Metal-free oxidative synthesis of quinazolinones via dual amination of sp^3 C–H bonds

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Electronic Supplementary Information

Content

General information

Unless otherwise indicated, all compounds and reagents were purchased from commercial suppliers and used without further purification. Melting points were measured with an X-4 melting point apparatus (Bei Jing Taike Co., Ltd.) and were uncorrected. ^{1}H-NMR and ^{13}C-NMR were recorded on a Bruker DPX 300 MHz or a Bruker AVANCE III 400 MHz spectrometer, respectively. 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).

General procedure for the synthesis of products

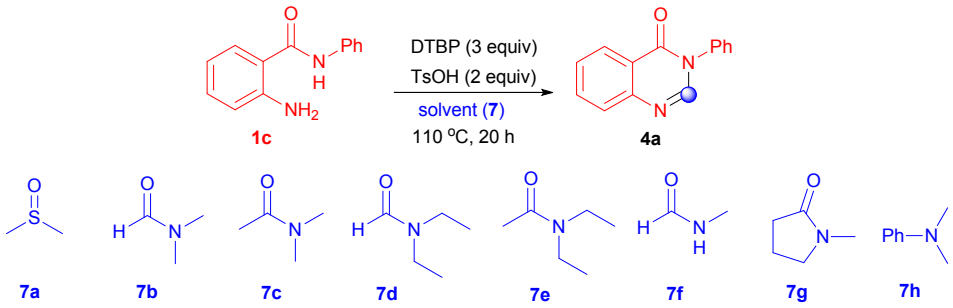
1. Synthesis of products 3

A mixture of 2-aminobenzamide **1** (or 2-aminobenzenesulfonamide, 0.3 mmol), TsOH (103 mg, 0.6 mmol), DTBP (165 μL, 0.9 mmol) and 2 mL methylarene **2** (for 2-methylnaphthalene, 2g was added) in 2 mL DMSO was stirred in a Schlenk tube at 110 °C. After stirring for 20 h, the reaction mixture was cooled to the room temperature, and diluted with ethyl acetate. The organic phase was washed with brine, dried over anhydrous Na_2SO_4, concentrated in vacuo and then purified by flash column chromatography on silica gel to afford the desired product **3**.

2. Synthesis of products 4

A mixture of 2-aminobenzamide **1** (0.3 mmol), TsOH (103 mg, 0.6 mmol), DTBP (165 μL, 0.9 mmol) in 2 mL DMA was stirred in a Schlenk tube at 110 °C. After stirring for 20 h, the reaction mixture was cooled to the room temperature, and diluted with ethyl acetate. The organic phase was washed with brine, dried over anhydrous Na_2SO_4, concentrated in vacuo and then purified by flash column chromatography on silica gel to afford the desired product **4**.

3. Optimization of reaction conditions for quinazolinones using solvent as carbon source (Table S1)[a]

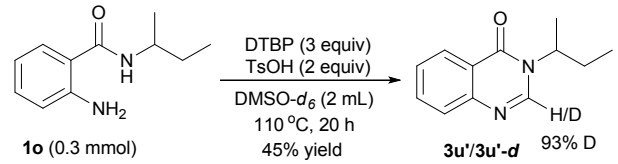


Entry	Solvent (**7**)	Yield (%)[b]
1	**7a**	24
2	**7b**	60
3	**7c**	**72**
4	**7d**	Nd.
5	**7e**	Nd.
6	**7f**	72
7	**7g**	16
8	**7h**	Nd.

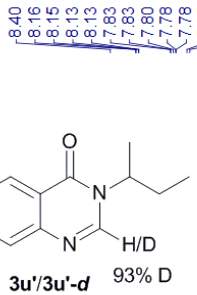
[a] Reaction conditions: **1c** (0.3 mmol), DTBP (0.9 mmol), TsOH (0.6 mmol), solvent **7** (2 mL), 110 °C, 20 h. [b] Isolated yield. Nd. = Not detected.

4. The ^{2}H-DMSO labeled experiment:

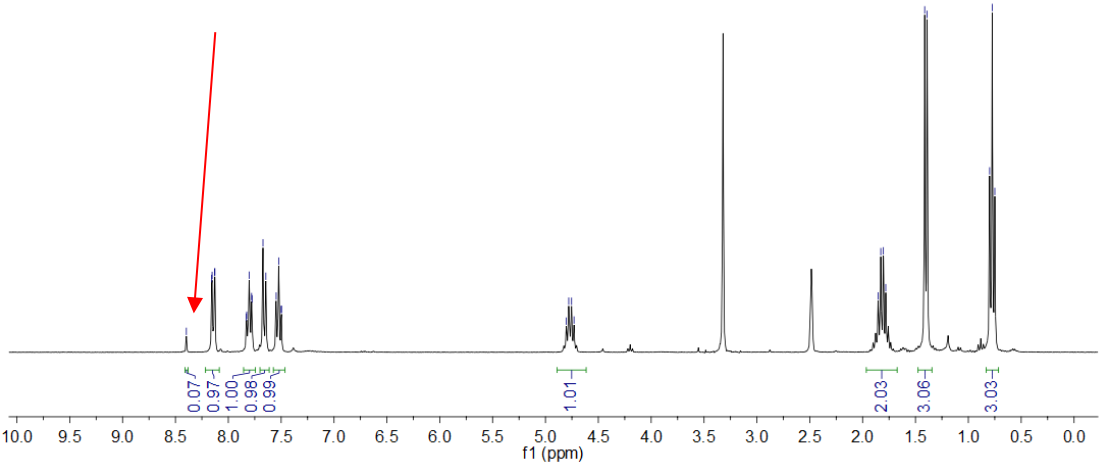
The below D-labeling experiment proved that the additional carbon atom in **3u'** was derived from DMSO.



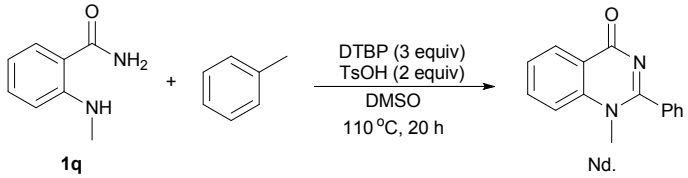
1o (0.3 mmol) **3u'/3u'-*d***



3u'/3u'-*d* 93% D

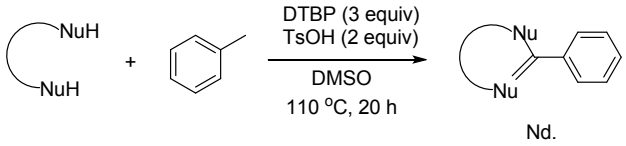


5. The failure examples:

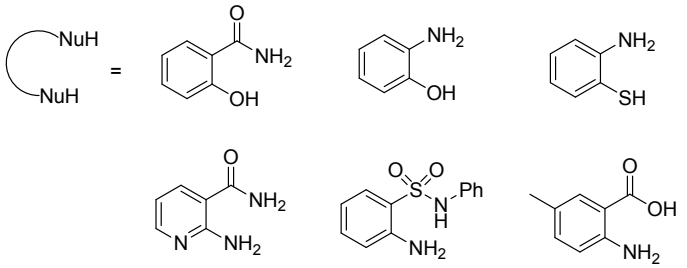


1q Nd.

We tested 2-(methylamino)benzamide (**1q**), but the desired product was not detected which indicated the sterically demanding *N*-methyl substituent inhibited the cyclization.

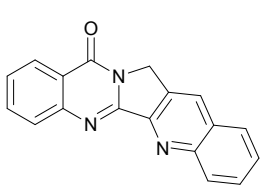


Nd.

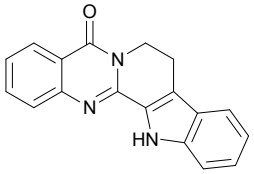


5% yield

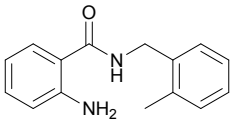
We investigated some substrates as shown above, but didn't obtain the corresponding products. However, 2-(aminomethyl)aniline could be converted to 2-phenylquinazoline in 5% yield with some unknown byproducts. We also tried the reaction of 2-aminobenzamide and ethylbenzene under standard conditions, but no aminated product was detected.



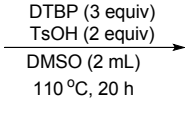
Luotonin A

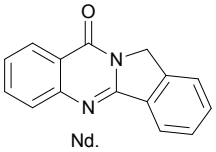


Rutaecarpine

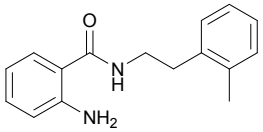


1r

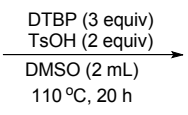


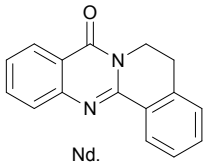


Nd.



1s

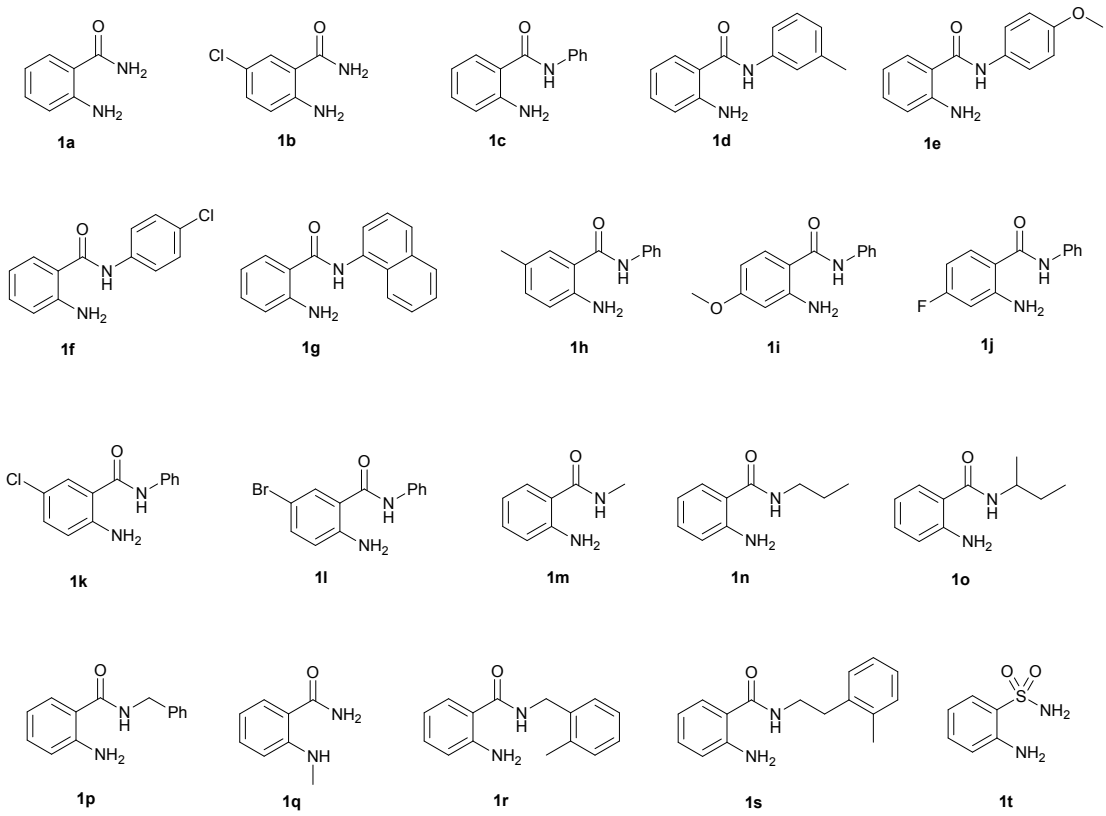




Nd.

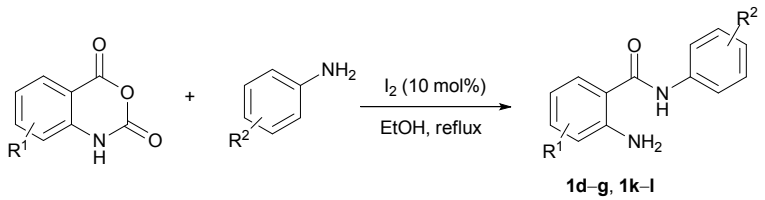
Luotonin A and Rutaecarpine are natural products containing the quinazolinone skeleton. Therefore, we tried to synthesize the analogous fused four-membered rings via intramolecular annulations, but we didn't obtain the corresponding products.

General procedure for the synthesis of substrates



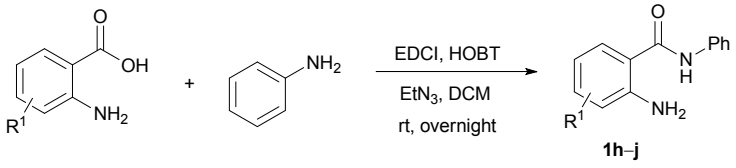
Substrates **1a**–**c**, **1m**, **1o**, **1t** are commercially available.

Synthesis of **1d**–**g**, **1k**–**l**[1]



Isatoic anhydride (5 mmol), aniline (5 mmol), and iodine (127 mg, 0.5 mmol) were added to EtOH (10 mL) and the mixture was heated at reflux in air. The progress of the reaction was monitored by TLC. Upon completion, the solvent was distilled off and the residue was diluted with EtOAc. The mixture was quenched by saturated $Na_2S_2O_3$ solution and then washed by brine. The organic layer was dried over anhydrous Na_2SO_4, concentrated and then purified by flash column chromatography on silica gel to afford the desired substrate.

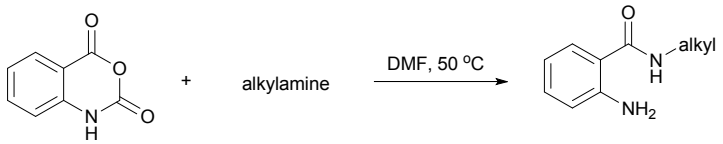
Synthesis of **1h**–**j**



2-Aminobenzoic acid (5 mmol), aniline (450 μL, 5 mmol), EDCI (1.06 g, 5.5 mmol), HOBT (0.74 g, 5.5 mmol) and EtN_3 (1.7 mL, 12.5 mmol) were added to DCM (25 mL) and the mixture was stirred at room temperature overnight. Upon completion, the solution was washed by saturated NH_4Cl solution.

The organic layer was dried over anhydrous Na_2SO_4, concentrated and then purified by flash column chromatography on silica gel to afford the desired substrate.

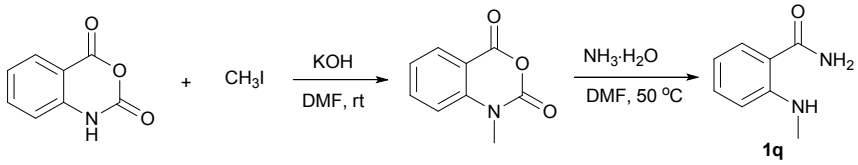
Synthesis of **1n**, **1p**, **1r–s**



1n, **1p**, **1r–s**

Isatoic anhydride (815 mg, 5 mmol) and alkylamine (5 mmol) were added to DMF (25 mL) and the mixture was stirred at 50 °C in air for 3 h. Upon completion, the solution was diluted with EtOAc, and then washed by brine. The organic layer was dried over anhydrous Na_2SO_4, concentrated and then purified by flash column chromatography on silica gel to afford the desired substrate.

Synthesis of **1q**

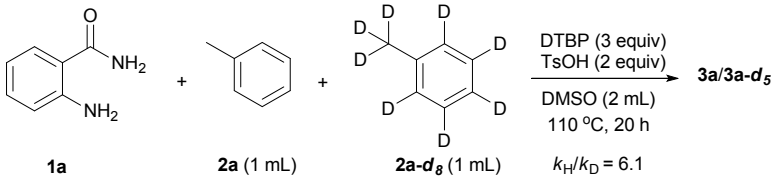


1q

Isatoic anhydride (1.63 g, 10 mmol), KOH (0.67 g, 12 mmol) and DMF (25 mL) were added to a Schlenk tube and then CH_3I (1.3 mL, 20 mmol) was added dropwise. The mixture was stirred at room temperature overnight. The solution was diluted with ethyl acetate, washed with diluted hydrochloric acid, saturated $NaHCO_3$, brine, and dried over anhydrous Na_2SO_4. The organic phase was concentrated in vacuo and then purified by flash column chromatography on silica gel to afford the methyl-substituted isatoic anhydride in 46% yield. The obtained intermediate (885mg, 5 mmol), 25% ammonia water (10 mL) and DMF (20 mL) were added to a Schlenk tube, heated at 50 °C for 30 min. The solution was then cooled to room temperature, diluted with ethyl acetate, washed with saturated NH_4Cl solution. The organic layer was dried over anhydrous Na_2SO_4, concentrated and then purified by flash column chromatography on silica gel to afford the desired substrate.

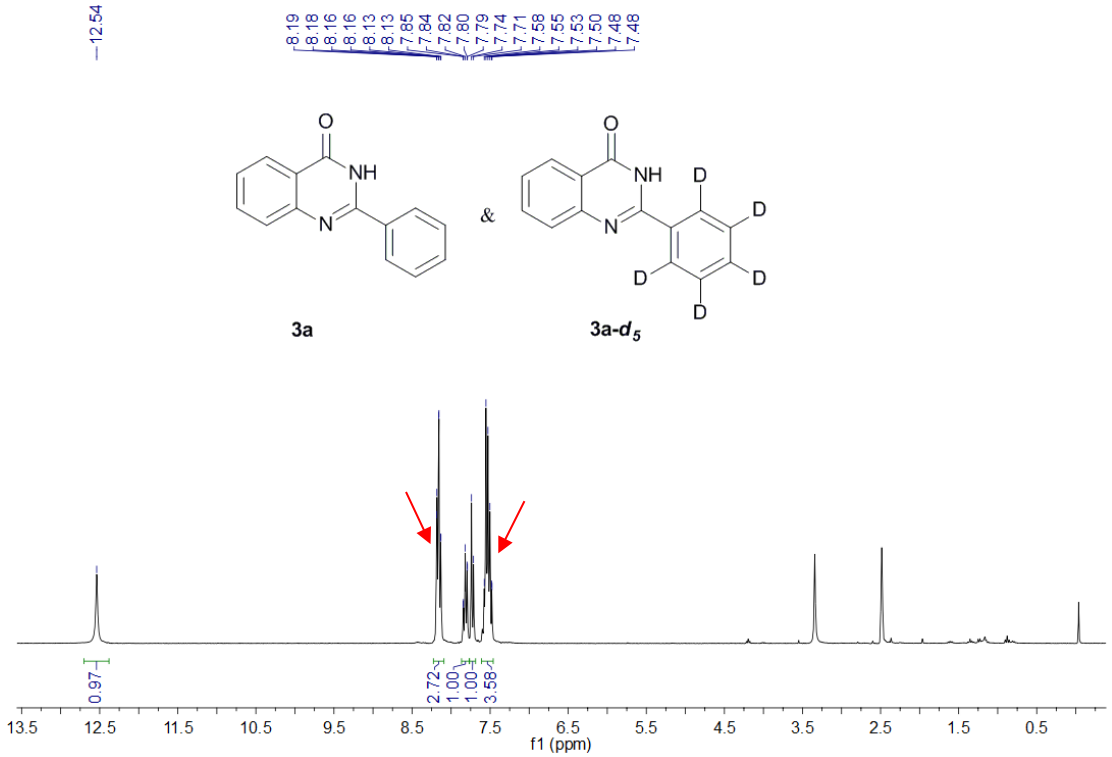
Control experiments on the reaction mechanism

1. Kinetics Isotope Effect (KIE)

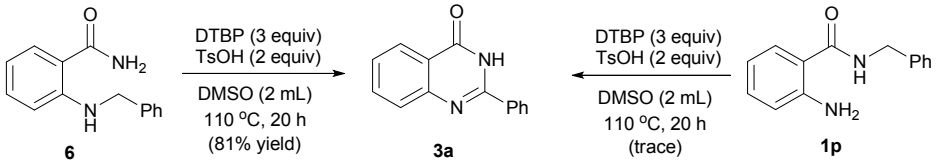


1a **2a** (1 mL) **2a-*d*$_8$** (1 mL) k_H/k_D = 6.1

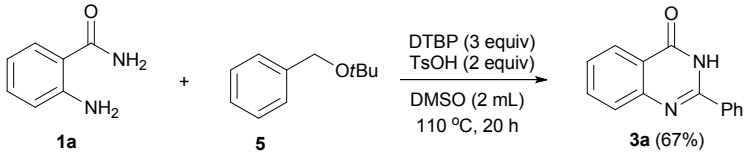
A mixture of 2-aminobenzamide **1a** (41 mg, 0.3 mmol), TsOH (103 mg, 0.6 mmol), DTBP (165 μL, 0.9 mmol), 1 mL toluene and 1 mL toluene-d_8 in 2 mL DMSO was stirred in a Schlenk tube at 110 °C. After stirring for 20 h, the reaction mixture was cooled to the room temperature, and diluted with ethyl acetate. The organic phase was washed with brine, dried over anhydrous Na_2SO_4, concentrated in vacuo and then purified by flash column chromatography on silica gel to afford the mixture of **3a** and **3a-*d*$_5$**. The ^{1}H NMR analysis showed that the ratio of **3a** to **3a-*d*$_5$** was 6.1:1 when compared with the standard ^{1}H NMR spectrum of **3a**, in which the integration of the peak at 7.64 – 7.45 ppm was 3.58 instead of 4.00.



2. Intermediate Experiments

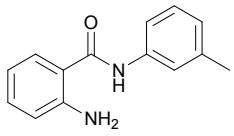


A mixture of 2-aminobenzamide **6** (68 mg, 0.3 mmol. **6** was prepared according to literature method[2].) or **1p** (68 mg, 0.3 mmol), TsOH (103 mg, 0.6 mmol) and DTBP (165 μL, 0.9 mmol) in 2 mL DMSO was stirred in a Schlenk tube at 110 °C. After stirring for 20 h, the reaction mixture was cooled to the room temperature, and diluted with ethyl acetate. The organic phase was washed with brine, dried over anhydrous Na_2SO_4, concentrated in vacuo. The reaction of **1p** produced trace amount of **3a** based on TLC analysis. The reaction residue of **6** was purified by flash column chromatography on silica gel to afford **3a** in 81% yield.



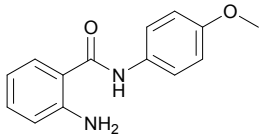
A mixture of 2-aminobenzamide **1a** (41 mg, 0.3 mmol), (*tert*-butoxymethyl)benzene **5** (148 mg, 0.9 mmol. **5** was prepared according to literature method[3].), TsOH (103 mg, 0.6 mmol), DTBP (165 μL, 0.9 mmol) in 2 mL DMSO was stirred in a Schlenk tube at 110 °C. After stirring for 20 h, the reaction mixture was cooled to the room temperature, and diluted with ethyl acetate. The organic phase was washed with brine, dried over anhydrous Na_2SO_4, concentrated in vacuo and then purified by flash column chromatography on silica gel to afford **3a** in 67% yield.

Substrate characterizations



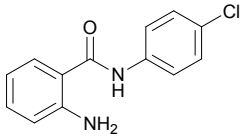
1d

*2-Amino-N-(m-tolyl)benzamide (**1d**)*[4]. 44% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (brs, 1H), 7.48 – 7.38 (m, 2H), 7.32 (d, *J* = 8.2 Hz, 1H), 7.27 – 7.19 (m, 2H), 6.95 (d, *J* = 7.5 Hz, 1H), 6.68 (t, *J* = 7.4 Hz, 2H), 5.46 (brs, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 148.9, 139.0, 137.7, 132.7, 128.8, 127.2, 125.3, 121.2, 117.6, 117.5, 116.8, 116.3, 21.5.



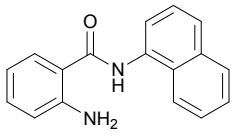
1e

*2-Amino-N-(4-methoxyphenyl)benzamide (**1e**)*[5]. 30% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (brs, 1H), 7.49 – 7.36 (m, 3H), 7.29 – 7.12 (m, 1H), 6.88 (d, *J* = 8.9 Hz, 2H), 6.68 (t, *J* = 8.3 Hz, 2H), 5.47 (brs, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 156.6, 148.8, 132.6, 130.8, 127.2, 122.6, 117.5, 116.8, 116.3, 114.2, 55.5.



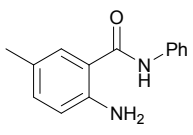
1f

*2-Amino-N-(4-chlorophenyl)benzamide (**1f**)*[4]. 50% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (brs, 1H), 7.51 (d, *J* = 8.7 Hz, 2H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.7 Hz, 2H), 7.28 – 7.21 (m, 1H), 6.70 (t, *J* = 7.7 Hz, 2H), 5.48 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 149.0, 136.4, 133.0, 129.4, 129.0, 127.1, 121.7, 117.6, 116.9, 115.8.



1g

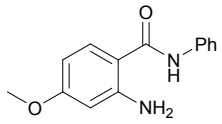
*2-Amino-N-(naphthalen-1-yl)benzamide (**1g**)*[6]. 24% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (brs, 1H), 7.93 – 7.81 (m, 3H), 7.73 (d, *J* = 8.3 Hz, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.55 – 7.43 (m, 3H), 7.33 – 7.25 (m, 1H), 6.78 – 6.70 (m, 2H), 5.55 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 149.3, 134.2, 132.9, 132.5, 128.8, 128.0, 127.4, 126.5, 126.3, 126.1, 125.7, 121.7, 121.2, 117.7, 116.9, 115.9.



1h

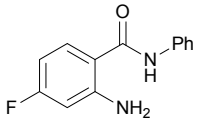
*2-Amino-5-methyl-N-phenylbenzamide (**1h**)*[7]. 35% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (brs, 1H), 7.65 – 7.51 (m, 2H), 7.36 (t, *J* = 7.9 Hz, 2H), 7.27 (s, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 7.08 (dd, *J* = 8.2,

1.6 Hz, 1H), 6.64 (d, J = 8.3 Hz, 1H), 5.28 (brs, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 146.5, 137.9, 133.7, 129.1, 127.3, 126.2, 124.4, 120.5, 117.8, 116.5, 20.4.



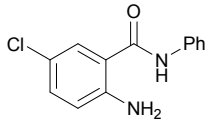
1i

2-Amino-4-methoxy-N-phenylbenzamide ***(1i)***. white solid, 24% yield, mp. 152–154 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (brs, 1H), 7.56 – 7.50 (m, 2H), 7.40 (d, J = 8.8 Hz, 1H), 7.35 (t, J = 7.9 Hz, 2H), 7.12 (t, J = 7.4 Hz, 1H), 6.27 (dd, J = 8.8, 2.5 Hz, 1H), 6.17 (d, J = 2.5 Hz, 1H), 5.70 (brs, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 163.2, 151.4, 138.0, 129.0, 128.9, 124.2, 120.5, 109.1, 104.3, 100.7, 55.2; MS (ESI): 243.10 $[M+H]^+$; HRMS (ESI) m/z calcd for $C_{14}H_{15}N_2O_2$ $[M+H]^+$ 243.1128, found 243.1126.



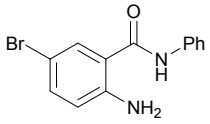
1j

2-Amino-4-fluoro-N-phenylbenzamide ***(1j)***. white solid, 39% yield, mp. 128–130 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (brs, 1H), 7.52 (dd, J = 8.5, 0.9 Hz, 2H), 7.47 – 7.39 (m, 1H), 7.34 (t, J = 8.0 Hz, 2H), 7.14 (t, J = 7.4 Hz, 1H), 6.54 – 6.12 (m, 2H), 5.68 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 165.5 (d, $J_{C\text{-}F}$ = 250.1 Hz), 151.3 (d, $J_{C\text{-}F}$ = 12.1 Hz), 137.6, 129.5 (d, $J_{C\text{-}F}$ = 11.2 Hz), 129.1, 124.6, 120.7, 112.5 (d, $J_{C\text{-}F}$ = 2.1 Hz), 104.2 (d, $J_{C\text{-}F}$ = 22.8 Hz), 103.2 (d, $J_{C\text{-}F}$ = 24.3 Hz); MS (ESI): 231.05 $[M+H]^+$; HRMS (ESI) m/z calcd for $C_{13}H_{12}FN_2O$ $[M+H]^+$ 231.0928, found 231.0927.



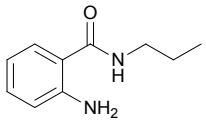
1k

2-Amino-5-chloro-N-phenylbenzamide ***(1k)***[8]. 44% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (brs, 1H), 7.59 – 7.50 (m, 2H), 7.42 (d, J = 2.4 Hz, 1H), 7.36 (t, J = 7.9 Hz, 2H), 7.22 – 7.11 (m, 2H), 6.64 (d, J = 8.7 Hz, 1H), 5.46 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 147.4, 137.5, 132.6, 129.1, 126.8, 124.8, 121.2, 120.7, 118.8, 117.2.



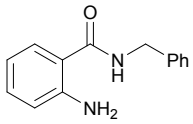
1l

2-Amino-5-bromo-N-phenylbenzamide ***(1l)***[9]. 46% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (brs, 1H), 7.60 – 7.49 (m, 3H), 7.36 (t, J = 7.9 Hz, 2H), 7.31 (dd, J = 8.7, 2.2 Hz, 1H), 7.16 (t, J = 7.4 Hz, 1H), 6.60 (d, J = 8.7 Hz, 1H), 5.49 (brs,2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 147.9, 137.5, 135.3, 129.7, 129.1, 124.8, 120.7, 119.1, 117.8, 107.9.



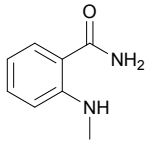
1n

*2-Amino-N-propylbenzamide (**1n**)*[10]. 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.23 – 7.16 (m, 1H), 6.77 – 6.56 (m, 2H), 6.11 (brs, 1H), 5.50 (brs, 2H), 3.37 (dd, *J* = 13.2, 6.9 Hz, 2H), 1.75 – 1.48 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 148.6, 132.1, 127.0, 117.3, 116.6, 116.5, 41.4, 22.9, 11.5.



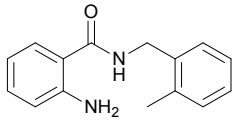
1p

*2-Amino-N-benzylbenzamide (**1p**)*[11]. 74% yield. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.76 (t, *J* = 5.7 Hz, 1H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.38 – 7.26 (m, 4H), 7.26 – 7.17 (m, 1H), 7.13 (t, *J* = 7.1 Hz, 1H), 6.68 (d, *J* = 8.0 Hz, 1H), 6.50 (t, *J* = 7.2 Hz, 1H), 6.41 (brs, 2H), 4.41 (d, *J* = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 168.8, 149.8, 139.9, 131.7, 128.2, 128.0, 127.1, 126.6, 116.4, 114.6, 114.4, 42.1.



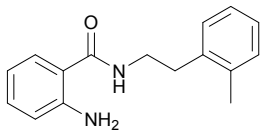
1q

*2-(Methylamino)benzamide (**1q**)*[12]. 69% yield. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.15 – 7.87 (m, 1H), 7.78 (brs, 1H), 7.57 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.26 (t, *J* = 7.2 Hz, 1H), 7.11 (brs, 1H), 6.60 (d, *J* = 8.3 Hz, 1H), 6.50 (t, *J* = 7.4 Hz, 1H), 2.75 (d, *J* = 5.1 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 171.6, 150.7, 132.6, 128.9, 113.8, 113.7, 110.5, 29.1.



1r

*2-Amino-N-(2-methylbenzyl)benzamide (**1r**)*[13]. 81% yield. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.63 (brs, 1H), 7.56 (d, *J* = 7.9 Hz, 1H), 7.28 – 7.18 (m, 1H), 7.18 – 7.06 (m, 4H), 6.69 (d, *J* = 8.2 Hz, 1H), 6.51 (t, *J* = 7.5 Hz, 1H), 6.39 (brs, 2H), 4.39 (d, *J* = 5.7 Hz, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 168.8, 149.7, 137.4, 135.3, 131.7, 129.8, 128.1, 127.1, 126.6, 125.6, 116.3, 114.6, 114.5, 40.2, 18.7.

