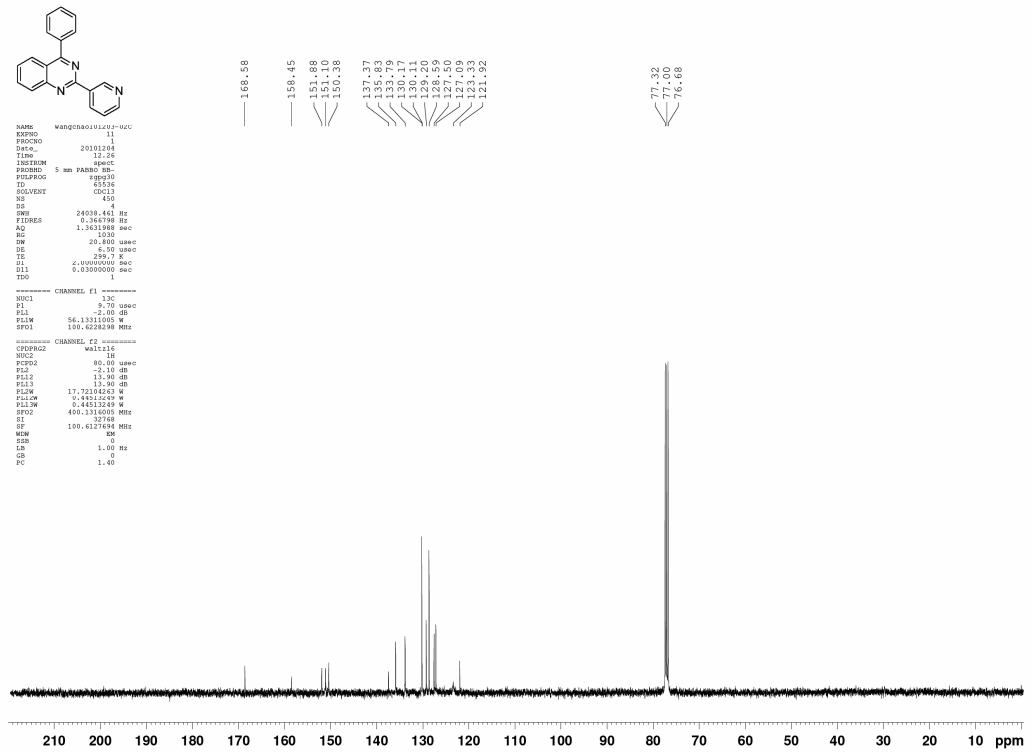

8.215
8.194
7.965
7.962
7.948
7.944
7.941
7.931
7.924
7.917
7.913
7.908
7.896
7.888
7.885
7.877
7.872
7.864
7.662
7.659
7.645
7.642
7.638
7.633
7.621
7.612
7.610
7.598
7.594
7.588
7.584
7.576
7.571
7.550
7.545
7.541
7.532
7.526
7.515
7.434
7.429
7.415
7.409
7.400
7.392
7.390
7.384
7.371
7.366
7.257
0.000
Cl
N
N
NAME wangchao101021-02H
EXPNO 10
PROCNO 1
Date_ 20101022
Time 8.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
PLW 22.90425682 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
4.04
1.10
2.98
1.01
2.06

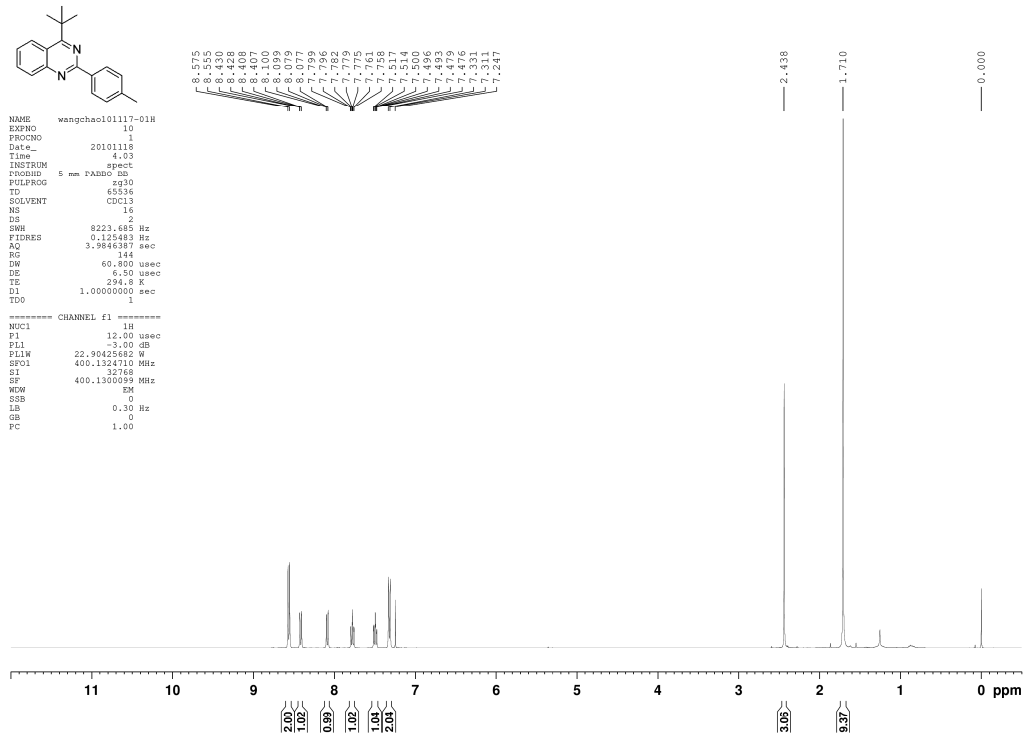

N
N
Cl
168.24
161.27
151.52
138.45
137.20
133.76
133.07
131.79
130.51
130.17
129.99
129.09
128.58
127.74
127.01
125.81
121.33
77.32
77.00
76.68
NAME wangchao101022-01C
EXPNO 11
PROCNO 1
Date 20101022
Time 20.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 724
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -2.00 dB
PLW 56.13311005 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.10 dB
PL12 13.90 dB
PL13 13.90 dB
PL2W 17.72104263 W
PL12W 0.44513249 W
PL13W 0.44513249 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127742 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