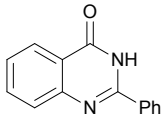


1s

*2-Amino-N-(2-methylphenethyl)benzamide (**1s**)*. white solid, 58% yield, mp. 129–131 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.32 (t, *J* = 5.5 Hz, 1H), 7.42 (d, *J* = 6.8 Hz, 1H), 7.22 – 7.04 (m, 5H), 6.67 (d,

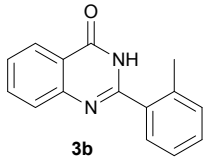
J = 8.0 Hz, 1H), 6.48 (t, *J* = 7.5 Hz, 1H), 6.39 (brs, 2H), 3.45 – 3.33 (m, 2H), 2.85 – 2.75 (m, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 168.8, 149.6, 137.7, 135.9, 131.5, 130.0, 129.1, 127.9, 126.2, 125.9, 116.3, 114.7, 114.5, 39.3, 32.8, 18.9; MS (ESI): 255.10 $[M+H]^+$; HRMS (ESI) m/z calcd for $C_{16}H_{19}N_2O$ $[M+H]^+$ 255.1492, found 255.1489.

Product characterizations



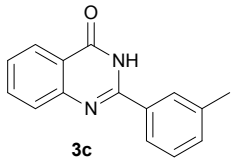
3a

2-Phenylquinazolin-4(3H)-one (***3a***)[14]. white solid, 81% yield, mp. 234–236 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.53 (brs, 1H), 8.16 (t, *J* = 7.7 Hz, 3H), 7.83 (t, *J* = 7.1 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.64 – 7.45 (m, 4H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 152.3, 148.7, 134.6, 132.7, 131.4, 128.6, 127.7, 127.5, 126.5, 125.8, 121.0; MS (ESI): 223.00 $[M+H]^+$.



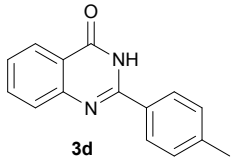
3b

2-(o-Tolyl)quinazolin-4(3H)-one (***3b***)[2]. white solid, 89% yield, mp. 216–218 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.43 (brs, 1H), 8.16 (d, *J* = 7.9 Hz, 1H), 7.86 – 7.78 (m, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.46 (m, 2H), 7.45 – 7.38 (m, 1H), 7.36 – 7.27 (m, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.7, 154.3, 148.7, 136.1, 134.4, 134.2, 130.5, 129.9, 129.1, 127.3, 126.6, 125.8, 125.7, 121.0, 19.5; MS (ESI): 236.95 $[M+H]^+$.



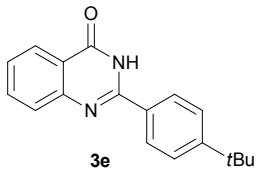
3c

2-(m-Tolyl)quinazolin-4(3H)-one (***3c***)[14]. white solid, 69% yield, mp. 221–223 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.46 (brs, 1H), 8.14 (dd, *J* = 7.9, 1.0 Hz, 1H), 8.01 (s, 1H), 7.96 (d, *J* = 7.0 Hz, 1H), 7.87 – 7.78 (m, 1H), 7.73 (d, *J* = 7.6 Hz, 1H), 7.54 – 7.45 (m, 1H), 7.45 – 7.33 (m, 2H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 152.3, 148.7, 137.9, 134.5, 132.6, 132.0, 128.5, 128.3, 127.5, 126.5, 125.8, 124.9, 121.0, 20.9; MS (ESI): 237.05 $[M+H]^+$.



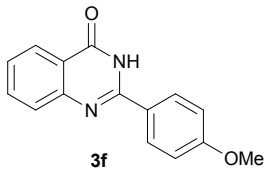
3d

2-(p-Tolyl)quinazolin-4(3H)-one (***3d***)[2]. white solid, 86% yield, mp. 241–243 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.44 (brs, 1H), 8.20 – 8.11 (m, 1H), 8.08 (d, *J* = 8.2 Hz, 2H), 7.89 – 7.76 (m, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.53 – 7.43 (m, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 152.2, 148.8, 141.4, 134.5, 129.9, 129.1, 127.6, 127.4, 126.3, 125.8, 120.9, 20.9; MS (ESI): 237.00 $[M+H]^+$.



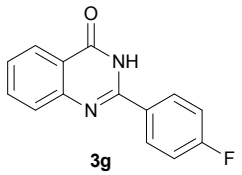
3e

*2-(4-(Tert-butyl)phenyl)quinazolin-4(3H)-one (**3e**)*[15]. white solid, 66% yield, mp. 239–242 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.47 (brs, 1H), 8.27 – 7.99 (m, 3H), 7.81 (t, J = 7.6 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.63 – 7.39 (m, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 154.3, 152.1, 148.8, 134.5, 129.9, 127.5, 127.4, 126.4, 125.8, 125.4, 120.9, 34.6, 30.9; MS (ESI): 279.00 $[M+H]^+$.



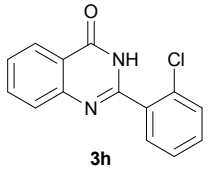
3f

*2-(4-Methoxyphenyl)quinazolin-4(3H)-one (**3f**)*[14]. white solid, 50% yield, mp. 248–251 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.39 (brs, 1H), 8.18 (d, J = 8.7 Hz, 2H), 8.12 (d, J = 8.0 Hz, 1H), 7.80 (t, J = 7.2 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.47 (t, J = 7.4 Hz, 1H), 7.07 (d, J = 8.7 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 161.8, 151.8, 148.9, 134.5, 129.4, 127.3, 126.1, 125.8, 124.8, 120.7, 114.0, 55.4; MS (ESI): 253.00 $[M+H]^+$.



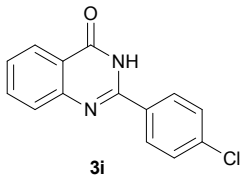
3g

*2-(4-Fluorophenyl)quinazolin-4(3H)-one (**3g**)*[15]. white solid, 74% yield, mp. 284–287 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.56 (brs, 1H), 8.30 – 8.19 (m, 2H), 8.14 (dd, J = 7.9, 1.1 Hz, 1H), 7.88 – 7.76 (m, 1H), 7.72 (d, J = 7.7 Hz, 1H), 7.57 – 7.46 (m, 1H), 7.38 (t, J = 8.9 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.0 (d, $J_{C\text{-}F}$ = 249.5 Hz), 162.2, 151.4, 148.6, 134.6, 130.3 (d, $J_{C\text{-}F}$ = 9.0 Hz), 129.2 (d, $J_{C\text{-}F}$ = 2.9 Hz), 127.4, 126.6, 125.8, 120.9, 115.6 (d, $J_{C\text{-}F}$ = 21.9 Hz); MS (ESI): 240.95 $[M+H]^+$.



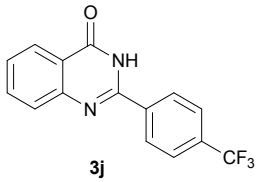
3h

*2-(2-Chlorophenyl)quinazolin-4(3H)-one (**3h**)*[14]. white solid, 26% yield, mp. 188–190 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.63 (brs, 1H), 8.17 (d, J = 7.1 Hz, 1H), 7.91 – 7.79 (m, 1H), 7.78 – 7.38 (m, 6H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 152.2, 148.6, 134.6, 133.8, 131.6, 131.5, 130.8, 129.6, 127.4, 127.2, 127.0, 125.8, 121.2; MS (ESI): 257.00 $[M+H]^+$.



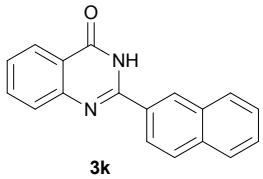
3i

2-(4-chlorophenyl)quinazolin-4(3H)-one (***3i***)[14]. white solid, 52% yield, mp. 298–300 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.58 (brs, 1H), 8.32 – 8.05 (m, 3H), 7.83 (t, J = 7.0 Hz, 1H), 7.73 (d, J = 7.7 Hz, 1H), 7.61 (d, J = 8.2 Hz, 2H), 7.52 (t, J = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 151.4, 148.5, 136.3, 134.6, 131.6, 129.6, 128.7, 127.4, 126.7, 125.9, 121.0; MS (ESI): 256.95 $[M+H]^+$.



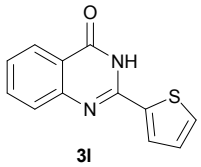
3j

2-(4-(Trifluoromethyl)phenyl)quinazolin-4(3H)-one (***3j***)[15]. white solid, 59% yield, mp. 285–288 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.75 (brs, 1H), 8.37 (d, J = 7.9 Hz, 2H), 8.16 (d, J = 7.7 Hz, 1H), 7.99 – 7.81 (m, 3H), 7.77 (d, J = 8.0 Hz, 1H), 7.55 (t, J = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.1, 151.2, 148.3, 136.6, 134.7, 131.1 (d, $J_{C\text{-}F}$ = 31.9 Hz), 128.7, 127.6, 127.1, 125.9, 125.5 (q, $J_{C\text{-}F}$ = 3.6 Hz), 123.9 (d, $J_{C\text{-}F}$ = 272.3 Hz), 121.1; MS (ESI): 291.00 $[M+H]^+$.



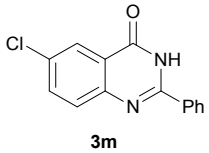
3k

2-(Naphthalen-2-yl)quinazolin-4(3H)-one (***3k***)[15]. yellow solid, 37% yield, mp. 248–251 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.65 (brs, 1H), 8.81 (s, 1H), 8.30 (d, J = 8.1 Hz, 1H), 8.18 (d, J = 7.4 Hz, 1H), 8.12 – 7.90 (m, 3H), 7.89 – 7.75 (m, 2H), 7.70 – 7.48 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 152.2, 148.8, 134.6, 134.1, 132.3, 129.9, 128.9, 128.14, 128.07, 127.9, 127.6, 127.5, 126.9, 126.6, 125.9, 124.5, 121.0; MS (ESI): 273.00 $[M+H]^+$.



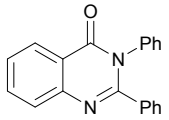
3l

2-(Thiophen-2-yl)quinazolin-4(3H)-one (***3l***)[14]. white solid, 40% yield, mp. 246–249 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.64 (brs, 1H), 8.22 (d, J = 2.9 Hz, 1H), 8.11 (d, J = 7.7 Hz, 1H), 7.85 (d, J = 4.5 Hz, 1H), 7.79 (t, J = 7.5 Hz, 1H), 7.63 (d, J = 8.1 Hz, 1H), 7.47 (t, J = 7.3 Hz, 1H), 7.22 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.8, 148.6, 147.8, 137.3, 134.7, 132.1, 129.4, 128.5, 126.9, 126.3, 126.0, 120.9; MS (ESI): 229.00 $[M+H]^+$.



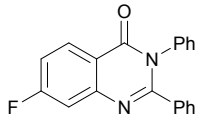
3m

6-Chloro-2-phenylquinazolin-4(3H)-one (***3m***)[14]. white solid, 46% yield, mp. 276–279 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.71 (brs, 1H), 8.16 (d, J = 6.7 Hz, 2H), 8.07 (d, J = 2.4 Hz, 1H), 7.85 (dd, J = 8.7, 2.5 Hz, 1H), 7.75 (d, J = 8.7 Hz, 1H), 7.61 – 7.49 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.3, 152.8, 147.5, 134.7, 132.4, 131.6, 130.7, 129.7, 128.6, 127.8, 124.8, 122.2; MS (ESI): 257.00 $[M+H]^+$.



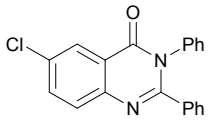
3n

*2,3-Diphenylquinazolin-4(3H)-one (**3n**)*[16]. white solid, 74% yield, mp. 168–170 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.22 – 8.14 (m, 1H), 7.94 – 7.84 (m, 1H), 7.76 (d, J = 7.9 Hz, 1H), 7.62 – 7.56 (m, 1H), 7.41 – 7.17 (m, 10H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 155.2, 147.2, 137.8, 135.6, 134.8, 129.5, 128.9, 128.8, 128.5, 128.1, 127.5, 127.4, 127.1, 126.4, 120.7; MS (ESI): 299.05 $[M+H]^+$.



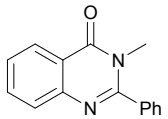
3o

*7-Fluoro-2,3-diphenylquinazolin-4(3H)-one (**3o**)*. white soild, 51% yield, mp. 207–209 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (dd, J = 8.8, 6.1 Hz, 1H), 7.46 (dd, J = 9.6, 2.5 Hz, 1H), 7.34 – 7.18 (m, 9H), 7.16 – 7.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8 (d, $J_{C\text{-}F}$ = 254.7 Hz), 161.6, 156.5, 149.6 (d, $J_{C\text{-}F}$ = 13.1 Hz), 137.4, 135.2, 130.0 (d, $J_{C\text{-}F}$ = 10.7 Hz), 129.6, 129.08, 129.06, 129.0, 128.6, 128.1, 117.7 (d, $J_{C\text{-}F}$ = 1.9 Hz), 116.1 (d, $J_{C\text{-}F}$ = 23.5 Hz), 113.1 (d, $J_{C\text{-}F}$ = 21.9 Hz); MS (ESI): 317.05 $[M+H]^+$; HRMS (ESI) m/z calcd for $C_{20}H_{14}FN_2O$ $[M+H]^+$ 317.1085, found 317.1078.



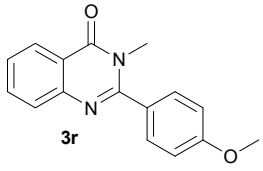
3p

*6-Chloro-2,3-diphenylquinazolin-4(3H)-one (**3p**)*[17]. white solid, 36% yield, mp. 232–234 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 1.9 Hz, 1H), 7.79 – 7.70 (m, 2H), 7.36 – 7.17 (m, 8H), 7.17 – 7.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 155.5, 146.0, 137.4, 135.2, 135.1, 133.1, 129.51, 129.45, 129.1, 129.02, 128.97, 128.6, 128.1, 126.5, 122.0; MS (ESI): 333.00 $[M+H]^+$.



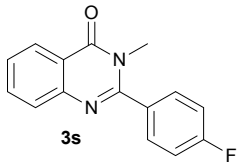
3q

*3-Methyl-2-phenylquinazolin-4(3H)-one (**3q**)*[16]. white solid, 82% yield, mp. 148–151 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.17 (dd, J = 7.9, 1.0 Hz, 1H), 7.87 – 7.78 (m, 1H), 7.69 – 7.62 (m, 3H), 7.58 – 7.50 (m, 4H), 3.35 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 156.1, 147.0, 135.4, 134.3, 129.8, 128.4, 128.2, 127.1, 126.8, 126.1, 120.1, 33.8; MS (ESI): 237.10 $[M+H]^+$.



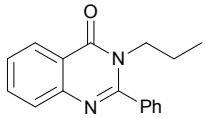
3r

*2-(4-Methoxyphenyl)-3-methylquinazolin-4(3H)-one (**3r**)*[18]. white solid, 57% yield, mp. 168–170 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.15 (d, J = 7.0 Hz, 1H), 7.87 – 7.74 (m, 1H), 7.70 – 7.57 (m, 3H), 7.52 (t, J = 7.5 Hz, 1H), 7.07 (d, J = 8.7 Hz, 2H), 3.83 (s, 3H), 3.39 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.8, 160.3, 156.0, 147.1, 134.2, 130.1, 127.6, 127.1, 126.6, 126.0, 119.9, 113.7, 55.3, 34.1; MS (ESI): 267.05 $[M+H]^+$.



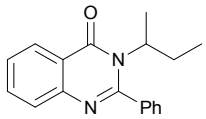
3s

*2-(4-Fluorophenyl)-3-methylquinazolin-4(3H)-one (**3s**)*. white solid, 57% yield, mp. 186–189 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.17 (dd, J = 8.0, 1.1 Hz, 1H), 7.87 – 7.79 (m, 1H), 7.77 – 7.70 (m, 2H), 7.66 (d, J = 7.7 Hz, 1H), 7.59 – 7.50 (m, 1H), 7.42 – 7.32 (m, 2H), 3.35 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.7 (d, $J_{C\text{-}F}$ = 247.3 Hz), 161.6, 155.3, 147.0, 134.3, 131.9 (d, $J_{C\text{-}F}$ = 3.3 Hz), 130.9 (d, $J_{C\text{-}F}$ = 8.6 Hz), 127.1, 126.9, 126.1, 120.1, 115.4 (d, $J_{C\text{-}F}$ = 21.9 Hz), 33.8; MS (ESI): 255.10 $[M+H]^+$; HRMS (ESI) m/z calcd for $C_{15}H_{12}FN_2O$ $[M+H]^+$ 255.0928, found 255.0923.



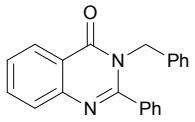
3t

*2-Phenyl-3-propylquinazolin-4(3H)-one (**3t**)*[19]. white solid, 46% yield, mp. 122–124 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 – 8.26 (m, 1H), 7.83 – 7.67 (m, 2H), 7.55 – 7.41 (m, 6H), 4.02 – 3.85 (m, 2H), 1.73 – 1.54 (m, 2H), 0.77 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 156.3, 147.2, 135.6, 134.3, 129.8, 128.8, 127.8, 127.5, 127.0, 126.8, 120.9, 47.5, 22.1, 11.2; MS (ESI): 265.10 $[M+H]^+$.



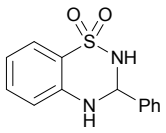
3u

*3-(Sec-butyl)-2-phenylquinazolin-4(3H)-one (**3u**)*[20]. colorless oil, 30% yield. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.16 (dd, J = 8.0, 1.1 Hz, 1H), 7.81 (ddd, J = 8.5, 7.2, 1.5 Hz, 1H), 7.63 (d, J = 7.7 Hz, 1H), 7.58 – 7.49 (m, 6H), 4.01 – 3.84 (m, 1H), 2.28 – 2.09 (m, 1H), 1.80 – 1.61 (m, 1H), 1.51 (d, J = 6.8 Hz, 3H), 0.59 (t, J = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 156.9, 146.5, 136.3, 134.3, 129.4, 128.6, 127.5, 126.92, 126.87, 125.9, 121.4, 59.2, 25.3, 17.6, 11.1; MS (ESI): 279.10 $[M+H]^+$.



3v

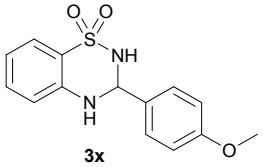
*3-Benzyl-2-phenylquinazolin-4(3H)-one (**3v**)*[19]. white solid, 87% yield, mp. 167–169 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.20 (d, J = 7.6 Hz, 1H), 7.91 – 7.83 (m, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.58 (t, J = 7.4 Hz, 1H), 7.53 – 7.34 (m, 5H), 7.27 – 7.11 (m, 3H), 6.94 – 6.79 (m, 2H), 5.17 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 156.1, 146.9, 136.7, 135.1, 134.7, 129.7, 128.4, 128.2, 128.0, 127.3, 127.2, 127.1, 126.4, 126.2, 120.4, 48.2; MS (ESI): 313.05 $[M+H]^+$.



3w

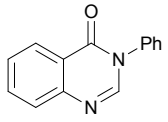
*3-Phenyl-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (**3w**)*[21]. white solid, 42% yield, mp.

129–132 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.87 (d, J = 12.1 Hz, 1H), 7.71 – 7.60 (m, 2H), 7.54 – 7.49 (m, 1H), 7.48 – 7.40 (m, 3H), 7.37 (brs, 1H), 7.34 – 7.26 (m, 1H), 6.90 (d, J = 8.3 Hz, 1H), 6.75 (t, J = 7.3 Hz, 1H), 5.77 (d, J = 12.1 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 143.9, 137.3, 132.8, 129.1, 128.5, 127.5, 123.7, 121.6, 116.7, 116.4, 68.4; MS (ESI): 261.05 $[M+H]^+$.



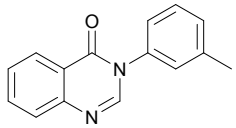
3x

*3-(4-Methoxyphenyl)-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (**3x**)*[21]. white solid, 30% yield, mp. 161–163 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.78 (d, J = 12.1 Hz, 1H), 7.57 (d, J = 8.7 Hz, 2H), 7.53 – 7.44 (m, 1H), 7.34 – 7.24 (m, 2H), 6.99 (d, J = 8.7 Hz, 2H), 6.88 (d, J = 8.2 Hz, 1H), 6.74 (t, J = 7.3 Hz, 1H), 5.71 (d, J = 12.0 Hz, 1H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.8, 143.9, 132.8, 129.5, 128.9, 123.7, 121.5, 116.6, 116.3, 113.8, 68.0, 55.2; MS (ESI): 290.95 $[M+H]^+$.



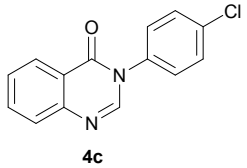
4a

*3-Phenylquinazolin-4(3H)-one (**4a**)*[22]. yellow solid, 72% yield, mp. 153–155 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.38 (d, J = 7.7 Hz, 1H), 8.15 (s, 1H), 7.87 – 7.71 (m, 2H), 7.63 – 7.48 (m, 4H), 7.46 – 7.39 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 147.8, 146.1, 137.5, 134.6, 129.6, 129.1, 127.7, 127.6, 127.2, 127.0, 122.4; MS (ESI): 223.10 $[M+H]^+$.



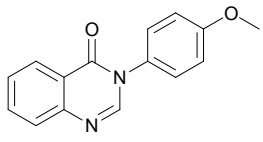
4b

*3-(m-Tolyl)quinazolin-4(3H)-one (**4b**)*[23]. white solid, 56% yield, mp. 146–148 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, J = 8.0, 0.9 Hz, 1H), 8.11 (s, 1H), 7.83 – 7.73 (m, 2H), 7.54 (ddd, J = 8.2, 6.9, 1.6 Hz, 1H), 7.43 (t, J = 7.7 Hz, 1H), 7.29 (d, J = 7.7 Hz, 1H), 7.25 – 7.19 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 147.9, 146.2, 139.8, 137.4, 134.6, 129.9, 129.5, 127.7, 127.61, 127.57, 127.2, 124.0, 122.4, 21.4; MS (ESI): 237.10 $[M+H]^+$.



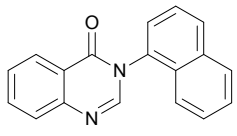
4c

*3-(4-Chlorophenyl)quinazolin-4(3H)-one (**4c**)*[22]. white solid, 47% yield, mp. 189–191 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, J = 8.0, 1.1 Hz, 1H), 8.09 (s, 1H), 7.84 – 7.78 (m, 1H), 7.77 – 7.73 (m, 1H), 7.59 – 7.49 (m, 3H), 7.42 – 7.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 147.8, 145.6, 135.9, 135.2, 134.8, 129.9, 128.4, 127.9, 127.7, 127.2, 122.2; MS (ESI): 257.00 $[M+H]^+$.



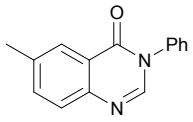
4d

*3-(4-Methoxyphenyl)quinazolin-4(3H)-one (**4d**)*[22]. yellow solid, 78% yield, mp. 210–212 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 7.9 Hz, 1H), 8.11 (s, 1H), 7.83 – 7.71 (m, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.33 (d, *J* = 8.7 Hz, 2H), 7.04 (d, *J* = 8.7 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 159.9, 147.9, 146.5, 134.5, 130.2, 128.2, 127.6, 127.1, 122.4, 114.8, 55.6; MS (ESI): 253.10 $[M+H]^+$.



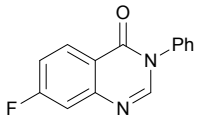
4e

*3-(Naphthalen-1-yl)quinazolin-4(3H)-one (**4e**)*[24]. white solid, 61% yield, mp. 142–144 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 7.9 Hz, 1H), 8.10 (s, 1H), 8.02 (d, *J* = 8.3 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.88 – 7.82 (m, 2H), 7.66 – 7.50 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 148.2, 146.9, 134.8, 134.4, 134.1, 130.3, 129.8, 128.7, 127.8, 127.79, 127.75, 127.3, 127.0, 126.0, 125.5, 122.4, 122.1; MS (ESI): 273.05 $[M+H]^+$.



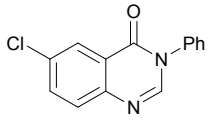
4f

*6-Methyl-3-phenylquinazolin-4(3H)-one (**4f**)*. white solid, 92% yield, mp. 123–126 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 8.08 (s, 1H), 7.67 (d, *J* = 8.3 Hz, 1H), 7.61 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.58 – 7.52 (m, 2H), 7.51 – 7.46 (m, 1H), 7.45 – 7.39 (m, 2H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8 145.8, 145.4, 138.0, 137.6, 136.0, 129.7, 129.1, 127.4, 127.1, 126.6, 122.1, 21.4; MS (ESI): 237.10 $[M+H]^+$; HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2O$ $[M+H]^+$ 237.1022, found 237.1019.



4g

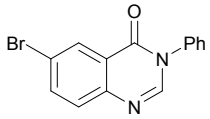
*7-Fluoro-3-phenylquinazolin-4(3H)-one (**4g**)*[22]. white solid, 89% yield, mp. 197–199 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (dd, *J* = 8.9, 6.1 Hz, 1H), 8.14 (s, 1H), 7.59 – 7.48 (m, 3H), 7.45 – 7.39 (m, 3H), 7.26 (td, *J* = 8.9, 2.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6 (d, $J_{C\text{-}F}$ = 255.0 Hz), 160.1, 150.1 (d, $J_{C\text{-}F}$ = 13.0 Hz), 147.3, 137.2, 130.0 (d, $J_{C\text{-}F}$ = 10.6 Hz), 129.7, 129.3, 127.0, 119.1 (d, $J_{C\text{-}F}$ = 2.1 Hz), 116.4 (d, $J_{C\text{-}F}$ = 23.4 Hz), 113.1 (d, $J_{C\text{-}F}$ = 22.0 Hz); MS (ESI): 241.10 $[M+H]^+$.



4h

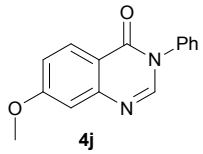
*6-Chloro-3-phenylquinazolin-4(3H)-one (**4h**)*[25]. white solid, 70% yield, mp. 198–199 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 1.1 Hz, 1H), 8.11 (s, 1H), 7.75 – 7.67 (m, 2H), 7.60 – 7.47 (m, 3H),

7.41 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 146.4, 146.3, 137.2, 135.0, 133.5, 129.7, 129.32, 129.26, 126.9, 126.5, 123.5; MS (ESI): 257.00 $[M+H]^+$.



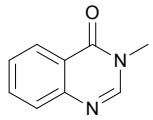
4i

*6-Bromo-3-phenylquinazolin-4(3H)-one (**4i**)*[26]. white solid, 72% yield, mp. 193–196 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, J = 2.2 Hz, 1H), 8.12 (s, 1H), 7.86 (dd, J = 8.7, 2.2 Hz, 1H), 7.63 (d, J = 8.7 Hz, 1H), 7.59 – 7.47 (m, 3H), 7.41 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 146.7, 146.5, 137.8, 137.2, 129.8, 129.7, 129.4, 129.3, 126.9, 123.8, 121.3; MS (ESI): 301.00 $[M+H]^+$.



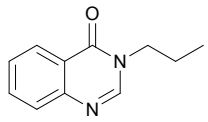
4j

*7-Methoxy-3-phenylquinazolin-4(3H)-one (**4j**)*. white solid, 30% yield, mp. 144–146 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 8.8 Hz, 1H), 8.10 (s, 1H), 7.57 – 7.52 (m, 2H), 7.50 – 7.45 (m, 1H), 7.45 – 7.39 (m, 2H), 7.14 (d, J = 2.4 Hz, 1H), 7.11 (dd, J = 8.8, 2.5 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 160.4, 150.1, 146.8, 137.5, 129.6, 129.0, 128.8, 127.1, 117.4, 115.8, 108.5, 55.8; MS (ESI): 253.05 $[M+H]^+$; HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2O_2$ $[M+H]^+$ 253.0972, found 253.0966.



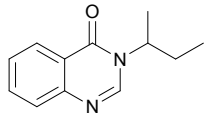
4k

*3-Methylquinazolin-4(3H)-one (**4k**)*[27]. white solid, 63% yield, mp. 111–112 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 7.8 Hz, 1H), 8.06 (s, 1H), 7.81 – 7.73 (m, 1H), 7.70 (d, J = 7.7 Hz, 1H), 7.54 – 7.46 (m, 1H), 3.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6, 148.2, 146.8, 134.2, 127.4, 127.3, 126.5, 122.0, 34.1; MS (ESI): 161.10 $[M+H]^+$.



4l

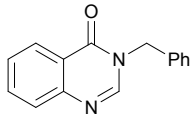
*3-Propylquinazolin-4(3H)-one (**4l**)*[28]. white solid, 54% yield, mp. 80–83 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, J = 8.0 Hz, 1H), 8.04 (s, 1H), 7.78 – 7.73 (m, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.52 – 7.48 (m, 1H), 4.00 – 3.95 (m, 2H), 1.89 – 1.79 (m, 2H), 1.01 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 148.1, 146.6, 134.1, 127.4, 127.2, 126.7, 122.2, 48.6, 22.6, 11.1; MS (ESI): 189.10 $[M+H]^+$.



4m (3u')

*3-(Sec-butyl)quinazolin-4(3H)-one ((**4m (3u')**)*[28]. yellow solid, 55% yield, mp. 71–73 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.41 (s, 1H), 8.14 (dd, J = 7.9, 1.0 Hz, 1H), 7.87 – 7.76 (m, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.53 (t, J = 7.1 Hz, 1H), 4.92 – 4.62 (m, 1H), 1.93 – 1.69 (m, 2H), 1.40 (d, J = 6.9 Hz, 3H), 0.78 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.1, 147.3, 145.6, 134.2, 127.1, 127.0,

126.3, 121.3, 51.6, 27.7, 19.4, 10.6; MS (ESI): 203.10 $[M+H]^+$.



4n

*3-Benzylquinazolin-4(3H)-one (**4n**)*[22]. white solid, 68% yield, mp. 86–89 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.11 (s, 1H), 7.74 (ddd, *J* = 8.3, 6.9, 1.5 Hz, 1H), 7.70 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.49 (ddd, *J* = 8.2, 6.9, 1.5 Hz, 1H), 7.37 – 7.29 (m, 5H), 5.19 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 148.1, 146.4, 135.8, 134.3, 129.0, 128.3, 128.0, 127.5, 127.4, 126.9, 122.2, 49.6; MS (ESI): 237.10 $[M+H]^+$.