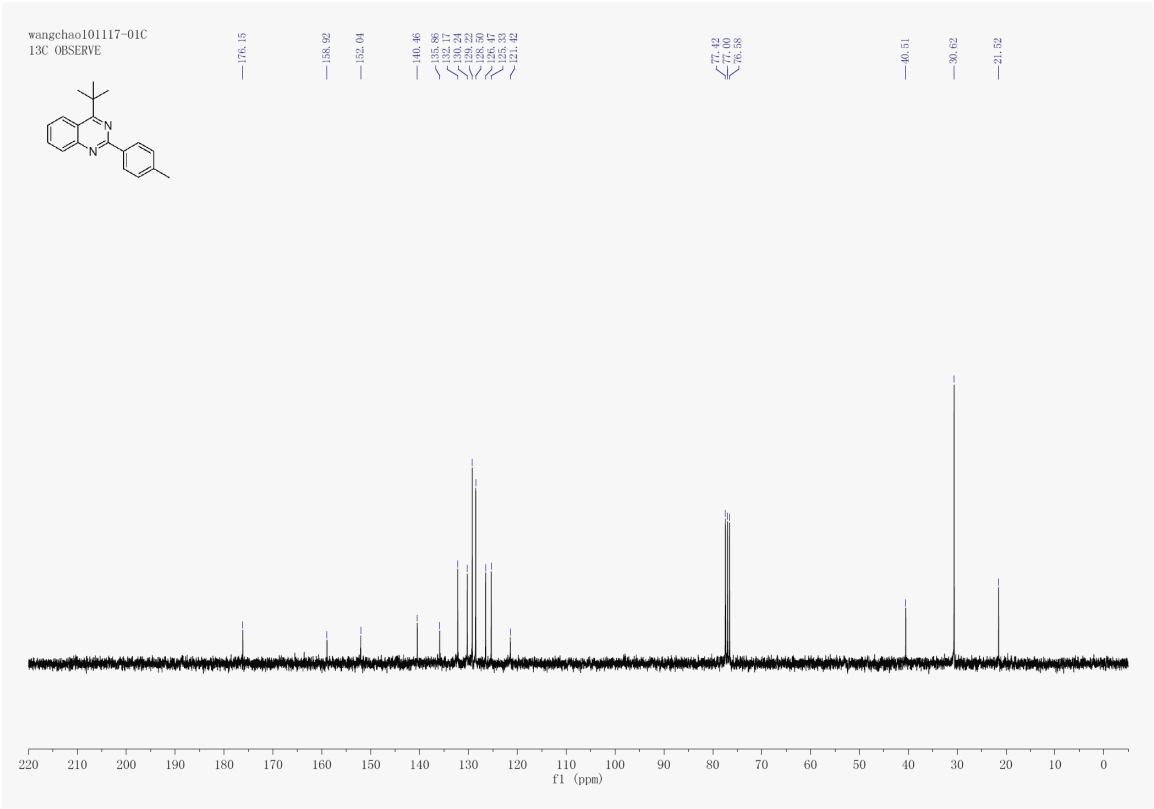

8.729
8.722
8.717
8.708
8.700
8.691
8.686
8.679
8.143
8.133
8.132
8.130
8.121
8.113
8.111
7.910
7.906
7.888
7.885
7.879
7.877
7.870
7.864
7.856
7.837
7.777
7.633
7.630
7.617
7.609
7.606
7.604
7.598
7.592
7.583
7.569
7.566
7.552
7.549
7.546
7.531
7.528
7.516
7.257
7.217
7.212
7.195
7.178
7.173
0.000
NAME wangchao100923-02H
EXPNO 10
PROCNO 1
Date_ 20100924
Time 9.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
PL1W 22.90425682 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00 2.01 3.06 3.00 1.07 2.02

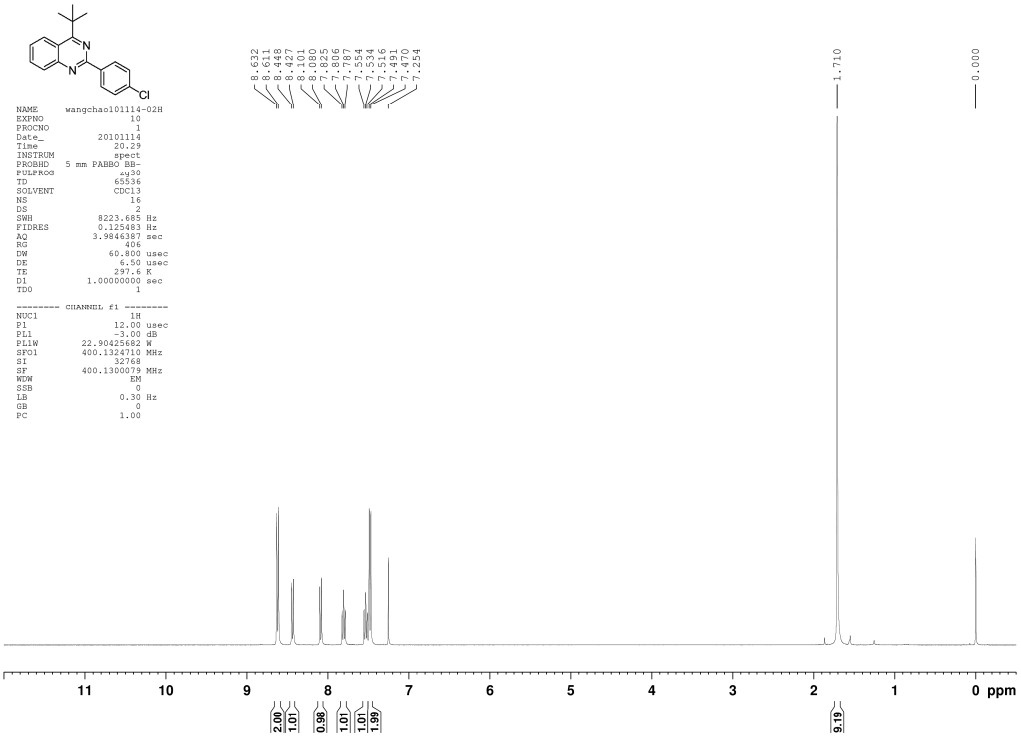

168.27
165.83
163.34
159.19
151.88
137.54
134.36
134.33
133.53
130.75
130.66
130.09
129.90
129.00
128.48
126.94
126.93
121.50
115.45
115.24
77.32
77.00
76.68
NAME wangchao100925-02C
EXPNO 11
PROCNO 1
Date_ 20100926
Time 3.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127766 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


9.903
8.945
8.925
8.750
8.180
8.166
8.159
8.147
7.939
7.920
7.901
7.883
7.878
7.620
7.611
7.604
7.552
7.571
7.455
7.261
0.000
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.87
1.00
0.99
1.97
3.21
4.21
1.29

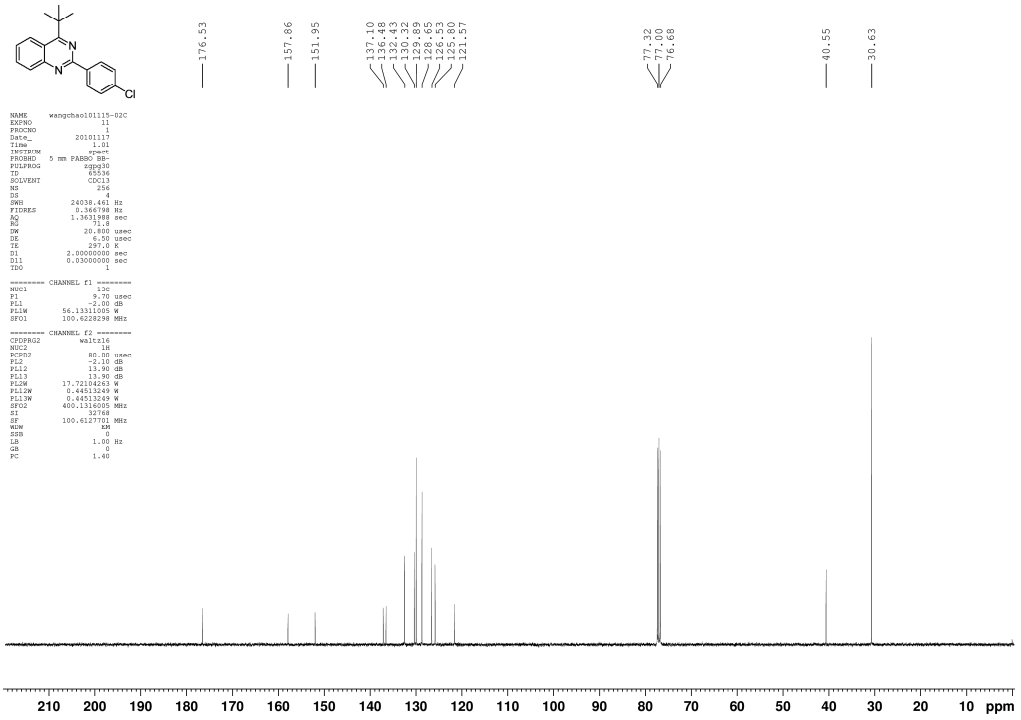

168.58
158.45
151.88
151.10
150.38
137.37
135.83
133.79
130.17
130.11
129.20
128.59
127.50
127.09
123.33
121.92
77.32
77.00
76.68
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


8.575
8.555
8.430
8.428
8.408
8.407
8.100
8.099
8.077
7.799
7.796
7.782
7.779
7.775
7.761
7.758
7.517
7.514
7.500
7.496
7.493
7.479
7.476
7.331
7.311
7.247
2.438
1.710
0.000
11
10
9
8
7
6
5
4
3
2
1
0 ppm
2.03
1.02
0.99
1.02
1.04
2.04
3.05
9.37