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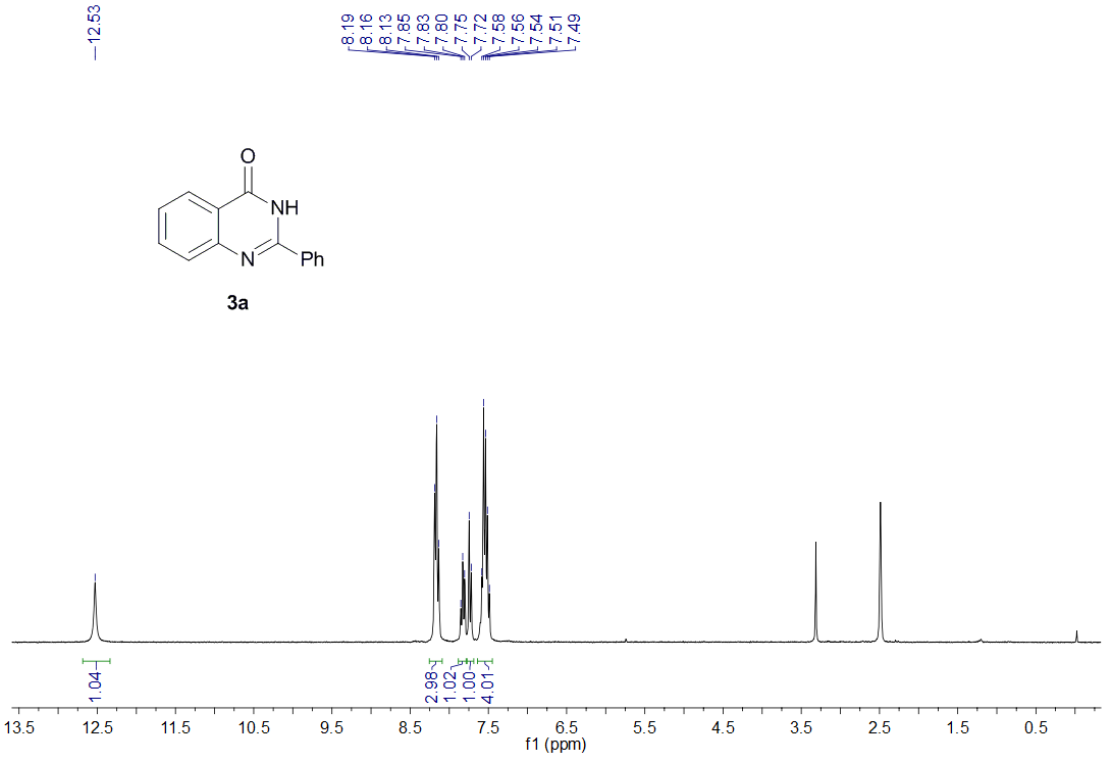
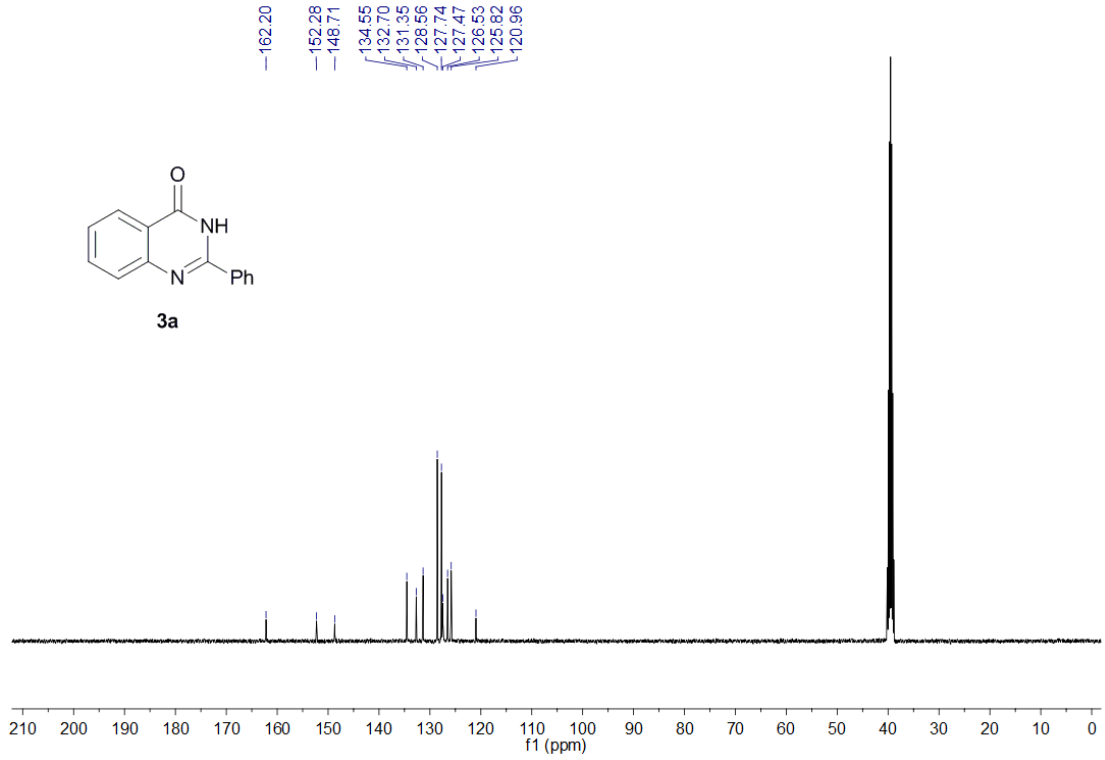
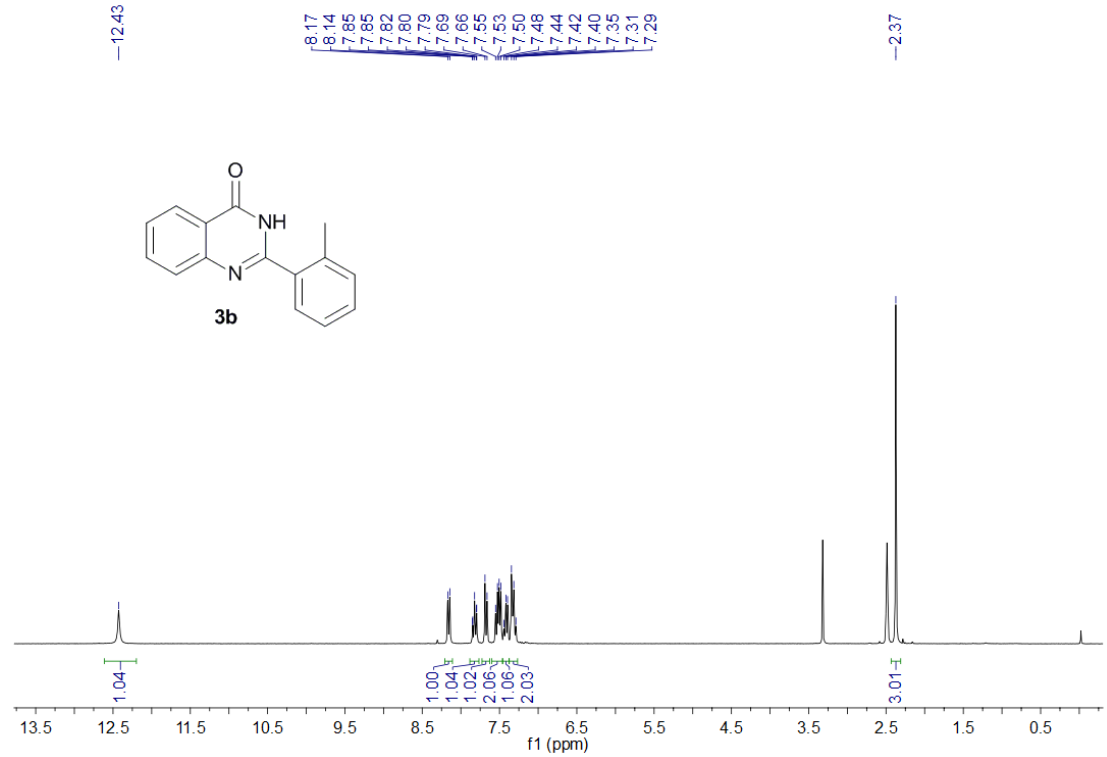
Spectral copies of ^{1}H- and ^{13}C-NMR of products