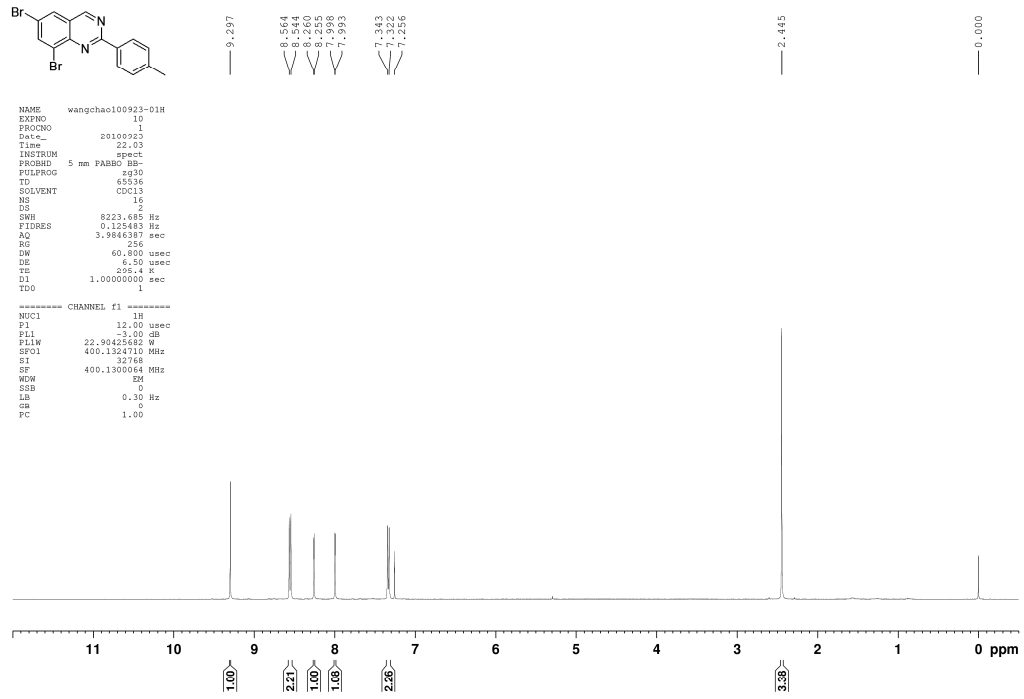

wangchao101117-01C
13C OBSERVE
176.15
158.92
152.04
140.46
135.88
132.17
130.24
129.22
128.50
126.47
125.33
121.42
77.42
77.00
76.58
40.51
30.62
21.52
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