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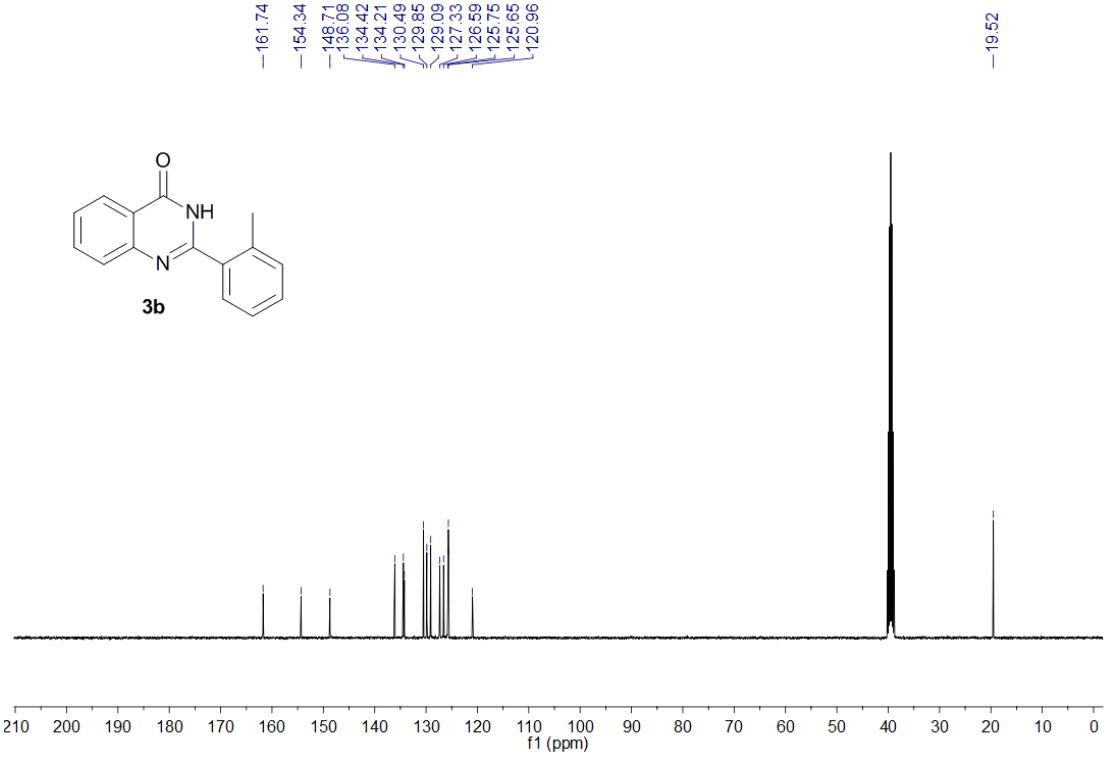
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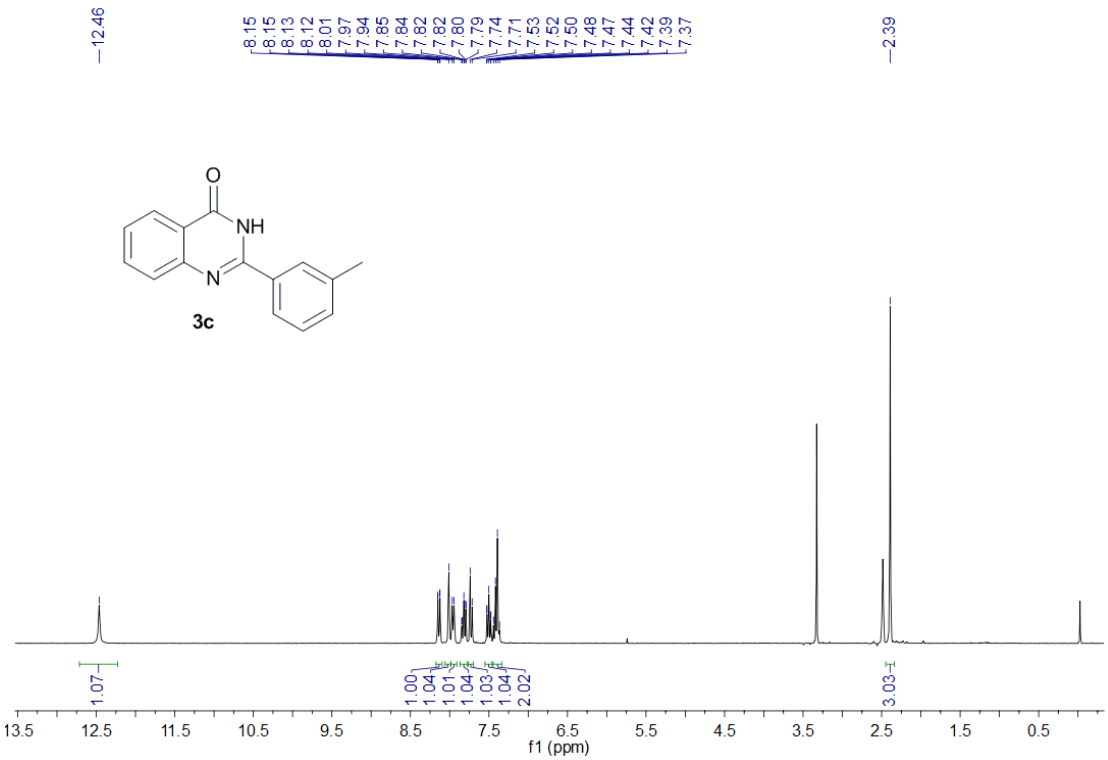
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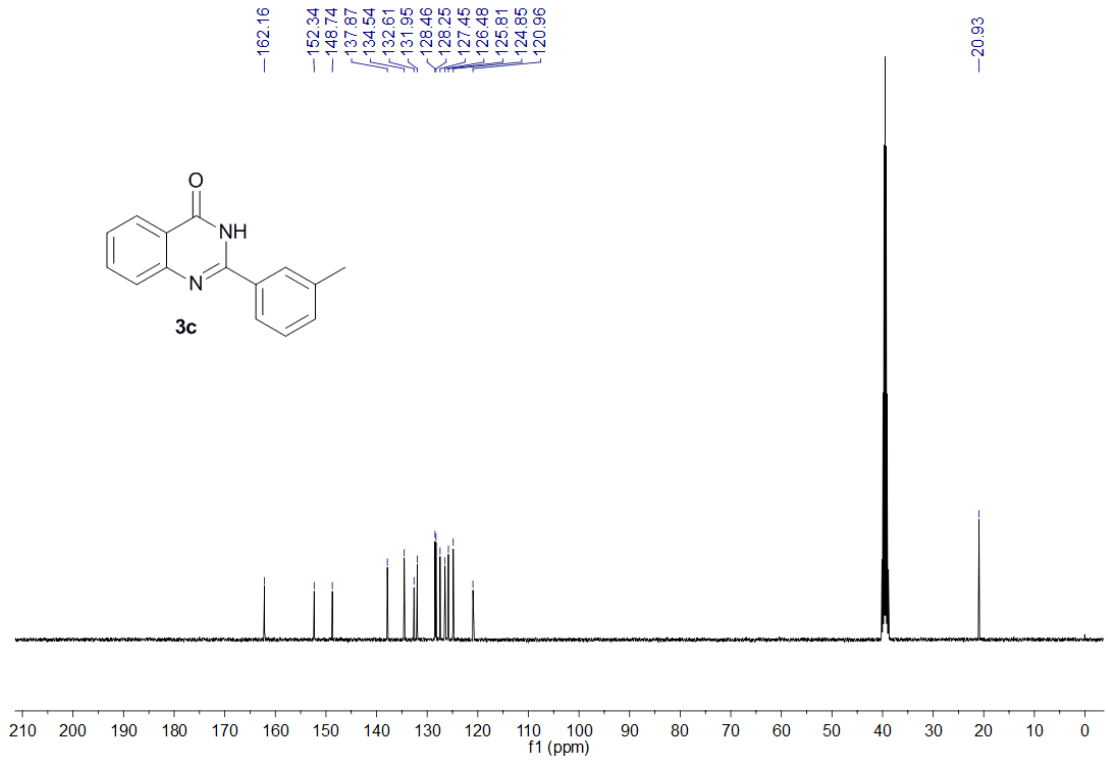
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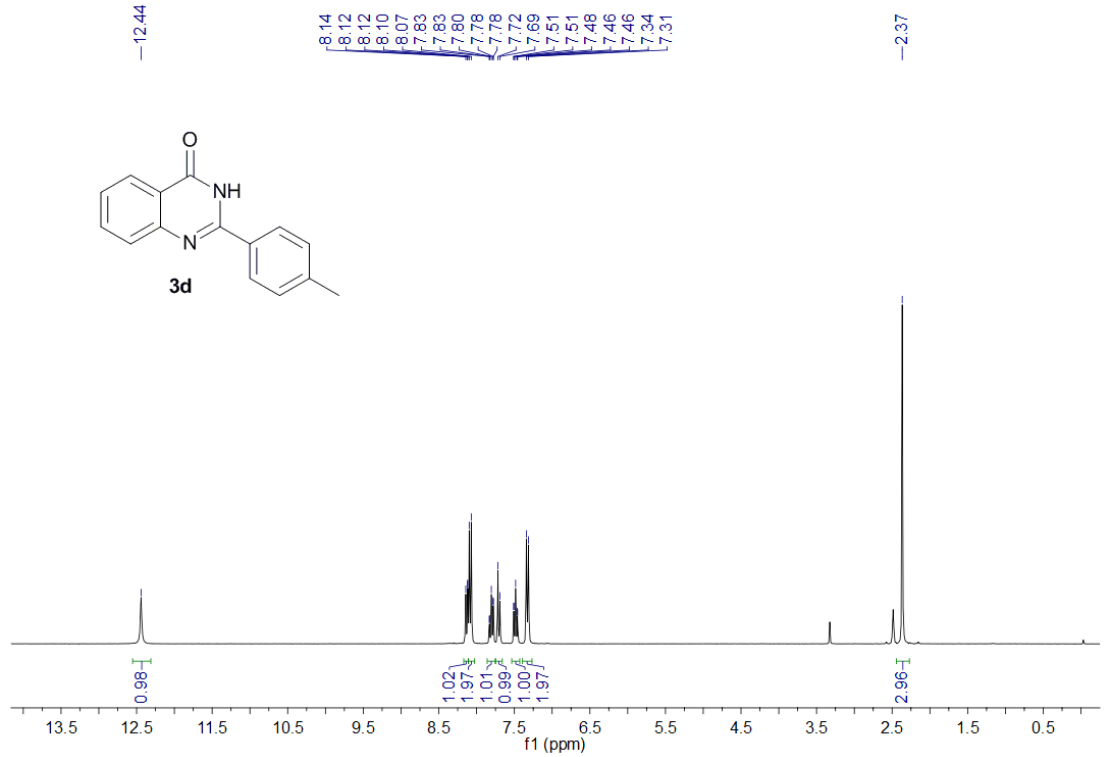
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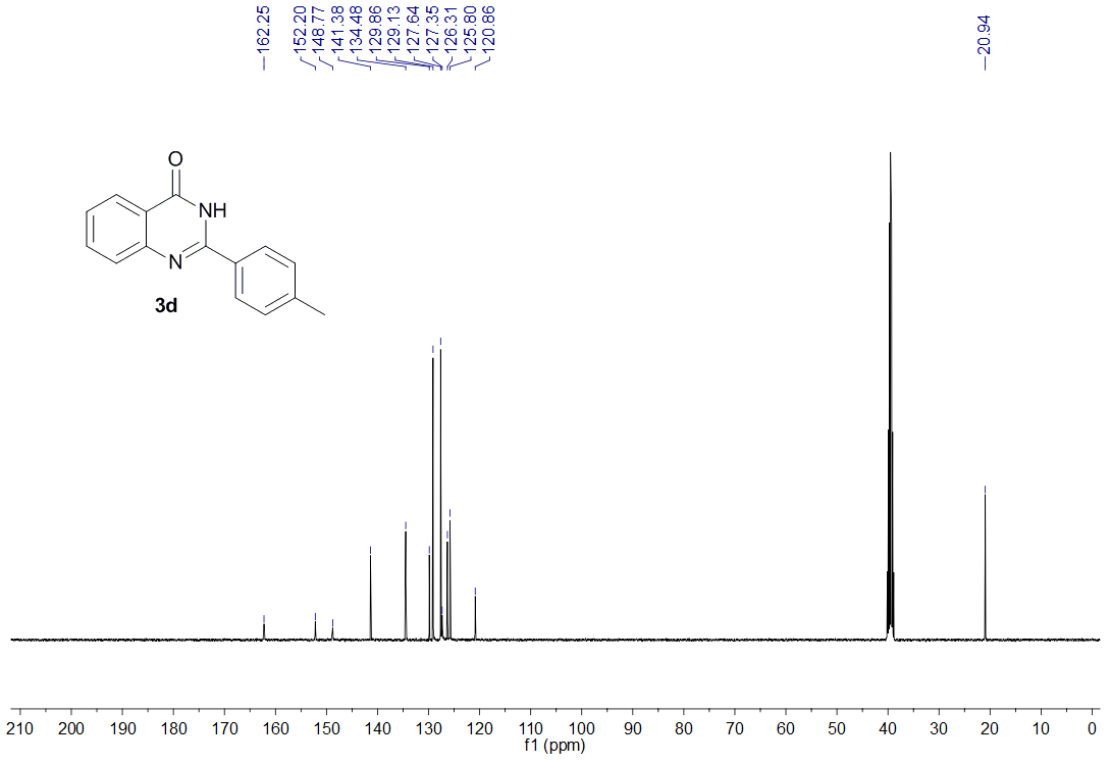
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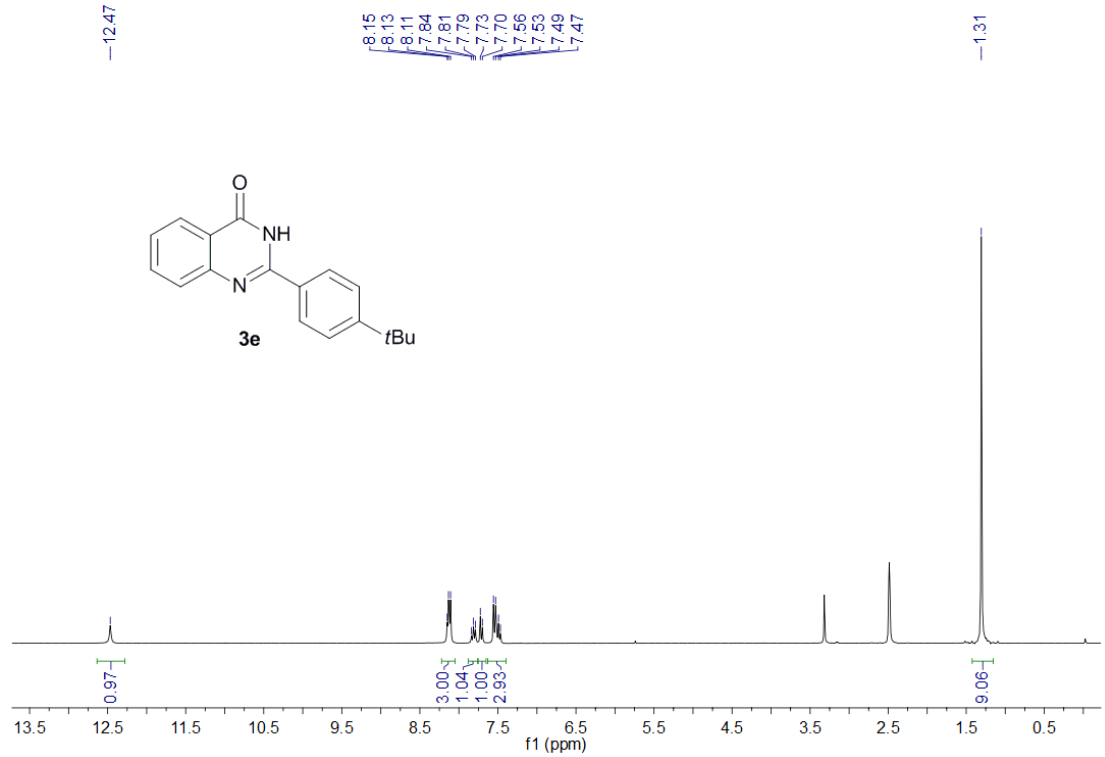
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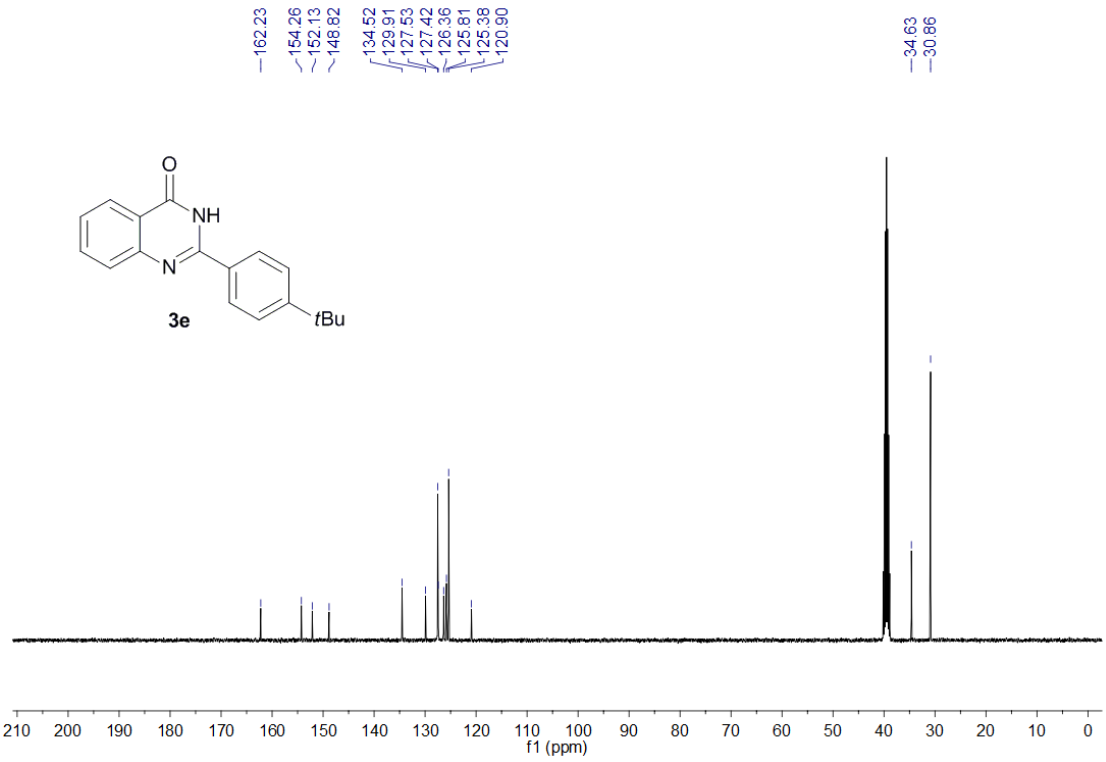
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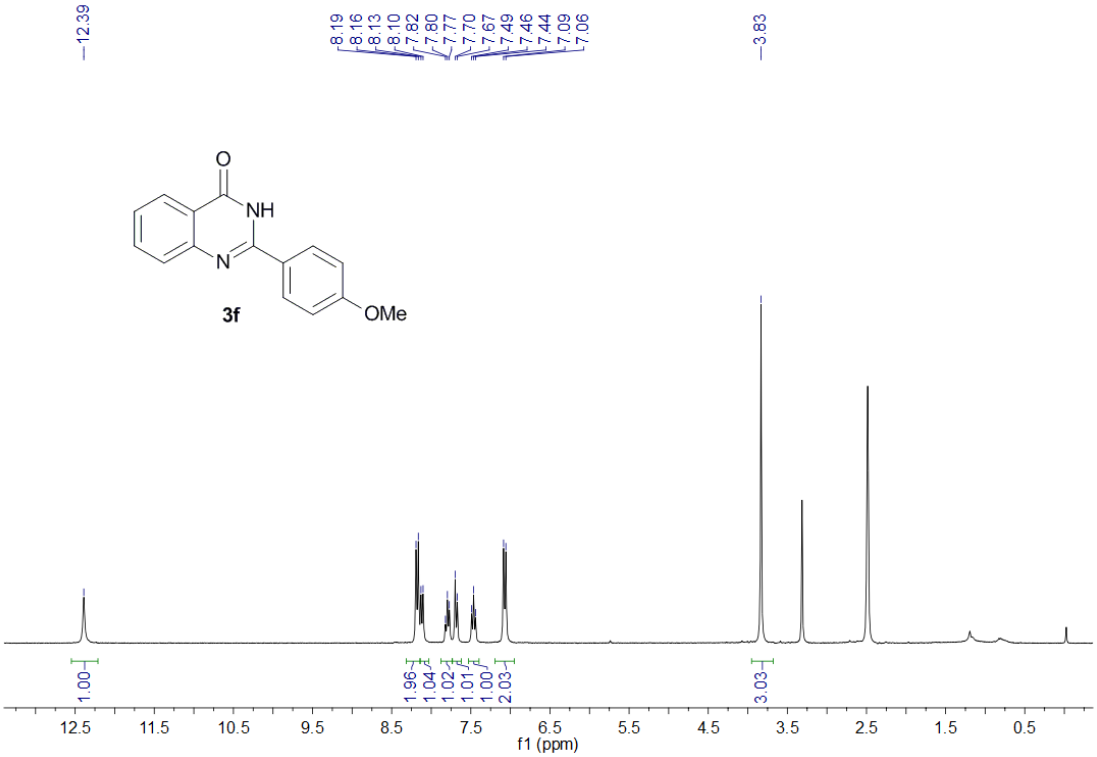
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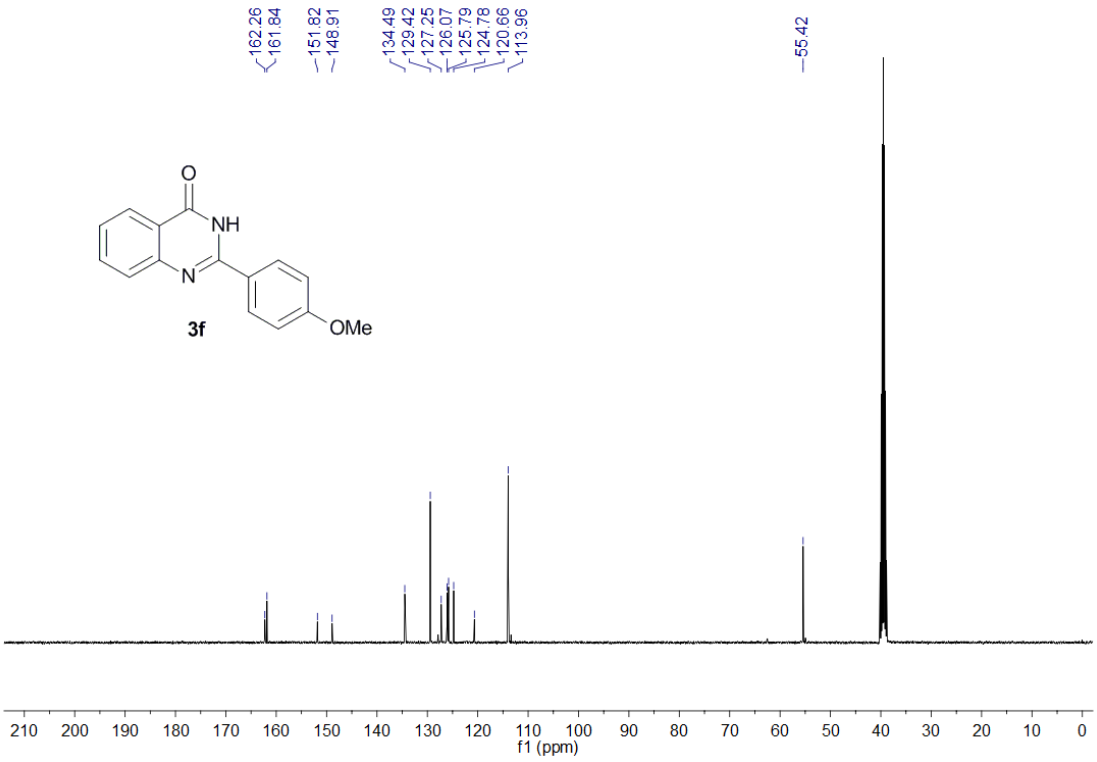
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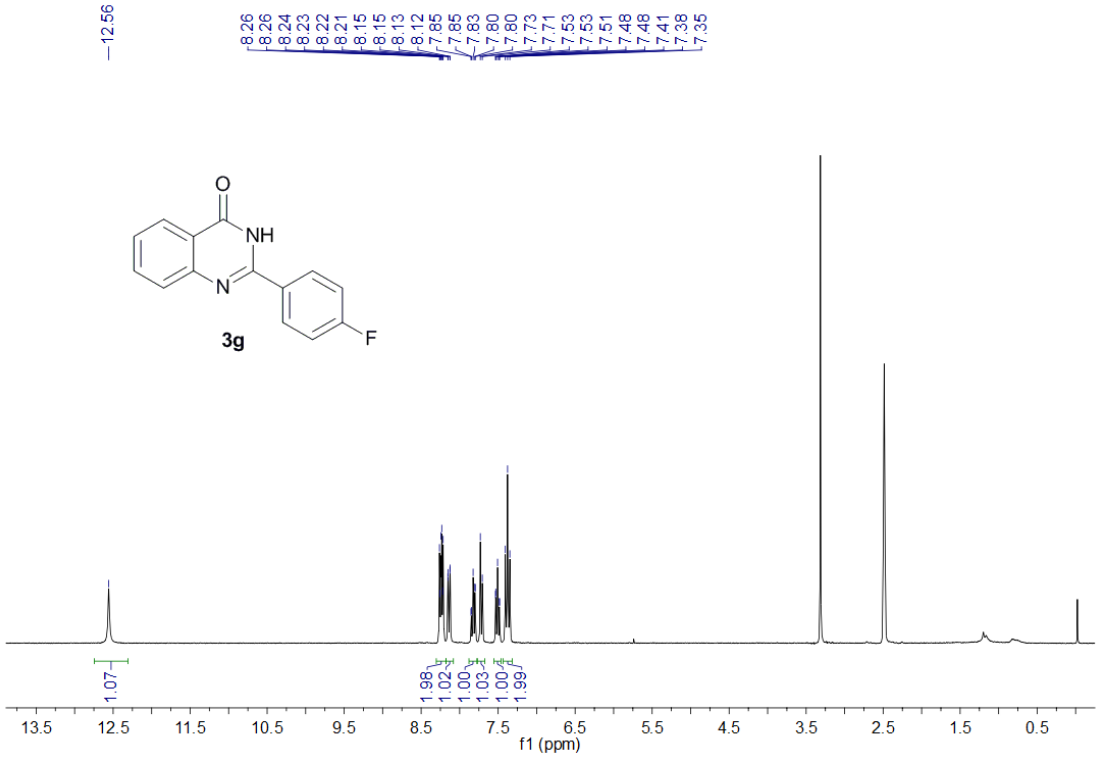
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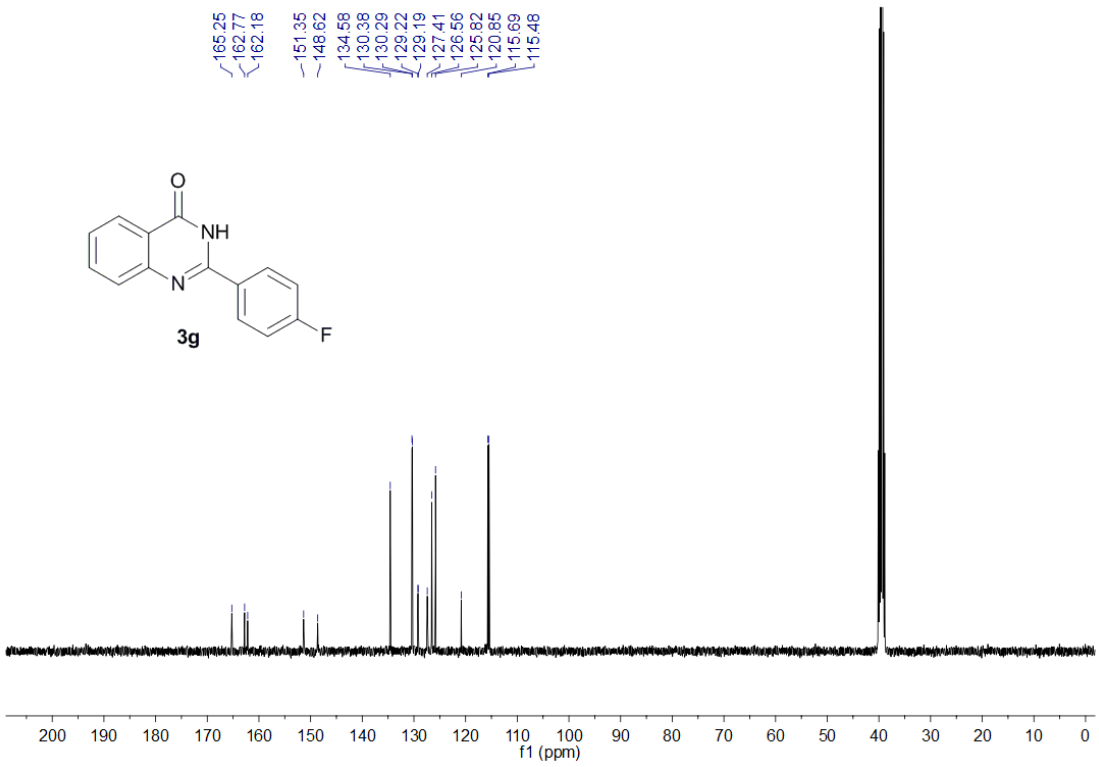
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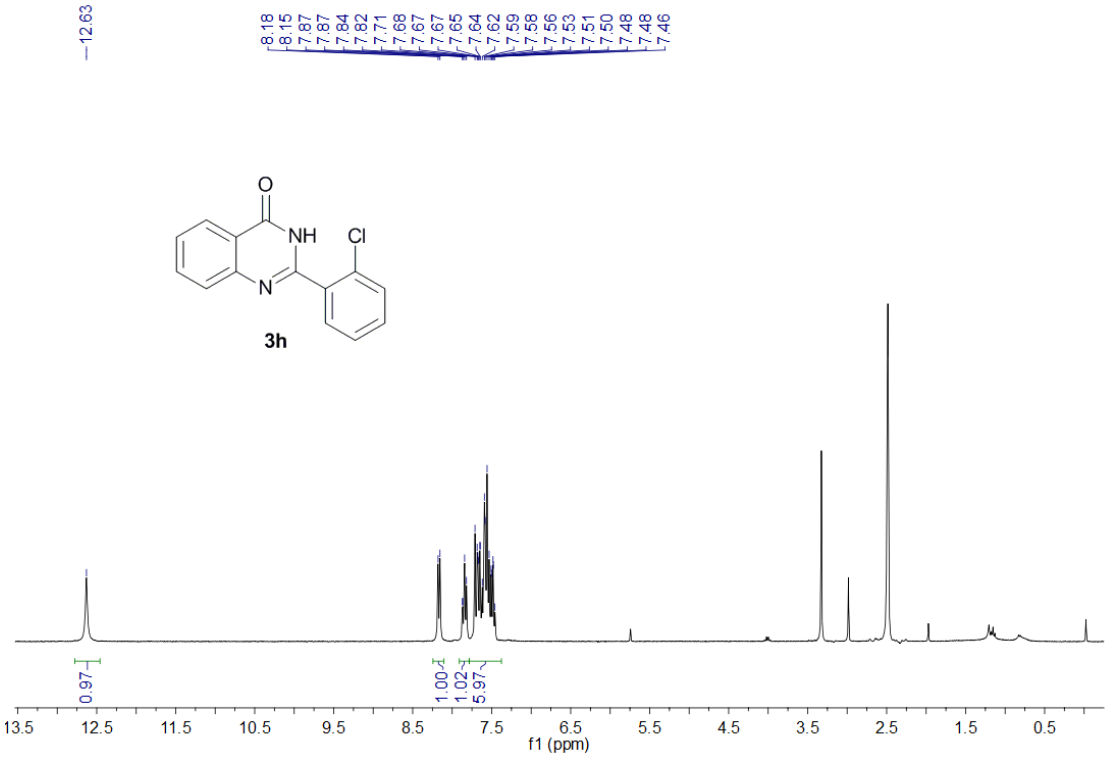
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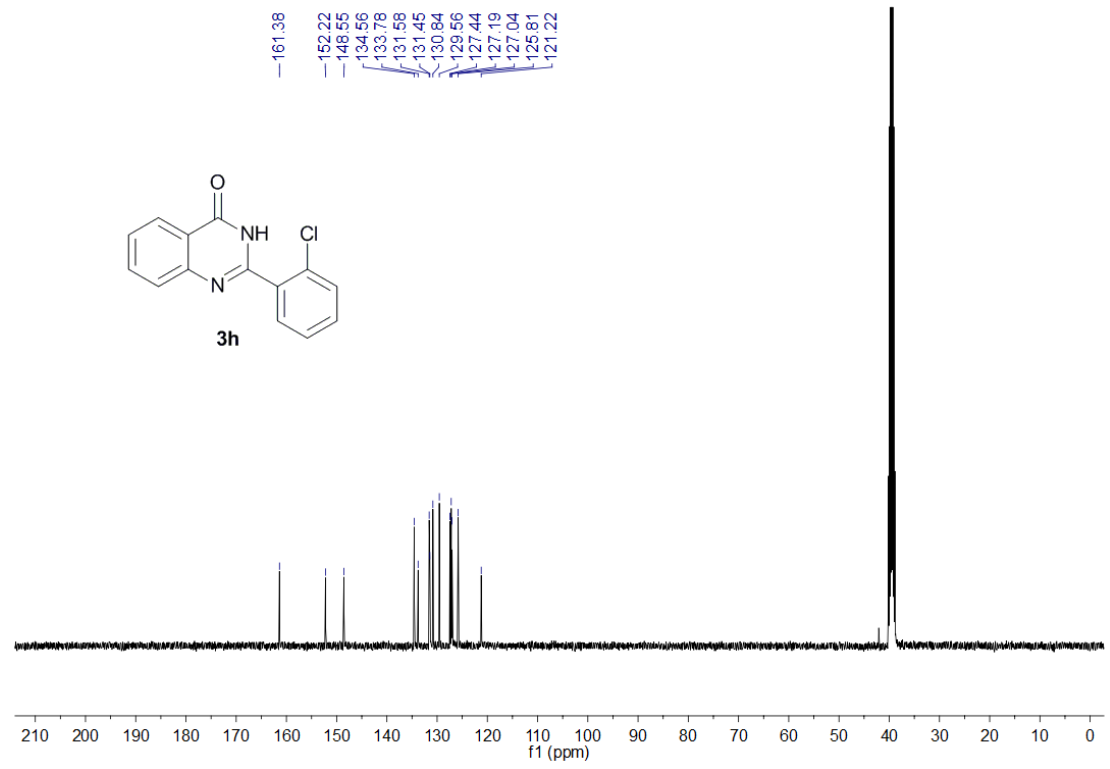
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130.84
129.56
127.44
127.19
127.04
125.81
121.22
O
NH
Cl
N
3h
210
200
190
180
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130
120
110
100
90
80
70
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50
40
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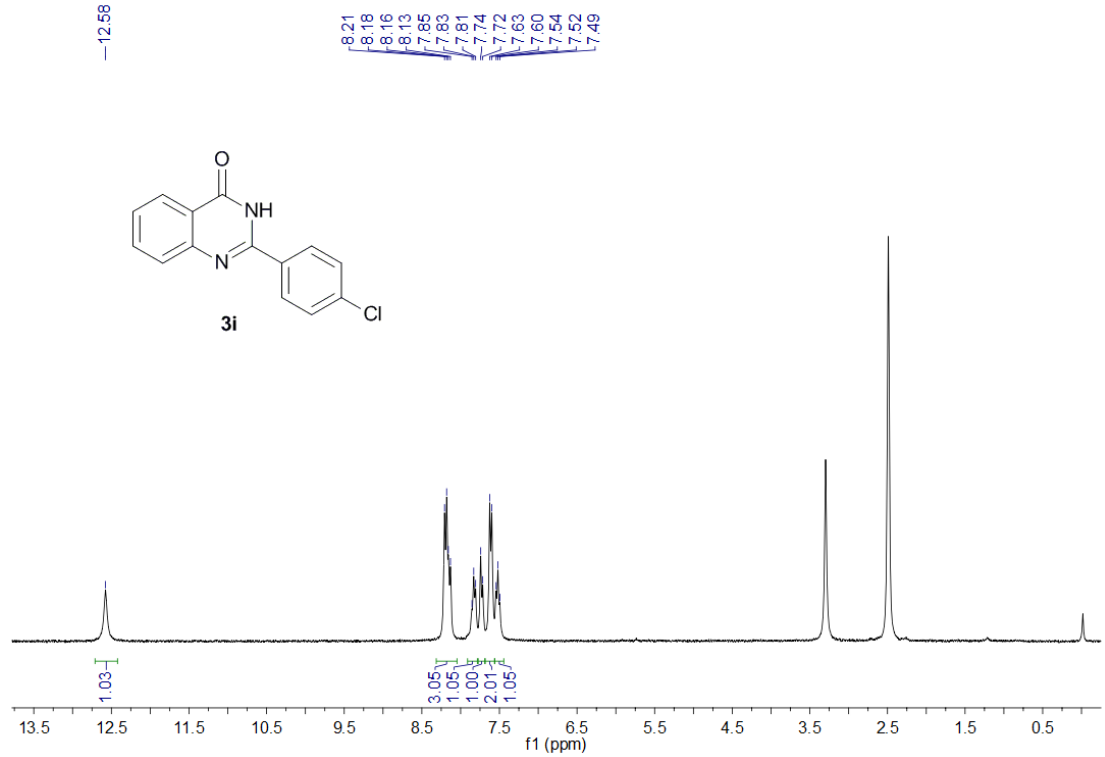
f1 (ppm)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7.54
7.52
7.49
O
NH
N
Cl
3i
1.03
3.05
1.05
1.00
2.01
1.05
13.5
12.5
11.5
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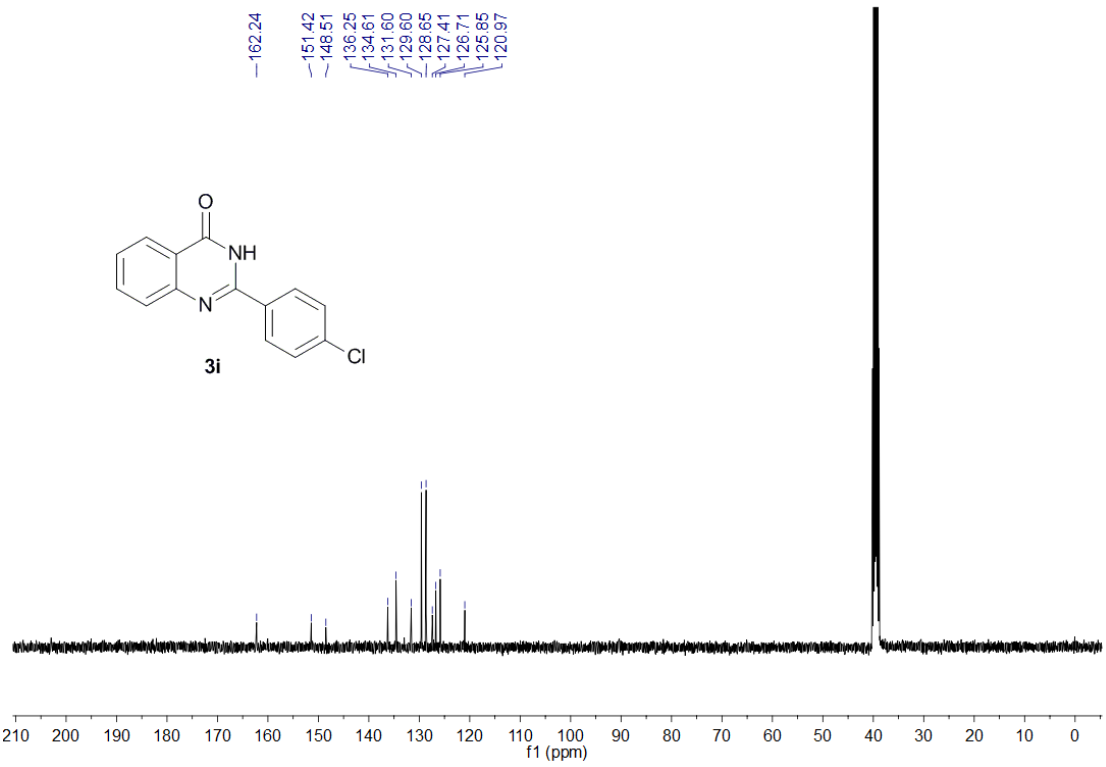
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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N
Cl
3i
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180
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50
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10
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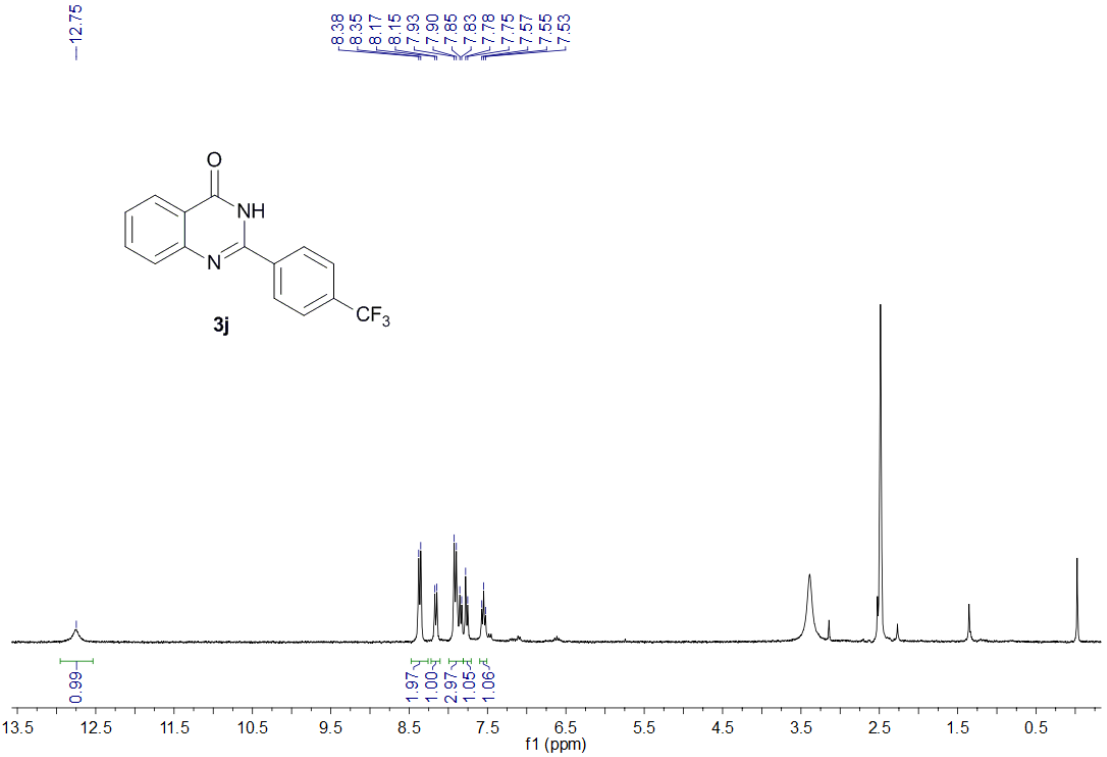
f1 (ppm)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7.78
7.75
7.57
7.55
7.53
O
NH
N
CF3
3j
0.99
1.97
1.00
2.97
1.05
1.06
13.5
12.5
11.5
10.5
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6.5
5.5
4.5
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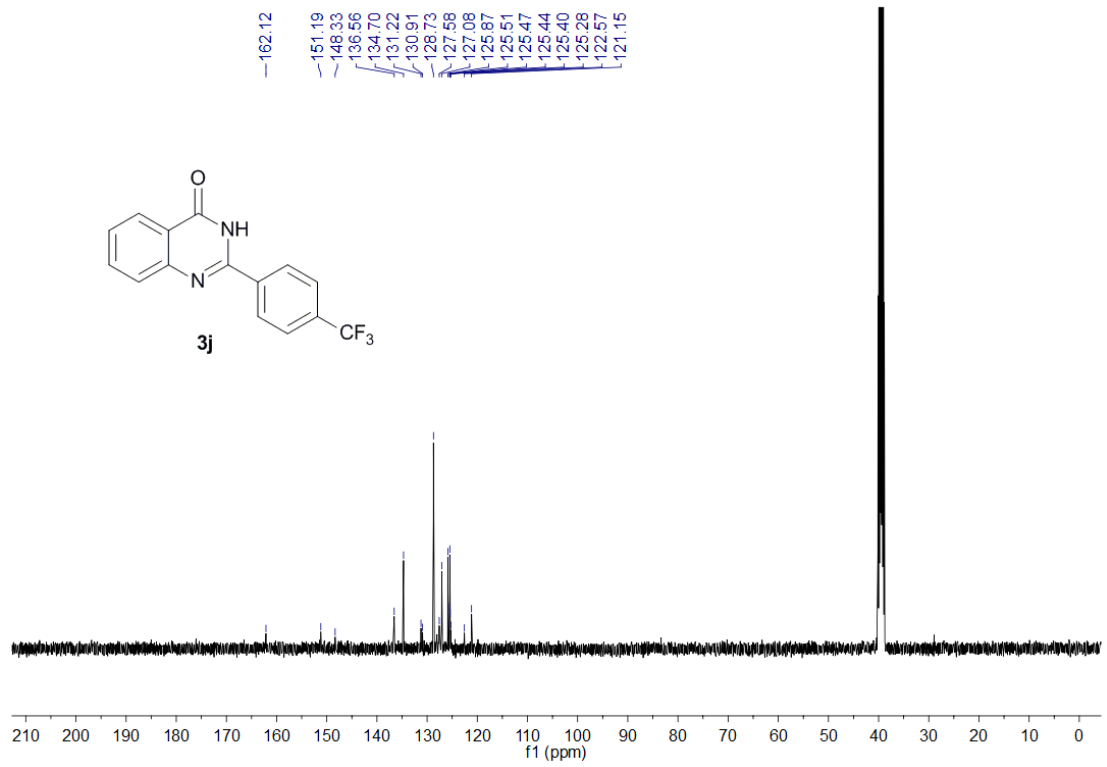
2.5
1.5
0.5
f1 (ppm)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125.51
125.47
125.44
125.40
125.28
122.57
121.15
O
NH
N
CF3
3j
210
200
190
180
170
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130
120
110
100
90
80
70
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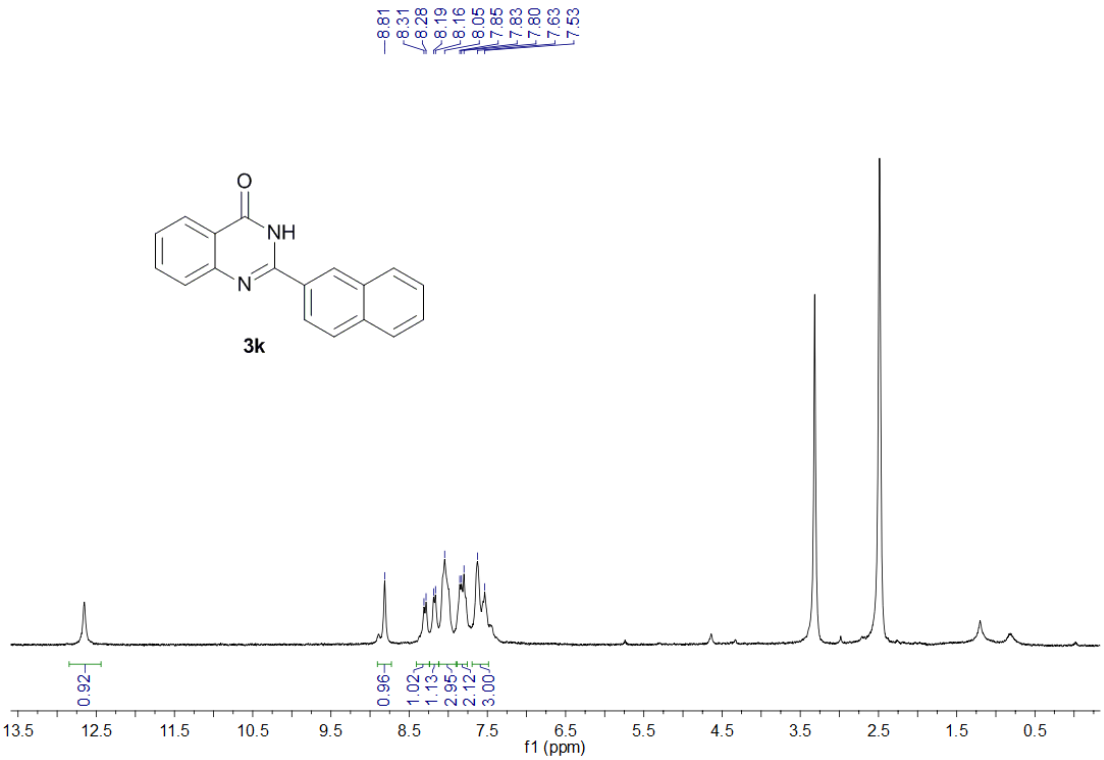
50
40
30
20
10
0
f1 (ppm)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8.19
8.16
8.05
7.85
7.83
7.80
7.63
7.53
O
NH
N
3k
0.92
0.96
1.02
1.13
2.95
2.12
3.00
13.5
12.5
11.5
10.5
9.5
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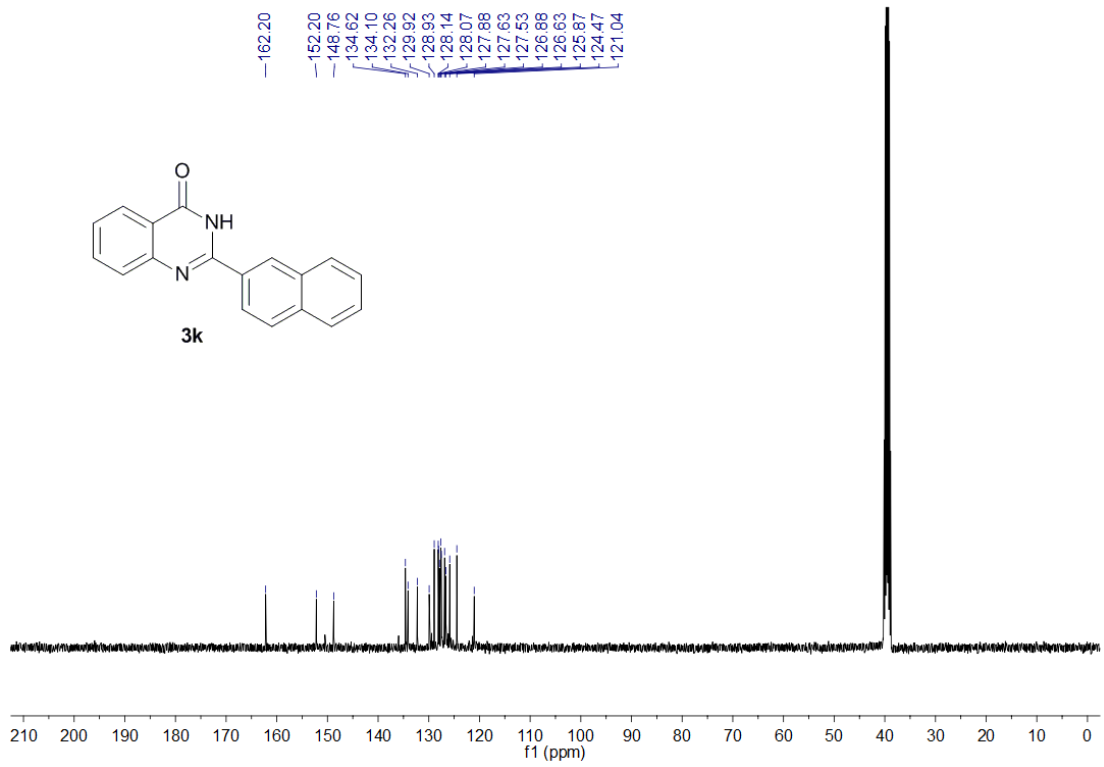
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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132.26
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128.14
128.07
127.88
127.63
127.53
126.88
126.63
125.87
124.47
121.04
O
NH
N
3k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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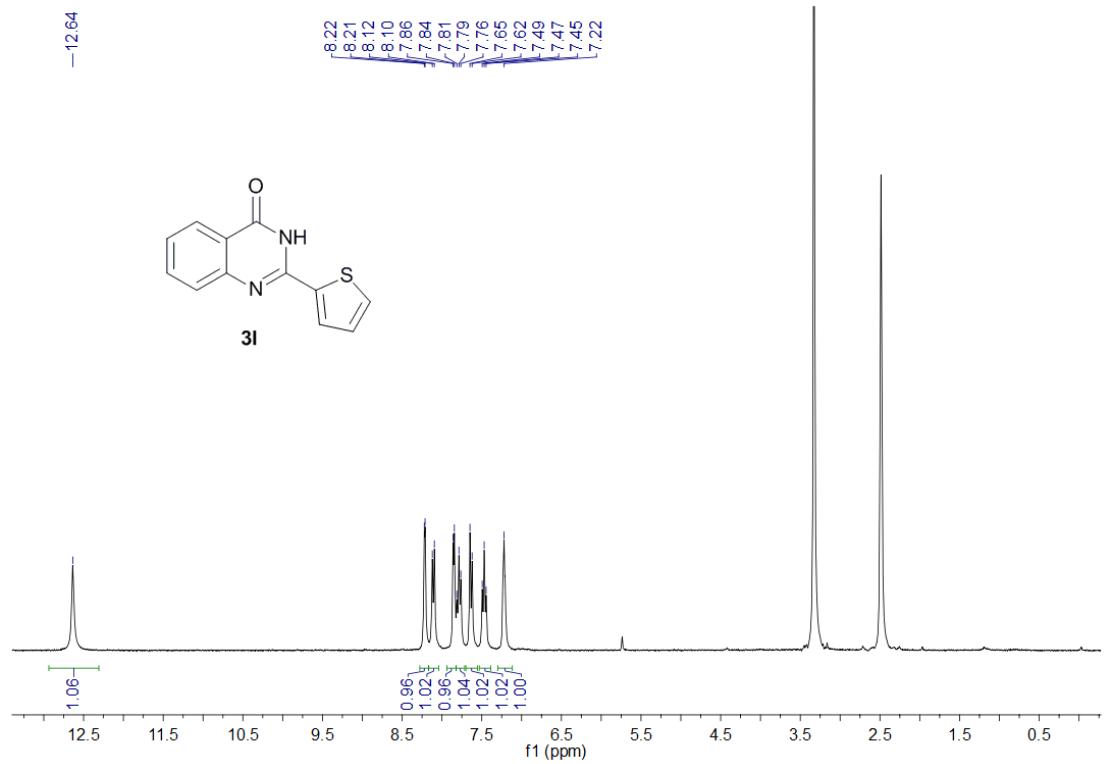
50
40
30
20
10
0
f1 (ppm)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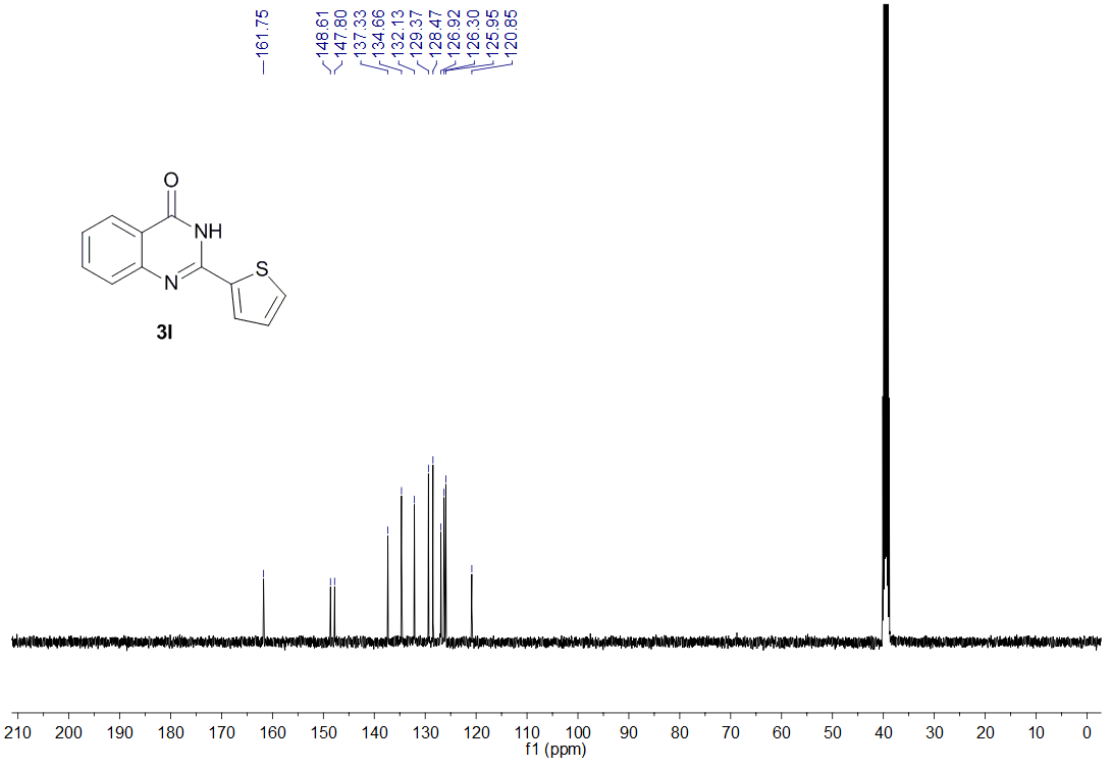
7.86
7.84
7.81
7.79
7.76
7.65
7.62
7.49
7.47
7.45
7.22
O
NH
N
S
3l
1.06
0.96
1.02
0.96
1.04
1.02
1.02
1.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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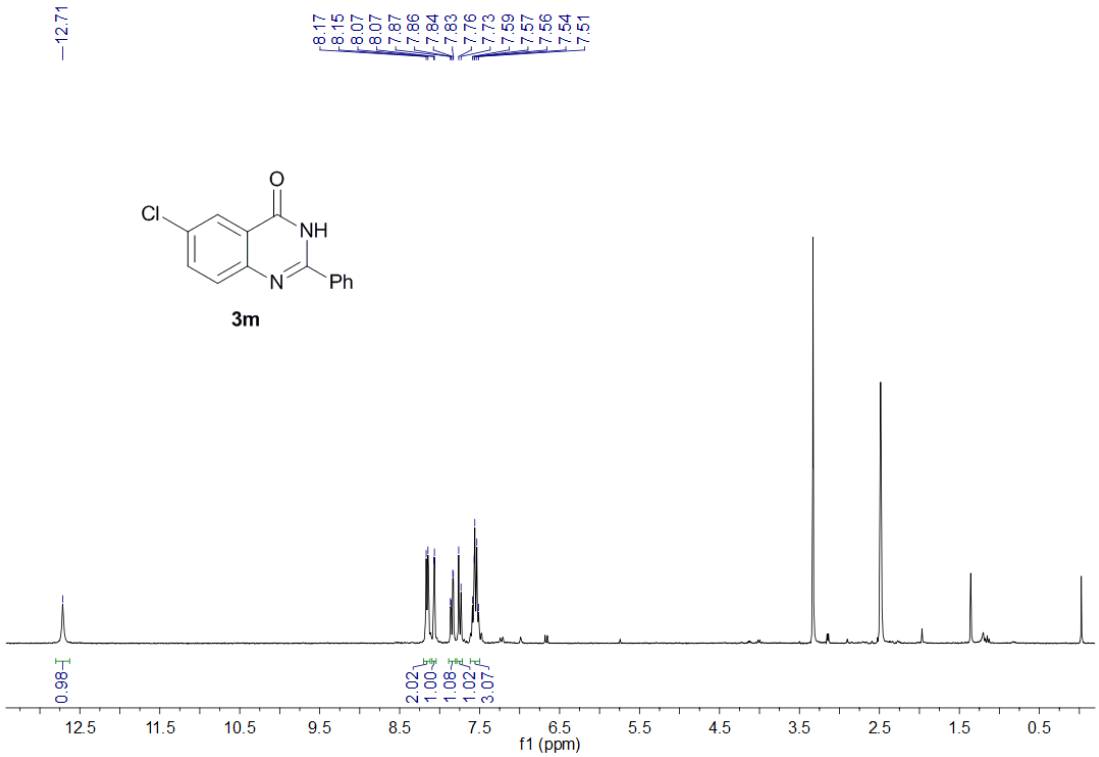
132.13
129.37
128.47
126.92
126.30
125.95
120.85
O
NH
N
S
3l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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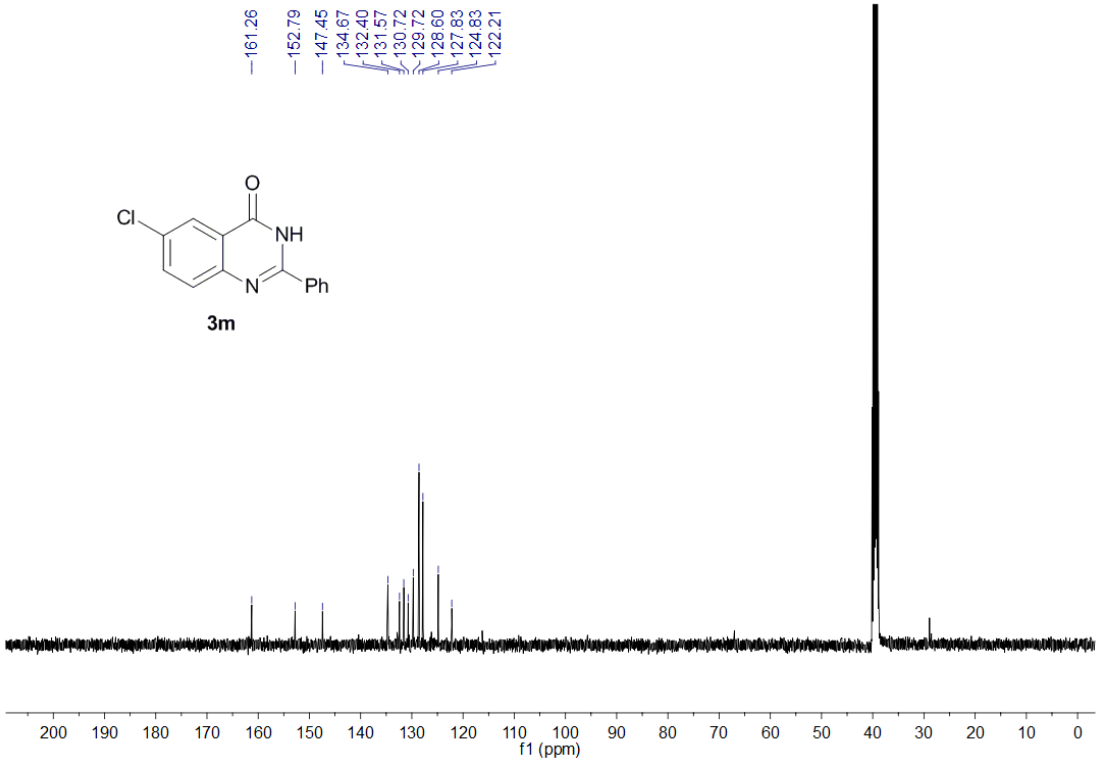
7.86
7.84
7.83
7.76
7.73
7.59
7.57
7.56
7.54
7.51
Cl
O
NH
N
Ph
3m
0.98
2.02
1.00
1.08
1.02
3.07
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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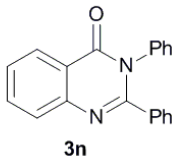
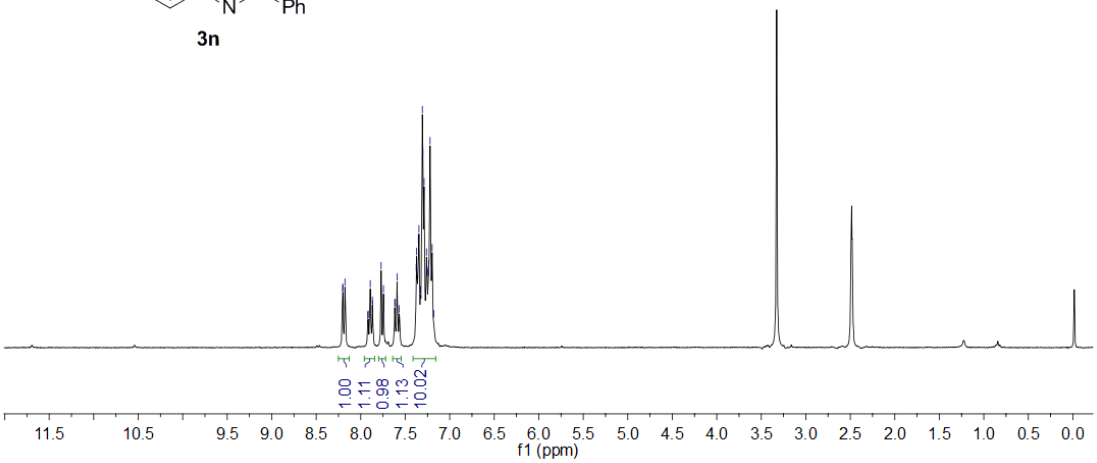
131.57
130.72
129.72
128.60
127.83
124.83
122.21
Cl
O
NH
N
Ph
3m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.20
8.20
8.18
7.92
7.92
7.89
7.87
7.87
7.77
7.74
7.62
7.62
7.59
7.57
7.38
7.37
7.35
7.35
7.33
7.31
7.30
7.29
7.26
7.25
7.24
7.24
7.22
7.20
7.18


O
N
Ph
N
Ph

3n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11.5
10.5
9.5
9.0
8.5
8.0
7.5
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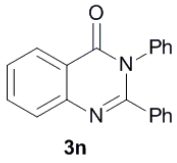
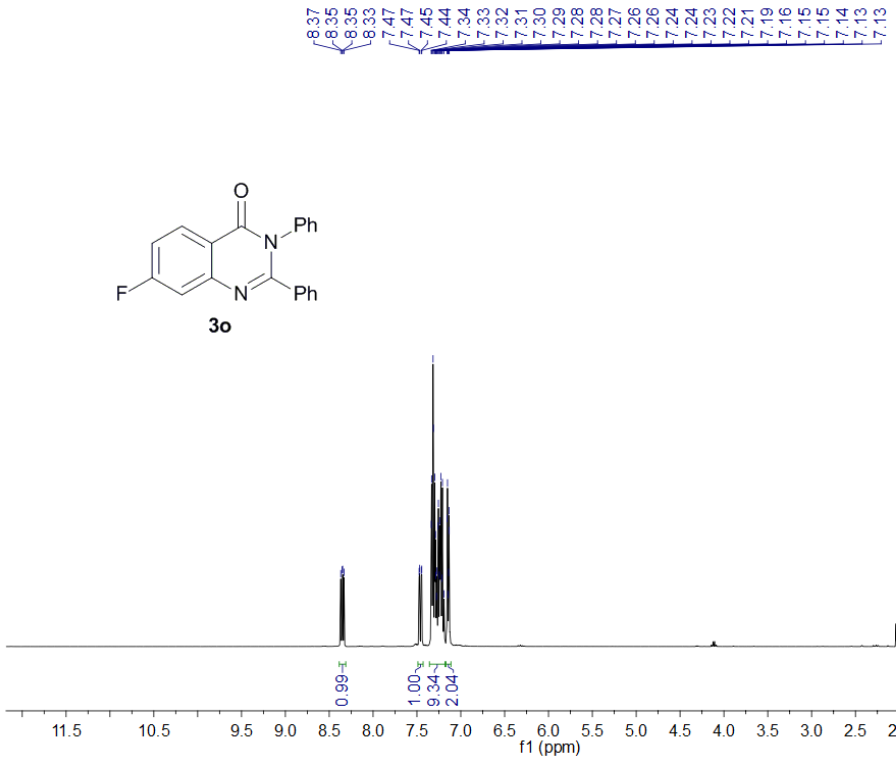
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.36
155.16
147.24
137.81
135.60
134.76
129.49
128.88
128.84
128.54
128.13
127.46
127.40
127.14
126.44
120.73


O
N
Ph
N
Ph

3n

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.37
8.35
8.35
8.33
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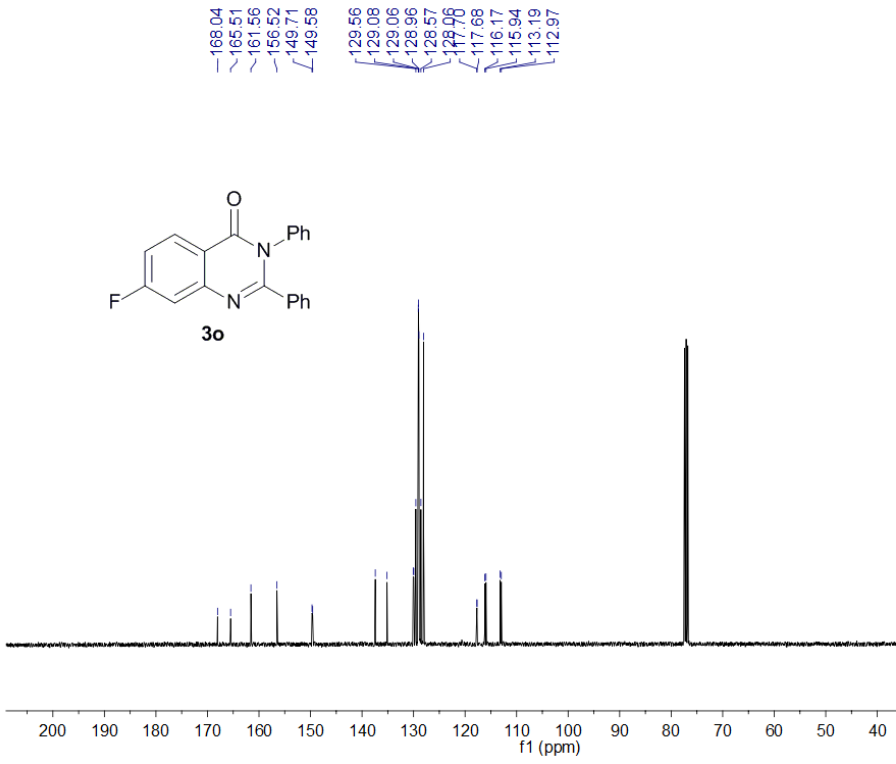
7.45
7.44
7.34
7.33
7.32
7.31
7.30
7.29
7.28
7.28
7.27
7.26
7.26
7.24
7.24
7.23
7.22
7.21
7.19
7.16
7.15
7.15
7.14
7.13
7.13
O
Ph
N
F
N
Ph
3o
0.99
1.00
9.34
2.04
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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165.51
161.56
156.52
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149.58
129.56
129.08
129.06
128.96
128.57
117.68
116.17
115.94
113.19
112.97
O
Ph
N
F
N
Ph
3o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.30
8.30
7.77
7.75
7.74
7.74
7.72
7.72
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.29
7.29
7.28
7.28
7.26
7.25
7.24
7.24
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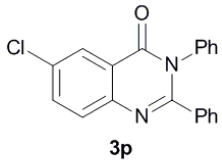
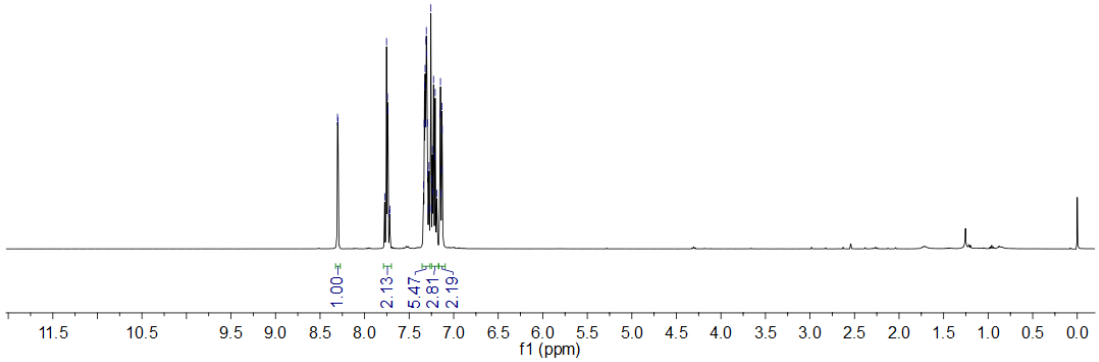
7.21
7.21
7.19
7.15
7.15
7.14
7.14
7.13
7.13


O
Cl
N
Ph
N
Ph

3p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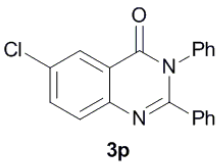
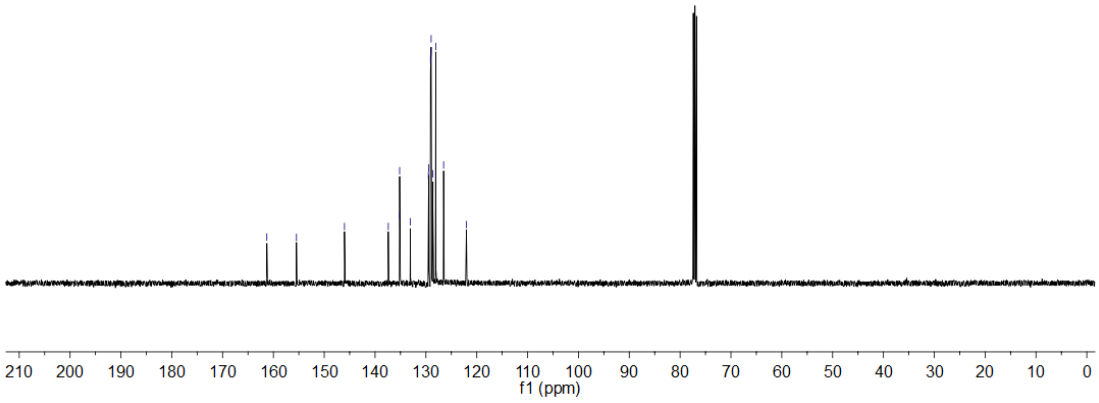
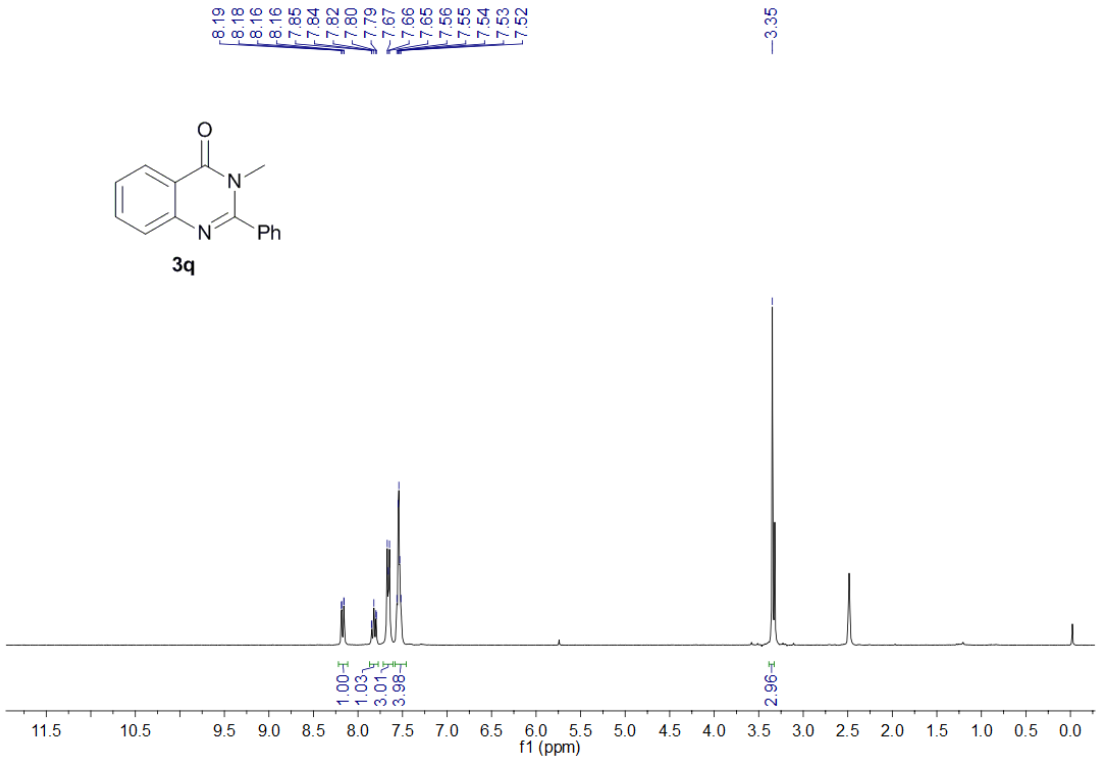
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.29
155.47
146.02
137.40
135.17
135.14
133.05
129.51
129.45
129.10
129.02
128.97
128.62
128.06
126.52
122.03


O
Cl
N
Ph
N
Ph

3p


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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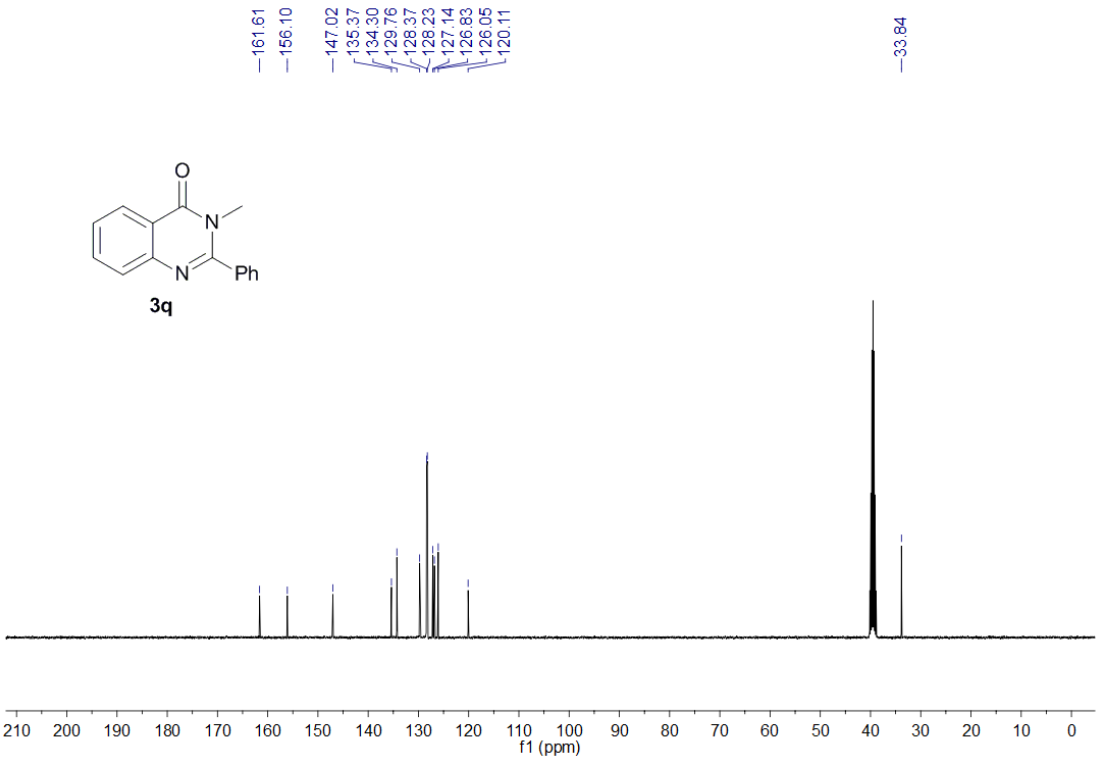
7.84
7.82
7.80
7.79
7.67
7.66
7.65
7.56
7.55
7.54
7.53
7.52
3.35
O
N
N
Ph
3q
1.00
1.03
3.01
3.98
2.96
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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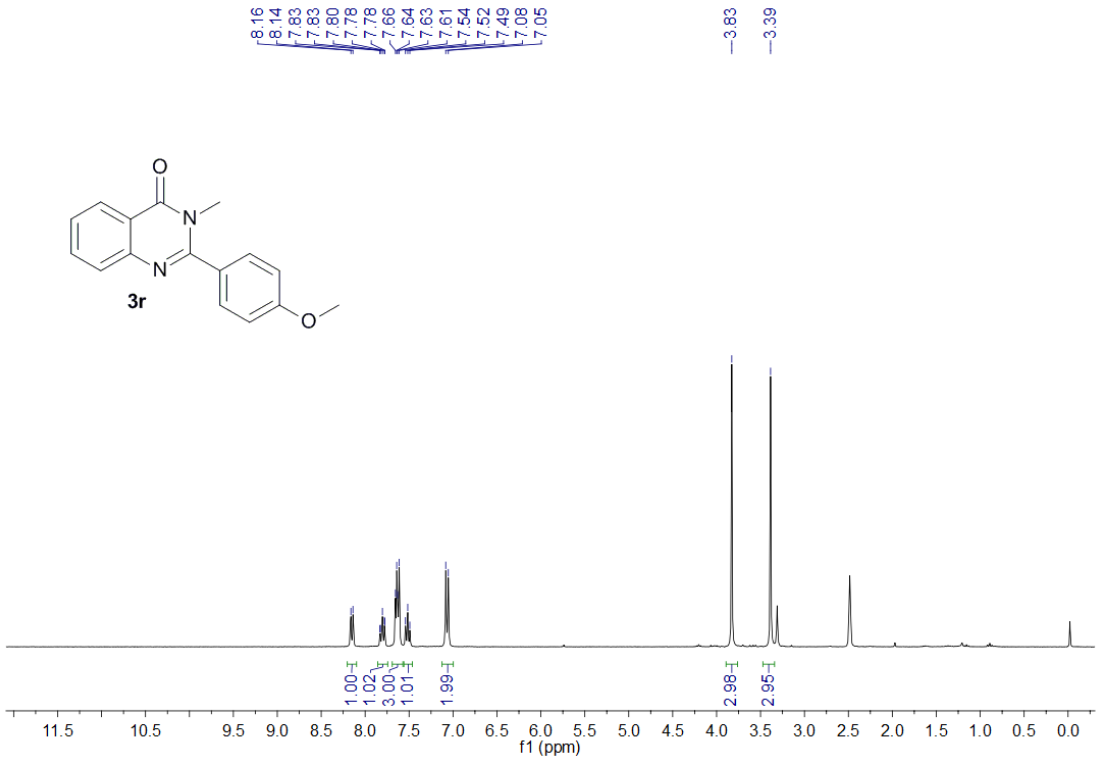
134.30
129.76
128.37
128.23
127.14
126.83
126.05
120.11
33.84
O
N
N
Ph
3q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.14
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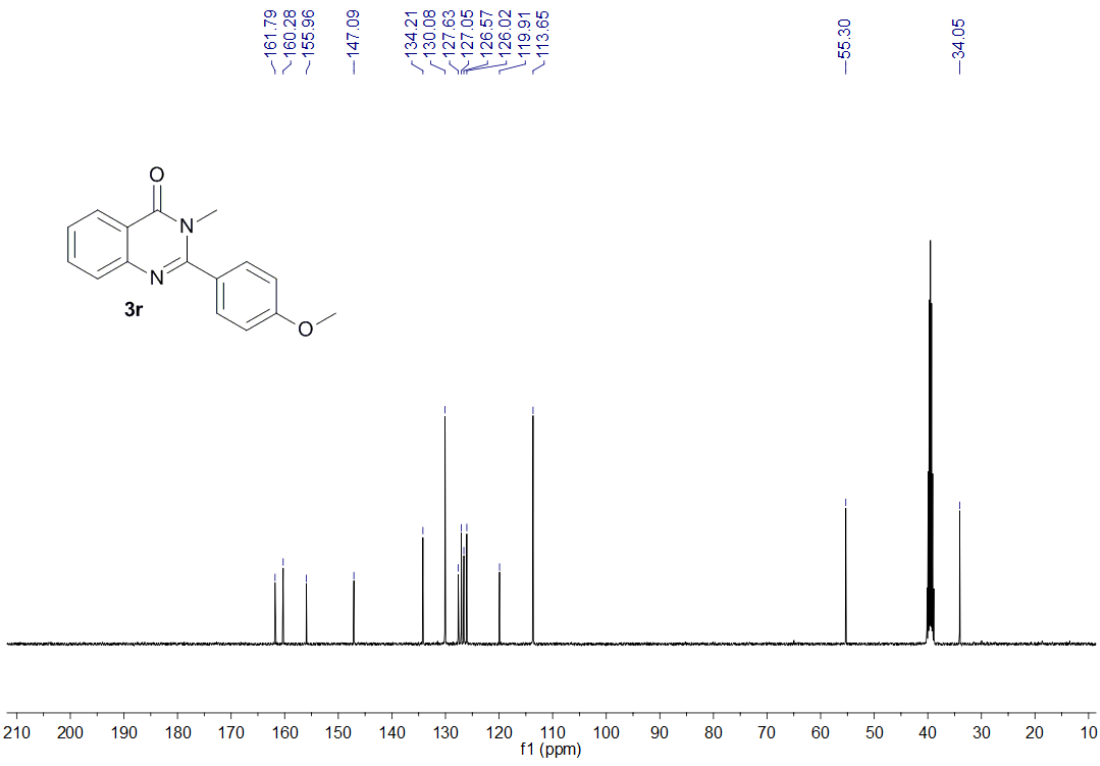
7.78
7.66
7.64
7.63
7.61
7.54
7.52
7.49
7.08
7.05
3.83
3.39
O
N
N
O
3r
1.00
1.02
3.00
1.01
1.99
2.98
2.95
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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147.09
134.21
130.08
127.63
127.05
126.57
126.02
119.91
113.65
55.30
34.05
O
N
N
O
3r
210
200
190
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120
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100
90
80
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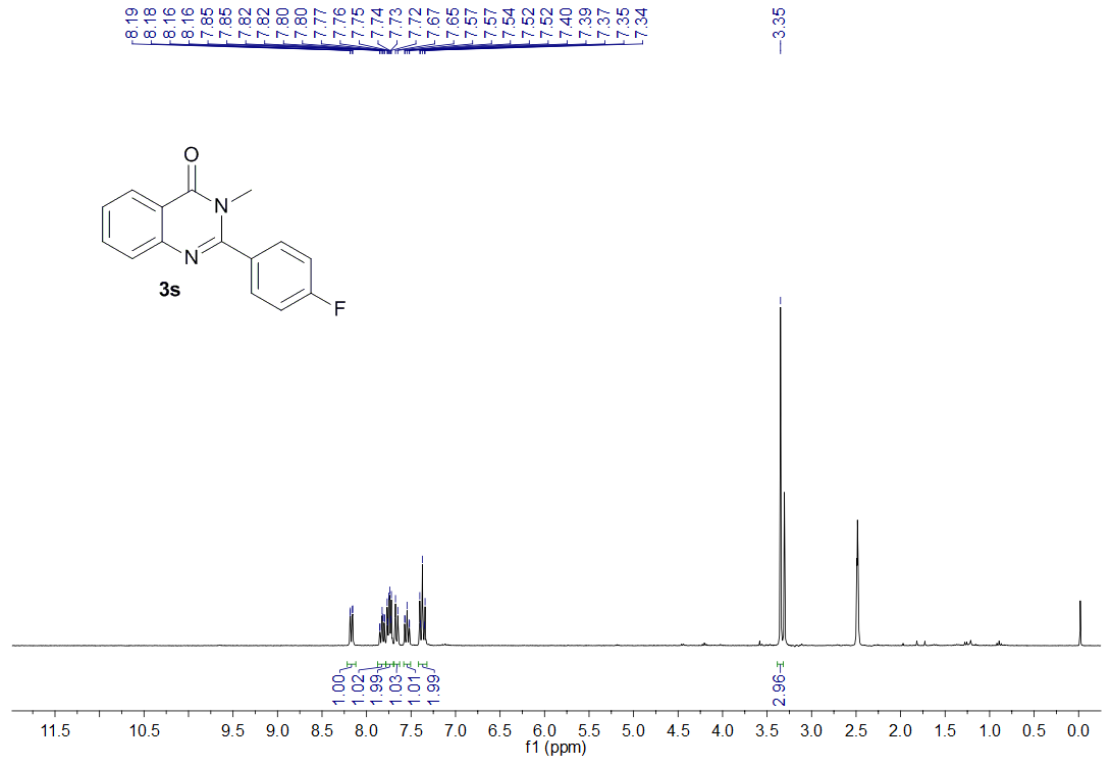
60
50
40
30
20
10
f1 (ppm)