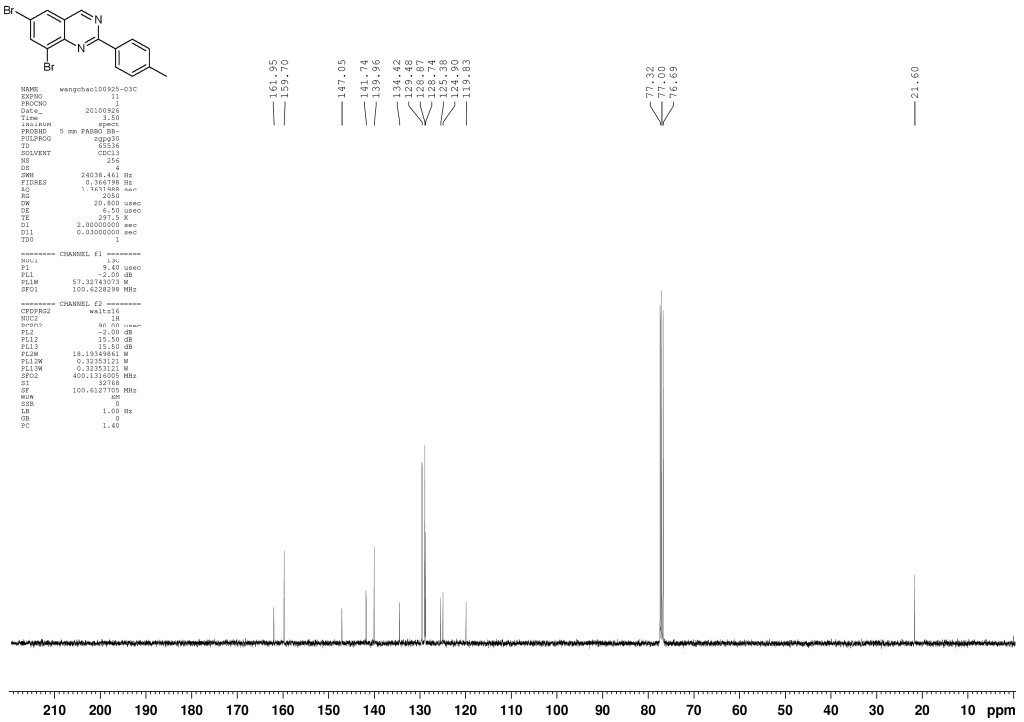


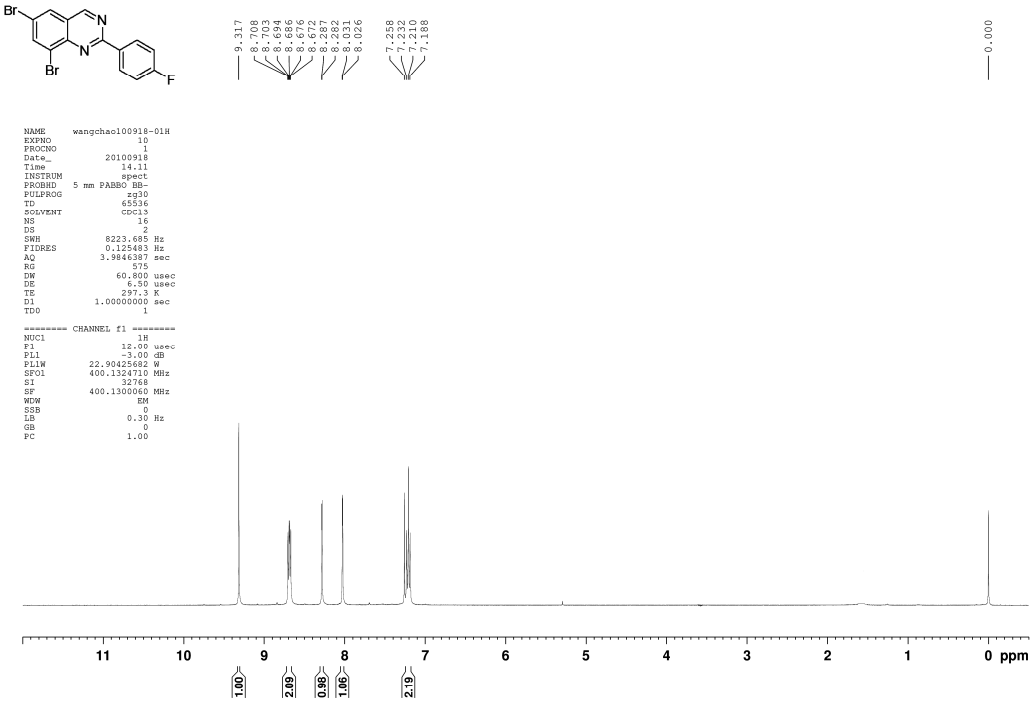

```
NAME          wangchao101114-02H
EXPNO                         10
PROCNO                         1
Date_                   20101114
Time                       20.29
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8223.685 Hz
FIDRES                 0.125483 Hz
AQ                     3.9846387 sec
RG                          406
DW                       60.800 usec
DE                        6.50 usec
TE                       297.6 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       12.00 usec
PL1                       -3.00 dB
PLW1                22.90425682 W
SFO1                400.1324710 MHz
SI                         32768
SF                  400.1300079 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
```