8.19
8.18
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8.16
7.85
7.85
7.82
7.82
7.80
7.80
7.77
7.76
7.75
7.74
7.73
7.72
7.67
7.65
7.57
7.57
7.54
7.52
7.52
7.40
7.39
7.37
7.35
7.34
3.35
O
N
N
F
3s
1.00
1.02
1.99
1.03
1.01
1.99
2.96
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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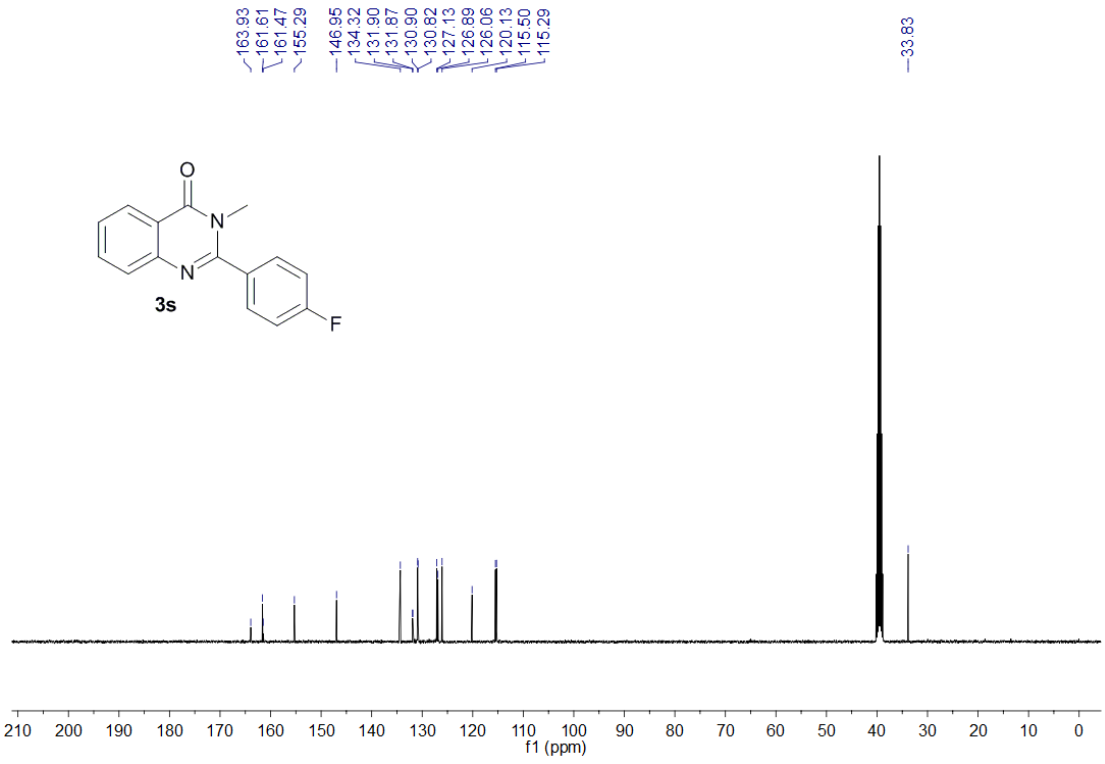
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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161.47
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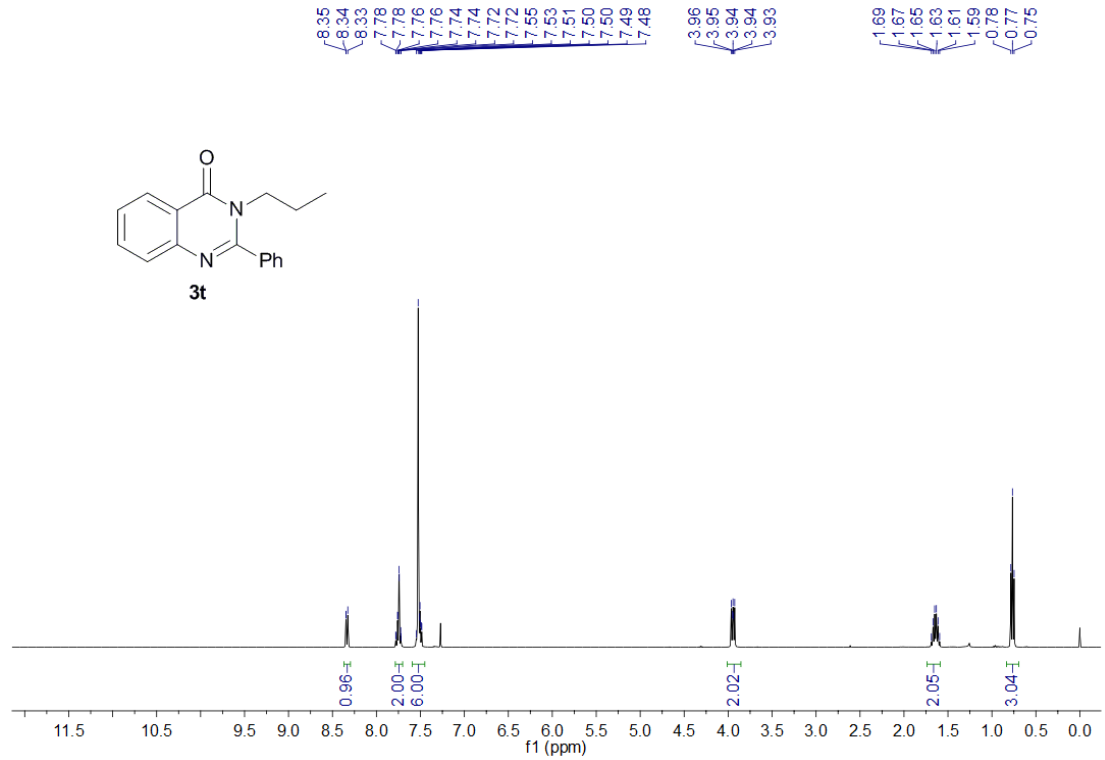
131.90
131.87
130.90
130.82
127.13
126.89
126.06
120.13
115.50
115.29
33.83
O
N
N
F
3s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.34
8.33
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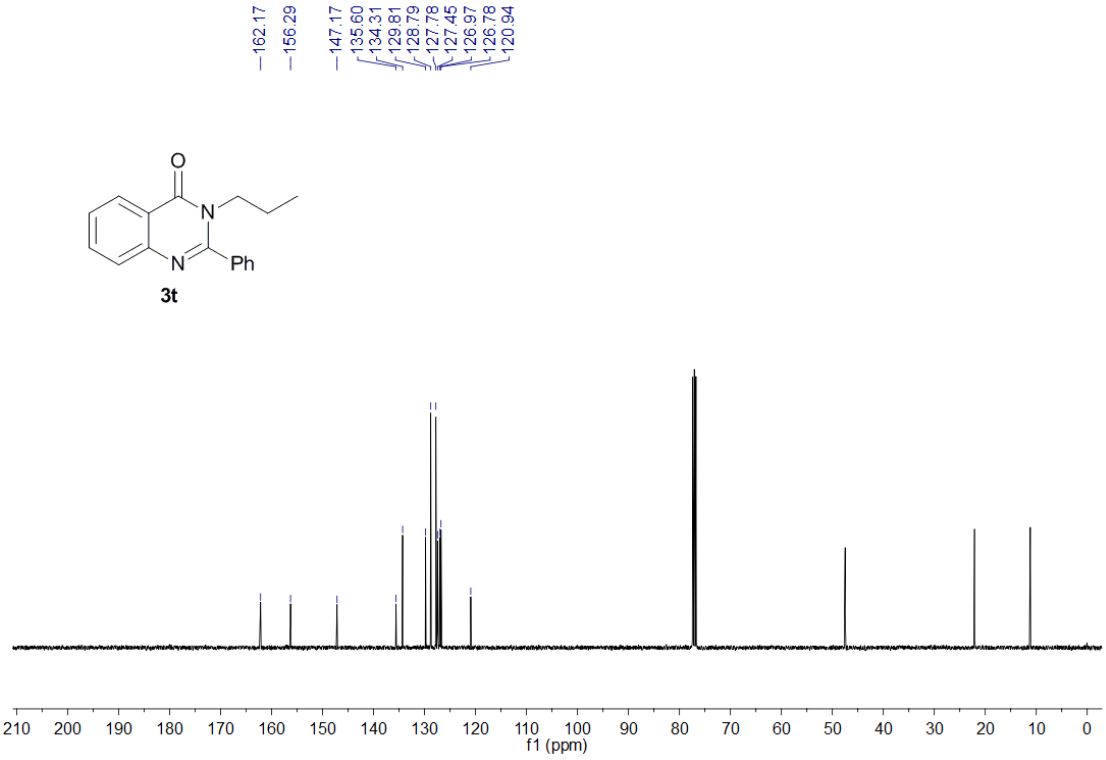
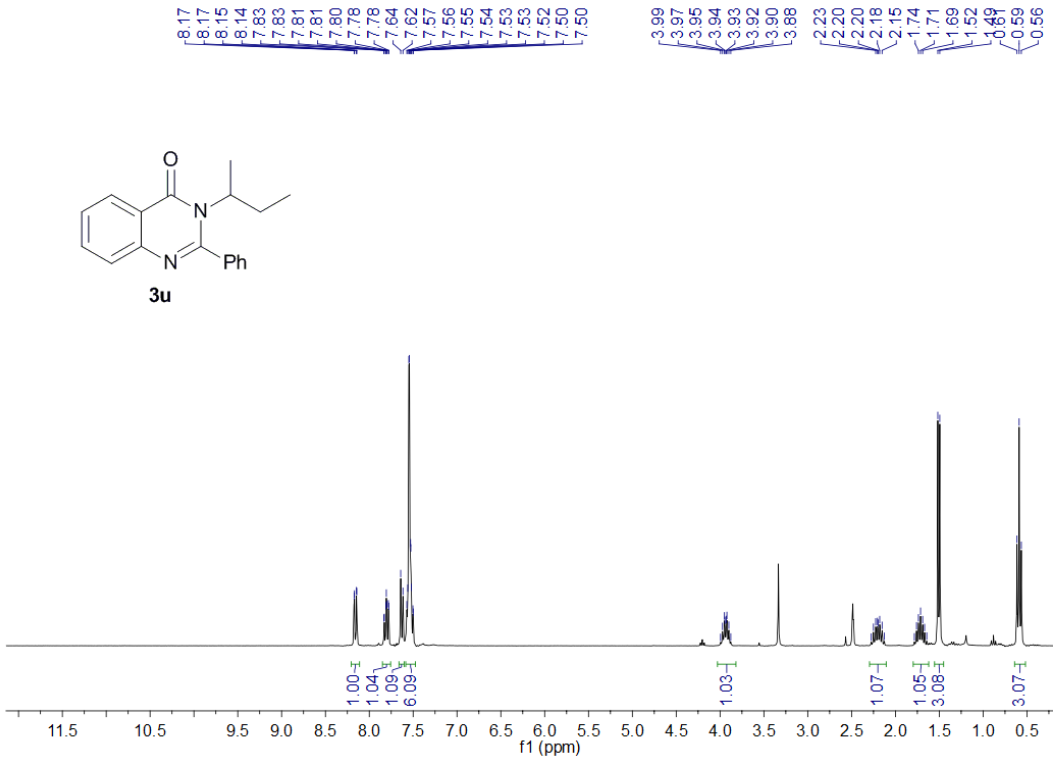
7.78
7.76
7.76
7.74
7.74
7.72
7.72
7.55
7.53
7.51
7.50
7.50
7.49
7.48
3.96
3.95
3.94
3.94
3.93
1.69
1.67
1.65
1.63
1.61
1.59
0.78
0.77
0.75
O
N
N
Ph
3t
0.96
2.00
6.00
2.02
2.05
3.04
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


162.17
156.29
147.17
135.60
134.31
129.81
128.79
127.78
127.45
126.97
126.78
120.94
O
N
N
Ph
3t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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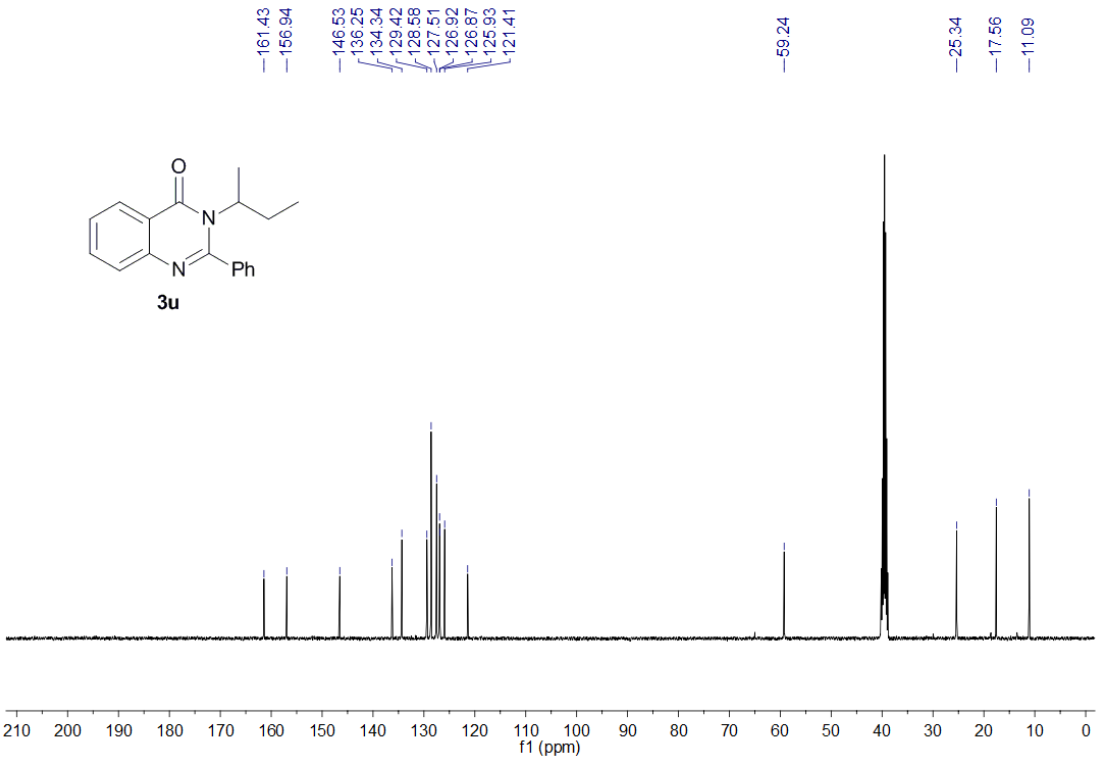
8.17
8.15
8.14
7.83
7.83
7.81
7.81
7.80
7.78
7.78
7.64
7.62
7.57
7.56
7.55
7.54
7.53
7.53
7.52
7.50
7.50
3.99
3.97
3.95
3.94
3.93
3.92
3.90
3.88
2.23
2.20
2.20
2.18
2.15
1.74
1.71
1.69
1.52
1.49
0.61
0.59
0.56
O
N
N
Ph
3u
1.00
1.04
1.09
6.09
1.03
1.07
1.05
3.08
3.07
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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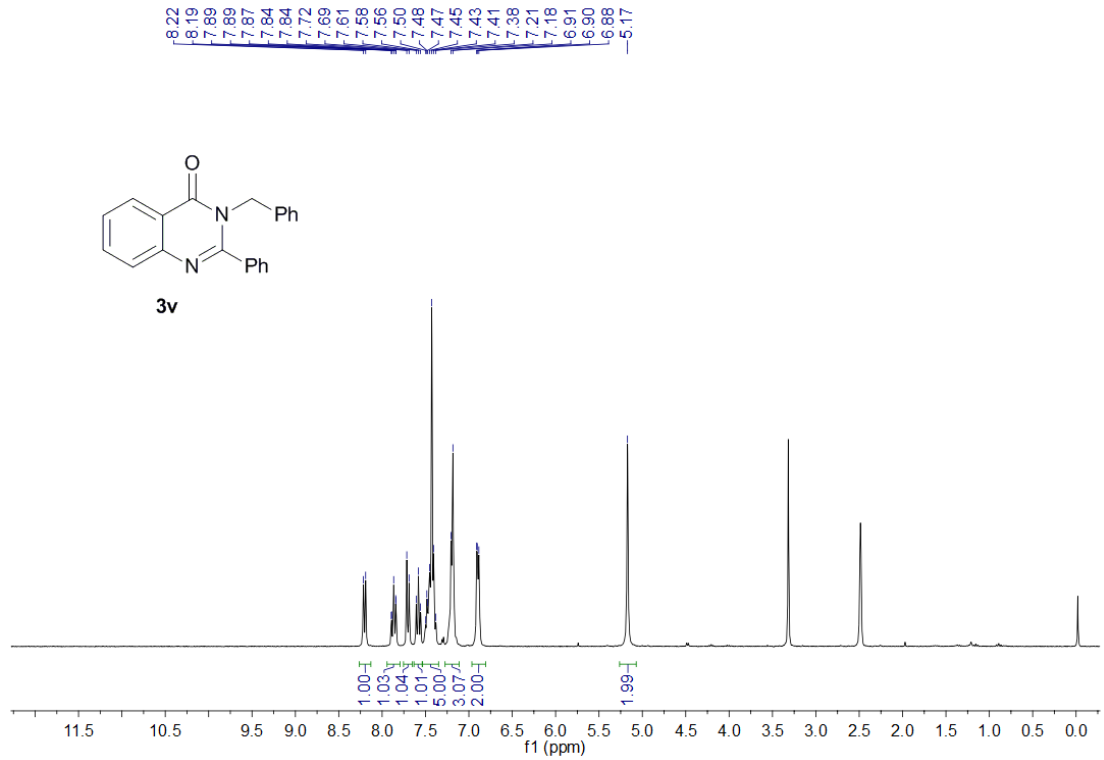
156.94
146.53
136.25
134.34
129.42
128.58
127.51
126.92
126.87
125.93
121.41
59.24
25.34
17.56
11.09
O
N
N
Ph
3u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.22
8.19
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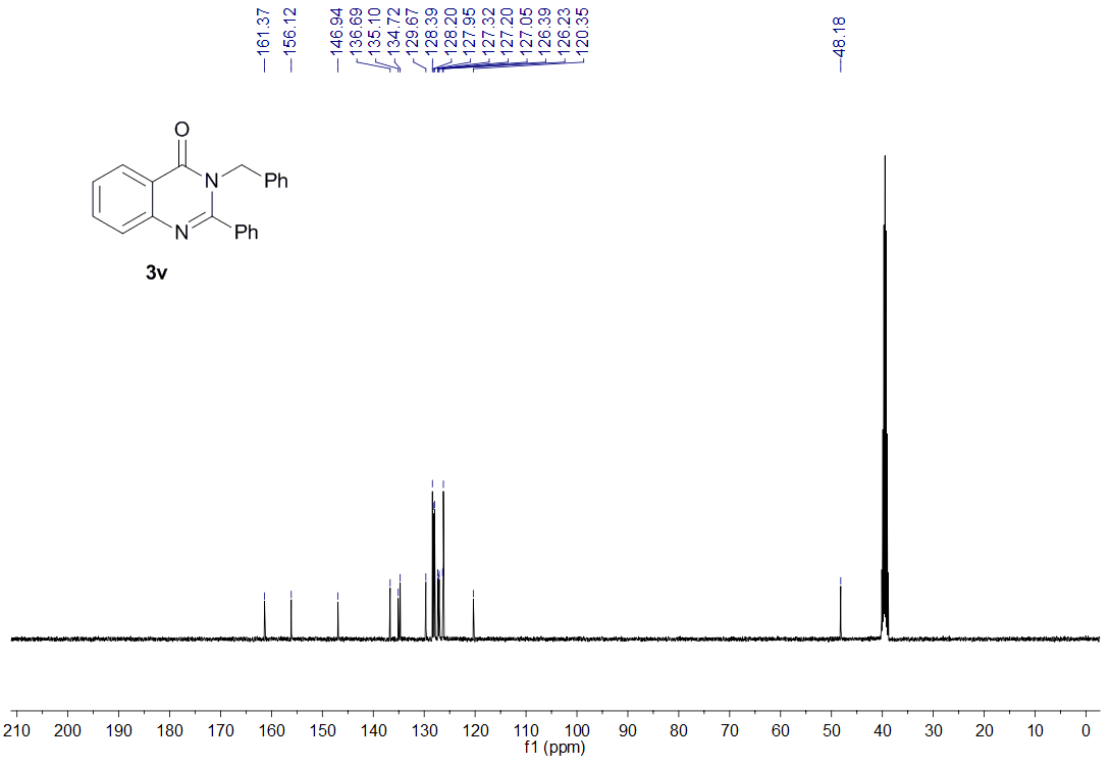
7.84
7.72
7.69
7.61
7.58
7.56
7.50
7.48
7.47
7.45
7.43
7.41
7.38
7.21
7.18
6.91
6.90
6.88
5.17
O
N
Ph
N
Ph
3v
1.00
1.03
1.04
1.01
5.00
3.07
2.00
1.99
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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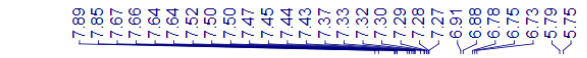
156.12
146.94
136.69
135.10
134.72
129.67
128.39
128.20
127.95
127.32
127.20
127.05
126.39
126.23
120.35
48.18
O
N
Ph
N
Ph
3v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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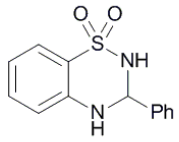
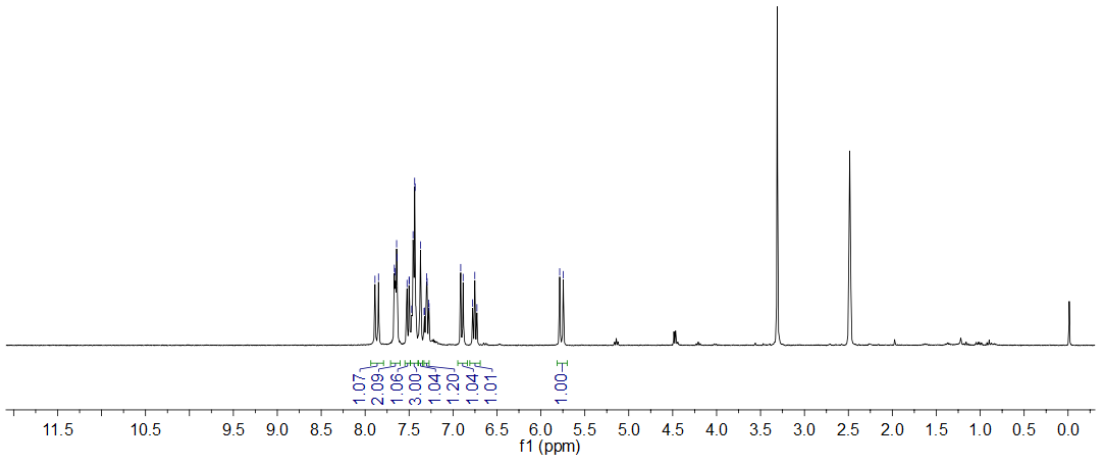
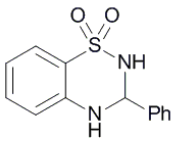
7.85
7.67
7.66
7.64
7.64
7.52
7.50
7.50
7.47
7.45
7.44
7.43
7.37
7.33
7.32
7.30
7.29
7.28
7.27
6.91
6.88
6.78
6.75
6.73
5.79
5.75


O
O
S
NH
N
H
Ph

3w

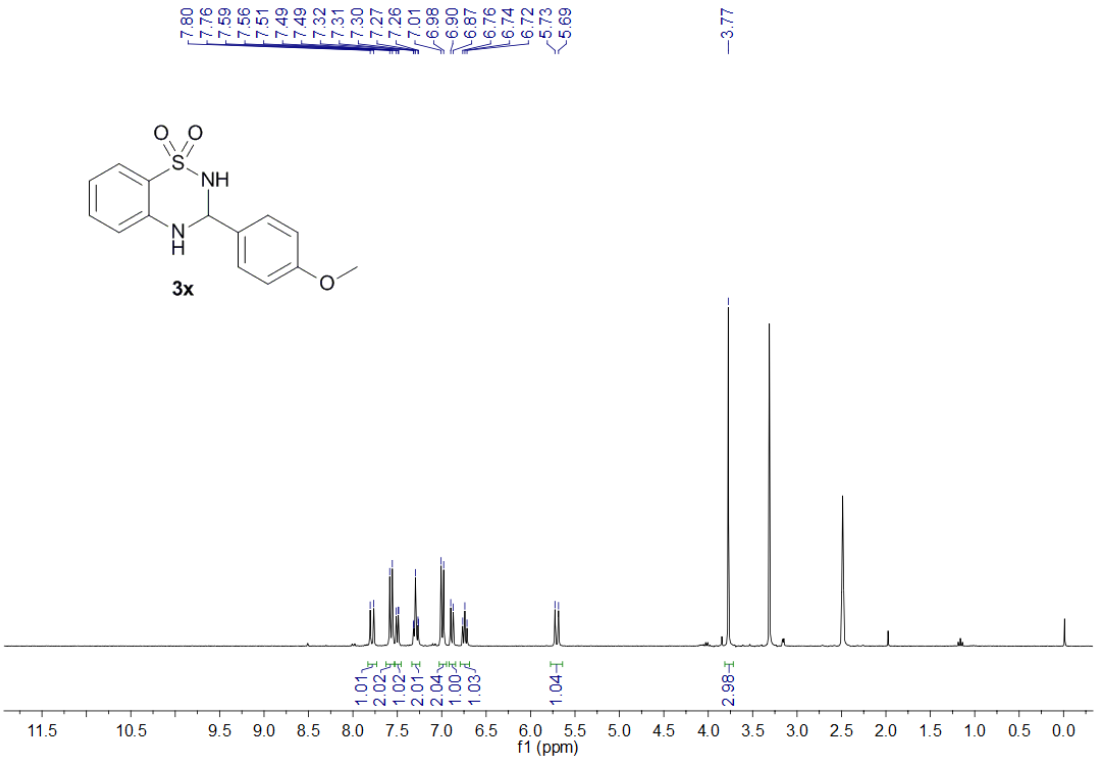

1.07
2.09
1.06
3.00
1.04
1.20
1.04
1.01
1.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

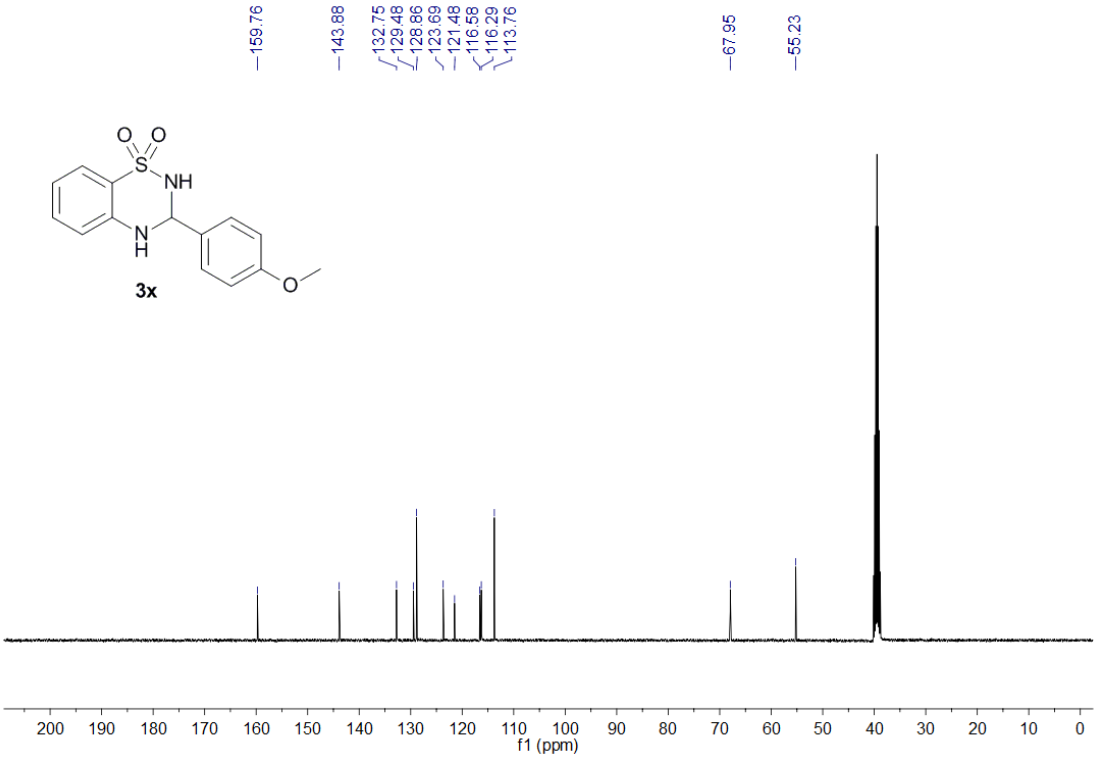

143.88
137.27
132.79
129.10
128.49
127.53
123.71
121.62
116.70
116.37
68.37

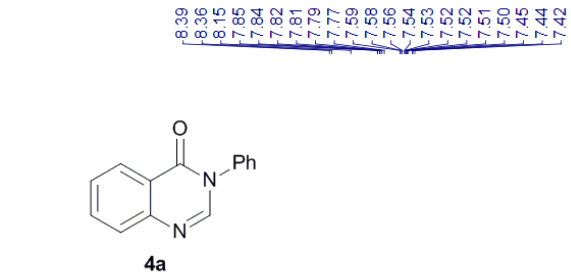

O
O
S
NH
N
H
Ph

3w

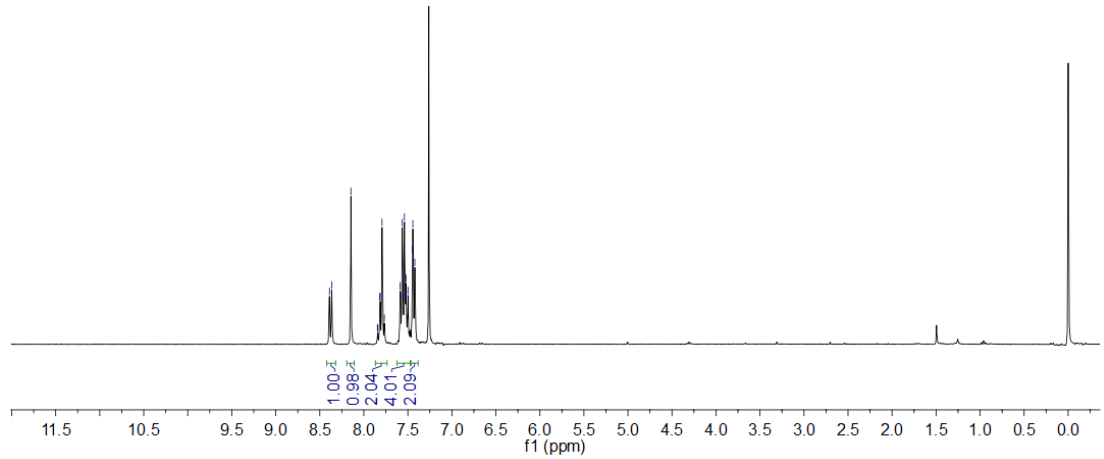
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

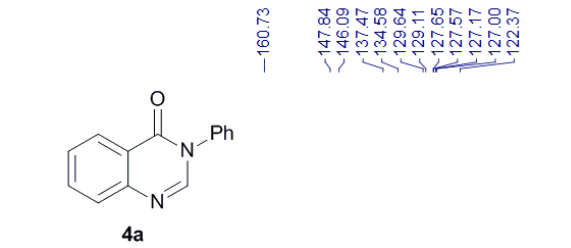

7.80
7.76
7.59
7.56
7.51
7.49
7.49
7.32
7.31
7.30
7.27
7.26
7.01
6.98
6.90
6.87
6.76
6.74
6.72
5.73
5.69
3.77
O
O
S
NH
N
H
O
3x
1.01
2.02
1.02
2.01
2.04
1.00
1.03
1.04
2.98
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


159.76
143.88
132.75
129.48
128.86
123.69
121.48
116.58
116.29
113.76
67.95
55.23
O
O
S
NH
N
H
O
3x
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

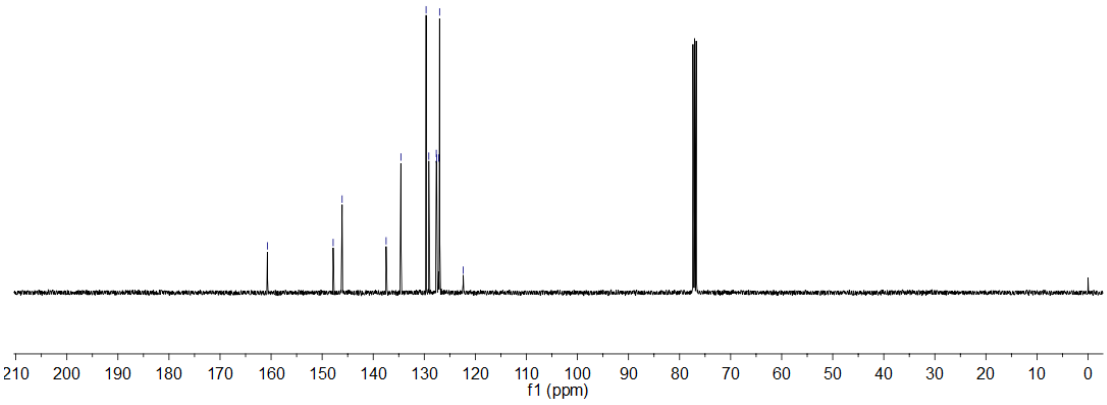

8.39
8.36
8.15
7.85
7.84
7.82
7.81
7.79
7.77
7.59
7.58
7.56
7.54
7.53
7.52
7.52
7.51
7.50
7.45
7.44
7.42
O
N
Ph
N

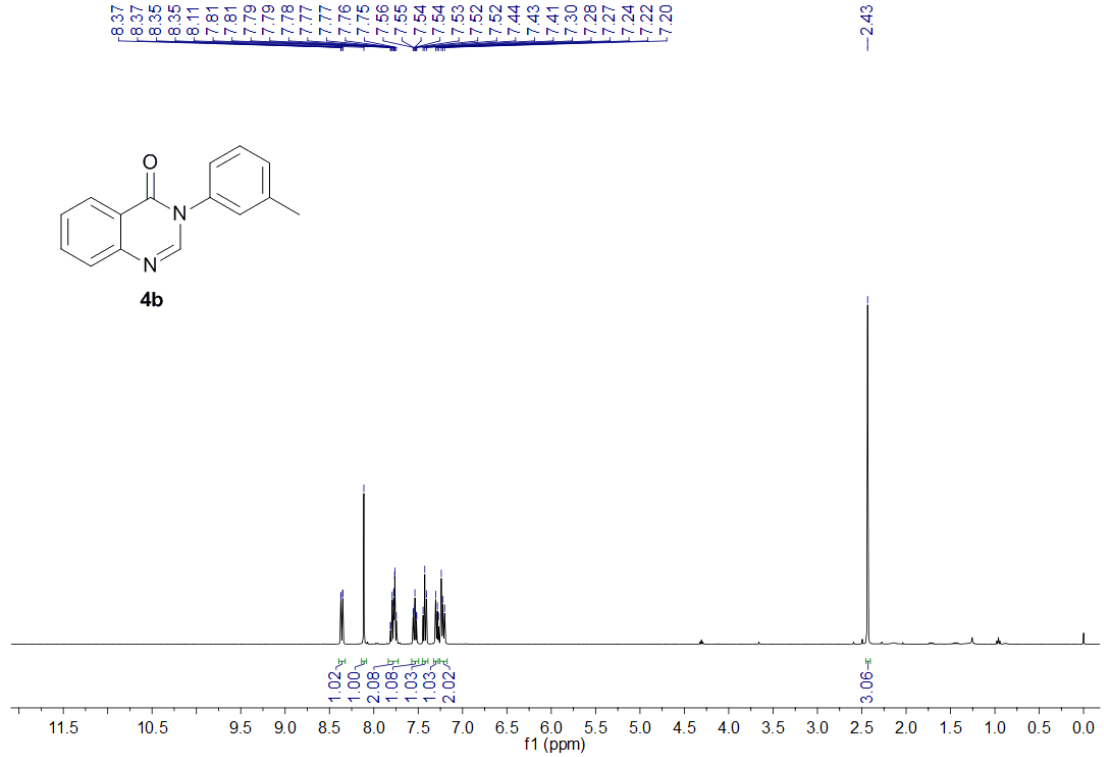
4a

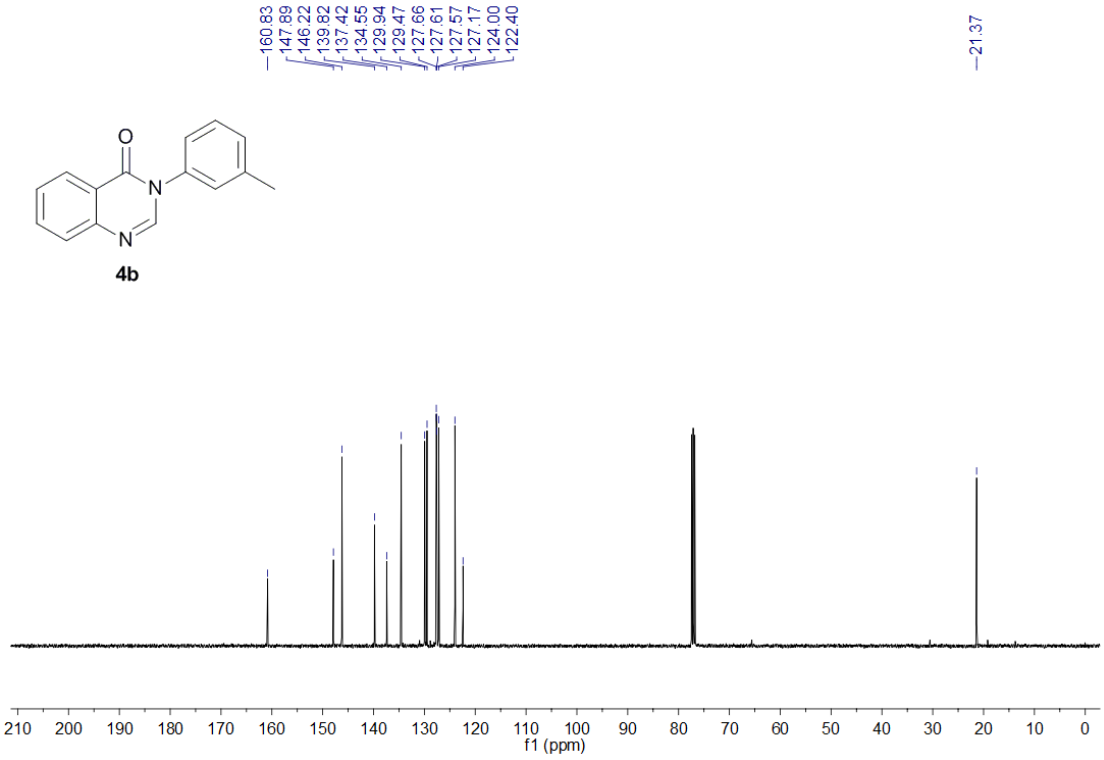

1.00
0.98
2.04
4.01
2.09
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.73
147.84
146.09
137.47
134.58
129.64
129.11
127.65
127.57
127.17
127.00
122.37
O
N
Ph
N

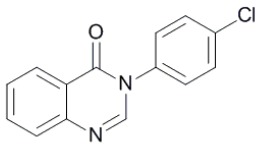
4a


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

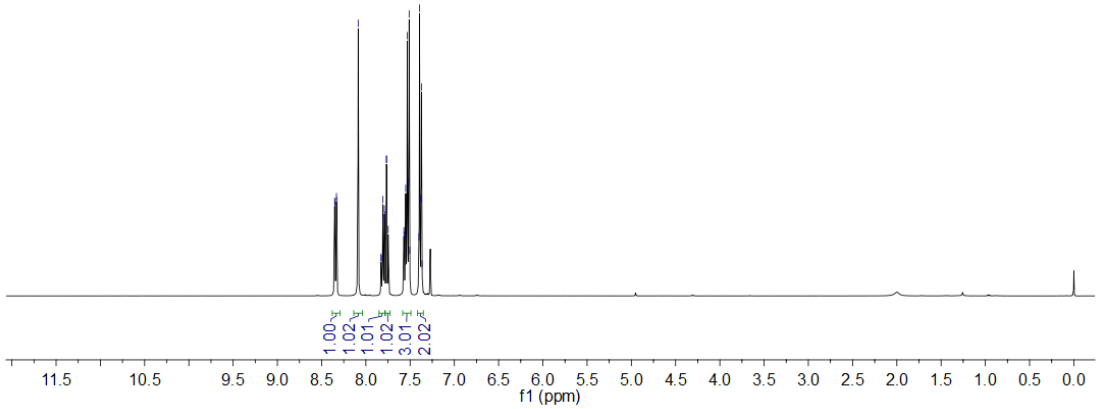

8.37
8.37
8.35
8.35
8.11
7.81
7.81
7.79
7.79
7.78
7.77
7.77
7.76
7.75
7.56
7.55
7.54
7.54
7.53
7.52
7.44
7.43
7.41
7.30
7.28
7.27
7.24
7.22
7.20
2.43
O
N
N
4b
1.02
1.00
2.08
1.08
1.03
1.03
2.02
3.06
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

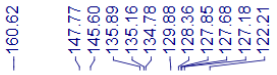

160.83
147.89
146.22
139.82
137.42
134.55
129.94
129.47
127.66
127.61
127.57
127.17
124.00
122.40
21.37
O
N
N
4b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.35
8.35
8.33
8.33
8.09
7.83
7.82
7.81
7.80
7.79
7.79
7.77
7.77
7.75
7.57
7.57
7.55
7.53
7.52
7.51
7.50
7.40
7.39
7.39
7.38
7.37
7.37


O
N
N
Cl

4c


1.00
1.02
1.01
1.02
3.01
2.02
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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145.60
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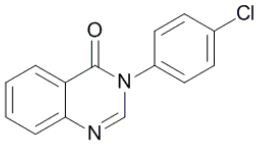
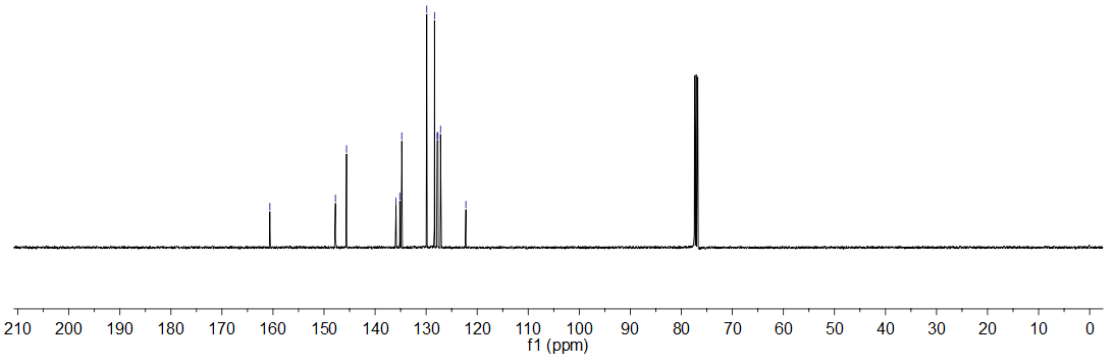
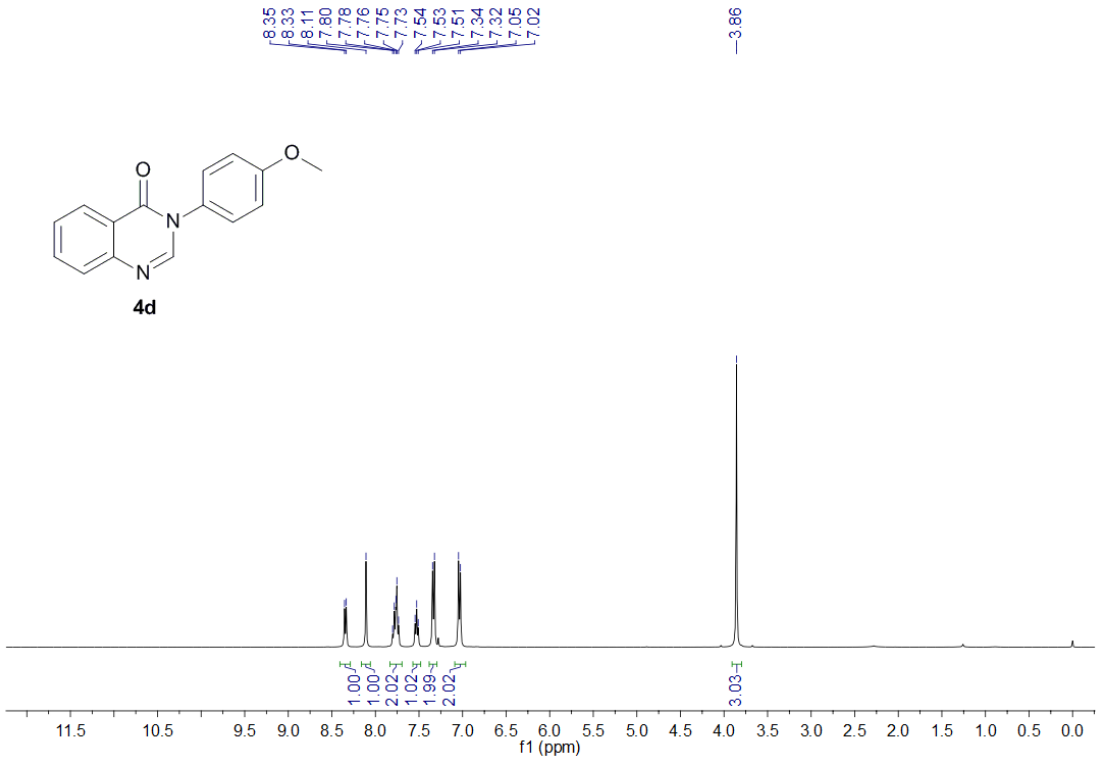
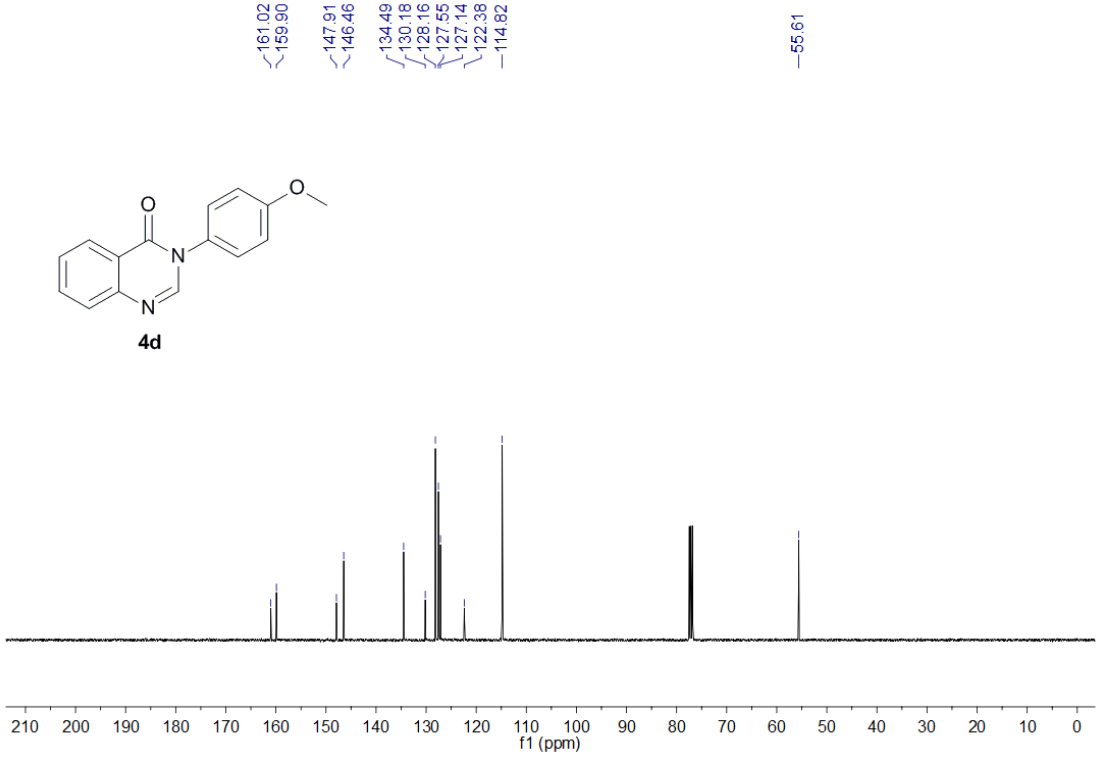
135.16
134.78
129.88
128.36
127.85
127.68
127.18
122.21


O
N
N
Cl

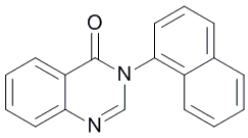
4c


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

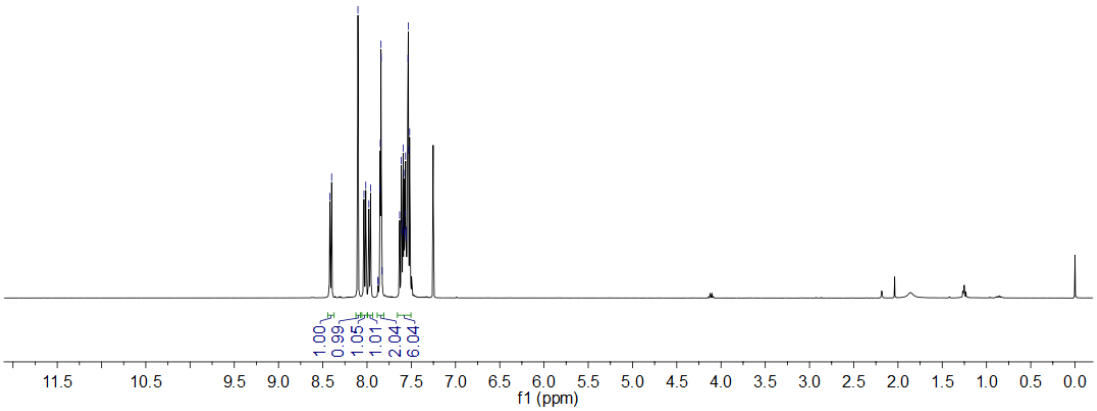

8.35
8.33
8.11
7.80
7.78
7.76
7.75
7.73
7.54
7.53
7.51
7.34
7.32
7.05
7.02
3.86
O
O
N
N
4d
1.00
1.00
2.02
1.02
1.99
2.02
3.03
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.02
159.90
147.91
146.46
134.49
130.18
128.16
127.55
127.14
122.38
114.82
55.61
O
O
N
N
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.42
8.40
8.10
8.03
8.01
7.98
7.96
7.88
7.87
7.86
7.85
7.84
7.84
7.83
7.63
7.61
7.60
7.60
7.59
7.58
7.58
7.58
7.57
7.56
7.56
7.56
7.54
7.53
7.53
7.52


O
N
N

4e


1.00
0.99
1.05
1.01
2.04
6.04
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.12
148.19
146.91
134.78
134.42
134.11
130.33
129.78
128.67
127.83
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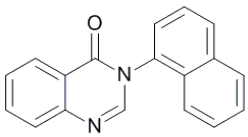
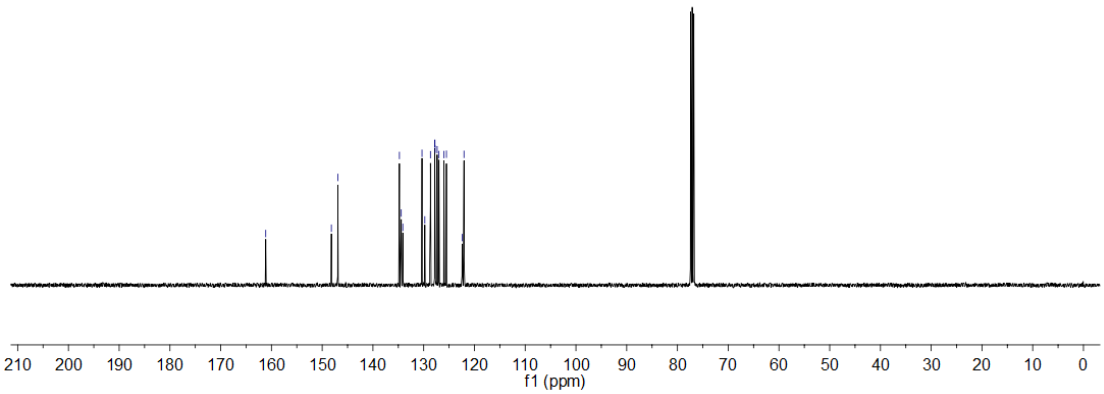
127.75
127.35
127.00
126.02
125.52
122.43
122.06


O
N
N

4e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200
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180
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160
150
140
130
120
110
100
90
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70
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50
40
30
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10
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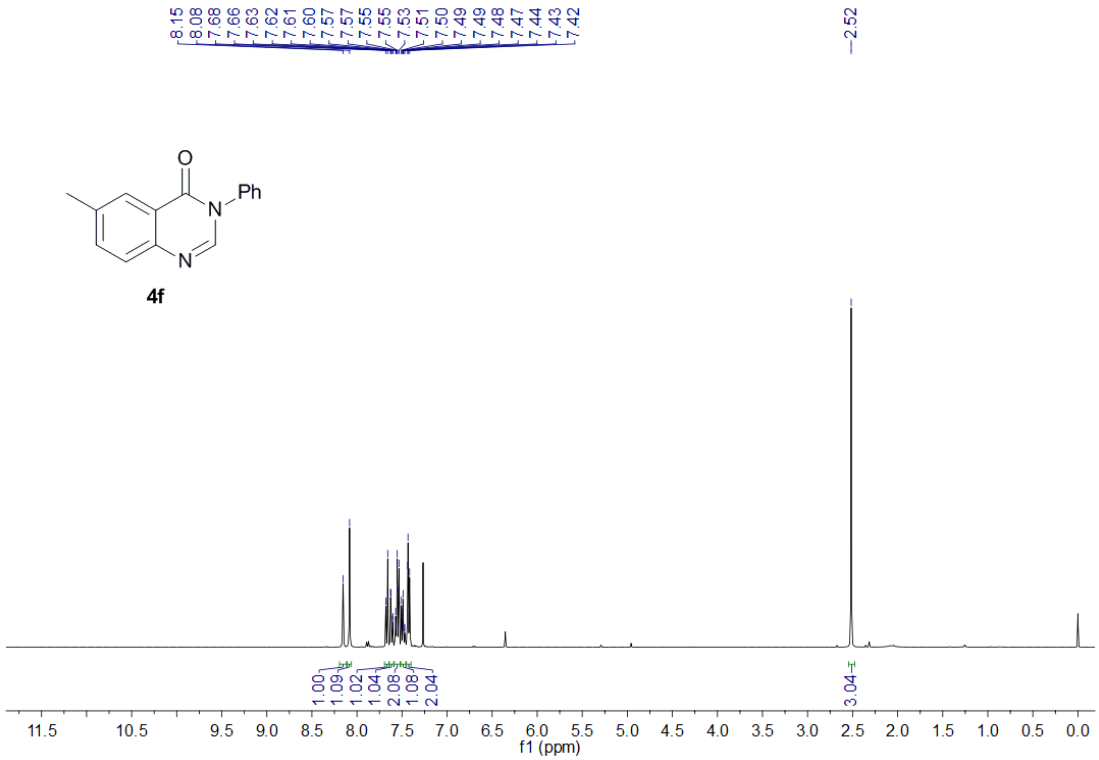
f1 (ppm)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8.08
7.68
7.66
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7.62
7.61
7.60
7.57
7.57
7.55
7.55
7.53
7.51
7.50
7.49
7.49
7.48
7.47
7.44
7.43
7.42
2.52
O
N
Ph
N
4f
1.00
1.09
1.02
1.04
2.08
1.08
2.04
3.04
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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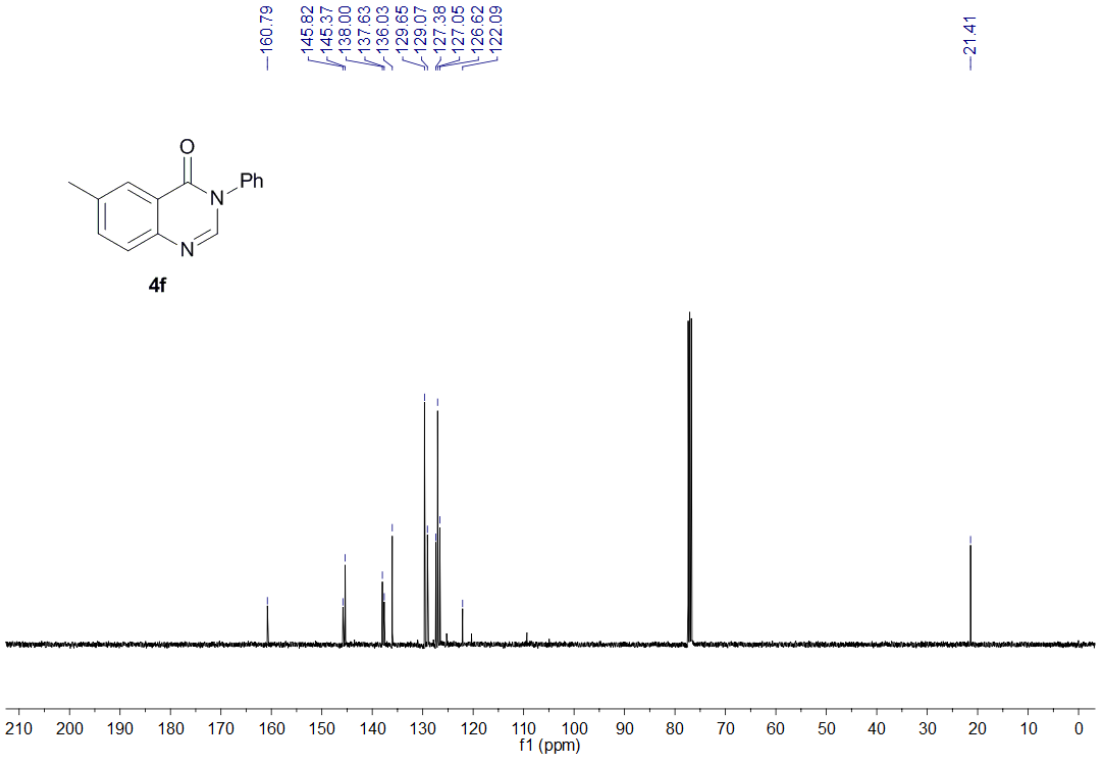
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.79
145.82
145.37
138.00
137.63
136.03
129.65
129.07
127.38
127.05
126.62
122.09
21.41
O
N
Ph
N
4f
210
200
190
180
170
160
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140
130
120
110
100
90
80
70
60
50
40
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10
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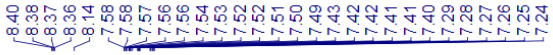
f1 (ppm)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7.57
7.56
7.56
7.54
7.53
7.52
7.52
7.51
7.50
7.49
7.43
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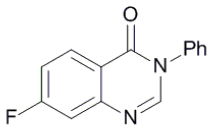
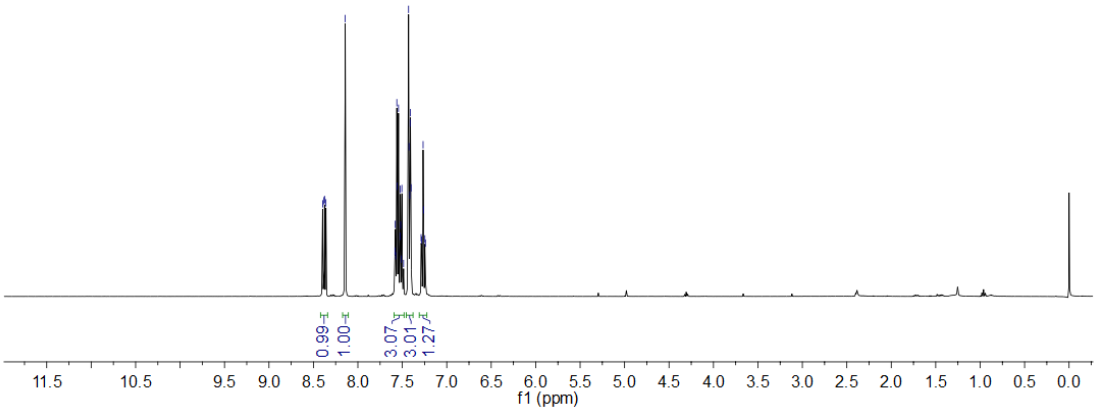
7.42
7.41
7.41
7.40
7.29
7.28
7.27
7.26
7.25
7.24


O
N
Ph
F
N

4g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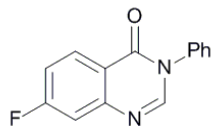
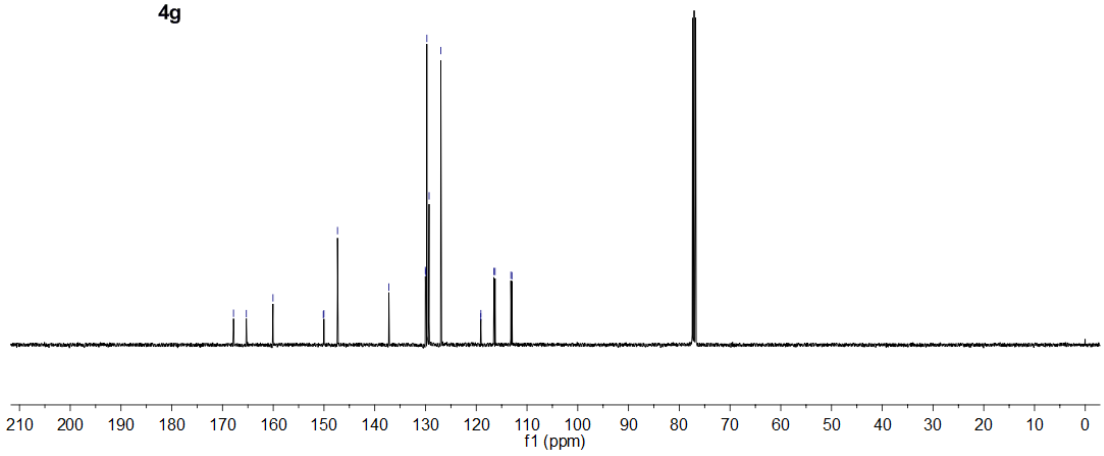
1.00
3.07
3.01
1.27
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


167.83
165.30
160.05
150.14
150.01
147.34
130.04
129.94
129.73
129.29
119.09
116.52
116.28
113.19
112.97