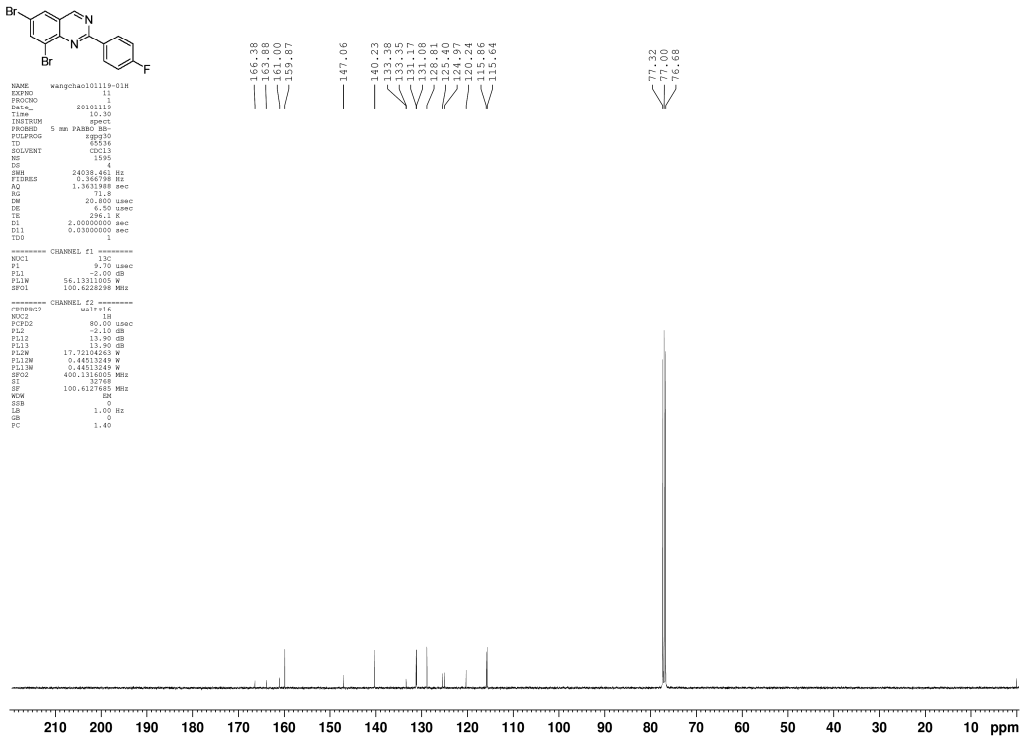


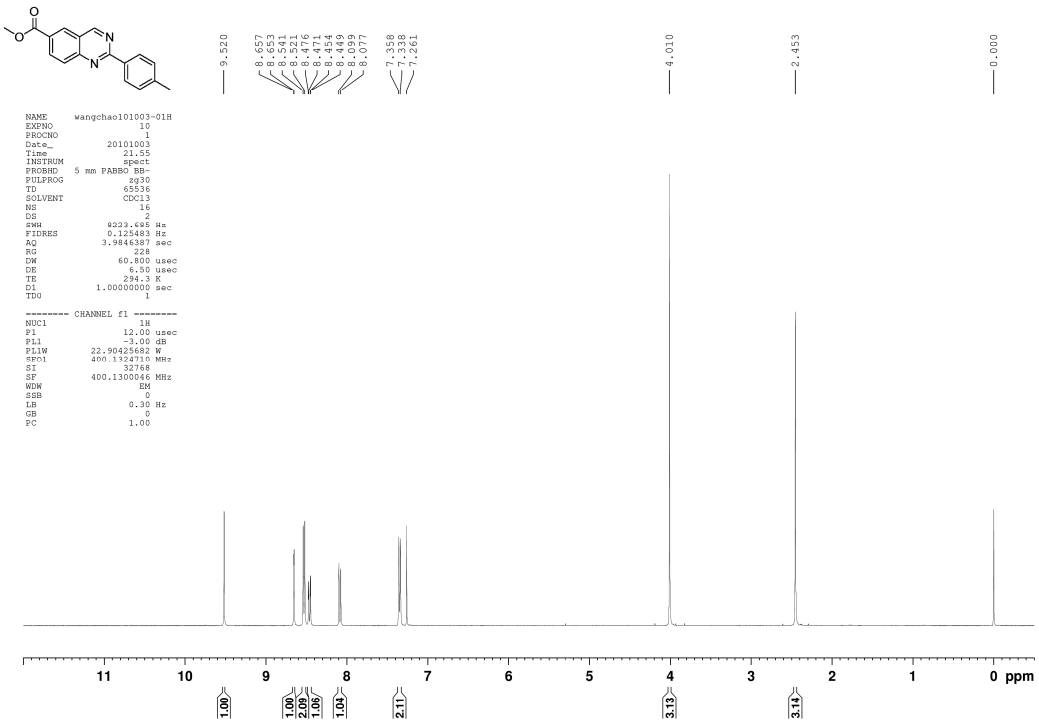

```
NAME          wangchao101115-02C
EXPNO                         11
PROCNO                         1
Date_                   20101117
Time                       11.01
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                          256
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.366798 Hz
AQ                     1.3631988 sec
RG                          181.8
DW                       20.800 usec
DE                        6.50 usec
TE                       297.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         13C
P1                        9.70 usec
PL1                      -2.00 dB
PLW1                56.13311005 W
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                    80.00 usec
PL2                      -2.10 dB
PL12                     13.90 dB
PL13                     13.90 dB
PL2W                17.72104263 W
PL12W                0.44513249 W
PL13W                0.44513249 W
SFO2                400.1316005 MHz
SI                         32768
SF                  100.6127701 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```

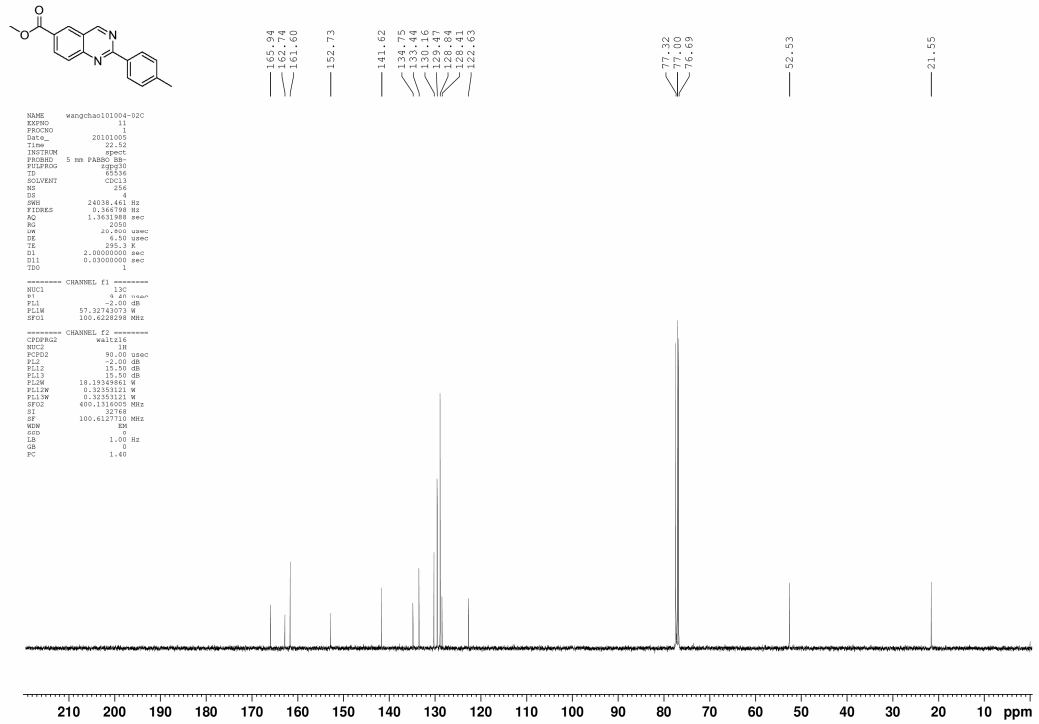

Br
N
N
Br
9.297
8.564
8.544
8.260
8.255
7.998
7.993
7.343
7.322
7.256
2.445
0.000
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
2.21
1.00
1.08
2.26
3.38


Br
N
N
Br
161.95
159.70
147.05