O
N
Ph
F
N

4g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200
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180
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150
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130
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110
100
90
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70
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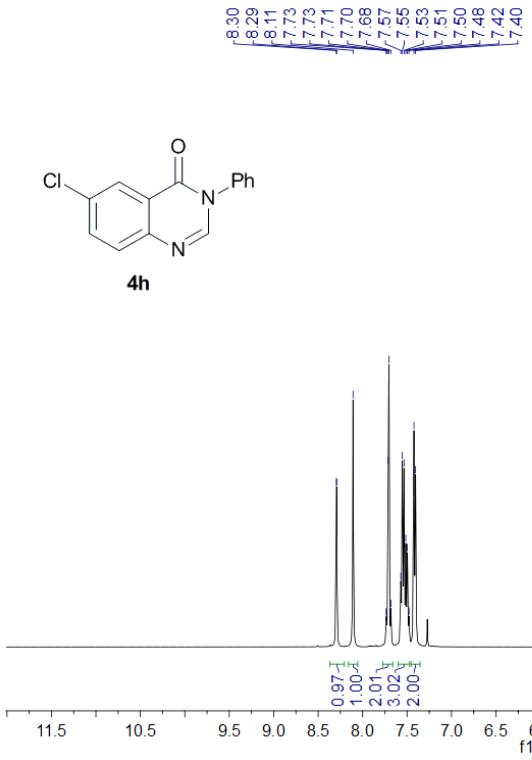
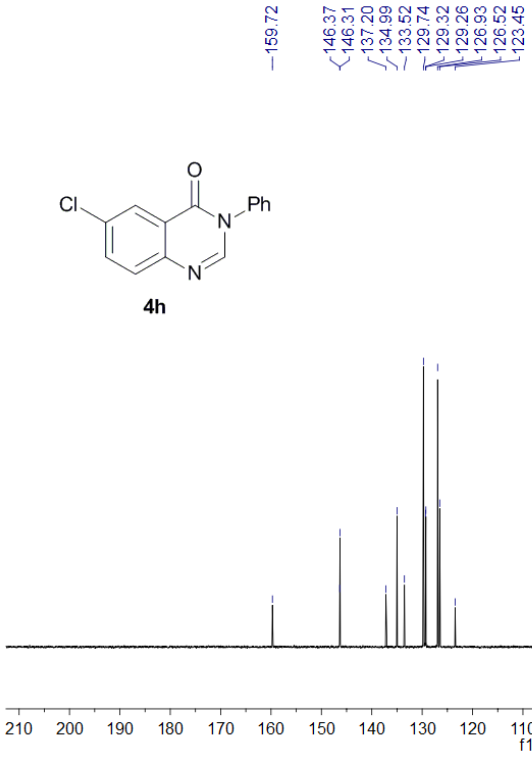
50
40
30
20
10
0
f1 (ppm)


8.30
8.29
8.11
7.73
7.73
7.71
7.70
7.68
7.57
7.55
7.53
7.51
7.50
7.48
7.42
7.40
O
Cl
N
Ph
N
4h
0.97
1.00
2.01
3.02
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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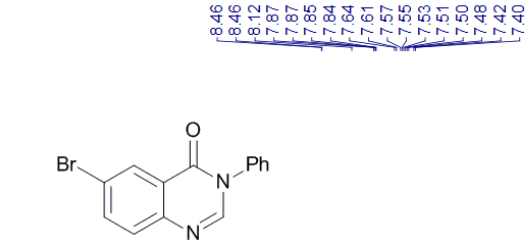
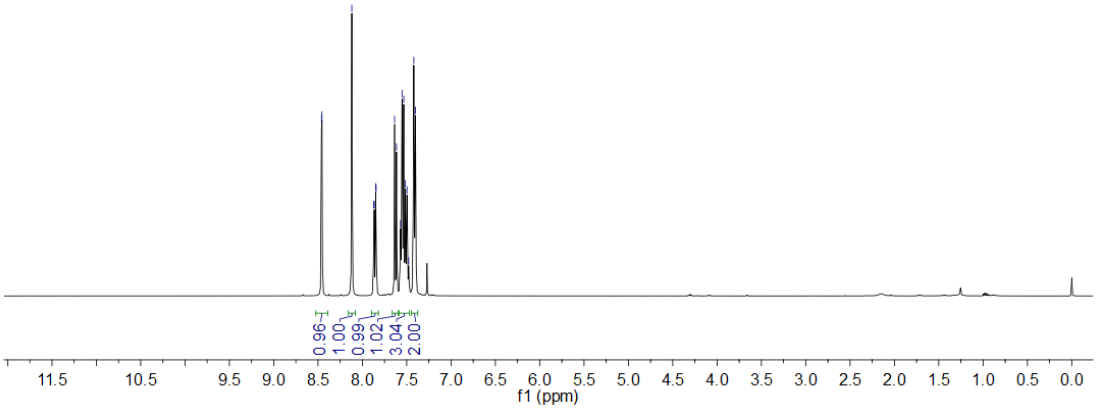
146.37
146.31
137.20
134.99
133.52
129.74
129.32
129.26
126.93
126.52
123.45
O
Cl
N
Ph
N
4h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.46
8.46
8.12
7.87
7.87
7.85
7.84
7.64
7.61
7.57
7.55
7.53
7.51
7.50
7.48
7.42
7.40
O
Br
N
Ph
N

4i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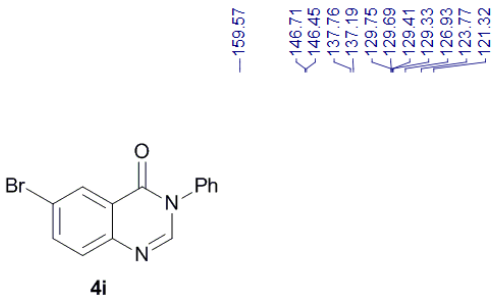
1.00
0.99
1.02
3.04
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


159.57
146.71
146.45
137.76
137.19
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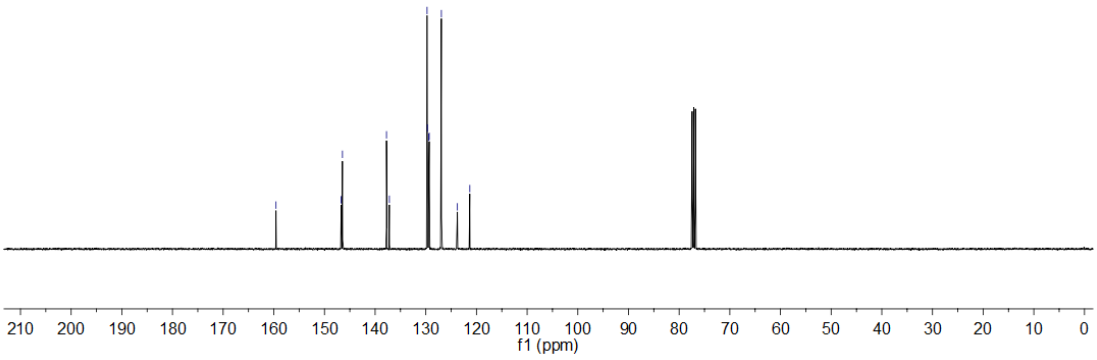
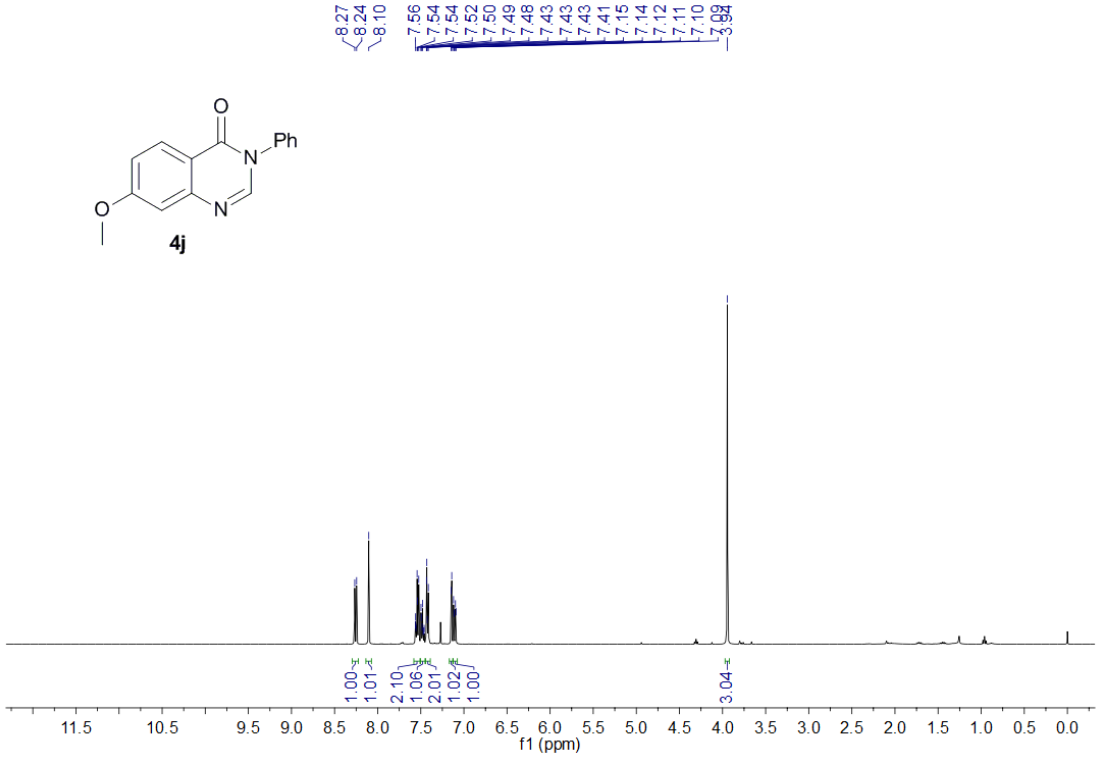
129.69
129.41
129.33
126.93
123.77
121.32
O
Br
N
Ph
N

4i


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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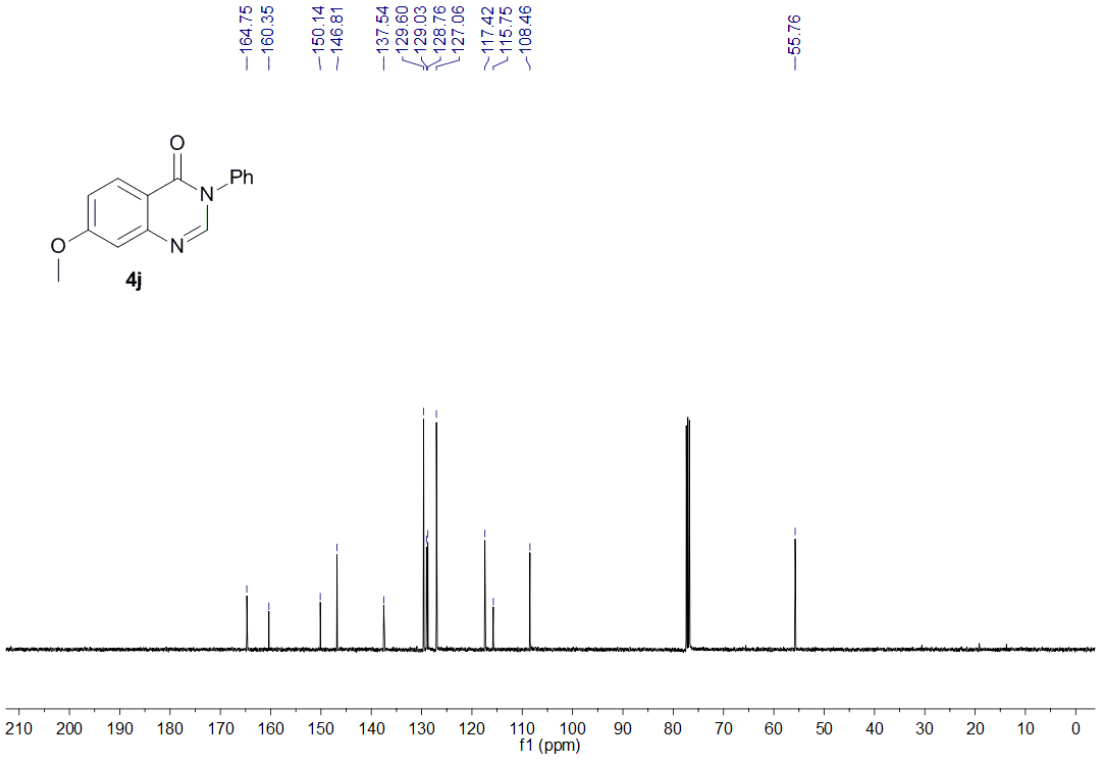
8.24
8.10
7.56
7.54
7.54
7.52
7.50
7.49
7.48
7.43
7.43
7.43
7.41
7.15
7.14
7.12
7.11
7.10
7.09
7.04
3.94
O
N
Ph
O
N
4j
1.00
1.01
2.10
1.06
2.01
1.02
1.00
3.04
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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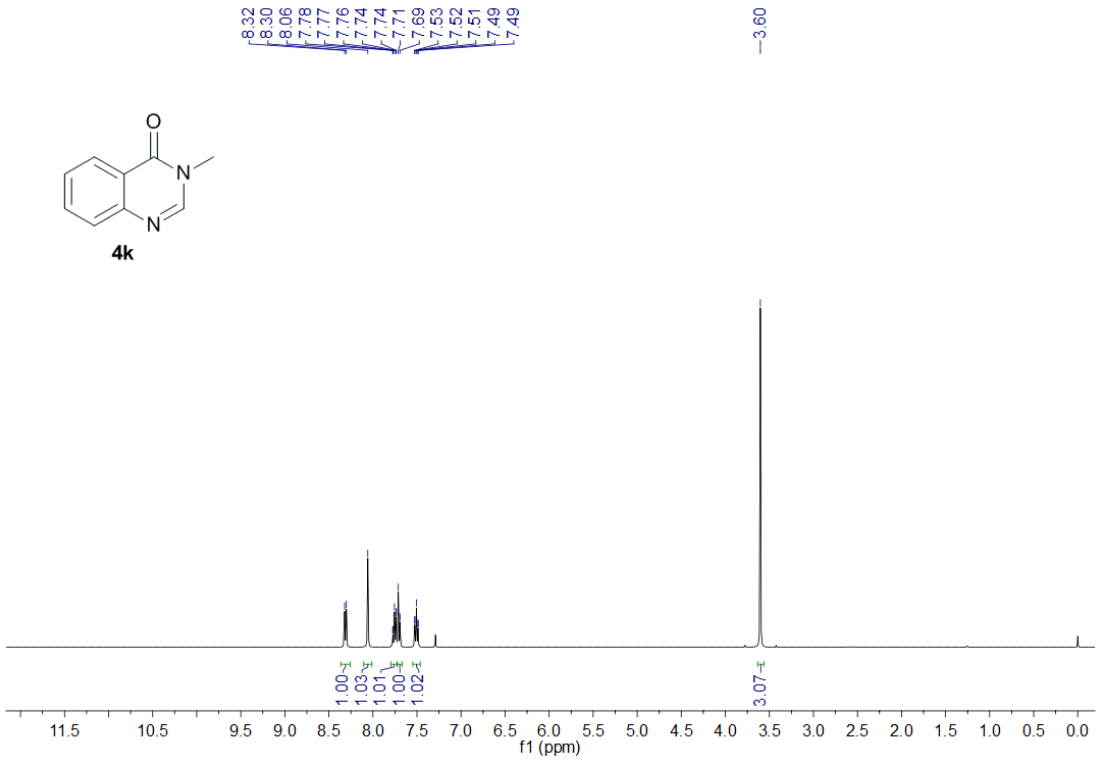
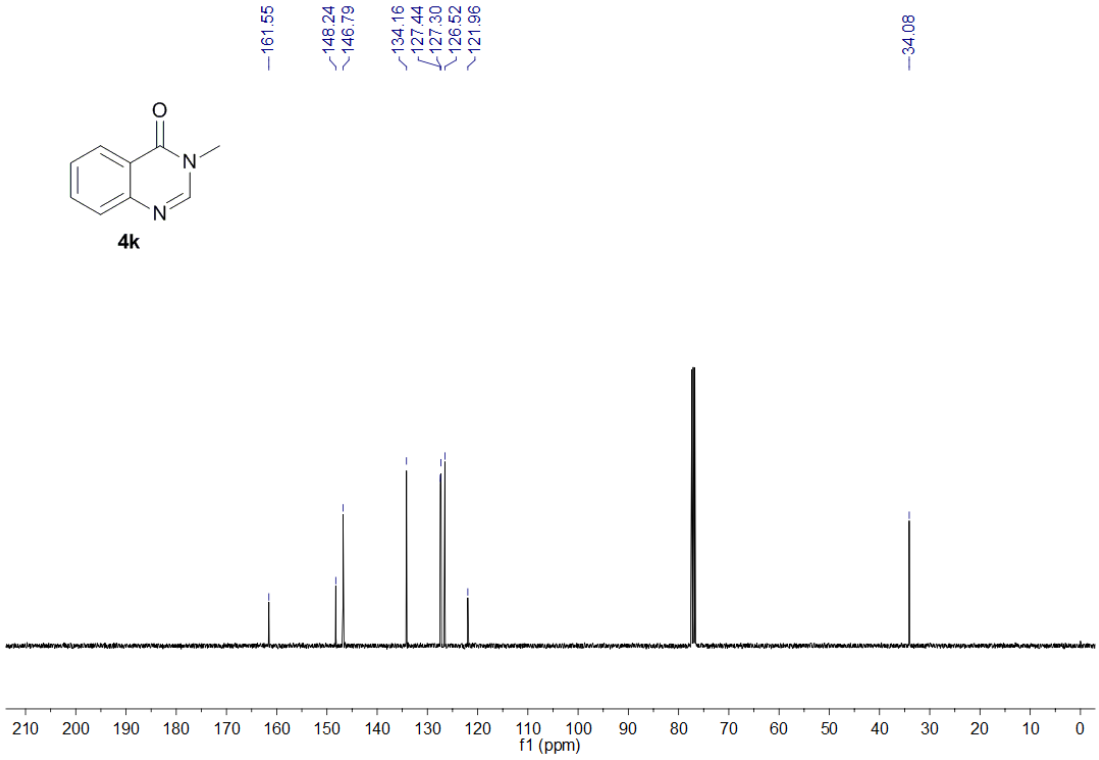
160.35
150.14
146.81
137.54
129.60
129.03
128.76
127.06
117.42
115.75
108.46
55.76
O
N
Ph
O
N
4j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.32
8.30
8.06
7.78
7.77
7.76
7.74
7.74
7.71
7.69
7.53
7.52
7.51
7.49
7.49
3.60
O
N
N
4k
1.00
1.03
1.01
1.00
1.02
3.07
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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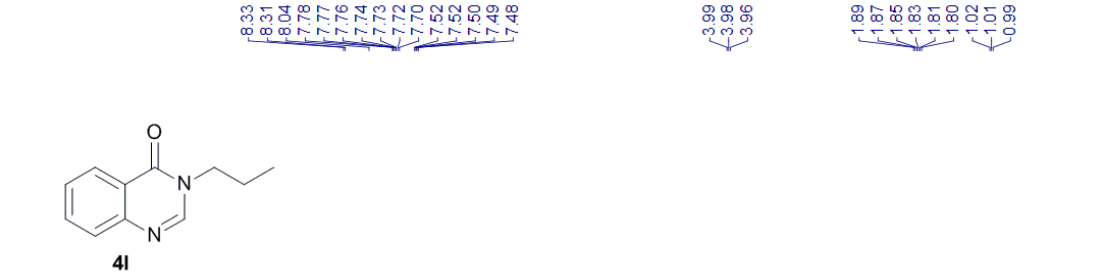
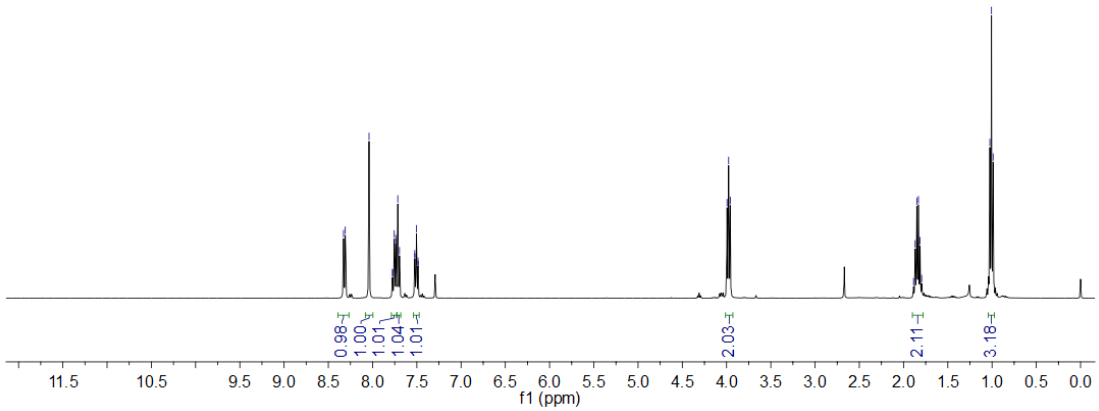
148.24
146.79
134.16
127.44
127.30
126.52
121.96
34.08
O
N
N
4k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.33
8.31
8.04
7.78
7.77
7.76
7.74
7.73
7.72
7.70
7.52
7.52
7.50
7.49
7.48
3.99
3.98
3.96
1.89
1.87
1.85
1.83
1.81
1.80
1.02
1.01
0.99

O
N
N

4l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1.01
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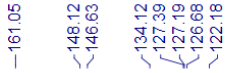
1.01
2.03
2.11
3.18
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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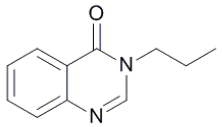
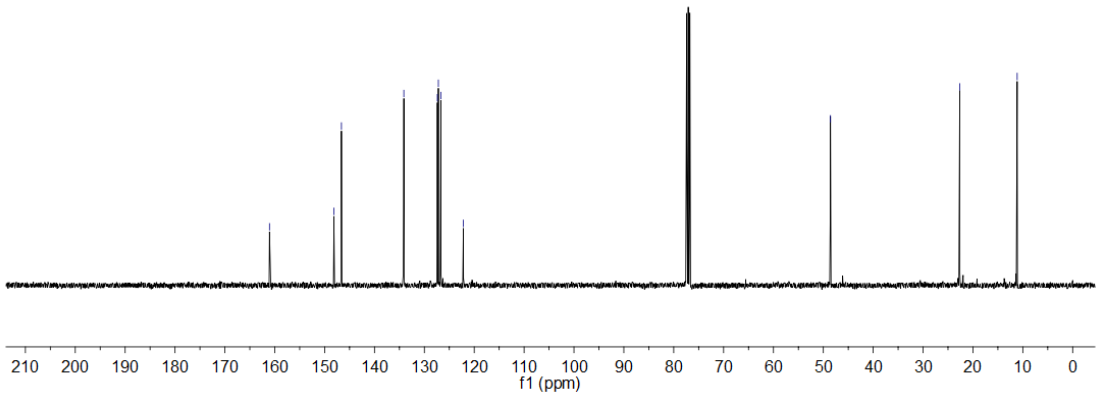
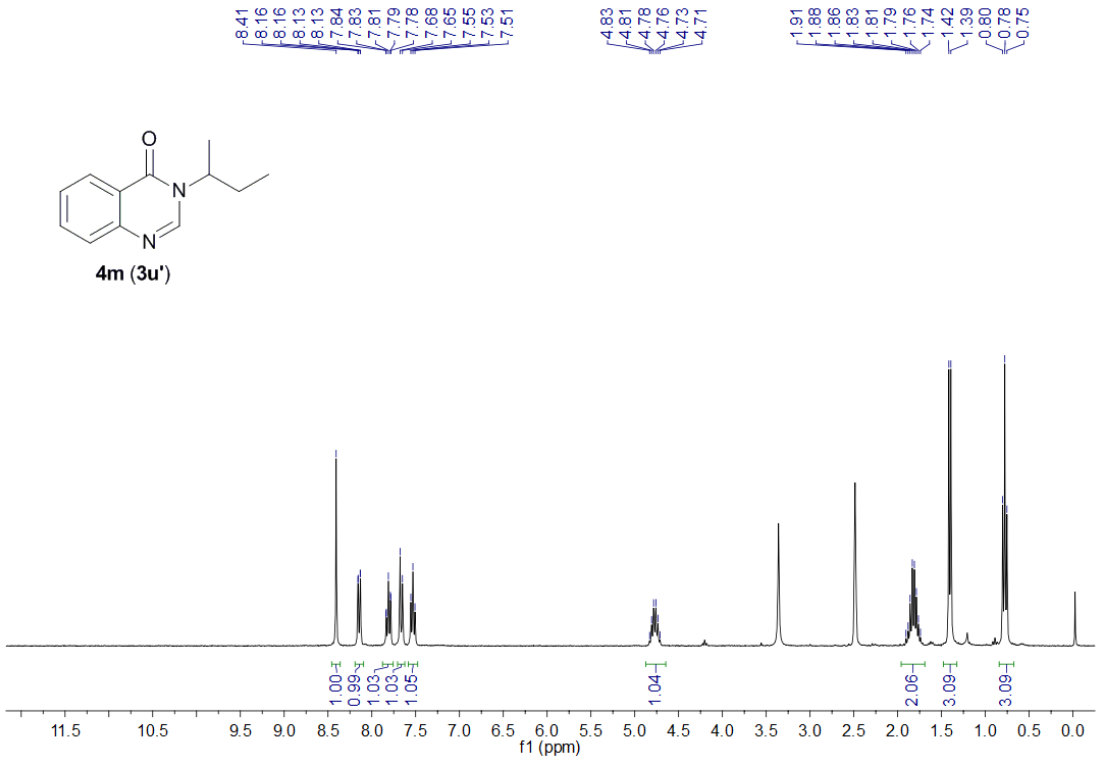
146.63
134.12
127.39
127.19
126.68
122.18
48.57
22.64
11.13


O
N
N

4l


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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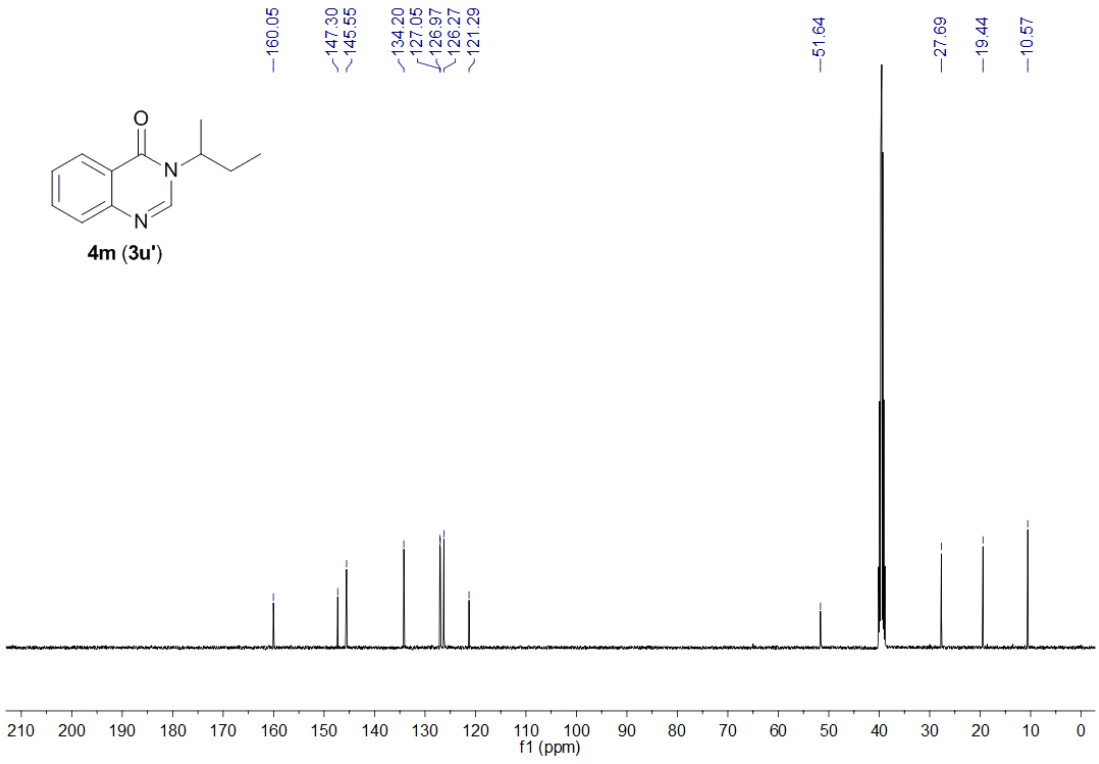
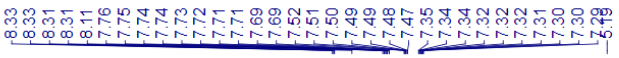
8.13
7.84
7.83
7.81
7.79
7.78
7.68
7.65
7.55
7.53
7.51
4.83
4.81
4.78
4.76
4.73
4.71
1.91
1.88
1.86
1.83
1.81
1.79
1.76
1.74
1.42
1.39
0.80
0.78
0.75
O
N
N
4m (3u')
1.00
0.99
1.03
1.03
1.05
1.04
2.06
3.09
3.09
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.05
147.30
145.55
134.20
127.05
126.97
126.27
121.29
51.64
27.69
19.44
10.57
O
N
N
4m (3u')
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.33
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8.31
8.31
8.11
7.76
7.75
7.74
7.74
7.73
7.72
7.71
7.71
7.69
7.69
7.52
7.51
7.50
7.49
7.49
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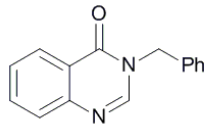
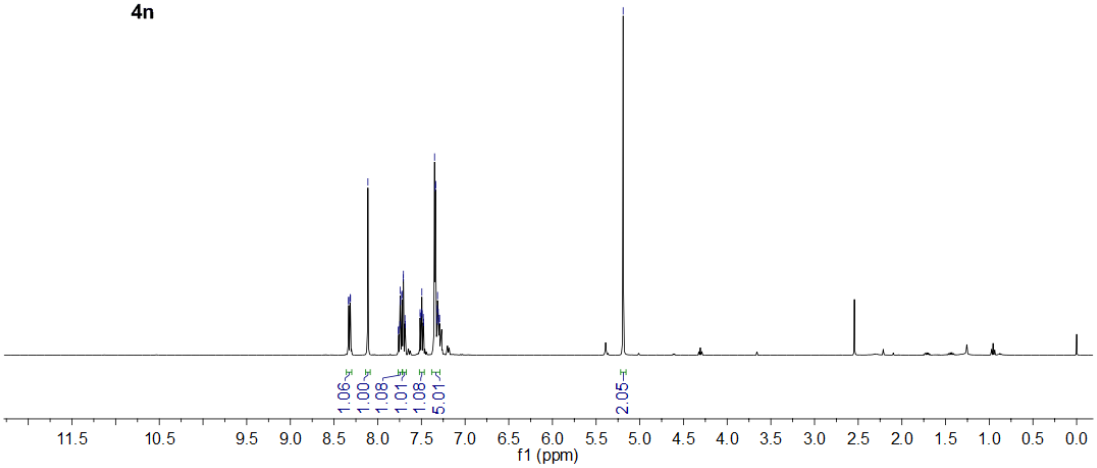
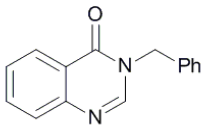
7.32
7.32
7.31
7.30
7.30
5.19


O
N
Ph
N

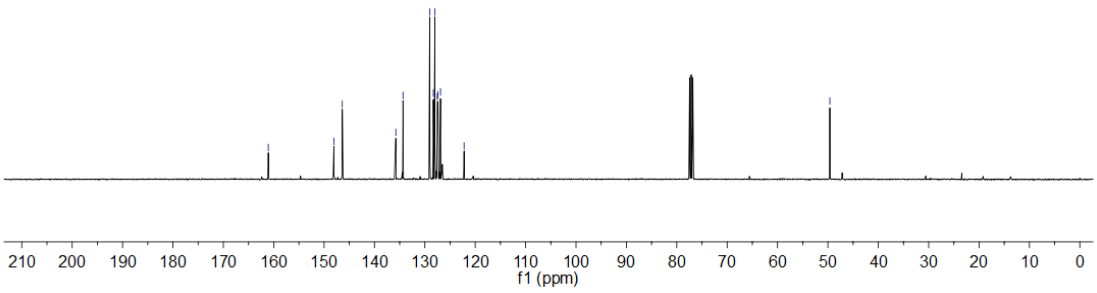
4n


1.06
1.00
1.08
1.01
1.08
5.01
2.05
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.08
148.05
146.39
135.77
134.33
129.04
128.32
128.01
127.53
127.40
126.89
122.21
49.61


O
N
Ph
N

4n


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)