141.74
139.96
134.42
129.48
128.07
128.74
125.38
114.00
119.83
77.32
77.00
76.69
21.60
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


Br
N
N
Br
F
9.317
8.708
8.703
8.694
8.686
8.676
8.672
8.267
8.262
8.031
8.026
7.258
7.232
7.210
7.188
0.000
NAME wangchao100918-01H
EXPNO 10
PROCNO 1
Date_ 20100918
Time 14.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 575
DW 60.800 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
PL1W 22.90425682 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 2.09 0.98 1.06 2.19


Br
N
N
Br
F
166.38
163.88
161.00
159.87
147.06
140.23
133.38
133.35
131.17
131.08
128.81
125.40
124.97
120.24
115.86
115.64
77.32
77.00
76.68
NAME wangchao101119-01H
EXPNO 11
PROCNO 1
Date_ 20101119
Time 10.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1595
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 71.8
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 80.00 usec
PL2 -2.10 dB
PL12 13.90 dB
PL13 13.90 dB
PL2W 17.72104263 W
PL12W 0.44513249 W
PL13W 0.44513249 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


9.520
8.657
8.653
8.541
8.521
8.476
8.471
8.454
8.449
8.099
8.077
7.358
7.338
7.261
4.010
2.453
0.000
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.00
2.09
1.06
1.04
2.11
3.13
3.14


165.94
162.74
161.60
152.73
141.62
134.75
133.44
130.16
129.47
128.84
128.41
122.63
77.32
77.00
76.69
52.53
21.55
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm